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Modèles biocinétiques de boues activées de type ASM : Analyse théorique et fonctionnelle, vers un jeu de paramètres par défaut

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HÉLÈNE HAUDUC

MODÈLES BIOCINÉTIQUES DE BOUES ACTIVÉES DE TYPE ASM : ANALYSE THÉORIQUE ET FONCTIONNELLE, VERS UN JEU DE PARAMÈTRES PAR DÉFAUT

Thèse présentée
à la Faculté des études supérieures de l'Université Laval
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DÉPARTEMENT DE GÉNIE CIVIL ET GÉNIE DES EAUX
FACULTÉ DES SCIENCES ET GÉNIE
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Résumé

La modélisation du fonctionnement des stations d'épuration est un outil largement utilisé notamment pour l'optimisation et la réhabilitation des ouvrages existants et le dimensionnement de nouvelles installations, par les ingénieurs et par les chercheurs. S'assurer d'une bonne qualité des modèles est donc primordial. Or, d'après les résultats d'une enquête internationale effectuée auprès de 96 utilisateurs potentiels de modèles, deux étapes dans l'utilisation des modèles sont considérées comme particulièrement délicates: le choix du modèle à utiliser parmi les modèles disponibles et l'étape de calage de ces modèles. Le travail présenté visait à fournir des éléments pour lever des obstacles à une utilisation plus généralisée des modèles biocinétiques à boues activées. Il a porté sur sept des modèles publiés : (1) ASM1, (2) ASM2d, (3) ASM3, (4) ASM3+BioP, (5) ASM2d+TUD, (6) Barker & Dold et (7) UCTPHO+.

Dans un premier temps, une analyse des **connaissances pratiques** des modèles a été effectuée afin d'améliorer le transfert des connaissances en modélisation. Une base de données de jeux de paramètres a été créée à partir d'études publiées et d'un questionnaire adressé aux utilisateurs de modèles. Cette base de données a notamment permis d'établir des fourchettes de valeurs utilisées pour l'ASM1 et l'ASM2d.

Puis, une analyse des **connaissances théoriques** ayant pour but d'aider les utilisateurs à mieux comprendre les sept modèles et à choisir le modèle adapté à leur projet a été réalisée. Les modèles étudiés ont d'abord été vérifiés et les erreurs de frappe et incohérences ont été corrigées. Les concepts de modélisation ont été comparés entre eux grâce à une nouvelle représentation graphique, et confrontés aux connaissances sur le fonctionnement biologique des boues activées afin de mettre en évidence les limites théoriques des modèles.

En dernier lieu, une méthodologie a été développée pour l'**obtention de jeux de paramètres par défaut** qui pourraient être utilisés comme valeurs initiales lors du calage des modèles. Pour cela, une procédure de calage multi-jeux de données a été élaborée. Cela nécessite au préalable le développement d'une procédure de calage automatisée et l'utilisation d'un critère de qualité permettant de définir l'arrêt de la procédure de calage. Une analyse est effectuée sur les critères de qualité utilisés en sciences de l'environnement.

Abstract

Mathematical modelling of activated sludge systems has become a widely accepted tool and is used in particular for optimization and upgrading of existing plants and for new facilities design, either by engineering and consulting companies, or university and research centers. Ensuring the adequate quality of modelling results is therefore essential. However, an international survey conducted among 96 potential users of activated sludge models (ASM) pointing to two main obstacles to the use of modelling: the selection of the model to use among the available models and the model calibration. The objective of this work was to provide elements to overcome these obstacles and to promote the wider use of biokinetic models for activated sludge systems. It focused on seven published models: (1) ASM1, (2) ASM2d, (3) ASM3, (4) ASM3+BioP, (5) ASM2d+TUD, (6) Barker & Dold and (7) UCTPHO+.

First, an analysis **of practical knowledge** on the models was performed to improve the transfer of modelling knowledge. A database of practical modelling applications from published case studies and from the answers of a questionnaire sent to model users was created. This database enables to establish ranges of parameter values commonly used for the ASM1 and ASM2d.

Then the theoretical knowledge on ASMs was analysed to help users to better understand the seven studied models and to select the model most appropriate to their project. The studied models were first verified and typing errors and inconsistencies have been corrected. The modelling concepts were compared to each other through a new graphical representation, and confronted with knowledge about the biology of activated sludge, in order to highlight the theoretical limits of each model.

Finally, a methodology has been developed to obtain default parameter values that could be used as initial values for model calibration. To this end, an automated calibration procedure that allows calibration on multiple data sets was proposed. Then, the quality criteria used in environmental sciences have been synthesised. These criteria are required to determine the best set of parameters based on the goodness-of-fit of the model and to compare results from different models.

Avant-Propos

Ces travaux de thèse ont été réalisés dans le cadre d'une collaboration entre Cemagref, l'institut de recherche en sciences et technologies pour l'environnement, et l'Université Laval (Québec, Canada). Au Cemagref, les travaux de thèse ont été effectués au sein de l'équipe Epure (Génie des processus épuratoires) de l'unité HBAN (Hydrosystèmes et bioprocédés) du groupement d'Antony (France), et dirigés par Sylvie Gillot. A l'Université Laval, ils ont été réalisés au sein du groupe de recherche model*EAU* du département de génie civil et de génie des eaux, et dirigés par Pr. Peter Vanrolleghem. Ces travaux s'inscrivent également dans le cadre d'une cotutelle établie entre l'Université Laval et l'école doctorale ABIES de l'Institut des Sciences et Industries du Vivant et de l'Environnement (AgroParisTech, Paris, France), dont Alain Bermond a assuré la correspondance pour ce projet. Ces travaux ont été également encadrés par Alain Héduit et Leiv Rieger.

Les travaux de thèse ont été développés en lien avec les travaux du Task Group « Good Modelling Practice » (TG-GMP, https://iwa-gmp-tg.cemagref.fr/) de l'International Water Association, dont l'objectif est d'élaborer une procédure de bonnes pratiques en matière de modélisation des boues activées. Ce groupe de travail est dirigé par Leiv Rieger et est composé de 6 autres membres : Sylvie Gillot, Günter Langergraber, Takayuki Ohtsuki, Andrew Shaw, Imre Takács et Stefan Winkler. Cette collaboration a fait l'objet de deux articles présentés dans la thèse :

- Hauduc H., Gillot S., Rieger L., Ohtsuki T., Shaw A., Takacs I., Winkler S. (2009) Activated sludge modelling in practice - An international survey, *Water Science and Technology*, **60**(8), 1943-1951.

  Cet article est basé sur l'analyse des réponses à un questionnaire aux utilisateurs effectifs et potentiels de modèles de type ASM. Ce questionnaire a été élaboré par les membres du TG-GMP. L'analyse des résultats et la rédaction de l'article ont été entièrement menées par moi-même, mais ont été affinées grâce à de nombreux échanges avec les co-auteurs. Cet article a été publié et est présenté au chapitre 2 de cette thèse.

- Hauduc H., Rieger L., Ohtsuki T., Shaw A., Takács I., Winkler S., Heduit A, Vanrolleghem P.A. and Gillot S. (In Press) Activated sludge modelling: Development and potential use of a practical applications database, *Water Science and Technology*, In Press.

  Cet article est basé sur l'analyse des réponses à un second questionnaire aux utilisateurs de modèles de type ASM et d'une revue de littérature extensive des applications de modélisation. Le questionnaire a été élaboré en collaboration avec les membres du TG-GMP. La synthèse bibliographique, la création de la base de données, l'analyse des résultats et la rédaction de l'article ont été entièrement menées par moi-même, mais ont été affinées grâce à de nombreux échanges avec les co-auteurs. Cet article a été accepté pour publication au mois de septembre, et est présenté au chapitre 3 de cette thèse. Quelques informations supplémentaires ont été ajoutées par rapport à l'article accepté.

Deux autres articles dont j'ai été la rédactrice principale ont été réalisés lors de ces travaux de thèse et sont intégrés dans la thèse :

- Hauduc H., Rieger L., Takacs I., Héduit A., Vanrolleghem P.A., and Gillot S. (2010) A systematic approach for model verification – Application on seven published Activated Sludge Models, *Water Science and Technology,* **61**(4), 825-839.

  Cet article a été publié et est présenté au paragraphe 4.2 de cette thèse.

- Hauduc H., Rieger L., Héduit A., Vanrolleghem P.A. and Gillot S. Critical review of activated sludge modelling: State of process knowledge, modelling concepts and limitations.

  Cet article est présenté au paragraphe 4.3. Cet article sera soumis au cours de l'hiver 2011. La version actuelle est présentée au paragraphe 4.3 de cette thèse.

Suite aux besoins émis par différents groupes de travail, de nouvelles règles pour nommer les variables d'état et les paramètres des modèles de traitement des eaux ont été établies. Les résultats ont été synthétisés dans un article par Corominas *et al.* (2010), dont je suis co-auteur. J'ai eu l'occasion de prendre part à ces discussions dès le début de ce groupe de travail. Plus précisément, ma contribution est l'application de la notation

normalisée pour les sept modèles étudiés. Elle a permis de corriger des règles ambiguës. Le tableau des paramètres du modèle est fourni en tant que matériel additionnel à l'article, et est disponible à l'adresse suivante: http://www.iwaponline.com/wst/06104/0912.xls. Cet article est mentionné au paragraphe 4.1 de cette thèse mais n'a pas été inclus dans sa globalité.

> Corominas L., Rieger L., Takács I., Ekama G., Hauduc H., Vanrolleghem P.A., Oehmen A., Gernaey K.V., van Loosdrecht M.C.M. and Comeau Y. (2010). New framework for standardized notation in wastewater treatment modelling. *Water Science and Technology*, **61**(4), 841-857.

Les travaux présentés au chapitre 5.4 de cette thèse et portant sur les critères de qualité des modèles fait l'objet d'une collaboration avec Dirk Muschalla (Post-doctorant, model*EAU*), Marc Neumann (Post-doctorant, model*EAU*) et Valentin Gamerith (doctorant, Technische Universität Graz, Autriche). La revue de littérature des critères de qualité a été réalisée par moi-même, mais discutée avec ces collaborateurs. L'élaboration d'une méthodologie pour tester l'applicabilité de ces critères au domaine du traitement des eaux usée a notamment été initiée lors de cette collaboration. Les travaux présentés au chapitre 5 de cette thèse utilisent le logiciel BlueM.Opt (Muschalla *et al.*, 2009), qui a été adapté pour le calcul des critères de qualités présentés dans la revue de littérature par Valentin Gamerith.

Je tiens à remercier sincèrement chacune des personnes citées pour leur contribution à ces travaux.

Remerciements

Au cours de ces trois années de doctorat, j'ai eu la chance de pouvoir rencontrer et travailler avec des personnes de différents horizons et de différents pays, que j'aimerais remercier ici.

Tout d'abord, j'aimerais remercier les membres de mon jury de thèse, et en premier lieu, le Pr. Serge Leroueil d'avoir accepté de présider ce jury. Je voudrais aussi tout particulièrement remercier le Pr. Eduardo Ayesa d'avoir accepté d'assister à une soutenance en français et pour ses remarques pertinentes, et Madame Evangelina Belia pour ses nombreux commentaires et son enthousiasme. Je remercie le Pr Paul Lessard, dont j'ai eu la chance de suivre les cours lors de mon passage à l'Université Laval, et dont j'ai apprécié la rencontre lors de mes séjours au Québec. Sa lecture attentive de cette thèse a permis de soulever de très intéressantes questions, parfois très philosophiques… J'adresse un grand merci au Pr Alain Bermond, dont j'ai suivi les cours en dernière année d'école à l'AgroParisTech, et qui a accepté d'être mon professeur référent auprès de l'école doctorale ABIES, bien que le sujet de cette thèse ne soit pas directement dans son domaine de recherche. Dans cette thèse en cotutelle, deux personnes ont joué un rôle prépondérant et auprès desquelles j'ai beaucoup appris : le Pr. Peter Vanrolleghem, qui a dirigé mes recherches à l'Université Laval, et Sylvie Gillot, qui a suivi mon travail en France. Je leur adresse toute ma gratitude pour leur accueil, leur soutien au cours de ces trois années, mais surtout pour la qualité de leur encadrement scientifique.

Deux autres personnes ont joué un grand rôle au cours de ces trois ans, et je voudrais les remercier chaleureusement. Tout d'abord, Alain Héduit, qui a assuré la direction de ma thèse par intérim, et qui m'a dispensé de nombreux et judicieux conseils. Aussi, je dois beaucoup à Leiv Rieger, qui a co-encadré mes travaux et m'a enseigné la rigueur germanique pour la rédaction d'articles.

Je ne voudrais pas oublier de citer dans ces remerciements toutes les personnes avec qui j'ai eu la chance de travailler. Je remercie Youri Amerlinck d'avoir participé aux comités de pilotage de ma thèse et d'avoir contribué à l'orientation de mes recherches. Je remercie également les membres du groupe de travail de l'IWA "Good Modelling Practice" non encore cités, pour leur accueil et leur contribution à mes travaux : Günter

Langergraber, Takayuki Ohotsuki, Andy Shaw, Imre Takács et Stefan Winkler. Je remercie également Yves Comeau, Lluis Corominas, Valentin Gamerith, Julien Laurent, Dirk Muschalla, Marc Neumann, Adrian Oehmen et Mark van Loosdrecht, avec qui j'ai eu la chance de travailler sur des publications.

Bien évidemment, dans ces quelques lignes, je ne peux oublier ceux qui ont rendu plus douces ces années de travail, à Québec comme à Paris : Arinala, Bertrand, Cyril, Fred, Giulia, Juan-Alberto, Kris, Lluis, Marc, Maria, Marie-Amélie, Santatra, et Thibault ; les Epurateurs, les petits poissons du bocal, les sudistes et les jardiniers du Cemagref. J'ai une pensée toute particulière pour Charlotte, Emmanuel et Lavinia, pour leur douce amitié qui a fait fondre plus vite qu'il n'y paraissait les quelques 5,58 mètres de neige de l'hiver québécois 2007-2008.

Je terminerais par remercier ceux sans qui ces longues études n'auraient pas été possibles, mes parents et ma famille qui m'ont toujours soutenue et bien plus au cours de ces longues années. Pour cela, ma reconnaissance est sans limites. Enfin, celui avec qui j'ai fais le pari fou d'organiser un mariage et deux thèses en une seule année, mon Thomas dont le soutien et les encouragements de tous les jours ont permis l'aboutissement de ces projets : MERCI.

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Articles dans revues scientifiques à comité de lecture

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Hauduc H., Rieger L., Takacs I., Héduit A., Vanrolleghem P.A., and Gillot S. (2010) A systematic approach for model verification – Application on seven published Activated Sludge Models, *Water Science and Technology,* **61**(4), 825-839.

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Hauduc H., Rieger L., Héduit A., Vanrolleghem P.A. and Gillot S. Critical review of activated sludge modelling: State of process knowledge, modelling concepts and limitations.

Corominas L., Rieger L., Takács I., Ekama G., Hauduc H., Vanrolleghem P.A., Oehmen A., Gernaey K.V., van Loosdrecht M.C.M. and Comeau Y. (2010). New framework for standardized notation in wastewater treatment modelling. *Water Science and Technology*, **61**(4), 841-857.

Conférences

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Hauduc H., Gillot S., Rieger L., Ohtsuki T., Shaw A., Takács I. and Winkler S. (2009) Activated Sludge Modelling in Practice - An International Survey. *MOSTforWATER Newsletter,* Mai 2009. http://www.mostforwater.com/Documents/Newsletter_200902.html#article_1

Autre

Hauduc H., Gillot S., Rieger L., Ohtsuki T., Shaw A., Takács I., Winkler S. (2009) Activated Sludge Modelling in Practice - International Surveys. *World Wide West*, April 27th 2009, Copenhagen, Denmark. (Journée des utilisateurs du logiciel WEST)

CHAPITRE 1 Introduction générale

Dans le souci de la préservation de notre environnement, les contraintes de rejet imposées aux industries et aux stations d'épuration municipales sont de plus en plus strictes au niveau mondial. Ainsi, la directive européenne relative au traitement des eaux résiduaires urbaines (91/271/CEE) a pour but de diminuer l'eutrophisation des milieux naturels et la pollution des ressources en eau par les nutriments (azote, phosphore) et les matières organiques. Pour cela, elle établit les exigences de traitement en fonction de la population raccordée à la station, et de la sensibilité du milieu récepteur. Au Canada, un projet de règlement équivalent, établi en vertu de la *Loi sur les pêches,* a récemment été proposé : le projet de *Règlement sur les effluents des systèmes d'assainissement des eaux usées* (Gazette du Canada, 2010).

1.1 Aperçu de la situation du traitement des effluents en Europe et au Canada

En Europe, le développement des stations d'épuration, l'augmentation de la proportion de population raccordée et l'amélioration du traitement des eaux résiduaires urbaines engagés depuis les années 1980 ont permis une diminution remarquable du volume de phosphore et de matières organiques dans les cours d'eau et les lacs. Cependant, malgré ces mesures, en 1998 seulement 2 pays de l'Union Européenne (Danemark et Autriche) étaient conformes à la directive eaux résiduaires urbaines (91/271/CEE). De plus, les stations d'épuration de nombreuses grandes villes (>150 000 Equivalents Habitants) n'atteignaient pas à cette date un niveau de traitement suffisant, et aucune amélioration n'avait été enregistrée en ce qui concerne la concentration des nitrates dans les eaux de surface (EEA, 2003). Ainsi, de nombreuses régions de l'Europe reçoivent encore un flux d'azote trop élevé (Figure 1-1).

Au Canada, 97% de la population était raccordée à un système de traitement des eaux usées en 1999. Cependant, le degré de traitement varie beaucoup, avec des traitements moins efficaces (traitements primaires ou secondaires) sur les côtes océaniques qu'à l'intérieur du territoire. De plus, les installations sont vieillissantes et deviennent insuffisantes avec l'accroissement de la population. Ainsi, malgré la forte proportion de

population reliée à un système de traitement des eaux résiduaires urbaines, une baisse de la qualité des eaux intérieures et côtières a été observée depuis les années 1990, ce qui a conduit notamment à des fermetures de plages, à des restrictions de la récolte des mollusques et des crustacés et à la dégradation des habitats aquatiques et des ressources halieutiques (Environnement Canada, 2001).

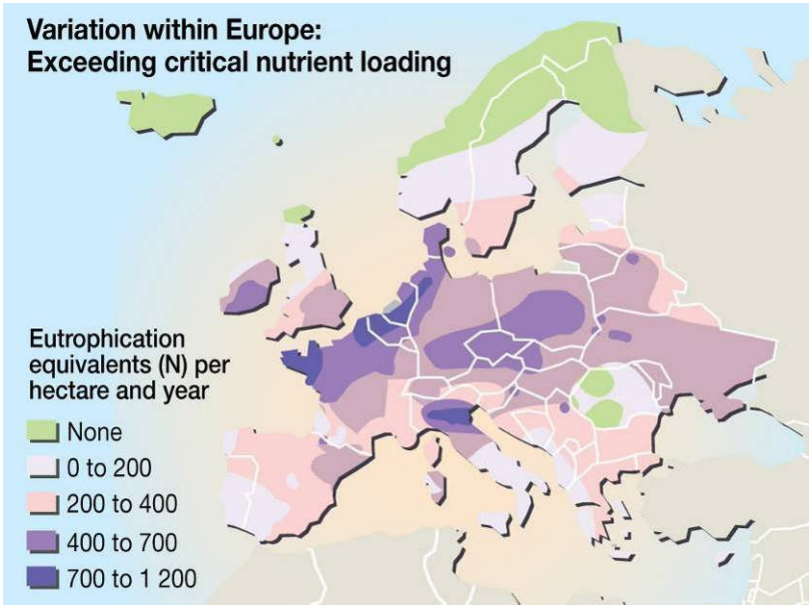


Figure 1-1. Variation des flux d'azote (kg/ha/an) rejetés en Europe (d'après Corcoran *et al.*, 2010; crédit : UNEP/GRID-Arendal)

Il est donc nécessaire de connaître et de maîtriser au mieux le fonctionnement des stations d'épuration afin d'en améliorer le fonctionnement et de réduire leur impact sur le milieu récepteur. Pour cela, la recherche se penche depuis une trentaine d'années sur 3 thématiques majeures :

- La compréhension du fonctionnement des boues activées (fonctionnement des populations bactériennes, phénomènes de compétition, comportement des micropolluants, production de gaz à effet de serre) (Gujer, 2006).
- La recherche et le développement de nouveaux procédés de traitement (plus efficaces, traitant les micropolluants, les flux de retour en tête de station du traitement des boues…) et de systèmes de contrôle en-ligne pour optimiser le traitement.
- La modélisation du fonctionnement des stations d'épuration, qui représente environ 20% des publications scientifiques concernant le traitement des eaux usées des vingt dernières années (voir Figure 1-2).

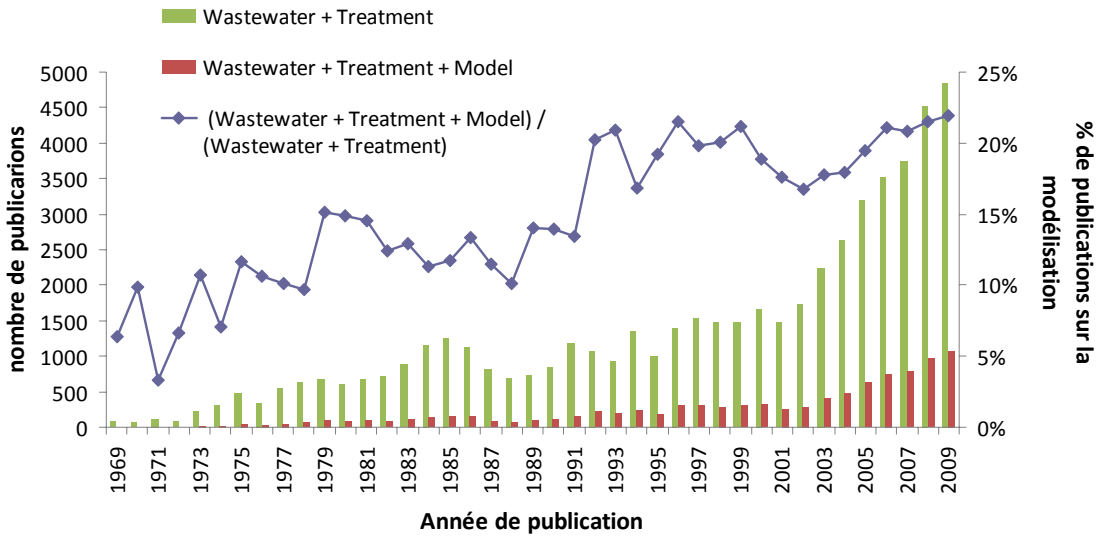


Figure 1-2. Évolution du nombre de publications concernant la modélisation (d'après la base de données Engineering Village www.engineeringvillage2.org ; mots clef : wastewater + treatment + model/ wastewater + treatment)

1.2 Les stations d'épuration (Steps) à boues activées

Le procédé dit à "boues activées" est basé sur le principe d'une culture bactérienne en suspension et aérée qui permet d'oxyder la matière organique, de stocker les nutriments (azote et phosphore) des eaux résiduaires dans la biomasse formée et de les éliminer. Ce procédé de traitement biologique des eaux résiduaires a été découvert au début du XXème siècle, et constitue le procédé le plus couramment utilisé pour le traitement des effluents urbains.

La Figure 1-3 reprend le principe général du procédé de traitement à boues activées. Les eaux usées collectées qui arrivent à la station d'épuration peuvent subir un traitement primaire, comme par exemple un dégrillage, un dégraissage et/ou une décantation primaire. Ces traitements permettent d'éliminer les éléments grossiers et difficilement dégradables par les bactéries.

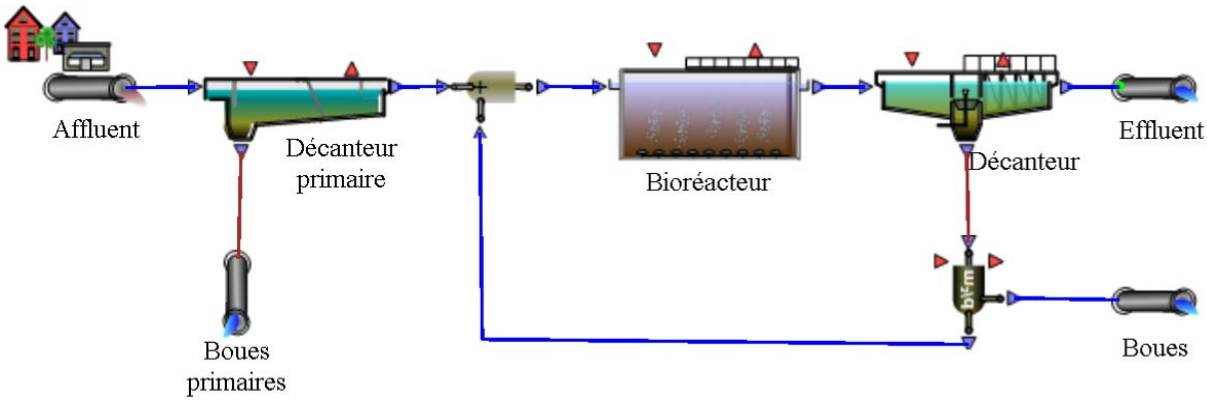


Figure 1-3. Principe du procédé de traitement des eaux usées à boues activées (Schéma réalisé à l'aide du logiciel WEST)

Le procédé par boues activées est un traitement dit secondaire des eaux usées. Son fonctionnement nécessite deux ouvrages principaux :

- un ou plusieurs **bioréacteurs** dans lesquels la matière organique et la pollution azotée et phosphorée des eaux résiduaires sont mis en contact avec une biomasse maintenue à concentration élevée et aérée. Grâce à l'oxygène qui leur est fourni, ces bactéries consomment la matière organique et les nutriments pour leur croissance. Ces micro-organismes forment des flocs, qui sont constitués de bactéries agrégées entre elles par des exo-polymères. Selon le niveau de traitement désiré, un ou plusieurs bassins sont utilisés, en parallèle ou en série, aérés ou non, ou avec une aération cadencée. En effet, la dénitrification (transformation des nitrates en diazote) nécessite un milieu anoxique, et la déphosphatation biologique nécessite une alternance de phase en anaérobiose et en aérobiose (voir paragraphe 4.4.5).

- Un **décanteur secondaire** dans lequel l'eau épurée est séparée de la biomasse. La décantation est facilitée par la formation des flocs. L'eau épurée est rejetée dans le milieu naturel par surverse, mais pourra au préalable subir un traitement tertiaire, selon le niveau de traitement requis. Les boues concentrées sont recirculées en tête du traitement biologique, afin de maintenir une concentration élevée de biomasse dans les bassins. Pour assurer une concentration constante de biomasse, la biomasse excédentaire produite est éliminée généralement à la sortie du décanteur. Ces boues biologiques pourront subir des traitements de réduction et/ou de stabilisation avant d'être éliminées.

1.3 Utilisation de la modélisation des stations d'épuration

En fonction des paramètres de fonctionnement de la station d'épuration (temps de séjour, temps d'aération, charge organique, âge des boues…) la modélisation permet de :

- simuler l'évolution des substrats d'intérêt (matière organique, azote, phosphore…) et de la biomasse bactérienne ;
- optimiser les performances du traitement en termes de qualité de l'eau en sortie, quantité de boues produites, dépense énergétique…
- prédire l'efficacité en cas de modification des conditions normales de fonctionnement (pluies en réseau unitaire, variation des températures, variation saisonnière de population, pollution accidentelle, apport d'influents atypiques…) et agir sur les paramètres de fonctionnement pour optimiser le traitement ;
- dimensionner les ouvrages des stations d'épuration lors de leur conception ou prédire l'efficacité d'un scénario de modification de l'installation.

La modélisation est donc un outil adapté à la conception de nouvelles stations, à l'optimisation et à la réhabilitation des stations existantes. Elle constitue également un outil très utilisé pour l'apprentissage et la formation au traitement des eaux usées. La modélisation permet en effet de mieux appréhender le fonctionnement de la station et les conséquences de la modification des paramètres de fonctionnement (Gernaey *et al.*, 2004).

Modéliser une station d'épuration nécessite en fait l'utilisation de plusieurs modèles (Gillot *et al.*, 2006):

- Un modèle hydrodynamique (représentant le comportement hydraulique de l'installation…),
- Un modèle d'aération,
- Des modèles pour les procédés physico-chimiques (variation du pH et de l'alcalinité, floculation, précipitation, décantation…),
- Des modèles biocinétiques (procédés biologiques),
- Un modèle de fractionnement : conversion des mesures réalisées sur l'affluent (DCO, NTK…) en variables d'état des modèles biocinétiques (fractions de substrat lentement et rapidement biodégradables…).

Les travaux de cette thèse portent particulièrement sur les modèles biocinétiques des boues activées.

1.4 Les modèles biocinétiques de boues activées (ASM)

Les modèles biocinétiques décrivent l'évolution des substrats d'intérêt des eaux usées sous l'action de réactions chimiques et de la biomasse bactérienne des boues activées. Une dizaine de modèles biocinétiques de boues activées ont été développés depuis le milieu des années 1960 (Gujer, 2006). Ils intègrent les phénomènes biologiques de croissance bactérienne par consommation de substrat organique ou minéral, d'hydrolyse et de mort bactérienne qui se produisent dans les bioréacteurs de la station d'épuration. Ces modèles sont dits de type Activated Sludge Models (ASM).

Pour construire des modèles adaptés aux objectifs et aux conditions de traitement, Vanrolleghem et Dochain (1998) proposent une méthodologie (Figure 1-4) basée sur les objectifs du modèle, sur les connaissances *a priori* du système à modéliser et sur les données disponibles.

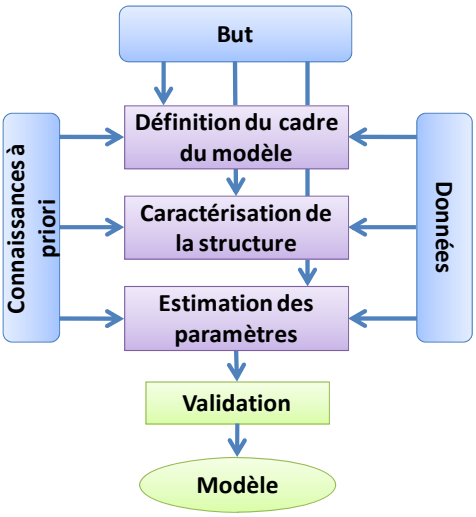


Figure 1-4. Étapes de construction d'un modèle (d'après Vanrolleghem and Dochain, 1998)

Dans cette étude, le cadre du modèle est le traitement biologique par boues activées, représenté par des variables d'état sur lesquelles sont effectuées des bilans de matières sous forme d'équations différentielles.

Depuis le modèle ASM1 (Henze *et al.*, 1987), les modèles biocinétiques sont représentés sous la forme d'une matrice de Gujer (ou matrice de Petersen, Takacs, 2005). Le principe de cette matrice peut être décrit à l'aide du modèle simpliste "ASM0" de croissance et décès de la biomasse hétérotrophe en conditions d'aérobiose (Table 1-1).

Table 1-1: Modèle de croissance et décès de la biomasse hétérotrophe en conditions d'aérobiose ASM0 (d'après Henze *et al.*, 2000a)

Continuité →

← Bilan de matière	Variable (i) Processus (j)	1 X_{OHO}	2 S_B	3 S_{O2}	Cinétique ρ_j
	1. Croissance	1	$-\frac{1}{Y_{OHO}}$	$-\frac{1-Y_{OHO}}{Y_{OHO}}$	$\frac{\mu_{OHO,Max}\, S_B}{K_{S_B,OHO}+S_B} X_{OHO}$
	2. Décès	-1		-1	$b_{OHO}.X_{OHO}$
		Biomasse (mgCOD/L)	Substrat (mgCOD/L)	Oxygène (-mgCOD/L)	

Chaque ligne de cette matrice représente un processus (ici 2 : croissance et décès), et chaque colonne une variable d'état (ici 3 : la biomasse, le substrat et l'oxygène). Chaque cellule contient le coefficient stœchiométrique ν_{ij} associé à la variable d'état i pour le processus correspondant j. La lecture en ligne doit permettre de vérifier la continuité du processus pour chacun des éléments, c'est-à-dire qu'il n'y a pas eu de création ou de perte de matière (voir paragraphe 4.3.2.1). La dernière colonne contient l'équation cinétique du processus ρ_j. La lecture en colonne du tableau permet d'écrire l'équation de bilan de matière de chacune des variables d'état i : $\text{Accumulation}_i = \text{entrée}_i + \text{réaction}_i - \text{sortie}_i$ avec $\text{réaction}_i = \Sigma \nu_{ij}\, \rho_j$.

Lorsque l'utilisateur choisit un modèle biocinétique qui a déjà été développé, il existe alors deux risques majeurs d'obtenir un modèle erroné : choisir un modèle non adapté au projet et caler de façon inadéquate le jeu de paramètres. En effet :

- Les modèles développés ne prennent pas tous en compte les mêmes phénomènes et réactions. Le choix du modèle dépend des objectifs du projet de modélisation et des conditions de traitement des eaux usées. Or, aucune étude n'a à l'heure

actuelle permis de comparer ces modèles et de guider l'utilisateur vers le modèle adéquate à la question posée.

- Peu de jeux de paramètres validés en fonction des domaines d'utilisation et des modèles sont disponibles. Or, le calage et la validation des modèles nécessitent l'acquisition d'un nombre important de données (fréquence, lieu et durée) sur la station d'épuration. Il est donc difficile et coûteux d'obtenir un modèle adapté à la station d'épuration.

Une prise de décision basée sur les résultats obtenus à l'aide d'un modèle non adapté ou mal calé peut avoir d'importantes conséquences sur la conception des ouvrages ou sur l'optimisation du procédé, et donc sur la qualité de l'effluent et sur les coûts de fonctionnement. Dans les deux cas, cela a un impact à la fois environnemental et économique.

L'objectif global de ce travail de thèse est d'apporter des éléments pour aider l'utilisateur dans le choix de son modèle et dans l'étape de calage. Ce travail de thèse a été développé en lien avec le groupe de travail IWA "Good Modelling Practice" (GMP-TG) (https://iwa-gmp-tg.cemagref.fr/) dont l'objectif est d'élaborer une procédure de bonnes pratiques en matière de modélisation des boues activées.

Les principaux axes de recherche ont été mieux définis à la suite de l'analyse des résultats d'une enquête effectuée auprès des utilisateurs effectifs et utilisateurs potentiels de ces modèles. Les résultats de cette enquête sont présentés dans le CHAPITRE 2 de la thèse. Les axes de recherche des travaux réalisés en sont déduits, ainsi que la démarche adoptée et le plan de la thèse. Les chapitres suivants sont présentés de manière identique : chaque chapitre débute par un résumé en français, le reste du chapitre étant rédigé en anglais. Ils intègrent un ou plusieurs articles publiés ou en voie de l'être, éventuellement complétés par des données non rapportées dans les articles. Enfin, une conclusion générale en français clôt cette thèse.

CHAPITRE 2 Activated sludge modelling: state of practical use

Le groupe de travail "Good Modelling Practice" (GMP-TG) de l'International Water Association (IWA) (https://iwa-gmp-tg.cemagref.fr/) élabore un guide pour l'utilisation des modèles à boues activées (ASM). Afin de connaitre les besoins des utilisateurs de modèles pour mieux y répondre, un questionnaire a été créé et envoyé en 2007 aux utilisateurs effectifs et potentiels de ces modèles. Les résultats de cette enquête ont fait l'objet d'un article présenté ci-après, et ont permis de préciser les objectifs de thèse.

i. Etat de l'utilisation pratique des modèles ASM

Les objectifs du questionnaire étaient (i) de mieux définir le profil des utilisateurs des modèles, (ii) d'identifier les outils et les procédures utilisés et (iii) de mettre en évidence les principales limites à l'utilisation des modèles de type ASM. Quatre-vingt-six réponses ont été reçues provenant du monde entier, et de plusieurs types d'organisation. Les utilisateurs de modèles ont un profil différent et une utilisation différente des modèles en Europe et en Amérique du Nord. Les nord-américains travaillent majoritairement pour des compagnies privées, alors que les européens sont majoritairement des universitaires. Ils ont pour la plupart acquis leurs connaissances en modélisation par eux-mêmes.

En Europe, les modèles sont utilisés pour l'optimisation du fonctionnement de stations existantes. En Amérique du Nord, ils représentent surtout un outil de conception et de dimensionnement. L'analyse du questionnaire a également montré que les étapes de "collecte de données", de "calage et validation" et de "simulation et interprétation des résultats" sont les plus coûteuses en temps du projet. Parmi la dizaine de modèles biocinétiques disponibles, l'ASM1 est le plus largement utilisé.

Les résultats ont mis en évidence les principaux verrous à l'utilisation des modèles et les principales requêtes pour l'amélioration des procédures de modélisation. Celles-ci portent principalement sur la normalisation des procédures de modélisation disponibles et sur un meilleur transfert des connaissances.

Ces résultats ont été publiés dans l'article suivant :

Hauduc, H., Gillot, S., Rieger, L., Ohtsuki, T., Shaw, A., Takacs, I., Winkler, S. (2009) Activated sludge modelling in practice - An international survey, *Water Science and Technology*, **60**(8), 1943-1951.

ii. Problématique et objectifs de la thèse

Les travaux réalisés rapportés dans cette thèse s'inscrivent pour partie dans les activités du groupe de travail GMP de l'IWA, et ont donc pour but principal de promouvoir les bonnes pratiques en matière de modélisation et de contribuer à rendre la modélisation des stations d'épuration plus accessible aux utilisateurs potentiels. Les deux problèmes pour la mise en place de modèles ASM, mis en exergue dans l'introduction (CHAPITRE 1), sont confirmés par les résultats du questionnaire, à savoir :

- **le choix du modèle** adéquat parmi les modèles biocinétiques disponibles. En effet, les utilisateurs de modèles n'ont pas toujours reçu de formation leur apportant les connaissances nécessaires au choix d'un modèle adapté à leurs objectifs.

- **l'étape de calage** du modèle qui a été soulignée comme étant une étape critique pour les utilisateurs de modèles de type ASM. Les jeux de paramètres publiés avec les modèles sont souvent utilisés comme valeurs initiales à l'étape de calage, or seul l'ASM1 présente ces valeurs comme des valeurs "par défaut" validées.

Les objectifs des travaux réalisés ont donc été fixés pour répondre à ces problématiques :

1. **Analyse des connaissances pratiques des modèles :** L'objectif est d'exploiter l'expérience pratique disponible pour la rendre accessible aux utilisateurs afin d'améliorer le transfert des connaissances en modélisation.

2. **Analyse des connaissances théoriques :** L'objectif est de développer une méthode pour faciliter la compréhension des modèles biocinétiques de stations d'épuration, et de définir les limites théoriques de ces modèles (hypothèses simplificatrices utilisées, processus non pris en compte…), ce qui aidera les utilisateurs à choisir le modèle adapté à leur projet.

3. **Méthodologie pour l'obtention d'un jeu de paramètres par défaut :** L'objectif est de mettre en place une méthodologie pour déterminer pour chacun des modèles un jeu de paramètre "par défaut" optimisé pour une grande diversité de conditions de fonctionnement. Ce jeu de paramètre par défaut pourra être utilisé comme point de départ à l'étape de calage.

La Figure 2-1 récapitule la problématique posée, les objectifs fixés et les résultats attendus pour le projet de thèse.

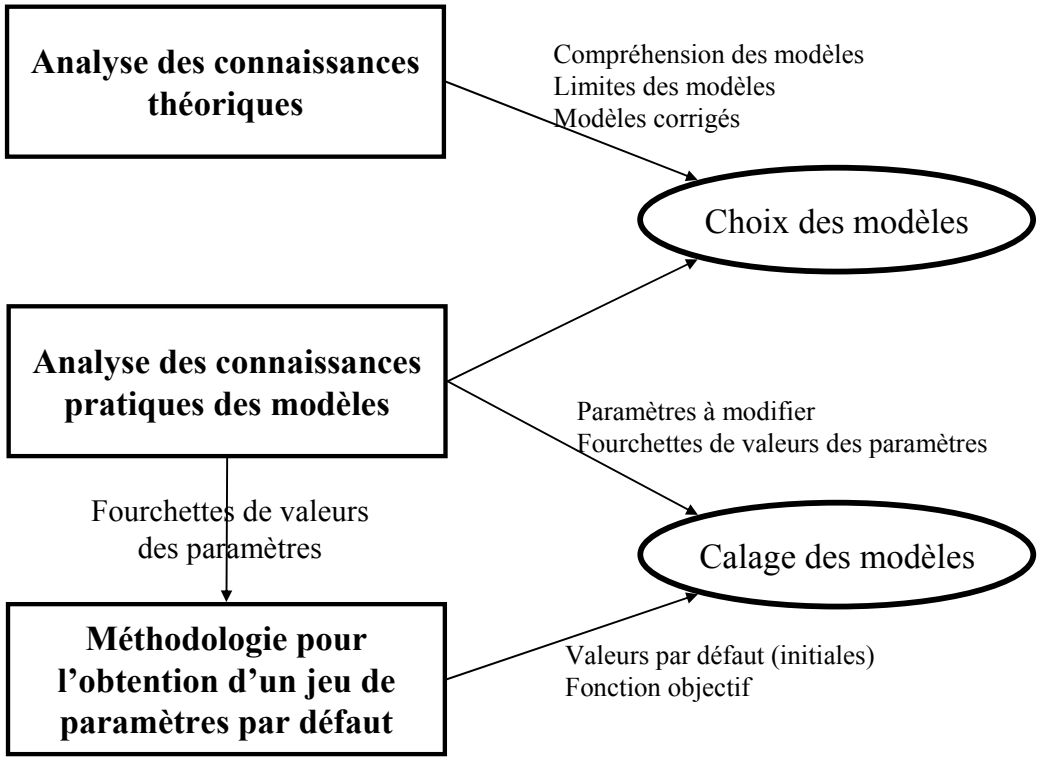


Figure 2-1. Synthèse et interactions de la problématique (à droite), des objectifs (à gauche) et des résultats attendus

Les travaux de recherche présentés se concentrent sur le traitement des eaux usées municipales. Les modèles retenus pour l'analyse sont les suivants :

- ASM1 (Henze *et al.*, 2000a)
- Barker & Dold model (New General) (Barker and Dold, 1997)
- ASM2d (Henze *et al.*, 2000b)
- ASM3 (Gujer *et al.*, 2000)
- ASM3+BioP (Rieger *et al.*, 2001)
- ASM2d+TUD (Meijer, 2004)
- UCTPHO+ (Hu *et al.*, 2007)

Ces modèles couvrent l'ensemble des processus modélisés en boues activées.

2.1 Activated Sludge Modelling in Practice - An International Survey[1]

2.1.1 Introduction

Activated Sludge Models (ASM) are now widely used for Wastewater Treatment Plant (WWTP) design, optimisation, operation and training. The decisions used in the design and optimisation of WWTPs have significant financial and environmental impacts; therefore they should be based on high quality models. Reaching the correct level of quality is thus a key topic for all model users.

A general framework for building and using activated sludge plant models is needed to increase the quality and efficiency of modelling projects. To this aim, the International Water Association (IWA) formed a Task Group on *Good Modelling Practice - Guidelines for Use of Activated Sludge Models* (GMP-TG) (https://iwa-gmp-tg.cemagref.fr/). Their assignment is to prepare a Scientific and Technical Report that proposes simple and effective procedures in the use of ASM-type models. The ultimate goal is to promote the correct use of ASM-type models by practitioners, and to overcome any major obstacles that prevent widespread use of Activated Sludge Modelling in practice.

A questionnaire was prepared by the GMP-TG and sent out in 2007 to benchmark and collect relevant information on the practical use of modelling. The objectives were threefold: (i) to better define the profile of ASM users, (ii) to identify the tools/procedures that are used (models, guidelines, protocols…) and (iii) to highlight the main limitations encountered while building and using ASM-type models.

[1] Hauduc, H., Gillot, S., Rieger, L., Ohtsuki, T., Shaw, A., Takacs, I., Winkler, S. (2009) Activated sludge modelling in practice - An international survey, *Water Science and Technology*, **60**(8), 1943-1951.

2.1.2 Methodology

2.1.2.1 The questionnaire

The questionnaire was divided into three main parts:

1. *Profile of the respondents*: the educational background of respondents, the type of organisation they are working for, etc.

2. *Questions to ASM users* (including 17 multiple choice and open questions): (i) biological models employed, procedures and platforms used; (ii) motivation for using models and typical pitfalls; and (iii) expectations for the IWA report.

3. *Questions to non-ASM users* (on the basis of 6 multiple choice and open questions): (i) reasons for not using ASMs; (ii) the main obstacles encountered; and (iii) expectations for model improvements.

For the analysis of this questionnaire, the answers of ASM users and non-users on the limitations of modelling projects and expectations were evaluated together.

2.1.2.2 The answers and the response rate

The questionnaire was sent out via several means: by e-mail lists, hand-outs in conferences and seminars, and downloads from partners' websites. 96 completed questionnaires were received but due to the open procedure used for distributing the questionnaire, it was impossible to calculate the response rate. 80% of the respondents were ASM users.

The representativeness of the answers is also unknown, because it is difficult to estimate the number of Activated Sludge Model users worldwide and different user categories may have responded at different rates. Two methods have been used to estimate the total number of ASM modellers worldwide:

- One of the questions referred to the number of ASM users in the company. Using this information alone it would be estimated that there are about 635 (±55) modellers, which is certainly less than the total in the world, since not every company or university has answered the questionnaire. It is difficult for people to know exactly how many people are using ASM models in their company.

- Numbers of sold licences of the latest versions of simulators were provided by some of the software companies. Summing those numbers led to a rough estimation of between 3000 and 5000 modellers worldwide.

2.1.2.3 The encoding

To analyse the results of this questionnaire, it was necessary to encode the answers. In fact the structure of the questionnaire was not appropriate to perform a simple analysis, due to the number of questions allowing free form responses, and because the respondents were allowed to answer several items for each multiple choice question.

The multiple choice question items were considered as a yes/no (coded with 1/0) question: yes if the item has been ticked. Items were created for the proposed topics in open questions. Then the questions were analysed as if they were multiple choice questions.

Several question and answer items were found to be similar among the questions asked to users and non users. As a result, several questions could be gathered into two main areas of concern: what are the obstacles in using wastewater treatment models and what are the expectations for improving modelling.

2.1.2.4 The statistics

Simple statistics were obtained by dividing the number of answers by the number of respondents to the question (96 for general questions, 76 for ASM user questions and 20 for non-ASM user questions). As discussed above, the respondents were allowed to tick several items per question which explains the overlaps in the histograms. To find correlations between the respondents' profiles (continent, organisation type) and their answers, the percentages of answers were calculated for each profile.

The confidence intervals on proportions were calculated with the Wilson interval (Brown *et al.*, 2001), that relies on only one approximation (Central Limit Theorem). According to Brown *et al.* (2001), for this type of questionnaire with few answers, the Wilson interval provides a more suitable interval than the more commonly used Wald interval, that relies on two approximations (CLT and observed proportion is used as an approximation of the true proportion in the population). Nevertheless, due to the

number of answers, the confidence intervals are quite large. Also, they are represented only on the graphs that merge all types of respondents to keep the graphs readable.

It is not possible to conclude on the significance of the results because of several shortcomings:

- the number of respondents is limited;
- the way the survey was sent out was not controlled to ensure a randomly sampled pool of respondents;
- the encoding of free answer question may have introduce some bias.

Nevertheless this study provides qualitative information on the trends in modelling.

2.1.3 Results and discussion

The results are presented in three parts according to the three main objectives of the questionnaire:

- Profile of Respondents
- Practical Use of ASMs
- Obstacles and Expectations for Use of ASMs

The discussion about each part follows the presentation of the results.

2.1.3.1 Profile of Respondents

2.1.3.1.1 Results

Among the 96 responses, 65% were returned from European countries and 20% from North America (see Figure 2-2). Other continents were under-represented, and South America, Africa, Asia and Australia have been merged during the evaluation of responses. Thus, the study focuses primarily on the differences between those North-American and European model users who responded.

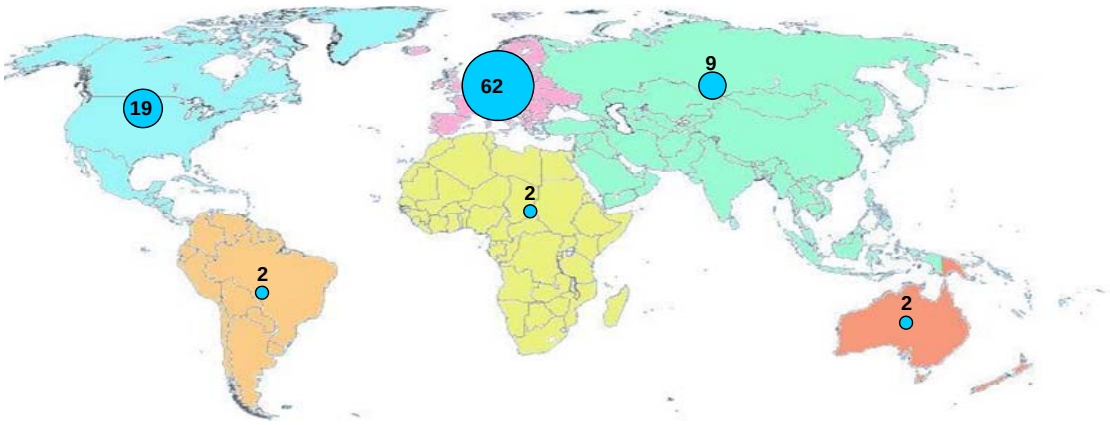


Figure 2-2. Number of answers per continent

Figure 2-3 is split into two parts. On the left is shown the distribution of the organisation types among respondents, and on the right the extrapolated distribution among the number of model users, calculated based on the given number of ASM users in the organisations. The respondents are mainly from universities and public research centres and from private companies. The distribution of the organisation type differs depending on whether the respondents are ASM users or non-users and on their continent (Figure 2-3). One should notice that:

- A greater proportion of non ASM users are from WWTPs and private companies compared to ASM users
- One third (33) of the total respondents are from European universities, which represents more than half of European respondents
- Two thirds of North American respondents are from private companies
- A similar proportion of modellers are seen in each category when comparing actual respondents (a) to the estimated number of modellers (b).
- The predominance of private companies in North America and of universities in Europe is even more important in the extrapolated distribution based on all model users within the organisations.

Since there is only one ASM user from WWTPs, that response is not taken into account when comparing response rates between organisation types.

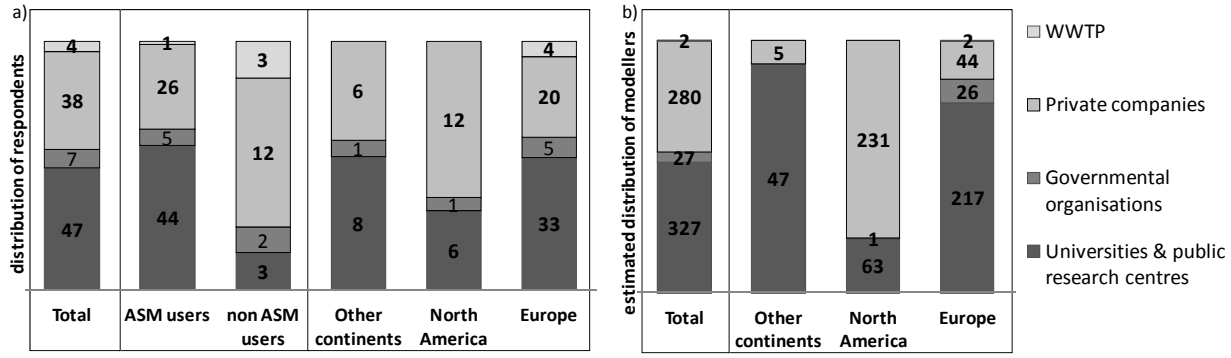


Figure 2-3. Distribution of organisation types among (a) the respondents and (b) the estimated number of model user

About 86% of the respondents have an engineering background, and their knowledge about modelling is acquired predominantly from self training (78%).

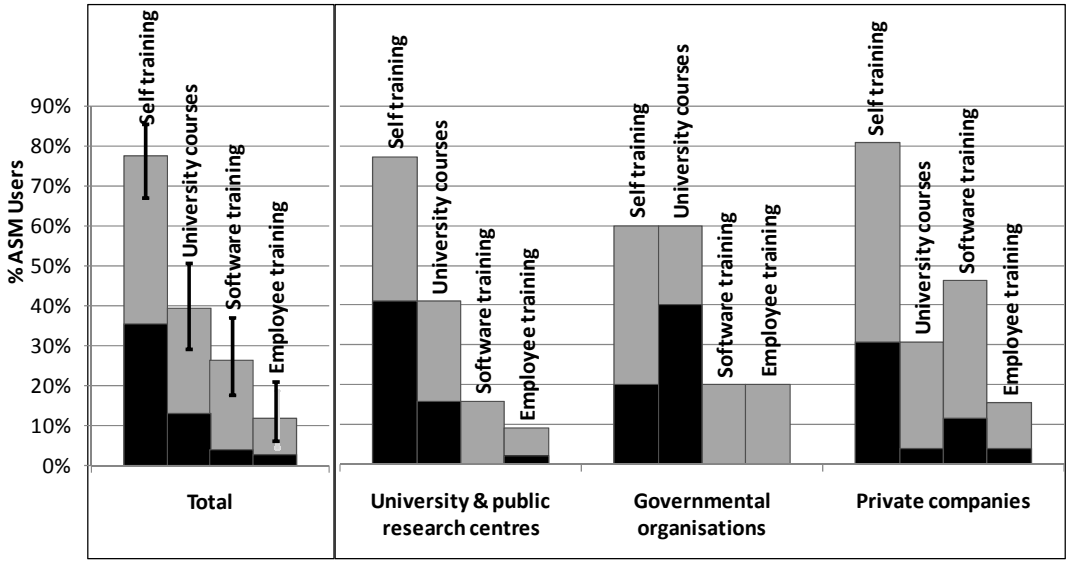


Figure 2-4. Source of knowledge of ASM users per organisation type

Figure 2-4 reveals that the source of knowledge varies among the organisation types. The portion of respondents who answered only one of the four items is indicated in black. Self training is always the main source of knowledge, and for a great proportion of people it is quoted as being their only source of knowledge. Private companies take much more advantage of training offered by software suppliers. Governmental employees using models are different in that they acquire their modelling of knowledge at university and employee training.

2.1.3.1.2 Discussion

The proportion of respondents from WWTPs and industry among non-ASM users reveals that they are interested in WWTP models since they have also answered the questionnaire but for several reasons (discussed below) they do not use them.

The large number of European respondents and especially those from universities is probably due to several factors: the way the questionnaire was distributed, the level of interest in the GMP-TG and the workload. The difference in proportion of European and North-American responses between private companies and universities can be interpreted that in Europe models are mostly a research subject whereas in North America they are predominantly used as an engineering tool in practice.

The engineering background of most of the respondents seems to confirm the hypothesis that wastewater treatment plant modelling is increasingly becoming an engineering tool. However, self training as main source of knowledge reveals a lack of university training and continuing education programs. Self training also includes knowledge transfer into work teams and learning by doing. Thus the proportion of respondents who have answered only one item is relevant. It shows that self training is the only source of knowledge for 31% of commercial ASM users. With limited opportunities in university courses, software providers seem to play an important role in transfer of modelling technology, especially among private companies.

2.1.3.2 Practical Use of ASMs

2.1.3.2.1 Results.

The main objectives cited for building and using a model are: optimisation (59%), design (42%) and prediction of future operations (21%). As shown in Figure 2-5, the modelling tasks differ depending on the organisation type:

- Optimisation (daily plant operation, control...) is the main objective regardless of the organisation type.
- Private companies use models for design (new plant design and expansion) more than any other organisation types.

- Universities are the only ones having a significant use of models for educational purposes.

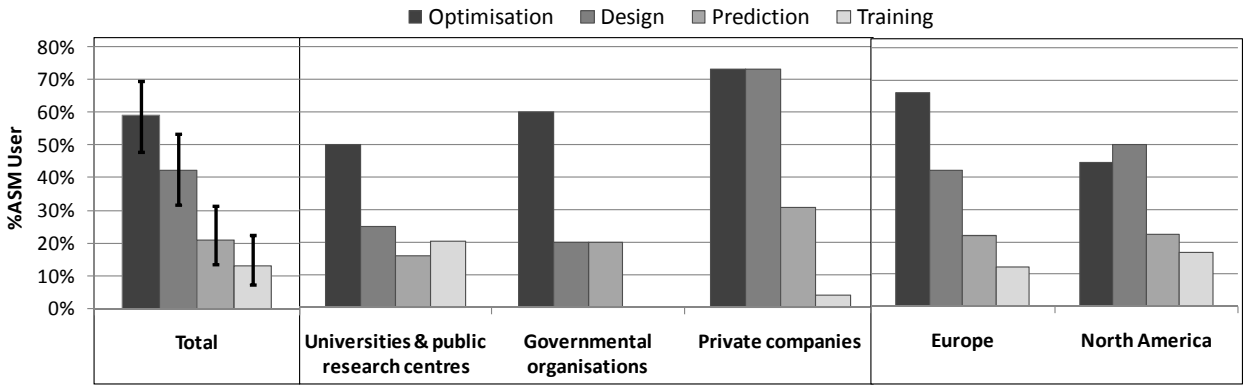


Figure 2-5. Main modelling objectives per organisation type

North-American and European users are using models in a slightly different way. Europeans are more concerned with daily plant operation and control strategies, while North-Americans use models more for plant design (and re-design).

Respondents were asked to state the time allocated to different modelling steps. Following the Good Modelling Practice protocol (http://www.modeleau.org/GMP_TG/UP.htm), the modelling steps that have been considered were:

1. Project definition
2. Data collection and reconciliation
3. Plant model set-up
4. Calibration/ validation
5. Simulation & results interpretation

The results presented in Figure 2-6 highlight the three most time consuming steps: data collection and reconciliation, calibration and validation, and simulation and results interpretation (including reporting). Time allocation for governmental organisations and universities is quite similar. Private and public organisations diverge most in the time spent on the calibration and validation step which is more important for public organisations, and on the simulation and result interpretation step, for which private companies spend more time than any other step.

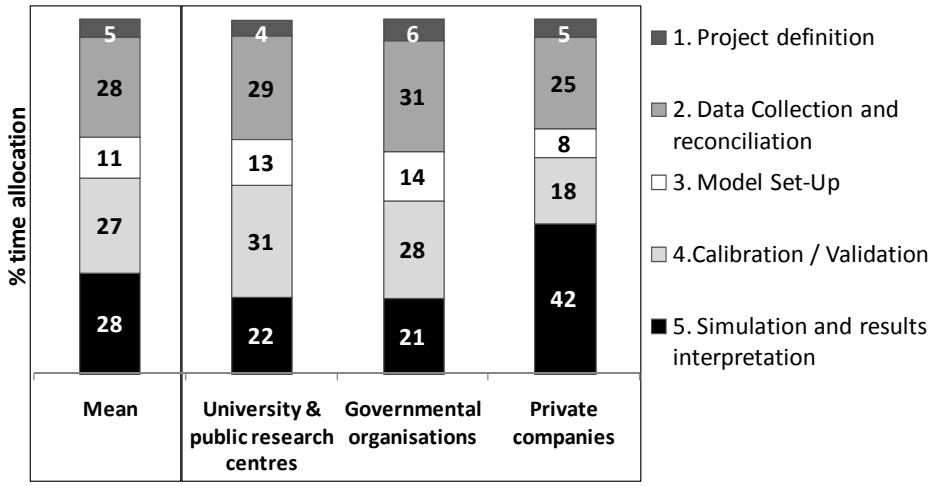


Figure 2-6. Time allocation of protocol steps for each organisation type

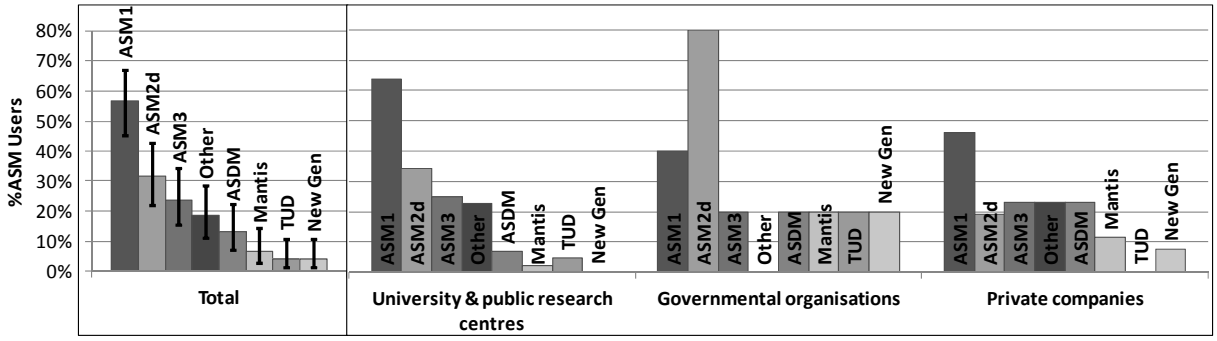


Figure 2-7. Models utilisation per organisation

To meet the modelling objectives (Figure 2-7):

- The most used biokinetics models are 1) ASM1 (Henze *et al.*, 1987) (57%) and 2) ASM2d (Henze *et al.*, 1999) (32 %).
- ASM3 (Gujer *et al.*, 1999) is used equally by each organisation type.
- ASM2d, TUD (Smolders *et al.*, 1995) and New General (Barker and Dold, 1997) are used much more by governmental organisations.
- Universities use mainly ASM1, whereas the preference for one particular model is less important among private companies.
- ASDM (BioWin, 2008) and Mantis (GPS-X, 2008) are much more used by governmental organisations and private companies than in universities.

2.1.3.2.2 Discussion

Consultants are mainly called upon for plant design studies and plant modifications, which is confirmed by these results. The difference between European and North-

American model use - that corresponds to the difference between universities and private companies - could be explained by the fact that in Europe the use of models by consultants is not widespread (see Figure 2-3) since design rules may be imposed (e.g.: the German design guideline ATV, 2000). On the contrary ASM-type modelling is often involved in the North-American WWTP design by consultants. Researchers are actually more concerned with optimisation, prediction and training. Many researchers often use virtual WWTPs as research tools, such as the IWA benchmarks models (COST/IWA benchmark, Jeppsson and Pons, 2004), as this is a relatively inexpensive way to carry out experiments.

The differences in time allocation between organisation types can be mostly explained by their aim in using models. Consultants are mainly using models in a practical way for design and optimisation, thus their major task is to deliver a report with reliable results to their customers. Universities and public research centres mainly use models for research, thus they aim for more detailed models and therefore spend more time on the data collection and reconciliation step and on calibration and validation. Also private companies likely spend less time on model set up, calibration and validation steps thanks to their modelling proficiency and use of typical modelling tasks developed through multiple modelling projects. Finally, consultants mainly use models for design and plant modifications, which do not require an extensive calibration step, as they use parameter sets from their modelling experience.

Another explanation for the limited use of ASM-type models in European engineering practice could be the typically small size of European consulting firms (with the UK as an exception) in comparison to the large and internationally operating North-American firms. The small size does not allow them to maintain critical level of modelling experience in-house. Since modelling is not a standard task yet, very few companies specialized in modelling exist in Europe.

The Mantis and New General models have a similar basis as ASM1. Mantis includes assimilative denitrification, whereas New General includes the Wentzel *et al.* (1992) Bio-P module. Consequently, these results show that ASM1 is the most used model type and many of its adaptations are used for specific processes.

2.1.3.3 Obstacles and Expectations for Use of ASMs

2.1.3.3.1 Results

Modelling projects are limited by a number of obstacles. To cope with these obstacles, respondents expressed several requests to facilitate the use of ASM-models in practice (see Figure 2-8). To keep the figure readable, only the proportion of all respondents is shown. The variation between profile types were included in the study, but are not shown.

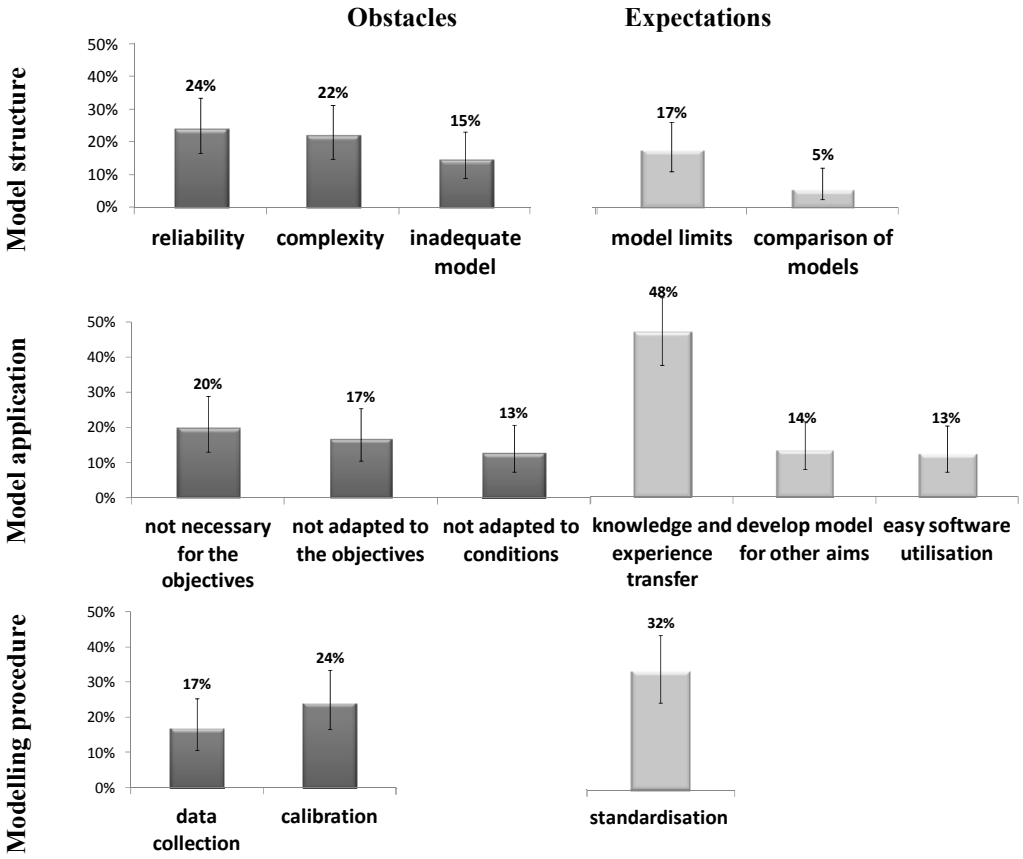


Figure 2-8. Obstacles and expectations

The items can be split into 4 topics:

- **Cost** (17% of respondents) **and time** (16% of respondents) are issues that could be seen as a related problem (not shown on Figure 2-8 for clarity). These obstacles are particularly strong among non-users and respondents from WWTPs.
- The **topic of model structure** is related to the theoretical and mathematical part of modelling. The obstacles expressed are the complexity of the models, the problems of reliability and non-adequacy of the model to simulate the behaviour

of the plant (for example they do not include precipitation phenomena or other specific processes). The expectations to overcome these obstacles are concerned with the definition of model limits and comparison of models. The problem of model reliability and the expectation to clearly state model limitations are quoted by both users and non-users. Comparison of models is not a high expectation among the respondents, but it is relevant to note that it is often requested by governmental organisations and universities, and not by private companies. Model complexity and inadequate models are considered problematic for all.

- **Model application** deals with the practical use of models and their implementation in software. This theme contains the most obstacles. For 20% of the respondents models are not necessary to reach their objectives, simpler methods can be used (e.g. mass balance). On the other hand, about 15% of the respondents claim that available models are not adapted to their objectives (i.e. the particular questions they want answers for). Furthermore, available models are sometimes not adapted to the operational conditions of the plant (for example higher temperature ranges). Consequently respondents, and especially non-ASM users (about 50% of them), are asking for the development of new models and strongly request better knowledge transfer (48%), including sharing case studies. Non-ASM users and respondents from WWTPs expect improvements in software to help carry out modelling steps.
- In the **modelling procedure**, data collection and calibration effort are the main obstacles. The three other modelling steps were not quoted by the respondents. Calibration effort is problematic for ASM users and represents an obstacle for using models among non-users. To solve these problems, people ask for a standardization of the procedures (32%). This expectation is quite important for all respondents, but especially for governmental organisations.

2.1.3.3.2 Discussion

Non-users, respondents from WWTPs and the category “other continents” (including South America, Africa and Asia) are more sensitive to the problems of cost, time demand and complexity of the models. That reveals a bias against models or a lack of knowledge on modelling. Actually, people have to be aware of the benefits of using

models to accept the associated cost. However, modelling requires a certain educational background which is difficult and time consuming to acquire after university studies. The high recurrence of the reliability problem and the expectation of clearer stated model limits show the lack of published technical studies on modelling results. Real and detailed examples would help to determine a realistic model prediction quality.

The reported obstacle by some that models are not required to reach the objectives reveals that these people prefer simpler methods over ASM-type models to meet their objectives. Non-ASM users particularly request the development of models for other aims but also for easier software. As the first statement is far less mentioned by other respondents, it seems that non-ASM users could have some bias or misinformation on model applications. As respondents from WWTPs also ask for more user-friendly software, this could reveal that currently available software is not straightforward for non-experienced people. But a contradiction remains between the wish to have models that cover an even larger number of processes and more user-friendly software despite the increased number of parameters and variables.

The questionnaire indicated that some users and non-users of the models (24%, see Figure 2-8) have reservations about the usefulness and accuracy of models. Two main misuses could be observed and corroborated by the results:

- Spending too much time on calibration without ensuring high quality data. For ASM users this is reflected by the time allocated to calibration. It is also a misconception from non-ASM users that calibration should be a big effort, although data collection does not seem to be a problem for them.

- Lacking methodology for the validation step. Modellers tend to use the independent validation data set for what is in effect a second calibration and not a validation at all. Consultants even often neglect the validation step altogether. The result is a model with a limited or unknown prediction capability, which could subsequently lead to a general mistrust in models.

2.1.4 Conclusion

This survey provided useful insights into the use of activated sludge models. It also pointed out the main limitations of modelling in the minds of users and the expectations of users for improvements.

Generally speaking, the majority of North-American and European modellers are using models in different ways. In Europe, models are most often used by researchers for optimisation purposes, while in North America most modellers are employed by private companies and carry out design studies. Modelling is an engineering tool, but a lack of relevant training has been highlighted. This study also reveals that models are sometimes not properly applied, probably due to a lack of knowledge and standardised procedures.

The development of standardised modelling procedures and better knowledge transfer by making some practical case studies available should address such obstacles as:

- the complexity (apparent or actual) of the model theories and modelling procedures,
- the time consuming steps and therefore the cost of modelling and
- the modellers' appreciation of the general reliability of the models.

2.2 Problem statement

Mathematical modelling of activated sludge systems is a widely accepted tool to optimize existing structures, to improve design and operation of wastewater treatment plants. The use of models to meet such challenges can not be envisaged without ensuring that their quality is adequate for different modelling objectives. To increase the quality of modelling studies, this thesis has selected to deal with two obstacles that have been raised in the introduction and in the analysis of the questionnaire: the choice of the appropriate models and the calibration of these models.

2.2.1 Model selection

Several biokinetic models are available. To our knowledge, published papers only compare two models side by side (Lubken *et al.*, 2003; Guisasola *et al.*, 2005) and are conducted on specific case studies. So far no project has compared the existing models for their concepts and their applicability for different treatment conditions. One can then wonder whether specific models may be better adapted to given objectives and whether these models give similar results, when subjected to a variety of process conditions.

In addition, these models require a lot of time and effort to set up, calibrate and use. Model users do not always have the necessary knowledge to establish a model suitable for their objectives. However, a good quality of the model is critical to support decisions appropriate to the economic and environmental project conditions.

2.2.2 Calibration step

The Good Modelling Practice task group defines five steps that should be followed in a modelling project:

1. Project definition
2. Data collection and reconciliation
3. Plant model set-up
4. Calibration/ validation
5. Simulation & results interpretation

The questionnaire analysis highlights that the model calibration step is a critical step for ASM type model users: at the expense of data collection, much energy is devoted to

calibration, which is perceived as a complicated and fastidious step. These models are furthermore nonlinear and the success of parameter estimation depends heavily on the values initially assigned. On the other hand, some parameters have little influence on the variables and thus it is often unnecessary to include them in the calibration step. Some are very influential, but can reach a non-physically meaning value through a purely mathematical calibration (Gernaey *et al.*, 2004).

Default parameter sets are often used as initial values for calibration step, or for a first approximation of the model results. However, a set of default parameters only exists for the ASM1 model. Nevertheless, users often use the values published with other models as default parameters, although these values are not validated (Langergraber *et al.*, 2004).

To facilitate the calibration step and ensure adequate quality for the modelling objectives, it would be useful to have default parameter sets to use as initial values in the calibration step, indications on parameters that should be included in the calibration step, and ranges of values within which these parameters can be changed.

2.3 Objectives of the thesis

This work is partly included in the GMP task group's activities (https://iwa-gmp-tg.cemagref.fr/). Therefore, the objectives of this research are to answer some of the questions and expectations highlighted in the analysis of the questionnaire submitted to the WWTPs effective and potential model users and to contribute to make the ASM modelling more accessible to them. To overcome the obstacles of model selection and calibration, three main objectives were defined:

- **Analysing the practical knowledge on models** to synthesise the practical experience available and make it accessible to users, and address the need for knowledge transfer required by models users. This includes an analysis of typical case studies, of the modelling procedure used (data reconciliation, model calibration and especially modified parameters and values used) and of the practical pitfalls in using models.

- **Analysing the theoretical knowledge** to synthesise the knowledge available on the studied models, highlight differences between the models concepts and draw the theoretical limits to their use. The aim is to help model users to better understand models and to be able to select the adequate model for their study.

- **Developping of a methodology to obtain default parameter sets** to facilitate the model calibration step for each model. Such methodology should help providing for each model a set of "default" parameter values optimized for a specific range of operating conditions.

Figure 2-9 summarises the issues raised, the objectives and deliverables of this work.

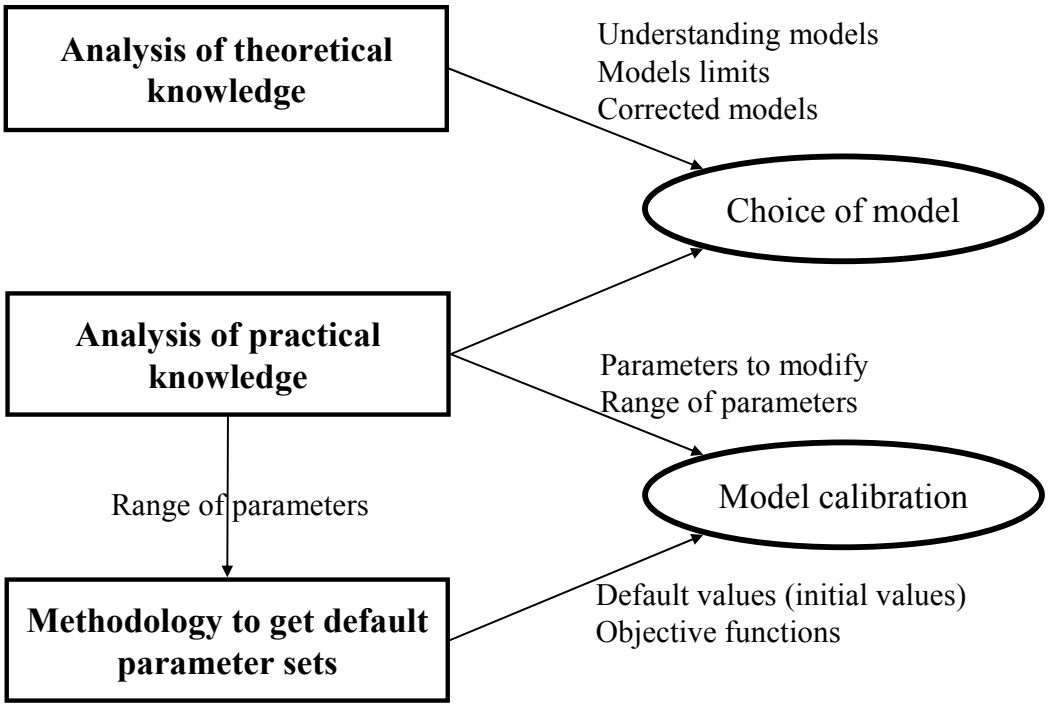


Figure 2-9. Synthesis and interactions of the issues (right), objectives (left) and results of the thesis

2.4 Delineation of the work

This research work focuses on the treatment of municipal wastewater. The models selected for the analysis are the following:

- ASM1 (Henze *et al.*, 2000a)
- Barker & Dold model (New General) (Barker and Dold, 1997)
- ASM2d (Henze *et al.*, 2000b)
- ASM3 (Gujer *et al.*, 2000)
- ASM3+BioP (Rieger *et al.*, 2001)
- ASM2d+TUD (Meijer, 2004)
- UCTPHO+ (Hu *et al.*, 2007)

These models integrate most of the processes and concepts modelled in activated sludge.

2.5 Outline of the thesis

The three research objectives are developed in the subsequent chapters of the thesis. The chapters 3 and 4, focusing on the state of practical and theoretical knowledge on models respecticely, are based on three published articles. The last objective, methodology to get default parameter sets, will be in the form of a dissertation chapter.

- **Chapter 3. Analysis of practical knowledge on models:** A database of practical applications that includes answers to a questionnaire and a literature review on published modelling projects has been built. The database is analysed to determine which biokinetic model parameters are usually changed by modellers, in which ranges, and what values are typically used. The questionnaire provides further information such as typical fractions (influent and sludge characteristics). Such information is useful in the data reconciliation step of the modelling exercice.

- **Chapter 4. Analysis of theoretical knowledge:** The models are first studied one by one and their stoichiometric continuity and kinetic consistency are verified. Then the modelling concepts used are compared and confronted to theoretical knowledge on the process mechanisms. This comparison highlights the theoretical limits to the use of the differents models studied.

- **Chapter 5. Methodology to get default parameter sets:** This part first describes the development of an automated calibration procedure that provides reproducible results, which can be used simultaneously on several data sets. This automated procedure requires the definition at least of one objective function that evaluates the quality of the calibration. Finally, the procedure is adapted to simultaneous multiple dataset calibration.

Finally, the conclusion of this document synthesises the main research results obtained.

CHAPITRE 3 Analysis of practical knowledge

Lors de la définition des besoins des utilisateurs des modèles (voir paragraphe 2.1), l'une des principales requêtes portait sur un meilleur transfert des connaissances en modélisation. L'objectif fixé pour ce travail était donc de recenser les connaissances pratiques sur l'utilisation des modèles à partir des réponses d'un second questionnaire et d'une revue de littérature. Cette analyse a fait l'objet d'un article. Le questionnaire a d'autre part permis de recenser les ratios typiques caractérisant l'influent et les boues activés utilisés. Ces résultats n'ont pas été inclus dans l'article mais sont présentés dans ce chapitre.

i. Développement et utilisation potentielle d'une base de données de projets de modélisation

Une base de données de projets de modélisation, contenant 77 jeux de paramètres, a été créée à partir i) des réponses à un questionnaire envoyé aux utilisateurs de modèles en 2008 pour fournir des informations pour le GMP-TG, et ii) d'une synthèse bibliographique de projets de modélisation publiés. La base de données est analysée afin de déterminer quels sont les paramètres du modèle biocinétique les plus souvent modifiés et les valeurs utilisées. Faute d'exemples suffisants pour chacun des modèles étudiés, seuls les résultats pour les modèles ASM1 et ASM2d ont pu être exploités en détail.

Concernant **l'ASM1**, le couple de paramètres ($\mu_{ANO,Max}$, b_{ANO}), le taux de croissance maximum et le taux de décès des autotrophes, est souvent modifié, alors que plusieurs études ont montré que fixer b_{ANO} à une valeur plus élevée que celle initialement proposée (0.17 d^{-1} au lieu de 0.10 d^{-1} à 20°C) permettait de ne pas modifier la valeur de $\mu_{ANO,Max}$ en cas de variation de l'âge de boues. D'autre part, certains utilisateurs ont modifié la structure du modèle en introduisant un rendement hétérotrophe plus faible en anoxie (0.54 g X_{OHO}.g X_{CB}^{-1} à 20°C). Enfin, les trois derniers paramètres remarquables dans la base de données sont des coefficients de demi-saturation, $K_{SB,OHO}$, $K_{NOx,OHO}$, et $K_{NHx,ANO}$, réputés fortement dépendre des conditions environnementales.

Pour **l'ASM2d**, les paramètres les plus modifiés sont exclusivement des paramètres cinétiques. Mais ce sont les paramètres qui concernent les PAO qui présentent la plus grande variabilité : le taux d'absorption des acides gras volatils (q_{PAO,VFA_Stor}) et le taux de stockage des polyP ($q_{PAO,PO4\_PP}$). Penya-Roja *et al.* (2002) suggèrent que ces fortes

variations sont dues au fait que le modèle ne prend pas en compte le stockage du glycogène.

Ces résultats devraient aider les utilisateurs de modèles dans l'étape de calage, en fournissant les valeurs des paramètres typiques comme point de départ et les fourchettes de valeur comme un guide. Toutefois, les valeurs proposées doivent être utilisées avec beaucoup de soin car elles ne prennent pas en compte les corrélations potentielles entre les paramètres.

Ces résultats on été partiellement inclus dans l'article suivant :

Hauduc H., Rieger L., Ohtsuki T., Shaw A., Takács I., Winkler S., Heduit A, Vanrolleghem P.A. and Gillot S. (in Press) Activated sludge modelling: Development and potential use of a practical applications database, *Water Science and Technology,* In Press.

ii. Autres résultats issus du questionnaire : les ratios typiques

Un autre objectif du deuxième questionnaire était de collecter des données sur les conditions de traitement des différentes zones géographiques, et notamment les ratios typiques caractérisant les eaux résiduaires et les boues activées. Bien que le manque de données n'ait pas permis de différencier les zones géographiques lors de l'analyse, les réponses correspondent dans l'ensemble aux valeurs trouvées dans la littérature, et peuvent être utilisées comme outil de validation et réconciliation des données.

3.1 Introduction

When analysing the requirements of the model users (see paragraph 2.1), a major request concerns a better transfer of modelling knowledge. Some model users have published the results of their modelling projects. However, published results are scattered and not always easily accessible (e.g.conference). In addition, the access to scientific journals is often limited to users from universities and research centres. Thus, the practical experience already published is difficult to access and synthesise by many water professionals.

The aim of this chapter is to contribute to the transfer of modelling knowledge by the development of a database of practical modelling applications and by getting inputs from model users through a second questionnaire.

3.2 Development and Potential Use of a Practical Applications Database[2]

3.2.1 Introduction

The International Water Association (IWA) Task Group on *Good Modelling Practice – Guidelines for use of activated sludge models* (GMP-TG, https://iwa-gmp-tg.cemagref.fr/) is collecting knowledge and experience on how to use activated sludge (AS) models in engineering practice. The group developed and sent out a first questionnaire to current and potential users of activated sludge models to better define the profile of ASM users and to identify the tools and procedures used. Ninety-six answers were received that provided useful insights into the use of activated sludge models and highlighted the main limitations of modelling and the expectations of users for improvements (Hauduc *et al.*, 2009). The calibration step was pointed out especially as one of the most time-consuming steps and is considered as an obstacle for widespread model use. Respondents also asked for better knowledge transfer.

[2] Hauduc H., Rieger L., Ohtsuki T., Shaw A., Takács I., Winkler S., Heduit A, Vanrolleghem P.A. and Gillot S. (in Press) Activated sludge modelling: Development and potential use of a practical applications database, *Water Science and Technology,* In Press.

A second, more detailed, questionnaire was sent out in 2008 to provide inputs for the GMP-TG report regarding typical parameter values and case studies from several countries and for different wastewater treatment conditions. In addition and as a second source of information, a literature review was carried out on published modelling projects. The objective of this work was to collect available experiences of practical applications using AS models. A database was constructed to synthesise the answers from the second questionnaire and literature data.

The database includes parameters for seven published activated sludge models: (1) ASM1 (Henze *et al.*, 2000a); (2) ASM2d (Henze *et al.*, 2000b); (3) ASM3 (Gujer *et al.*, 2000); (4) ASM3+BioP (Rieger *et al.*, 2001); (5) ASM2d+TUD (Meijer, 2004); (6) Barker & Dold model (Barker and Dold, 1997); (7) UCTPHO+ (Hu *et al.*, 2007). In order to keep this chapter readable, these references will not be repeated each time. Prior to this parameter study, all models were analysed for typos and errors (Hauduc *et al.*, 2010).

3.2.2 Method

3.2.2.1 Source of data

3.2.2.1.1 Questionnaire

In order to completely describe each modelling study, the questionnaire asked for the objectives of the project, the description of the wastewater treatment plant (WWTP) and the parameter set used for the biokinetic model. The questionnaire was sent out in 2008 to the respondents of the first survey, to the attendees of the WWTmod2008 seminar in Mont-St-Anne, QC, Canada, and could be downloaded from GMP-TG sponsor websites.

Probably due to the higher complexity of this questionnaire, only 28 answers were received, among which 17 were usable for this study (i.e. at least one model parameter set provided).

3.2.2.1.2 Literature review on published modelling projects

In order to have a homogeneous database, only published modelling projects applied to full-scale WWTPs or pilot plants with a major domestic wastewater influent were selected. The review includes 50 articles containing 59 parameter sets.

3.2.2.2 Database description

3.2.2.2.1 Structure

In order to store all the information in an efficient way, a database composed of three main tables was constructed:

1. **Parameter sets**: model, country, temperature, parameter values
2. **WWTP description**: information on influent, wastewater characteristics, processes and environmental conditions
3. **Model users**: user information.

These tables are linked by common information, such as the code of the modeller or the WWTP (Figure 3-1), which ensures traceability of information.

The information included in the database and an overview of the forms is presented in ANNEXE 1.

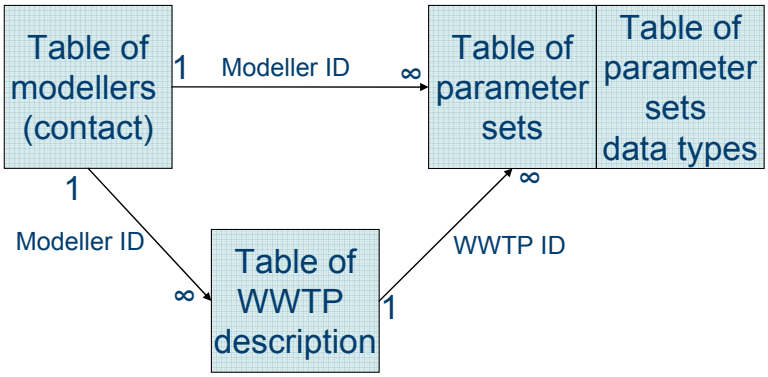


Figure 3-1. Database structure

To limit the number of fields in the parameter sets table, the parameters of all models were renamed with the standardised notation of Corominas *et al.* (2010), therefore allowing the parameters that are similar between models to be compared directly.

3.2.2.2.2 Classification of parameter sets

Two classes of model parameter sets were distinguished:

- **Optimised parameter sets** obtained for a specific modelling project. These parameter sets were provided with the description of the WWTP under study. Parameter values may have different sources (see below).
- **Proposed new default parameter sets** based on personal expertise. These parameters were used as starting points for the calibration step during the project and given with an approximate number of WWTPs on which this experience was gained.

Figure 3-2 summarises the distribution of the 76 parameter sets over these two classes and over their origin.

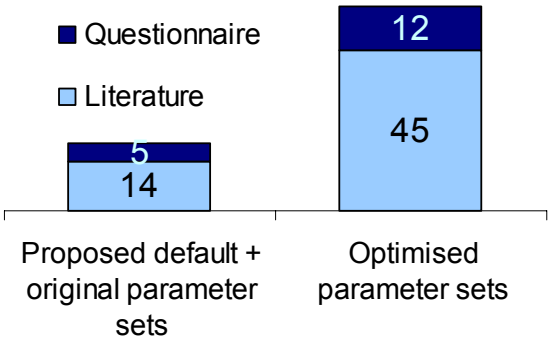


Figure 3-2. Distribution of parameter sets by type and origin

3.2.2.2.3 Sources of parameter values.

According to the way it was obtained, a parameter value could be qualified as:

- **Original**: value given in the original publication of the model;
- **New Default**: value given in a proposed new default parameter set;
- **Measured**: value is obtained using a dedicated experimental protocol;
- **Calibrated**: value is changed either using a manual or an automatic procedure to fit simulation results to the data collected on the WWTP.

3.2.2.2.4 Temperature adjustment.

For comparison purposes, the parameter values were standardised at 20°C. The correction factor was either provided with the dataset or extracted from the original publication. However, for ASM1 and ASM2d original publications, the kinetic parameters are given at 10°C and 20°C. The correction factor θ_{pow} has thus been recalculated following the equation $k_{10°C}=k_{20°C}*\theta_{pow}^{10-20}$.

3.2.2.3 Database analysis

The database was analysed for the three topics described below and represented on Figure 3-3.

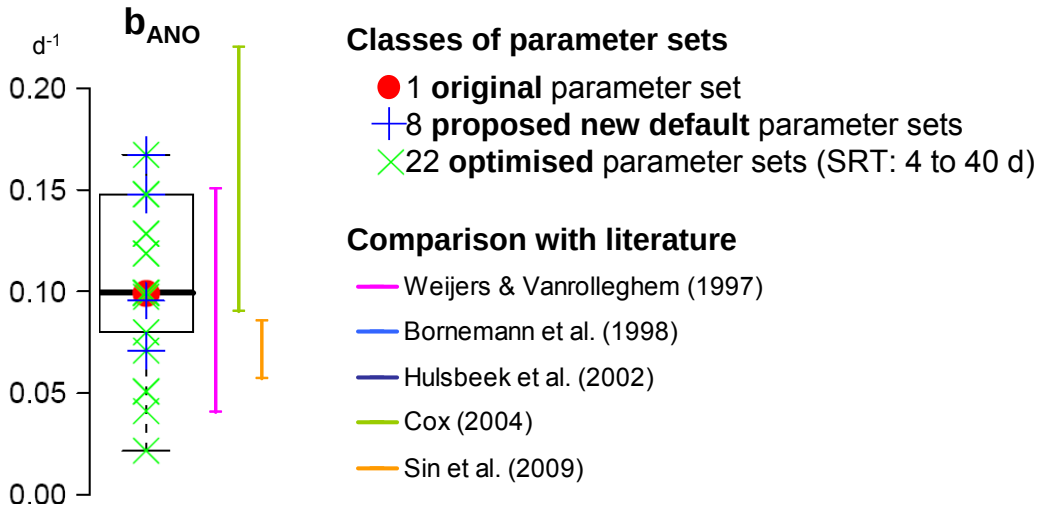


Figure 3-3. Analysis of parameter sets from the database: the example of b_{ANO}

Original/proposed new default parameter sets: The proposed default parameter sets (in blue + in Figure 3-3) are compared to the original ones (in red ●). The parameter values differences are identified and discussed.

Parameters changed in modelling projects: The optimised parameter set values are then considered (in green X). Most often changed parameters (in more than 50% of the projects) are highlighted.

Parameter ranges and statistics: For each model the median value (bold line in Figure 3-3), variables have been calculated:

- The median values, which should not be misinterpreted as new default parameters, because the median values are not from a single parameter set and some parameters may be correlated (e.g. growth and decay rate),
- The 25th and 75th percentiles (bottom and top of the box). These percentiles have been chosen to exclude extreme values and to obtain a representative range of the typical parameter values,
- The variability (V), the difference between the two percentiles divided by the median.

These results are discussed and confronted to the knowledge on parameter values and parameter ranges of other published overview studies.

3.2.3 Results

3.2.3.1 Modelling project characteristics

The database contains 76 parameter sets, which can be differentiated into 57 optimised parameter sets and 19 proposed new default parameter sets, and distributed as shown in Figure 3-4. ASM1 and ASM2d are the models most represented in the database.

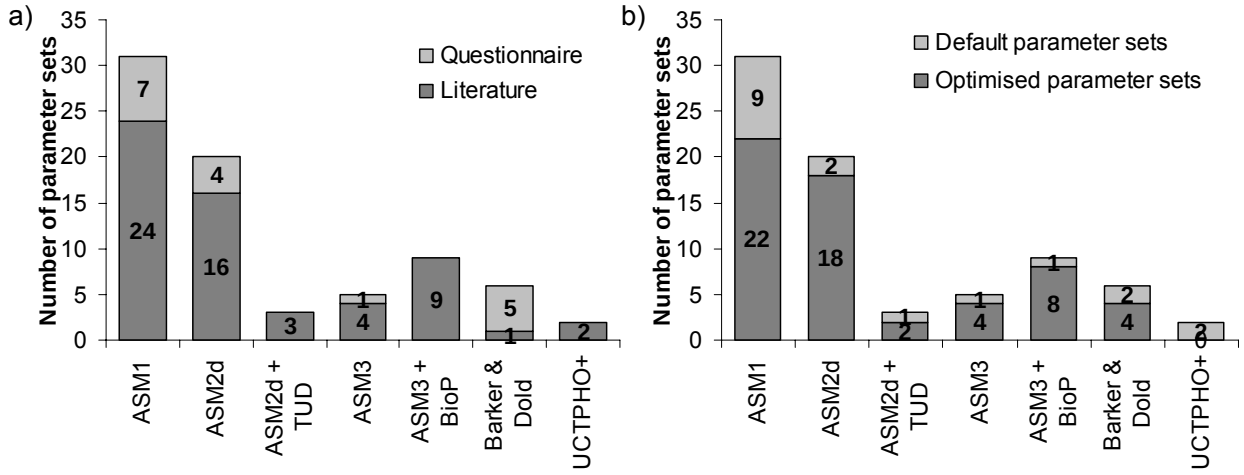


Figure 3-4**.** Distribution of parameter sets per model and a) per source and b) per class of parameter set

The following paragraphs describe the main information extracted from the current database for ASM1 and ASM2d. An insufficient number of modelling studies is available for the other models, thus no comments are given on the results for these models. However, synthesis tables are presented in the ANNEXE 1 for ASM3, ASM3+BioP and Barker & Dold model. Concerning ASM2d+TUD and UCTPHO+, no additional modelling projects than those in the original publication were found, the tables are thus not presented.

3.2.3.2 ASM1

3.2.3.2.1 Data description.

The database contains 31 parameter sets for ASM1, of which 9 are "proposed new default parameter" sets and 22 are "optimised parameter sets" from specific modelling

projects. The modelling studies were mainly carried out at full scale WWTPs (19) mostly in Europe (18), with only 1 application in North-America and 3 in Asia. The sludge ages of the specific modelling projects are between 4 and 40 days.

Table 3-2 presents the main results extracted from the database including the original and the proposed new default parameter sets. Basic statistics for optimised parameter sets comprise the number of values for each parameter (n), if the parameter has been modified in more than 50% of the cases (Modif. >50%), the median value (Med.), the 25^{th} and 75^{th} percentiles and the variability (V). The proposed new default parameter sets are by definition based on several simulation studies and therefore present more experience than single studies. Consequently, they are presented on the same level as the median of all the optimised parameter sets.

Original/proposed new default parameter set: Only 3 parameters (out of 26) have not been changed compared to the original value: the autotrophic growth yield (Y_{ANO}), the fraction of particulate unbiodegradable organics generated in biomass decay ($f_{XU\_Bio,lys}$) and the nitrogen content of unbiodegradable organics generated in biomass decay (i_{N_XUE}).

A change in ASM1 model structure for the ordinary heterotrophic yield (Y_{OHO}) value by introducing an ordinary heterotrophic yield under anoxic conditions is suggested in three of the proposed new default parameter sets.

Parameters changed in modelling projects (compared to original values): for each parameter set, a majority of parameters are kept at their default values. Only the autotrophic growth yield (Y_{ANO}) is always kept at its original value. Nine parameters were changed in more than half of the modelling studies: 6 temperature correction factors, the heterotrophic yield (Y_{OHO}) and the autotrophic growth and decay rate pair ($\mu_{ANO,Max}$, b_{ANO}).

Only a few parameter sets contain measured parameters (Stamou *et al.*, 1999; Makinia and Wells, 2000; Petersen *et al.*, 2002a; Nuhoglu *et al.*, 2005). Most of the measured values are close to the values used in other modelling projects, except for Stamou *et al.* (1999) who determined very low values for the heterotrophic and autotrophic growth related parameters.

Table 3-1.Synthesis of database results for ASM1, only modified parameters are mentioned. Parameter values are standardised at a temperature of 20°C.

Parameter *	Unit	Description	Original parameter set		Optimised parameter sets						Proposed new default parameters
			Notation	Value (a)	n	Modif >50%	Med.	Perc. 25%	Perc. 75%	V (%)	Parameter sets: b / c / d / e / f / g / h / i
Stoichiometric parameters											
Y_{OHO}	g X_{OHO}.g XC_B^{-1}	Yield for X_{OHO} growth	Y_H	**0.67**	26	X	**0.67**	0.62	0.67	7	0.6*(c;i)* $Y_{OHO.Ox}$: 0.67 and $Y_{OHO.Ax}$: 0.54 (b;f;h)
Conversion coefficient											
i_{N_XBio}	g N.g X_{Bio}^{-1}	N content of biomass (X_{OHO}, X_{PAO}, X_{ANO})	$i_{X,B}$	**0.086**	31		**0.086**	0.079	0.086	8	0.08*(c;g)*
Kinetic parameters											
Hydrolysis											
$q_{XCB\_SB,hyd}$	g XC_B.g X_{OHO}^{-1}.d^{-1}	Maximum specific hydrolysis rate	k_h	**3**	31		**3**	2.2	3	26	2*(c)* / 2.21*(i)* / 5.2*(g)*
$\theta_{qXCB\_SB,hyd}$	-	Temperature correction factor for $q_{XCB\_SB,hyd}$	θ_{kh}	**1.116**	11	X	**1.116**	1.072	1.12	4	1.072*(f)*
$K_{XCB,hyd}$	g XC_B.g X_{OHO}^{-1}	Half-saturation coefficient for XC_B/X_{OHO}	K_X	**0.03**	30		**0.03**	0.03	0.03	0	0.02*(c)* / 0.17*(g)* / 0.15*(i)*
$\theta_{KXCB,hyd}$	-	Temperature correction factor for $K_{XCB,hyd}$	θ_{KX}	**1.116**	10	X	**1.116**	1.116	1.12	0	1*(f)*
$\eta_{qhyd,Ax}$	-	Correction factor for hyd. under anoxic cond.	η_h	**0.4**	31		**0.4**	0.4	0.5	25	0.5*(g)*/ 0.6*(d)* $n_{qhyd.An}$: 0.75*(d)*
Ordinary Heterotrophic Organisms											
$\mu_{OHO,Max}$	d^{-1}	Maximum growth rate of X_{OHO}	μ_H	**6**	31		**6**	5.7	6	6	4*(d)* / 5.7*(g)*
$\theta_{\mu OHO,Max}$	-	Temperature correction factor for $\mu_{OHO,Max}$	$\theta_{\mu H}$	**1.072**	11	X	**1.072**	1.071	1.09	2	
$\eta_{\mu OHO,Ax}$	-	Reduction factor for anoxic growth of X_{OHO}	η_g	**0.8**	31		**0.8**	0.8	0.8	0	0.6*(c)*
$K_{SB,OHO}$	g S_B.m^{-3}	Half-saturation coefficient for S_B	K_S	**20**	31		**20**	10	20	50	5*(d)* / 10*(g)*
b_{OHO}	d^{-1}	Decay rate for X_{OHO}	b_H	**0.62**	31		**0.62**	0.61	0.62	2	0.4*(d)* / 0.41*(i)* / 0.5*(c)* / 0.53*(g)*
θ_{bOHO}	-	Temperature correction factor for b_{OHO}	θ_{bH}	**1.12**	11	X	**1.1**	1.029	1.12	8	1.029*(f)*/ 1.071*(c;d)*
$K_{O2,OHO}$	g S_{O2}.m^{-3}	Half-saturation coefficient for S_{O2}	K_{OH}	**0.2**	31		**0.2**	0.2	0.2	0	0.05*(f)* / 0.1*(i)*
$K_{NOx,OHO}$	g S_{NOx}.m^{-3}	Half-saturation coefficient for S_{NOx}	K_{NO}	**0.5**	31		**0.5**	0.1	0.5	80	0.1*(f)* / 0.2*(i)*
Autotrophic Nitrifying Organisms											
$\mu_{ANO,Max}$	d^{-1}	Maximum growth rate of X_{ANO}	μ_A	**0.8**	30	X	**0.8**	0.66	0.9	30	0.77*(i)* / 0.82*(g)*/ 0.85*(c)* / 0.9*(b; d)*
$\theta_{\mu ANO,Max}$	-	Temperature correction factor for $\mu_{ANO,Max}$	$\theta_{\mu A}$	**1.103**	14	X	**1.103**	1.059	1.11	5	1.059*(f; h)*/ 1.072*(b)*
b_{ANO}	d^{-1}	Decay rate for X_{ANO}	b_A	**0.5-0.15**	30	X	**0.1**	0.08	0.15	70	0.07*(g)* / 0.096*(i)* / 0.17*(b; f; h)*
θ_{bANO}	-	Temperature correction factor for b_{ANO}	θ_{bA}	**1.072**	12	X	**1.07**	1.029	1.072	4	1.027*(f; h)* / 1.083*(d)* / 1.103*(c)*
q_{am}	m^3.g $X_{CB,N}^{-1}$.d^{-1}	Rate constant for ammonification	k_a	**0.08**	29		**0.08**	0.07	0.08	12	0.05*(g)* / 0.16*(i)*
θ_{qam}	-	Temperature correction factor for q_{am}	θ_{ka}	**1.072**	11		**1.07**	1.07	1.07	0	1.071*(d; c)*
$K_{O2,ANO}$	g S_{O2}.m^{-3}	Half-saturation coefficient for S_{O2}	K_{OA}	**0.4**	31		**0.4**	0.4	0.4	0	0.2*(f)* / 0.5*(c)* / 0.75*(i)*
$K_{NHx,ANO}$	g S_{NHx}.m^{-3}	Half-saturation coefficient for S_{NHx}	K_{NH}	**1**	31		**1**	0.75	1	25	0.1*(f)* / 0.5*(d)*

a: Henze *et al.* (2000a); b, c: 2 answers from the questionnaire; d: Bornemann *et al.* (1998); e: Hulsbeek *et al.* (2002); f: Marquot (2006); g: Spanjers *et al.* (1998); h: Choubert *et al.* (2009b); i: Grady *et al.* (1999).

*Standardised notation from Corominas *et al.* (2010) is used. n: number of parameter values in the database.

Please refer to the appendix for the parameter definitions.

Parameter ranges and statistics: All median values are the same as in the original parameter set. The variability is quite narrow (<33%), except for the half-saturation coefficients for substrate ($K_{SB,OHO}$) and nitrate ($K_{NOx,OHO}$) and the autotrophic decay rate (b_{ANO}).

3.2.3.2.2 Discussion

Original vs. proposed new default parameter sets: The need to change the ASM1 model structure by introducing a heterotrophic yield under anoxic conditions ($Y_{OHO,Ax}$) to properly model the nitrate and COD consumption was experimentally proven by Orhon *et al.* (1996). A new default value of 0.54 g X_{OHO}.g XC_B^{-1} is proposed by Choubert *et al.* (2009a), based on full-scale modelling studies.

The change of the maximum autotrophic growth rate ($\mu_{ANO,Max}$) and decay rate (b_{ANO}) is discussed in Dold *et al.* (2005). The authors showed that it was no longer necessary to modify $\mu_{ANO,Max}$ when the sludge retention time (SRT) varies if a higher b_{ANO} value is used (experimentally measured to 0.19 ±0.4 d^{-1}). Choubert *et al.* (2009b) proposed the values of $\mu_{ANO,Max}$=0.8 d^{-1} and b_{ANO}=0.17 d^{-1} at 20°C as new default values validated on 13 full-scale WWTPs in France.

Parameters changed in modelling projects (compared to original values): Similar to the proposed new default parameter sets a reduced heterotrophic growth rate (Y_{OHO}) is often associated with plants with anoxic and/or anaerobic zones. This confirms the need to differentiate aerobic and anoxic growth yields.

The couple ($\mu_{ANO,Max}$, b_{ANO}) is modified in most studies. However, in the analysed modelling projects a high maximum growth rate was not always compensated by a high decay rate.

In addition, the temperature correction factor values are sometimes re-evaluated in the course of a project. They are deduced from the parameter determination at a different temperature and therefore include measurement uncertainties.

Parameter ranges and statistics: The ranges provided by the 25th and 75th percentiles of the database are generally in agreement with other overview studies, which ranges were not included in the database (Weijers *et al.*, 1996; Bornemann *et al.*, 1998; Hulsbeek *et*

al., 2002; Cox, 2004; Sin *et al.*, 2009). However, the ranges from the database differ from these studies for the following parameters:

- $\mu_{OHO,Max}$ and b_{OHO} ranges proposed by Weijers and Vanrolleghem (1996) are wider (respectively 2-10 d^{-1}; 0.1-1.5 d^{-1});

- $K_{SB,OHO}$, b_{OHO} and $K_{NHx,ANO}$ in Bornemann et al. (1998) have different and not overlapping ranges (respectively 1-5 g $S_B.m^{-3}$; 0.3-0.5 d^{-1}; 0.1-0.7 g $S_{NHx}.m^{-3}$);

- The median values provided by Cox (2004) are quite different from the database ones (up to 100% of relative difference); whereas the 25th and 75th percentiles are in agreement. An exception is for the heterotrophic growth and decay rates ($\mu_{OHO,Max}$, b_{OHO}) and the half-saturation coefficient for substrate ($K_{SB,OHO}$), for which the ranges provided by Cox (2004) are not overlapping the database ones (respectively 2.06-4.69 d^{-1}; 0.2-0.6 d^{-1}; 2.54-7.06 g $S_B.m^{-3}$);

- Sin *et al.* (2009) provided "uncertainties" (or better variabilities) based on expert knowledge. Two parameter variabilities ($\mu_{ANO,Max}$, b_{ANO}) are narrower than the observed variability in this study (respectively 5% and 25%) and 8 much wider (50% of variability for i_{N_XBio}, $K_{O2,OHO}$, q_{am}, $K_{NHx,ANO}$; 25% of variability for $K_{XCB,hyd}$, $\mu_{OHO,Max}$, $\eta_{\mu OHO,Ax}$, $K_{O2,ANO}$).

It is noticeable that the above mentioned parameters correspond to the ones with the largest variability in Table 3-1 and/or to those modified in more than 50% of the cases, although the observed variations of these parameters are often lower than those provided in these studies.

Finally, all of the overview studies present a parameter range or an "uncertainty" for the autotrophic yield (Y_{ANO}), whereas its value was modified in none of the 22 modelling projects.

3.2.3.2.3 Conclusion.

Results concerning ASM1 are summarised in Table 3-2. This table includes the main parameters that are highlighted by at least one of the four areas of study. The box-plots corresponding to these parameters are presented in ANNEXE 1.

Table 3-2. Summary of results for ASM1

	default ≠ original	modified >50%	large ranges	ranges ≠ literature
b_{ANO}	**X**	**X**	**X**	**X**
$\mu_{ANO, Max}$	**X**	**X**		
Y_{OHO}	**X**	**X**		
$K_{SB,OHO}$	**X**		**X**	**X**
$K_{NOx,OHO}$	**X**		**X**	
$K_{NHx,ANO}$	**X**			**X**

Regarding ASM1, six parameters have been pointed out as subject to changes: Y_{OHO}, $K_{SB,OHO}$, $K_{NOx,OHO}$, $\mu_{ANO,Max}$, b_{ANO} and $K_{NHx,ANO}$. In addition to the variability of Y_{OHO}, $\mu_{ANO,Max}$ and b_{ANO} already discussed, the three other parameters are half-saturation coefficients, suspected to depend on environmental conditions. These results are supported by the literature data although the chosen 25th and 75th percentiles provide a narrower range for some of the parameters than specified in literature.

3.2.3.3 ASM2d

3.2.3.3.1 Data description.

The database contains 20 parameter sets for ASM2d, of which 2 are "proposed new default parameter sets" and 18 are "optimised parameter sets" from specific modelling projects. The modelling studies were mainly carried out in Europe (16), with only two applications in Asia; and mainly on full scale WWTPs (12). Table 3-3 synthesises the main results for ASM2d. The sludge ages of the specific modelling projects are between 7 and 22 days.

Table 3-3.Synthesis of database results for ASM2d model, only modified parameters are mentioned.

Parameter values are standardised at a temperature of 20°C.

Parameter*	**Unit**	**Original notation**	**Original parameter set**	**Optimised parameter sets**					
Parameter sets			**j**	**n**	**Modif. >50%**	**Median**	**Perc. 25%**	**Perc. 75%**	**V (%)**
Kinetic parameters									
Hydrolysis									
$\eta_{qhyd,Ax}$	-	η_{NO3}	**0.60**	20		0.60	0.60	0.80	33
$\eta_{qhyd,A\eta}$	-	η_{fe}	**0.40**	20		0.40	0.20	0.40	50
Ordinary Heterotrophic Organisms									
$\mu_{OHO,Max}$	d^{-1}	μ_H	**6.0**	20	X	6.0	4.0	6.0	33
$\eta_{\mu OHO,Ax}$	-	η_{NO3}	**0.8**	20		0.8	0.8	0.8	0
Phosphorus Accumulating Organisms									
q_{PAO,VFA_Stor}	$g\ X_{Stor}.g\ X_{PAO}^{-1}.d^{-1}$	q_{PHA}	**3**	20	X	3.4	3.0	6.0	90
$q_{PAO,PO4\_PP}$	$g\ X_{PP}.g\ X_{PAO}^{-1}.d^{-1}$	q_{PP}	**1.50**	20	X	1.50	1.50	3.30	120
$\mu_{PAO,Max}$	d^{-1}	μ_{PAO}	**1.00**	20		1.00	1.00	1.04	4
$\theta_{\mu PAO,Max}$	-	$\theta_{\mu PAO}$	**1.041**	3		1.041	1.041	1.058	2
m_{PAO}	d^{-1}	b_{PAO}	**0.20**	20	X	0.20	0.15	0.20	25
b_{PP_PO4}	d^{-1}	b_{PP}	**0.20**	20	X	0.20	0.15	0.20	25
b_{Stor_VFA}	d^{-1}	b_{PHA}	**0.20**	20	X	0.20	0.15	0.20	25
Autotrophic Nitrifying Organisms									
$\mu_{ANO,Max}$	d^{-1}	μ_{AUT}	**1.00**	20	X	1.00	1.00	1.15	15
b_{ANO}	d^{-1}	b_{AUT}	**0.15**	20		0.15	0.15	0.16	7
$K_{NHx,ANO}$	$g\ S_{NHx}.m^{-3}$	K_{NH4}	**1.00**	20	X	1.00	0.50	1.00	50

j: Henze *et al.* (2000b). Please refer to the appendix for the parameter definitions.

*Standardised notation from Corominas *et al.* (2010) is used. n: number of parameter values in the database.

Original vs. proposed new default parameter sets: Only the original parameter set is presented. A new default parameter set was proposed by Cinar *et al.* (1998) but it concerns in fact ASM2 and not ASM2d.

Parameters changed in modelling projects (compared to original values): The majority of the parameters are kept at their original values, from which 33 (of the 83 parameters) have never been changed:

- 4 of the 11 stoichiometric parameters: the inert fractions generated in hydrolysis and biomass decay processes ($f_{SU\_XCB,hyd}$, $f_{XU\_Bio,lys}$); the yield of polyphosphate storage per organic stored compound used (Y_{PHA_PP}) and the autotrophic growth yield (Y_{ANO}).

- 7 of the 15 conversion coefficients: i_{N_SF}, i_{N_XBio}, i_{P_SF}, i_{P_SU}, i_{TSS_XCB}, $i_{TSS\_XPAO,PHA}$ and $i_{TSS\_XPAO,PP}$.

- 22 of the 57 kinetic parameters: the alkalinity half-saturation parameters ($K_{Alk,OHO}$, $K_{Alk,PAO}$, $K_{Alk,ANO}$); heterotrophic half-saturation parameters for nutrients ($K_{NHx,OHO}$, $K_{PO4,OHO}$); autotrophic half-saturation parameters for nutrients ($K_{PO4,ANO}$); 5 phosphorus accumulating organism half-saturation parameters (K_{S,fPP_PAO}, $K_{O2,PAO}$, $K_{NOx,PAO}$, $K_{NHx,PAO}$, $K_{PO4,PAO,upt}$); the half-saturation parameters for dissolved oxygen and nitrates in the hydrolysis process ($K_{O2,hyd}$, $K_{NOx,hyd}$); 6 of the 12 temperature correction factors ($\theta_{q\_XCB\_SB,hyd}$, $\theta_{\mu\_OHO,Max}$, $\theta_{q\_SF\_Ac,Max}$, θ_{b_OHO}, $\theta_{\mu\_ANO,Max}$, θ_{b_ANO}); and the chemical phosphorus precipitation parameters ($q_{P,pre}$, $q_{P,red}$, $K_{Alk,pre}$).

Two types of modelling studies could be distinguished:

- Studies with a calibrated parameter subset (12 studies). These are mainly composed of kinetic parameters;

- Studies with measured parameters (6 studies), among which 4 studies use the calibration protocol of Penya-Roja *et al.* (2002) (Penya-Roja *et al.*, 2002; Ferrer *et al.*, 2004; Garcia-Usach *et al.*, 2006). This protocol is based on batch tests that allow the measurement of many stoichiometric and kinetic coefficients for autotrophs, ordinary heterotrophs and phosphorus accumulating organisms.

Among the 18 modelling studies, 8 parameters - all of which are kinetic parameters - were changed in more than half of the cases: the heterotrophic and autotrophic maximum growth rates ($\mu_{OHO,Max}$, $\mu_{ANO,Max}$), the autotrophic half-saturation coefficient for ammonia ($K_{NHx,ANO}$), the rate constants for volatile fatty acids (VFA) uptake (q_{PAO,VFA_Stor}) and for polyphosphate storage ($q_{PAO,PO4\_PP}$) of the PAO and their storage pools' decay (m_{PAO}, b_{PP_PO4}, b_{Stor_VFA}).

Parameter ranges and statistics: The median values are the same as the original publication values except for the rate constant for VFA uptake (q_{PAO,VFA_Stor}). The ranges of kinetic parameter values between 25th and 75th percentiles are quite narrow (<33%), except for the reduction factor for hydrolysis under anaerobic conditions ($\eta_{qhyd,A\eta}$), for the rate constants for VFA uptake (q_{PAO,VFA_Stor}) and polyphosphate storage ($q_{PAO,PO4\_PP}$) and the half-saturation coefficient for ammonia ($K_{NHx,ANO}$).

3.2.3.3.2 Discussion

Parameters changed in modelling projects (compared to original values): Among the eight parameters that were changed most, two have a particularly wide range of values: the rate constants for VFA uptake (q_{PAO,VFA_Stor}) and polyphosphate storage ($q_{PAO,PO4\_PP}$). Furthermore, the users of the Penya-Roja *et al.* (2002) protocol observed large parameter ranges for PAO growth and polyphosphates storage yields (Y_{PAO}, $Y_{PP\_Stor,PAO}$). This could indicate a problem in the ASM2d model structure, such as the simplification of not taking into account glycogen storage and glycogen accumulating organisms in ASM2d (Penya-Roja *et al.*, 2002).

Another explanation could be that the ASM2d model describes polyphosphate uptake and the growth of PAOs as two independent kinetic processes. However, experimental results show that oxidation of organic stored compounds provides energy for both PAO growth and polyphosphate storage (Wentzel *et al.*, 1989). Consequently, PAO growth and polyphosphate storage yield are linked and depend on the oxidation of organic stored compounds. Therefore some models link both yields to energy production (in metabolic models, e.g.: Meijer, 2004) or model PAO growth and polyphosphate storage as a single process (Barker & Dold model, UCTPHO+). Fixing the ratio between growth and phosphate storage would then assist ASM2d calibration.

Parameter ranges and statistics: Based on expert knowledge, Brun *et al.* (2002) assigned an uncertainty to each parameter. The database is in agreement with the low uncertainties (between 5% and 20%) attributed to stoichiometric parameters and conversion coefficients parameters by Brun *et al.* (2002). In Brun *et al.* (2002), high uncertainty is attributed to kinetic parameters (between 20% and 50% of uncertainty), which are overestimated based on the database results for all the parameters, except for the reduction factors for hydrolysis under anoxic and anaerobic conditions ($\eta_{qhyd,Ax}$, $\eta_{qhyd,An}$), the rate constants for VFA uptake (q_{PAO,VFA_Stor}) and polyphosphate storage ($q_{PAO,PO4\_PP}$).

3.2.3.3.3 Conclusion.

Results concerning ASM2d are summarised in Table 3-4.

Table 3-4. Summary of results for ASM2d

	default ≠ original	modified >50%	large ranges	ranges ≠ literature
$\mu_{OHO,\ Max}$		**X**	**X**	
$\mu_{ANO,Max}$		**X**		
q_{PAO,VFA_Stor}		**X**	**X**	**X**
$q_{PAO,PO4\_PP}$		**X**	**X**	**X**
m_{PAO}, b_{PP_PO4}, b_{Stor_VFA}		**X**		
$K_{NHx,ANO}$		**X**	**X**	

The main potential pitfalls in calibrating ASM2d seem to come from the determination of the rate constants for VFA uptake (q_{PAO,VFA_Stor}) and polyphosphate storage ($q_{PAO,PO4\_PP}$). These two parameters are used in organic compound storage and consumption processes, and their high variability could indicate a problem in the model structure leading to difficulties in the calibration process.

3.2.4 Discussion

3.2.4.1 Inter-model comparison

In both ASM1 and ASM2d, few parameters have been changed in more than half the cases considered. This shows that either model users are in most cases relying on the

original values, or that the model outputs are not sensitive to these parameters. In an inter-model comparison taking into account the results for other models presented in the appendix (ASM3, ASM3+BioP, ASM2d+TUD, Barker & Dold), the following parameters are most often modified:

- growth and decay rates of autotrophs,
- PAO storage processes rates,
- Heterotrophic half-saturation coefficients for substrate and oxygen
- Autotrophic half-saturation coefficient ammonia.

The half-saturation coefficients are thought to be dependent on specific environmental conditions.

Several modelling protocols suggest measuring some kinetic and stoichiometric parameters: WERF (Melcer *et al.*, 2003), BIOMATH (Vanrolleghem *et al.*, 2003)and HSG (Langergraber *et al.*, 2004). However, in current practice few, if any, biokinetic parameters are measured

3.2.4.2 Limitations of modelling project articles

The large literature review on modelling projects revealed that important information is often missing from these articles to enable them to be fully used. Lacking information included:

- information on plant: tank configuration, tank dimensions, aeration time;
- information on environmental conditions: temperature, rain events, diurnal variations;
- information on measurement campaign: duration, number of samples, measurement methods;
- information on influent characteristics and characterisation method used;
- method used for data validation and reconciliation;
- method used to optimise the parameter set: protocol, parameters set to original value;
- temperature for which the optimised parameter set is provided.

This lack of information prevents further analysis of the database, such as an investigation of correlations. It also makes it difficult to evaluate the quality of the modelling projects. Thus, the modelling projects included in the database had to be

considered to be of equal quality. The differences within parameter values therefore are supposed to be linked to the WWTP conditions and not to a wrong calibration or poor data quality.

It should also be noted that there seems to be a lack of (published) experimental data with respect to parameter values. If parameters were measured it is often difficult to evaluate the results due to missing information on the measurement method.

3.2.4.3 Potential use of the database

A number of correlations were searched for in the database including: correlations between parameters; between changed values; between parameters and WWTP conditions (Food/Microorganism ratio, nitrogen loads, Sludge Retention Time). No significant correlations were found which is probably due to the limited number of datasets.

The database has been designed to allow future extensions with new data sets. A larger database could allow further analysis to:

- determine model parameter ranges and typical values to define current practice and help model users in the calibration step for the commonly used models;
- provide a synthesis of practical modelling experiences that could help model users to find appropriate case studies similar to their simulation project;
- examine correlations between changes in parameter values and WWTP conditions;
- determine practical model limits from various modelling experiences;
- identify research needs.

3.3 Typical fractions

The second objective of the questionnaire 2 was to collect data on the typical process conditions occurring in wastewater treatment plants located in different geographical areas. One of the questions focused on typical fractions, i.e. the relationships between the magnitude of COD, BOD, nitrogen, phosphorus and TSS measured in raw influent, in settled wastewater and in the mixed liquor. Some of these ratios are subject to change according to geographical areas, depending on e.g. climate, lifestyle, type of sewerage system. These ratios are very useful in the data reconciliation and validation step. They help to highlight outlier values and to correct them if required. The results are presented in Table 3-5, and exclusively concern municipal wastewater.

Table 3-5. Synthesis of typical values from the second questionnaire

	Ratio	Unit	nb	mean	*Std%*	median	min	max
Raw influent	**N_T/COD_T**	g N/g COD	12	**0.095**	*17%*	**0.091**	0.050	0.150
	NH_4/N_{TK}	g N/g N	13	**0.684**	*8%*	**0.670**	0.500	0.900
	P_T/COD_T	g P/g COD	12	**0.016**	*22%*	**0.016**	0.007	0.025
	PO_4/P_T	g P/g P	12	**0.603**	*16%*	**0.600**	0.390	0.800
	COD_T/BOD_5	g COD/g BOD	12	**2.060**	*11%*	**2.050**	1.410	3.000
	COD_S/COD_T	g COD/g COD	13	**0.343**	*29%*	**0.350**	0.120	0.750
	TSS/COD_T	g TSS/g COD	12	**0.503**	*18%*	**0.500**	0.350	0.700
	COD_X/VSS	g COD/g VSS	11	**1.690**	*12%*	**1.600**	1.300	3.000
	VSS/TSS	g SS/g SS	12	**0.740**	*20%*	**0.800**	0.300	0.900
	BOD_5/BOD_∞	g BOD/g BOD	7	**0.655**	*7%*	**0.650**	0.580	0.740
	Alkalinity	Mol_{eq}/L	11	**5.173**	*35%*	**5.000**	1.500	9.000
Primary effluent	**N_T/COD_T**	g N/g COD	9	**0.134**	*35%*	**0.120**	0.050	0.360
	NH_4/N_{TK}	g N/g N	11	**0.755**	*4%*	**0.750**	0.430	0.900
	N_T/COD_T	g P/g COD	9	**0.023**	*25%*	**0.023**	0.010	0.060
	PO_4/P_T	g P/g P	10	**0.741**	*12%*	**0.750**	0.500	0.900
	COD_T/BOD_5	g COD/g BOD	9	**1.874**	*31%*	**1.900**	0.500	3.000
	COD_S/COD_T	g COD/g COD	10	**0.449**	*31%*	**0.495**	0.150	0.750
	TSS/COD_T	g TSS/g COD	9	**0.380**	*21%*	**0.400**	0.180	0.560
	COD_X/VSS	g COD/g VSS	9	**1.718**	*14%*	**1.700**	1.400	3.500
	VSS/TSS	g SS/g SS	9	**0.794**	*7%*	**0.800**	0.700	0.909
	BOD_5/BOD_∞	g BOD/gBOD	6	**0.644**	*10%*	**0.656**	0.533	0.760
	Alkalinity	Mol_{eq}/L	9	**5.711**	*40%*	**6.000**	1.500	9.000
Activated sludge	**COD_T/VSS**	g COD/g SS	9	**1.434**	*7%*	**1.420**	1.266	1.600
	N_T/COD_T	g N/g COD	7	**0.073**	*35%*	**0.060**	0.045	0.116
	P_T/COD_T	g P/g COD	7	**0.020**	*64%*	**0.015**	0.010	0.044
	VSS/TSS	g SS/g SS	10	**0.739**	*8%*	**0.750**	0.650	0.900

nb: number of answers ; Std%: standard deviation in %

The limited number of answers prevents the analysis of the effect of the geographical areas. These numbers are given from the respondent expertise, and are not necessarily linked to a particular project. Furthermore, to properly study these numbers, other information is missing, e.g. the characteristics of the sewers (combined or separated), whether the ratios were given for dry weather or wet weather conditions, and the characteristics of primary treatment.

These numbers are in agreement with literature data (Table 3-6), particularly those presented by Pons *et al.* (2004) for European wastewaters. The data presented in Table 3-6 for this reference correspond to the mean of values for the different countries, and the minimum and maximum values among the countries.

Table 3-6. Ratios from literature

Reference		**Ratio**	typical value (std%)	min	max
(Metcalf & Eddy *et al.*, 2003)	RI	**COD_T/BOD_5**		1.25	3.333
	PE	**COD_T/BOD_5**		1.667	2.500
(Melcer *et al.*, 2003)	RI	**$NH4/N_{TK}$**		0.500	0.750
	RI	**PO4/PT**		0.500	0.850
(Pons *et al.*, 2004)	RI	**N_T/COD_T**	0.095 (17%)	0.069	0.113
	RI	**P_T/COD_T**	0.016 (21%)	0.013	0.022
	RI	**TSS/COD_T**	0.530 (14%)	0.480	0.641
	RI	**COD_T/BOD_5**	2.305 (13%)	1.890	2.667

RI: Raw Influent; PE: Primary Effluent

In conclusion, the ratios extracted from the second questionnaire could be used for the data reconciliation and validation step.

3.4 Conclusion

This chapter purposes a synthesis of available practical knowledge on parameter values and typical ratios gathered in a database that combines experience from modelling projects and expert knowledge. The database was analysed to extract relevant information in terms of model parameters: Which parameters have often been changed and in which range of values. For now this database provides parameter ranges and typical values for ASM1 and ASM2d. However, these parameters should be used with great care since they are the result of averaging practical experience without taking into account parameter correlations or specific environmental conditions.

Concerning **ASM1**, 6 parameters have been pointed out as subject to change:

- the heterotrophic yield Y_{OHO}, for which the model structure should be modified to take into account an aerobic and an anoxic value;
- the maximum autotrophic growth and decay rates, $\mu_{ANO,Max}$ and b_{ANO}, which are linked. Using a higher value of b_{ANO} (0.17 d^{-1} at 20°C) seems to fix $\mu_{ANO,Max}$ (0.8 d^{-1} at 20°C).
- half-saturation coefficients $K_{SB,OHO}$, $K_{NOx,OHO}$, and $K_{NHx,ANO}$, suspected to depend on environmental conditions are highly variable.

As far as **ASM2d** is concerned, the parameters modified in most cases are:

- the heterotrophic and autotrophic growth rates, $\mu_{OHO,Max}$ and $\mu_{ANO,Max}$,
- rate constants for VFA and polyphosphates uptake, q_{PAO,VFA_Stor} and $q_{PAO,PO4\_PP}$, that could indicate a model structure problem;
- PAO and storage pools decay parameters, m_{PAO}, b_{PP_PO4} and b_{Stor_VFA},
- the half-saturation coefficient for ammonia $K_{NHx,ANO}$.

Typical fractions provided in the questionnaire were also provided. Typical numbers and ranges of values extracted can be used to guide the data reconciliation and validation step. However, the number of data provided so far is too limited to analyse the differences in fraction values between geographical areas.

Despite the amount of collected information, no correlation was established between the model parameters. More modelling projects are required to expand the database. This could be envisaged by making the database available online, with the possibility to input new projects. This would however require a specific procedure to verify the quality of the data.

CHAPITRE 4 Analysis of theoretical knowledge

L'enquête auprès des utilisateurs de modèles (2.1) a montré que 22% d'entre eux trouvent les modèles trop complexes et 24% n'ont pas confiance en leur modèle. De plus, 78% des utilisateurs de modèles ont acquis leurs connaissances en modélisation partiellement ou totalement par auto-formation. D'autre part, bien que les modèles publiés soient tous représentés sous le même format (matrice de Gujer), ils utilisent une notation différente qui les rend difficilement lisibles. Par conséquent, la plupart des utilisateurs ne maitrise que très peu de modèles (souvent seulement l'ASM1) et n'est donc pas en mesure de choisir le modèle adéquat à leur cas d'étude.

L'objectif de ce chapitre est de faciliter la compréhension des modèles aux utilisateurs, de leur fournir les moyens de vérifier les erreurs mathématiques des modèles, et de leur permettre d'effectuer un choix éclairé du modèle adéquat à leur projet d'étude.

i. Notation

Suite aux besoins émis par différents groupes de travail, de nouvelles règles pour nommer les variables d'état et les paramètres des modèles de traitement des eaux ont été établies. Les résultats ont été synthétisés dans un article par Corominas *et al.* (2010), avec lequel est fourni un tableau de traduction des anciennes notations pour les sept modèles étudiés.

Corominas L., Rieger L., Takács I., Ekama G., Hauduc H., Vanrolleghem P.A., Oehmen A., Gernaey K.V. and Comeau Y. (2010) New framework for standardized notation in wastewater treatment modelling. *Water Science and Technology*, **61**(4), 841-857.

ii. Vérification des modèles

La qualité des résultats de simulation peut être impactée par des erreurs dans les modèles publiés ou par leur implémentation dans les logiciels de simulation. Pour cela une méthode systématique est proposée pour vérifier les modèles publiés et implémentés dans les logiciels de simulation. Les publications originales des sept modèles étudiés ont été vérifiées de cette façon, ce qui a permis de déceler des erreurs de frappe, des inconsistances ou des variables non prises en compte dans les coefficients stœchiométriques ou cinétiques. Les erreurs trouvées dans la cinétique et la stœchiométrie des sept modèles sont détaillées. De plus une feuille de calcul reprenant les matrices de Gujer corrigées des modèles est fournie en matériel additionnel.

Ces résultats ont été publiés dans l'article suivant :

Hauduc H., Rieger L., Takacs I., Héduit A., Vanrolleghem P.A., and Gillot S. (2010) A systematic approach for model verification – Application on seven published Activated Sludge Models, *Water Science and Technology* **61**(4) 825-839.

iii. Comparaison théorique des modèles

Une revue critique des modèles étudiés est effectuée processus par processus. Neufs processus ont été distingués et sont listés dans le Tableau 4-1.

Tableau 4-1. Liste des processus et des modèles considérés

Processus	ASM1	Barker & Dold	ASM2d	ASM3	ASM3+ BioP	UCTPHO+	ASM2d+ TUD
Hydrolyse	X	X	X	X	X		X
Fermentation		X	X			X	X
Croissance des OHO	X	X	X	X	X[1]	X[2]	X
Croissance des ANO	X	X	X	X	X	X	X
Décès des OHO & ANO	X	X	X	X	X	X	X
Stockage des PHA		X	X		X	X	X
Stockage des PolyP		} X[3]	X		X	} X[3]	X
Croissance des PAO			X		X		X
Décès des PAO		X	X		X	X	X

[1] Incluant le stockage des PHA par les OHOs; [2] Incluant l'adsorption et l'hydrolyse; [3] Incluant le stockage des polyP.

Pour chacun de ces processus, une brève synthèse bibliographique est suivie par la comparaison des concepts de modélisation. Une nouvelle représentation graphique des processus a été développée pour permettre aux utilisateurs de mieux comprendre les concepts des modèles et leurs différences.

La comparaison des connaissances théoriques avec les concepts de modélisation permet en outre de mettre en relief le degré de simplification de chaque concept, et donc de mettre en avant les limites théoriques des modèles.

Les résultats seront soumis sous la forme d'une revue critique au mois de septembre :

Hauduc H., Rieger L., Héduit A., Vanrolleghem P.A. and Gillot S. Critical review of activated sludge modelling: State of process knowledge, modelling concepts and limitations.

4.1 Introduction

The questionnaire analysed in paragraph 2.1 highlights three main obstacles concerning the selection of the model structure, i.e. the theoretical and mathematical part of modelling: i) modellers do not trust their model, ii) the models are too complex, and iii) the available models are not always adequate to the modellers' objectives, which the means that the models do not include adequate description of some processes to simulate the WWTP behaviour. Moreover, this questionnaire points out that modellers acquire their modelling knowledge mainly by self-learning.

Consequently, the aim of this chapter is to provide tools to help model users i) to better understand published models, ii) to get an error-free model, whether they implement a published model or develop their own model, iii) to help selecting the adequate model for their project, depending on the theoretical limits of each of the available models.

The development of a standardised model notation, preliminary step to compare models, is first presented. Then, a tool to verify models is developed and applied to the seven models envisaged in this thesis. Finally, the modelling concepts of the seven studied models are compared and their level of simplification regarding the theoretical knowledge on biological processes is analysed.

4.2 Standardised notation[3]

A number of activated sludge models has been published since the 70's, with an increasing complexity (Gujer, 2006). These models have been developed by different research groups, which use different ways of naming state variables and parameters. A framework for model description has been first established by Grau *et al.* (1982a; 1982b; 1987). However, this framework was not adapted to the development of new and more complex models. It results for example in models with the same parameters being named differently and vice versa. Consequently, learning a new model is sometimes like learning a new language.

The need of a new framework for standardised notation arose from several groups, including the GMP-TG (https://iwa-gmp-tg.cemagref.fr/), so that a working group was formed at the 1st IWA/WEF Wastewater Treatment Modelling Seminar (WWTmod2008). The results of these discussions have been synthesised by Corominas *et al.* (2010). The principle of this notation is to agree on a few "main symbols" that describe the particle size of the state variables or the parameter types (growth rate, half-saturation coefficient…). To clarify the meaning of the state variable or parameter, subscripts are introduced in a specific order and using standardised abbreviations. The main rules for building state variables and parameters names are synthesised in Figure 4-1.

This standardised notation was used throughout the thesis, except in part of the chapter on model verification (4.3) to help traking errors on the original publications. Correspondance with original notation can be found in the following link: http://www.iwaponline.com/wst/06104/0912.xls and in ANNEXE 1.

[3] Corominas L., Rieger L., Takács I., Ekama G., Hauduc H., Vanrolleghem P.A., Oehmen A., Gernaey K.V. and Comeau Y. (2010) New framework for standardized notation in wastewater treatment modelling. *Water Science and Technology*, **61**(4), 841-857.

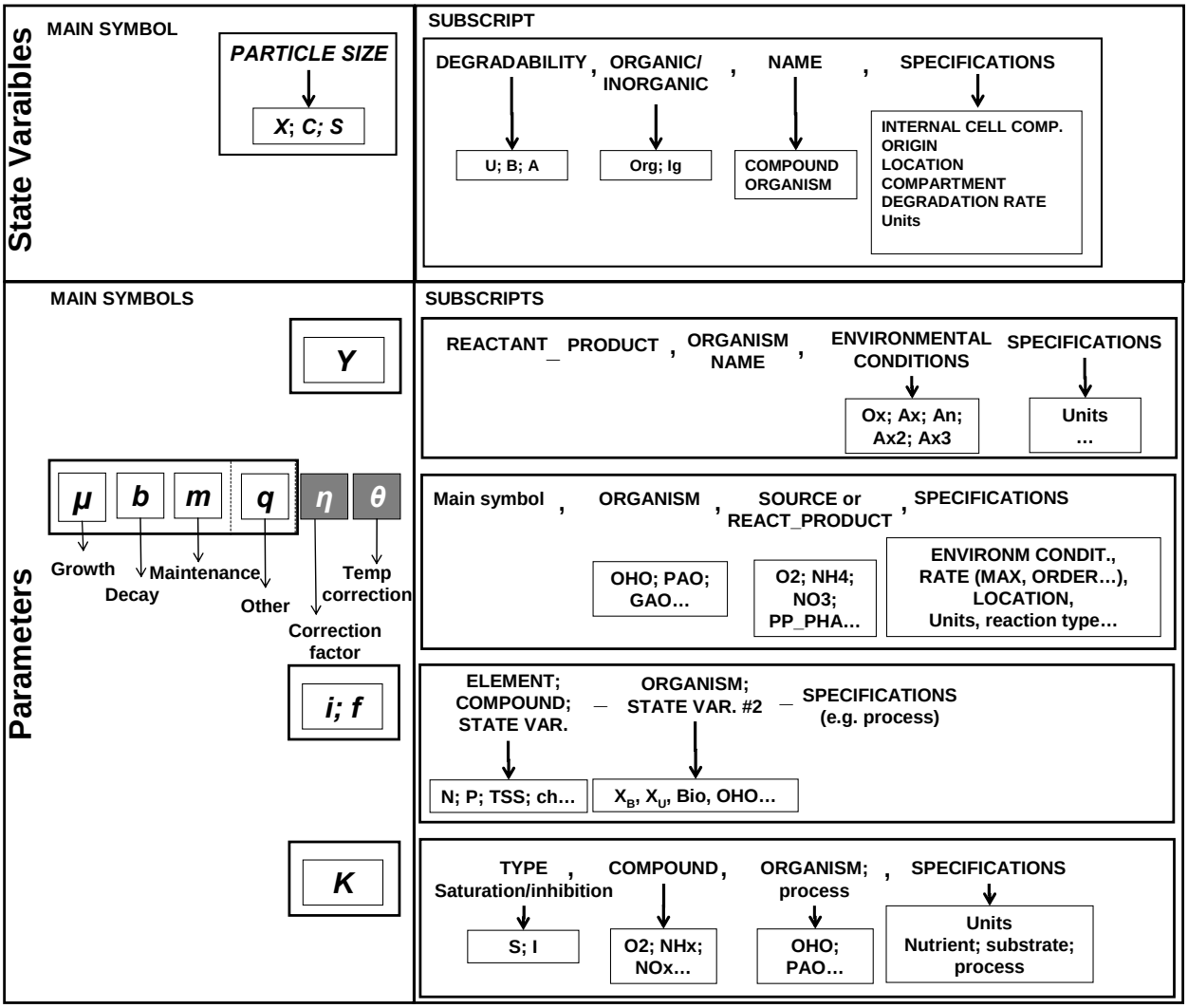


Figure 4-1. Notation framewok for naming state variables and parameters (from Corominas *et al.*, 2010)

4.3 A systematic approach for model verification – Application on seven published Activated Sludge Models[4]

4.3.1 Introduction

The quality of simulation results can be affected by several error sources (Refsgaard *et al.*, 2007): i) context and framing; ii) input uncertainty; iii) model structure uncertainty; iv) parameter uncertainty and v) model technical uncertainty, e.g. model implementation errors. Gernaey *et al.* (2006) detailed the error sources when models are implemented into a simulation software: i) simplification of the original model; ii) typing errors; iii) incomplete model description in the paper; iv) scattered description of the model in the paper; v) misinterpretation of the model description; vi) errors when coding model; vii) general programming bugs.

Surprisingly no error report has been published, except for ASM2d and ADM1 in Gernaey *et al.* (2006). Tracking those errors is indeed difficult and time consuming for model users, and the potential publication formats are not adapted to publish such information. Furthermore, some typing errors seem to appear or disappear following the version of the papers describing a given model (e.g.: ASM2d where typing errors appeared in the paper Henze *et al.* (2000b) compared to previous publications: Henze *et al.* (1998) and Henze *et al.* (1999)). This work aims thus to provide i) a systematic approach to track typing errors and inconsistencies in models, ii) a thorough list of errors in the commonly used activated sludge model publications and iii) the corrected Gujer Matrices (also called Petersen Matrix, Takacs, 2005) in original and new standardised notation format (Corominas *et al.*, 2010) in a spreadsheet (see http://www.iwaponline.com/wst/06104/0898.xls). The work does not intend to address model structure problems linked either to modelling concepts or to simplifications used in the models.

Seven of the most commonly used activated sludge models have been investigated: (1) ASM1 (Henze *et al.* (1987); republished in Henze *et al.* (2000a)); (2) ASM2d (Henze *et al.* (1999); republished in Henze *et al.*, (2000b)); (3) ASM3 (Gujer *et al.* (1999);

[4] Hauduc H., Rieger L., Takacs I., Héduit A., Vanrolleghem P.A., and Gillot S. (2010) A systematic approach for model verification – Application on seven published Activated Sludge Models, *Water Science and Technology,* **61**(4), 825-839.

corrected version published in Gujer *et al.* (2000)); (4) ASM3+Bio-P (Rieger *et al.*, 2001); (5) ASM2d+TUD (Meijer, 2004); (6) New General (Barker and Dold, 1997); (7) UCTPHO+ (Hu *et al.*, 2007). To keep the chapter readable, those references will not be repeated each time.

4.3.2 How to track typing errors and inconsistencies in model development and software implementation

Before using or implementing a published model or when developing a new model one should first verify the model by checking the continuity of the stoichiometry and the consistency of the kinetic rate expressions. Because typing errors could stem from the original model publication or could occur during software implementation, this step should be done directly in the simulation software (simulator). However, not all simulators provide adequate tools to track such errors.

One way of verifying model implementations would consist in performing a ring test between several simulators with independent implementations (by several modellers). The simulation results for the same modelling project are compared to verify the model implementations. This method was chosen by the BSM task group to validate the implementation of their settling and biokinetic models, and ASM1 in particular (Jeppsson *et al.*, 2007; Copp *et al.*, 2008). The study revealed errors in the model codes, in the simulator codes and in the aeration models of the evaluated simulators. However, this task necessitates considerable effort and different simulators, which is not usually available to ASM users.

A method to automatically isolate model implementation errors by comparison of two independent model implementations has been developed by Yuan *et al.* (2003). Next to detection of model implementation errors, a method based on so-called Feature Matrices has been developed also to diagnose the errors and point to the probable location of the error in the model code. However this promising method has not yet been implemented in any simulator.

The following paragraphs propose functionalities of model editors to allow for model verification. Some alternative ways to track errors are also suggested. However this methodology will not allow for the detection of numerical problems that could appear due to programming errors in simulators or wrong numerical solver settings. These

errors should be fixed by the simulator developers through the above mentioned ring test for example.

4.3.2.1 How to track stoichiometric discontinuities

As state variables are typically expressed in terms of COD, elements (e.g. N, P) or charge, a composition matrix (Gujer and Larsen, 1995) was developed complementary to the Gujer Matrix (Henze *et al.*, 1987). It contains the required conversion coefficients for all state variables (in rows) to check the continuity for conservatives (e.g. COD, elements and charge) and observables (e.g. TSS) (in columns) for each process. The conversion coefficients to obtain the COD content of a state variable can be calculated from the theoretical COD of each atomic element and the charges (Table 4-2). This is illustrated in Table 4-3.

Table 4-2. Theoretical COD of main elements and electrical charge (from Gujer and Larsen, 1995)

Element description	**Symbol**	**Oxidation number**	**Theoretical COD (g COD.mol^{-1})**	**Molecular weight (g.mol^{-1})**
Negative charge	(-)	+1	+8	-
Positive charge	(+)	-1	-8	-
Carbon	C	+4	+32	12
Nitrogen	N	-3	-24	14
Hydrogen	H	+1	+8	1
Oxygen	O	-2	-16	16
Sulphur	S	+6	+48	32
Phosphorus	P	+5	+40	31
Iron	Fe	+3	+24	55.8

Table 4-3. Explanation and exact values of the main coefficients used in ASM-type models

Description	Symbol	Calculation	Exact value*	Unit
Conversion factor for NO_3^- into COD	i_{COD_NOx}	(-24+3*(-16)+8) g COD.mol^{-1} / 14 g N.mol^{-1}	-64/14	g COD.g N^{-1}
Conversion factor for N_2 into COD	i_{COD_N2}	(-24*2) g COD.mol^{-1} / (14*2) g N.mol^{-1}	-24/14	g COD.g N^{-1}
Stoichiometric factor for NO_3^- reduction to N_2 (amount of COD provided by reduction)	$i_{NOx,N2}$	(64-24) g COD.mol^{-1} / 14 g N.mol^{-1}	40/14	g COD.g N^{-1}
Conversion factor for NH_4^+ into charge	i_{Charge_NHx}	1 Charge.mol^{-1} / 14 g N.mol^{-1}	1/14	Charge.g N^{-1}
Conversion factor for NO_3^- into charge	i_{Charge_NOx}	-1 Charge.mol^{-1} / 14 g N.mol^{-1}	-1/14	Charge.g N^{-1}
Conversion factor for Ac (CH_3COO^-) in charge	i_{Charge_Ac}	-1 Charge.mol^{-1}/ (2*32+3*8-2*16+8)g COD.mol^{-1}	-1/64	Charge.g COD^{-1}
Conversion factor for PolyP into charge $(K_{0.33}Mg_{0.33}PO_3)_n$	i_{Charge_PP}	K^+ and Mg^{2+} not considered: $(PO_3)_n^-$ -1 Charge.mol^{-1} / 31 g P.mol^{-1}	-1/31	Charge.g P^{-1}
Conversion factor for PO_4^{3-} into charge	i_{Charge_PO4}	PO_4^{3-}: 50% $H_2PO_4^-$ + 50% HPO_4^{2-} (-1-2) Charge.mol^{-1} / (2*31) g P.mol^{-1}	-1.5/31	Charge.g P^{-1}
Conversion factor for MeP ($FePO_4$) in P	i_{P_MeP}	$FePO_4$: 55.8+31+4*16=150.8 g.mol^{-1} 31 g P.mol^{-1}/ 150.8 g TSS.mol^{-1}	31/ 150.8	g P.g TSS^{-1}
Stoichiometric coefficients for precipitation and redissolution of PO_4^{3-} (ASM2d)	$f_{MeOH\_PO4,MW}$	$Fe(OH)_3 + PO_4^{3-} \rightleftharpoons FePO_4 + 3HCO_3^-$	-106.8 /31	-
	$f_{MeP\_PO4,MW}$	$Fe(OH)_3$: 55.8+3*16+3=106.8 g.mol^{-1} $FePO_4$: 55.8+31+4*16=150.8 g.mol^{-1} Normalised on PO_4^{3-} (=31g P.mol^{-1})	150.8 /31	-

*The molecular weights used are rounded values (e.g. 12 g C.mol C^{-1} instead of 12.0107 g C.mol C^{-1}) but as the same value is used for each element in the model, the continuity is verified (which is not the case when rounding ratios, since the rounding error is different for each ratio).

The continuity check is carried out by multiplying (analytically or numerically) the stoichiometric matrix with the composition matrix as shown in Figure 4-2. The resulting matrix should contain only zeros, or near zeros in case of rounding problems.

ASM1 Composition Matrix

		elements		
		COD	N	Charge
1	S_i	1	0	0
2	S_s	1	0	0
3	X_i	1	0	0
4	X_s	1	0	0
5	$X_{B,H}$	1	0,086	0
6	$X_{B,A}$	1	0,086	0
7	X_p	1	i_{ci}	0
8	S_o	-1		0
9	S_{NO}	-4,57	1	-0,071
10	S_{NH}	0	1	0,071
11	S_{ND}	0	1	0
12	X_{ND}	0	1	0
13	S_{ALK}	0	0	-1
14	S_{N2}	-1,71	1	0

ASM1 Gujer Matrix
(S_{N2} has been added for continuity)
i: state variable
j: process
v_{ij}: stoichiometric coefficient (calculated from parameter values of Henze *et al.*, 2000)

	i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	
j		S_i	S_s	X_i	X_s	$X_{B,H}$	$X_{B,A}$	X_p	S_o	S_{NO}	S_{NH}	S_{ND}	X_{ND}	S_{ALK}	S_{N2}	
1	Aerobic growth of heterotrophs		-1,49			1			-0,49		-0,09			-0,006		0E-15 0E-15 0E-15
2	Anoxic growth of heterotrophs		-1,49			1				-0,17	-0,09			0,006	0,172	0E-15 0E-15 0E-15
3	Aerobic growth of autotrophs						1		-18,04	4,17	-4,25			-0,60		0E-15 0E-15 0E-15
4	Decay of heterotrophs				0,92	-1		0,08	v_{ji}				0,081			
5	Decay of autotrophs				0,92		-1	0,08					0,081			$\Sigma_i v_{ji}.i_{ci} = 0$ E-15
6	Ammonification of soluble organic N										1	-1		0,07		
7	Hydrolysis of entrapped organics		1		-1											0E-15 0E-15 0E-15
8	Hydrolysis of entrapped organic N											1	-1			0E-15 0E-15 0E-15

Figure 4-2. How to check continuity of Gujer Matrix

The common way to check continuity is a numerical analysis starting with default parameter values. For this study the tolerance is set to 10^{-15}. The numerical analysis is an option available in most simulators, or can be performed using spreadsheets (see http://www.iwaponline.com/wst/06104/0898.xls).

However, when some parameters are fixed to zero (e.g. $f_{SU\_XB,hyd}$, the fraction of inert COD generated in hydrolysis in ASM2d, ASM3, ASM3+Bio-P and ASM2d+TUD), a stoichiometric coefficient could be forgotten without any impact on continuity (see hydrolysis process in ASM3+Bio-P and processes 5 to 12 in UCTPHO+). Furthermore, errors could be compensated by other parameter values (e.g. when using rounded values everywhere in the model). Thus, another check has to be done by changing parameter values one after the other to track any discontinuity. To change values of parameters calculated from elemental molecular weights (see Table 4-3), the molecular weight of the element has to be changed for all the concerned parameters at once.

A better way to track discontinuity that stems from numerical problems is to use a symbolic analysis. Symbolic analysis allows re-calculating stoichiometric coefficients from the basic stoichiometric coefficients (e.g. yields) and the composition matrix. The symbolic analysis could be carried out by appropriate tools such as Maple (Maplesoft).

4.3.2.2 How to track kinetic inconsistencies

Some simulators provide the kinetic rates in symbolic form, which allows an easy check of the proper implementation (mainly parentheses errors). However, it is not possible to track kinetic inconsistencies in model editors so far. A tool to check kinetic rate expressions that could be implemented in simulators is proposed. This tool is based on four questions that modellers should answer for every process:

- Which are the consumed components (every state variable with a negative stoichiometric coefficient)? For every consumed component the kinetic rate expression should include a limitation function (e.g. Monod term). Concerning alkalinity, see the discussion in the chapter "Common published errors".
- Which biomass is involved in the process as biocatalyst? The kinetic rate expression is typically proportional to this biomass concentration.
- Are other components required for the process (e.g. an electron acceptor that is not consumed: Oxygen in ASM2d aerobic hydrolysis)? The kinetic rate expression should include a limitation function for those components (e.g. Monod term).
- Are other components inhibitory (e.g. oxygen in an anoxic process)? The kinetic rate expression should include an inhibitory function for those components (e.g. inhibitory Monod term).

In the attached spreadsheet (see http://www.iwaponline.com/wst/06104/0898.xls) it is proposed to perform this analysis by colouring the Gujer Matrix cells with different colours for each question. The two first questions could be easily automated in a model editor through the stoichiometric values of the Gujer Matrix. Nevertheless, the two last questions must involve the model developer to indicate electron acceptor conditions of the processes and inhibitors. This kind of matrix should be provided in model publications and implemented in simulators. With those pieces of information, model editors should be able to automatically check whether the kinetic rate expression includes a term for each coloured component.

In the presented work, the kinetic rate expressions were checked carefully to ensure that i) every reactant of the process is limiting (to stop a reaction when a reactant is limiting and to prevent the calculation of negative concentrations); ii) every switching function or kinetic parameter is coherent; and iii) kinetic rate expressions are consistent from one model to another.

4.3.3 Common published errors

4.3.3.1 Rounding parameters

An error that occurs systematically and that may hinder the continuity of a model is to round parameters to 2 significant figures or even to use rounded and "exact values" of parameters (i.e. fractions in calculated parameters, see Table 4-3) in the very same model. To avoid an accumulation of rounding problems, it is recommended to keep "exact values" everywhere in the model.

The "exact values" of conversion coefficients can be calculated from theoretical (conceptual) COD of elements as defined by Gujer and Larsen (1995) (Table 4-2) and from molecular weights (periodic table of elements). Table 4-3 summarizes the main conversion coefficients, their calculation explanation and their exact values to be used in ASM-type models.

4.3.3.2 Temperature adjustment of kinetic parameters

Kinetic parameter values depend on temperature. Three different ways have been proposed to provide temperature adjustment of kinetic parameters (with θ being the temperature adjustment coefficient, $k_{20°C}$ the kinetic coefficient at 20°C and k_T the kinetic coefficient at temperature T):

- In ASM1 and ASM2d, kinetic parameters are given at 10 and 20°C
- In ASM3, ASM3+Bio-P and ASM2d+TUD, θ values are provided using the following equation: $k_T=k_{20°C}*e^{\theta*(T-20)}$
- In New General and UCTPHO+, θ values are provided using: $k_T=k_{20°C}*\theta^{T-20}$

The two last equations are similar: the temperature adjustment e^{θ} in equation $k_T=k_{20°C}*e^{\theta*(T-20)}$ is equivalent to θ in the equation $k_T=k_{20°C}*\theta^{T-20}$. It is thus easy to convert temperature coefficient from one equation to the other. Unfortunately the same

symbol (θ) is given to these two different parameters. As suggested in Corominas *et al.* (2010), an extended notation should be used. The first parameter could be noted θ_{exp} and the second one θ_{pow}. Then $\theta_{pow}=\exp(\theta_{exp})$. However, it should be easier for model comparison to use a single temperature adjustment equation among the modelling community. The second equation ($k_T=k_{20°C}*\theta_{pow}^{T-20}$) is chosen in this work as it is the simplest one and the most commonly used (Vavilin, 1982).

4.3.3.3 Impact of alkalinity on kinetic rates

Alkalinity is introduced in several models to guarantee the continuity in ionic charge of the biological processes, and to predict possible pH changes. Alkalinity is usually measured in molar concentration of HCO_3^- or in concentration of $CaCO_3$ (1 mol $HCO_3^-.m^{-3}$=50 g $CaCO_3.m^{-3}$). Low alkalinity concentration causes unstable pH, which could reach inhibiting levels (Henze *et al.*, 2000a). Three ways to deal with alkalinity have been proposed in the models:

- Alkalinity is not taken into account in the model at all (New General and UCTPHO+);
- Alkalinity is taken into account in the stoichiometry but does not limit the kinetic rates (ASM1);
- Alkalinity is taken into account in both stoichiometry and kinetic rates (ASM2d, ASM3, ASM3+Bio-P and ASM2d+TUD).

For the latter models, the stoichiometric coefficients for alkalinity were compared using the parameter sets from the original publications (see http://www.iwaponline.com/wst/06104/0898.xls). Those calculations reveal two major problems that are illustrated through practical examples:

- **the use of alkalinity as a limiting factor for kinetic rates is not consistent**. Table 4-4 summarises models that involve alkalinity. For each process, it is checked whether alkalinity is consumed or produced and whether alkalinity is considered as a limiting factor or not. It reveals that alkalinity is a limiting factor for all processes in those models where alkalinity is consumed, except in process 11, 21 and 15 of ASM2d+TUD (see paragraph concerning ASM2d+TUD below). Alkalinity may also be considered as a limiting factor or not in the processes where it is produced.

Table 4-4. The use of alkalinity as a limiting factor for kinetic rates. Stoichiometric coefficients have been calculated with published parameter values

	Nb of processes	Nb of proc. with: -Alk **consummed** -Alk **limiting**	Nb of proc.with: -Alk **produced** -Alk **limiting**	Nb of proc. with: -Alk **consummed** -Alk **not limiting**	Nb of proc. with: -Alk **produced** -Alk **not limiting**	Nb of proc. without Alk. stoichiom.
ASM2d	21	8	7	0	6	
ASM3	12	2	1	0	8	1
ASM3+Bio-P	23	6	4	0	11	2
ASM2d+TUD	22	3	4	3	12	

– **the stoichiometric coefficients for alkalinity highly depend on parameter values** (e.g. yield values or conversion coefficients that change the proportions of consumed or released nutrients). To illustrate this point, a test has been carried out on ASM2d+TUD by changing two stoichiometric parameter values (i_{NBM} and i_{NSF}). Table 4-5 shows that these parameter values impact the sign of the stoichiometric coefficient of alkalinity. Thus, a process that consumes alkalinity with one parameter set could produce alkalinity with another parameter set.

Table 4-5. Examples of changes in stoichiometric coefficient values of ASM2d+TUD depending on parameter values

Processes	**Default parameter values**		**Tested parameter values**	
	parameter value	Alkalinity stoich.coeff. sign	parameter value	Alkalinity stoich.coeff. sign
Process 15	i_{NBM}=0.07	-	i_{NBM}=0.08	+
Processes 1, 2, 3	i_{NSF}=0.03	+	i_{NSF}=0.045	-
Process 4	i_{NSF}=0.03	-	i_{NSF}=0.045	+

The way of inclusion of alkalinity in the kinetic rates is a structural model problem and therefore out of the scope of this chapter. The reason to discuss it was to raise awareness of inconsistencies. Hence, the kinetic rates for alkalinity in the attached spreadsheets have not been changed (see http://www.iwaponline.com/wst/06104/0898.xls).

4.3.4 Typing errors, inconsistencies and gaps in published models

During the checks performed on the stoichiometric continuity and the evaluation of the kinetic rate expressions, several implementation errors and inconsistencies were identified. They are presented below for each model and separated into 3 different error

types: i) typing errors; ii) inconsistencies when it is not clearly an error but a potentially risky simplification; and iii) gaps in stoichiometry and kinetics due to oversight or purposeful omission to keep the model simple.

4.3.4.1 ASM1

ASM1 was first published in 1987 by Henze *et al.* This first version contained other errors than the 2000a version but these errors are not discussed here.

4.3.4.1.1 Inconsistencies

There is no term in the kinetic rate expression to model nutrient (ammonia) limitation in the heterotrophic growth process, which could induce negative ammonia concentration values (Table 4-6).

Table 4-6. Inconsistencies in kinetic rate expressions in ASM1 model publication (Henze *et al.*, 2000a)

Process	Description	Missing Monod term	Correct Monod Term
1, 2	Heterotrophic growth	Ammonia limitation	$\frac{S_{NH}}{K_{NH,H} + S_{NH}}$

The coefficient $K_{NH,H}$ is introduced and the same default value as in ASM2d is chosen (0.05 g $S_{NH4}.m^{-3}$).

4.3.4.1.2 Gaps

In order to close mass balances, N_2 should be included in the Gujer Matrix in process 2 (anoxic growth of heterotrophic biomass). This variable is only useful to verify the model continuity but has no impact on model results.

To perform a full nitrogen balance, variables S_{NI} (soluble non-biodegradable organic nitrogen) and X_{NI} (particulate non-biodegradable organic nitrogen) should be estimated in the influent. As non-biodegradable compounds, they do not appear in the Gujer Matrix. S_{NI} should be added to total soluble nitrogen in the effluent and X_{NI} should be added to total nitrogen in activated sludge.

4.3.4.2 ASM2d

4.3.4.2.1 Typing errors

Table 4-7 summarises ASM2d typing errors. Those typing errors have previously been pointed out by Gernaey *et al.* (2006).

Table 4-7. Typing errors in ASM2d model publication (Henze *et al.*, 2000b)

Process	Description	Kinetic or stoichiometry	Wrong	Correct
6, 7	Anoxic growth of heterotrophs on S_F and S_A	Kinetic rate	$\frac{K_{NO3}}{K_{NO3}+S_{NO3}}$	$\frac{S_{NO3}}{K_{NO3}+S_{NO3}}$
7	Anoxic growth of heterotrophs on S_A	Stoichiometry of S_{N2}	$-\frac{1-Y_H}{40/14.Y_H}$	$\frac{1-Y_H}{40/14.Y_H}$
8	Fermentation	Kinetic rate	K_F	K_{fe}
11	Aerobic storage of X_{PP}	Kinetic rate	K_{PP}	K_{IPP}
13,14	Aerobic and anoxic growth of X_{PAO}	Stoichiometry of X_{PHA}	$-1/Y_H$	$-1/Y_{PAO}$

Stoichiometric coefficients for S_O, S_{NH4}, S_{N2}, S_{NO3}, S_{PO4}, S_{ALK} and X_{TSS} are not given in detail, so that users have to apply continuity equations to implement them. The corrected matrix provided in the attached spreadsheet details these coefficients (see http://www.iwaponline.com/wst/06104/0898.xls).

4.3.4.2.2 Inconsistencies

The same parameter name is given to many kinetic parameters common for hydrolysis, precipitation, heterotrophic, phosphorus-accumulating and nitrifying organisms processes, although some of these parameters have different values in the parameter set provided in the publication (e.g.: η_{NO3}(hydrolysis)=0.6 and η_{NO3}(heterotrophs)=0.8). A suffix (respectively: HYD, PRE, H, PAO, AUT) has been added to these parameters to avoid any confusion. These problems are fixed when defining extended symbols using the standardised notation (Corominas *et al.*, 2010).

4.3.4.3 ASM3

4.3.4.3.1 Typing errors

The original publication (Gujer *et al.*, 1999) had several typing errors. The corrected version (Gujer *et al.*, 2000) should be used.

The coefficient $i_{SS,STO}$ is missing in the parameter list, the same default value as in ASM3+Bio-P is chosen (0.6 g TSS.g $XStor^{-1}$).

Stoichiometric coefficients for S_O, S_{NH4}, S_{N2}, S_{NOx}, S_{PO4}, S_{ALK} and X_{TSS} are not given in detail, so that users have to apply continuity equations to implement them. The corrected matrix provided in the attached spreadsheet details these coefficients (see http://www.iwaponline.com/wst/06104/0898.xls).

4.3.4.4 ASM3 + Bio-P

4.3.4.4.1 Typing errors

Table 4-8 summarises ASM3+Bio-P typing errors.

4.3.4.4.2 Inconsistencies

The kinetic parameter $K_{NO,A}$ is missing: the kinetic rate in process 12 (Anoxic endogenous respiration) uses $K_{NO,H}$.

Table 4-8. Typing errors in ASM3+Bio-P model publication (Rieger *et al.*, 2001)

Process	Description	Kinetic or stoichiometry	Wrong	Correct
1	Hydrolysis	Stoichiometry of S_I	No coefficient	f_{SI}
1	Hydrolysis	Stoichiometry of S_{PO4}	$i_{P,XS}$-$i_{P,SS}$	-(1-f_{SI})*$i_{P,SS}$-f_{SI}*$i_{P,SI}$+$i_{P,XS}$
8, 9	Aerobic and anoxic respiration of internal storage	Kinetic rate	b_H	b_{Sto}
11, 12	Aerobic and anoxic endogenous respiration of X_{AUT}	Kinetic rate	$K_{O,H}$	$K_{O,A}$
P9, P11	Anoxic lysis of X_{PP} and anoxic respiration of X_{PHA}	Kinetic rate	$\frac{S_{NO}}{K_{NO,PAO}}$	$\frac{S_{NO}}{K_{NO,PAO}+S_{NO}}$

4.3.4.5 ASM2d+TUD

4.3.4.5.1 Typing errors

Table 4-9 summarises ASM2d+TUD typing errors.

Table 4-9. Typing errors in ASM2d+TUD model publication (Meijer, 2004)

Process	Description	Kinetic or stoichiometry	Wrong	Correct
5, 7, 10, 12	OHO growth on S_A and PAO growth on S_A	Kinetic rate	K_A	K_{Ac}
21	Autotrophic growth	Stoichiometry of X_{TSS}	$-i_{TSS,BM}$	$i_{TSS,BM}$
21	Autotrophic growth	Kinetic rate	K_O	$K_{A,O}$
21	Autotrophic growth	Kinetic rate	K_{PO}	S_{PO}

4.3.4.5.2 Inconsistencies

The kinetic check reveals missing Monod terms to ensure consistency with the process. Table 4-10 summarises ASM2d+TUD inconsistencies in kinetic rate expressions.

Another theoretical inconsistency was identified in the anoxic glycogen formation process (process 15). This process turns PAO matter into glycogen and uses nitrate as the energy source. However, PAO matter is more oxidised than glycogen and no compound with reducing power is used in this process. To match the continuity mathematically, it results in a production of nitrate and a consumption of N_2. Note that this inconsistency has a negative effect on denitrification. As this is a structural inconsistency, the process has not been changed and no kinetic limitation function has been added for N_2 in the attached spreadsheet (see http://www.iwaponline.com/wst/06104/0898.xls).

As in ASM2d, the same parameter name is given to many kinetic parameters common for hydrolysis and organisms processes. A suffix has been added to these parameters to avoid any confusion.

Table 4-10. Inconsistencies in kinetic rate expressions in ASM2d+TUD model publication (Meijer, 2004)

Process	Description	Missing Monod term	Correct Monod Term
1	Aerobic hydrolysis	Oxygen limitation	$\frac{S_O}{K_O + S_O}$

4.3.4.6 New General (Barker and Dold, 1997)

4.3.4.6.1 Typing errors

The unit of K_{SP} (Saturation constant for $P_{PP\text{-}LO}$) should be g $P.m^{-3}$ instead of g $P.g\ COD^{-1}$.

4.3.4.6.2 Inconsistencies

In the kinetic rate expressions of processes 1 to 8 (growth on S_{BSC} or S_{BSA}) there is no substrate preference switch function (as e.g. in ASM2d) such as $S_{BSC}/(S_{BSC}+S_{BSA})$. This substrate preference switch function avoids that the heterotrophic specific growth rate increases above a maximum value if both substrates are present in high concentration (Henze *et al.*, 2000b). Even if Barker and Dold (1997) specify that the S_{BSA} concentration entering the anoxic and aerobic zones is usually very low, this substrate preference switch function could be added to enhance the robustness of the model. The preference switch function $S_{BSC}/(S_{BSC}+S_{BSA})$ is proposed (as e.g. used in ASM2d and in ADM1 (Batstone *et al.*, 2002)), other function types are described in Dudley *et al.* (2002).

The kinetic check reveals other missing Monod terms to ensure consistency with the stoichiometry of the process. Table 4-11 summarises New General inconsistencies in kinetic rate expressions.

Table 4-11. Inconsistencies in kinetic rate expressions in New General model publication (Barker and Dold, 1997)

Process	Description	Missing Monod term	Correct Monod term
1 to 4	Heterotrophic growth on S_{BSC}	Substrate preference switch function	$\frac{S_{BSC}}{S_{BSC}+S_{BSA}}$
5 to 8	Heterotrophic growth on S_{BSA}	Substrate preference switch function	$\frac{S_{BSA}}{S_{BSC}+S_{BSA}}$
15	Fermentation of S_{BSC} to S_{BSA} (Anaerobic growth)	Phosphate and ammonia limitation	$\frac{N_{H3}}{K_{NA}+N_{H3}}\cdot\frac{P_{O4}}{K_{LP,GRO}+P_{O4}}$
16	Autotrophic growth	Phosphate limitation	$\frac{P_{O4}}{K_{LP,GRO}+P_{O4}}$
20 and 21	Aerobic growth of PAO, PO_4 limited	$P_{PP\text{-}LO}$ limitation (phosphorus source in case of PO_4 depletion)	$\frac{P_{PP-LO}}{K_{XP}+P_{PP-LO}}$

4.3.4.6.3 Gaps

In order to keep the continuity, N_2 (processes 2, 4, 6, 8, 22 and 27) should be included in the Gujer Matrix as a state variable. As in ASM1, this variable is only useful to verify the model continuity but has no impact on model results.

The "COD losses" mentioned in Barker and Dold (1997) (processes 11, 12, 15 and 36) have been detected based on experimental data. It is modelled through the introduction of an efficiency parameter in hydrolysis processes (11, 12) and a yield parameter in fermentation and sequestration processes (15, 36). However the fate of the resulting COD is not described by the model and leads to a lack of continuity. In the model ASDM (as implemented in BioWin, 2008), the "COD loss" is considered to be due to H_2 gas formation (Kraemer *et al.*, 2008). A state variable S_H is therefore added to the model (Table 4-12).

In processes 3, 4, 7, 8, 19 and 21, there is another discontinuity for COD that is not mentioned in the paper, due to the potential use of NO_3^- as a nitrogen source by heterotrophs. Indeed, when NO_3^- is used as a nitrogen source, the fate of the oxygen content of NO_3^- is not considered. The O_2 stoichiometric coefficient should be lower for growth with NO_3^- as nitrogen source than O_2 consumption for growth with NH_3 (Grady *et al.*, 1999).

To match the continuity of aerobic processes (3, 7, 19 and 21), the authors suggest to decrease the oxygen stoichiometric coefficient by subtracting the COD content in the consumed nitrates (Table 4-12). This correction is not possible for anoxic processes (4 and 8). The proposed solution is to consider that more substrate is needed for the same growth: the stoichiometric coefficient of the substrate (S_{BSC} or S_{BSA}) is increased by the COD consumed when using nitrates as nitrogen source (Table 4-12).

Polyphosphate accumulating organisms (PAOs) (Z_P in the model's notation) do not have the same nitrogen content as autotrophs (Z_A) and heterotrophs (Z_H) ($f_{N,ZP}$=0.07 and $f_{N,ZA}$ and $f_{N,ZH}$=0.068). In the decay process, all organisms turn into endogenous mass (Z_E) that has the same nitrogen content as the biomass it comes from ($f_{N,ZEP}$=0.07 and $f_{N,ZEA}$ and $f_{N,ZEH}$=0.068). Thus, the model structure allows different nitrogen fractions for the endogenous masses. However all the biomasses are turned into a single Z_E, which only has a single nitrogen fraction. Consequently, with the published parameter values, there is a lack in nitrogen continuity of -5.10^{-4} g N for processes 23, 27 and 31 (aerobic, anoxic and anaerobic decay of PAOs). All biomass nitrogen fractions $f_{N,ZEP}$, $f_{N,ZEA}$ and $f_{N,ZEH}$ should be corrected with the same value. A value of 0.07 g N.g COD^{-1} is proposed.

4.3.4.7 UCTPHO+

4.3.4.7.1 Typing errors

Table 4-13 summarises UCTPHO+ typing errors.

4.3.4.7.2 Inconsistencies

The kinetic check reveals some missing Monod terms to ensure consistency with the stoichiometry of the processes Table 4-14 summarises UCTPHO+ inconsistencies in the kinetic rate expressions.

Table 4-12. Gaps in stoichiometry in New General model publication (Barker and Dold, 1997)

Process	Description	Gap in stoichiometry	Corrected stoichiometry*
2, 4, 6, 8	Anoxic growth of heterotrophs	S_{N2} variable	$(1-Y_{H.ANOX})/(i_{NOx,N2}*Y_{H.ANOX})$
22	Anoxic growth of PolyP organisms	S_{N2} variable	$(1-Y_P)/(i_{NOx,N2}*Y_P)$
27	Anoxic decay of PolyP organisms	S_{N2} variable	$(1-f_{EP.P}-f_{ES.P})/i_{NOx,N2}$
11	Anoxic hydrolysis of stored/enmeshed COD	S_H variable	$(1-E_{ANOX})/i_{COD\_SH}$
12	Anaerobic hydrolysis of stored/enmeshed COD	S_H variable	$(1-E_{ANA})/i_{COD\_SH}$
15	Fermentation of S_{BSC} to S_{BSA}	S_H variable	$(1-(1-Y_{H,ANA})*Y_{AC}-Y_{H,ANA})/i_{COD\_SH}$
36	Sequestration of S_{CFA} by PolyP organisms	S_H variable	$(1-Y_{PHB})/i_{COD\_SH}$
3, 7	Aerobic growth of heterotrophs on S_{BSC} / S_{BSA} with N_{O3}	Oxygen from consumed N_{O3} not include in S_O	$-(1-Y_{H.AER})/Y_{H.AER} - i_{COD\_NOx}*f_{N.ZH}$
19, 21	Aerobic growth of PolyP organisms on S_{PHB} with N_{O3} without and with P_{O4} limited	Oxygen from consumed N_{O3} not include in S_O	$-(1-Y_P)/Y_P - i_{COD\_NOx}*f_{N.ZP}$
4, 8	Anoxic growth of heterotrophs on S_{BSC} / S_{BSA} with N_{O3}	Different yield for S_{BSC} or S_{BSA} consumption with N_{O3}	$-1/Y_{H.ANOX} + i_{COD\_NOx}*f_{N.ZH}$

*The new parameters and variables introduced in this study are named according to the standardised notation rules (Corominas *et al.*, 2010) and thus may not be consistent with the original model notation. The conversion factors are described in Table 4-3.

Table 4-13. Typing errors in UCTPHO+ model publication (Hu *et al.*, 2007)

Process	Description	Kinetic or stoichiometry	Wrong	Correct
14, 17	Heterotrophic and autotrophic decay	Stoichiometry of X_{ENM}	$f_{XI,H}$	$f_{XE,H}$
14, 17	Heterotrophic and autotrophic decay	Stoichiometry of S_{NH4}	No coefficient	$i_{NBM}-(1-f_{XE-H})*i_{NENM}-f_{XE-H}*i_{NXE}$ or $i_{NBM}-(1-f_{XE-NIT})*i_{NENM}-f_{XE-NIT}*i_{NXE}$
5 to 8	Heterotrophic growth on S_F	Stoichiometry of S_{PO4}	$-i_{PBM}$ No P contained in S_F	$-i_{PBM}+i_{PSF}/Y_{H1}$ or $-i_{PBM}+i_{PSF}/Y_{H2}$
9 to 12	Heterotrophic growth on X_{ads}	Stoichiometry of S_{PO4}	$-i_{PBM}$ No P contained in X_{ads}	$-i_{PBM}+i_{PENM}/Y_{H1}$ or $-i_{PBM}+i_{PENM}/Y_{H2}$
15	Conversion of S_F to S_A	Stoichiometry of S_{PO4}	No coefficient	i_{PSF}
18	Aerobic growth of X_{PAO} on X_{PHA} with S_{NH4}	Stoichiometry of S_{PO4}	No coefficient	$-i_{PBM}-Y_{PP1}/Y_{PAO1}$
24, 27, 30	Decay of X_{PAO}	Stoichiometry of S_{NH4}	In coefficients A, B and C, nitrogen fraction of X_E is i_{NBM} instead of i_{NXE}	A: $i_{NBM}-f_{XE.PAO}*i_{NXE}-f_{SI.PAO}*i_{NSI}$ B: $i_{NBM}-f_{XE.PAO}*i_{NXE}-f_{SI.PAO}*i_{NSI}-i_{NENM}*(1-\eta_{PAO})*(1-f_{XE.PAO}-f_{SI.PAO})$ C: $i_{NBM}-f_{XE.PAO}*i_{NXE}-f_{SI.PAO}*i_{NSI}-i_{NENM}*(1-f_{XE.PAO}-f_{SI.PAO})$
14, 17, 24, 27, 30	OHO, ANO and PAO decay	Stoichiometry of S_{PO4}	$i_{PBM}*(1-f_{XE})$ P fraction of X_E is i_{PBM} instead of i_{PXE}	$i_{PBM}-f_{XE.H}*i_{PXE}$ or $i_{PBM}-f_{XE.NIT}*i_{PXE}$ or $i_{PBM}-f_{XE.PAO}*i_{PXE}$
24, 27, 30	Decay of X_{PAO}	Stoichiometry of S_{PO4}	$i_{PBM}-f_{XE.PAO}*i_{PXE}$ No P contained in S_I	$i_{PBM}-f_{XE.PAO}*i_{PXE}-f_{SI.PAO}*i_{PSI}$
14, 17, 26, 27, 29, 30, 32	OHO and ANO decay, anoxic and anaerobic PAO decay, X_{PHA} lysis	Stoichiometry of S_{PO4}	No P contained in X_{ENM}	Depends on X_{ENM} stoichiometry: $v_{ij,XENM}*i_{PENM}$ should be added (see http://www.iwaponline.com/wst/06104/0898.xls)

Table 4-14. Inconsistencies in kinetic rate expressions in UCTPHO+ model publication (Hu *et al.*, 2007)

Process	Description	Missing Monod term	Correct Monod Term
1 to 4	Heterotrophic growth on S_A	Substrate preference switch function	$\frac{S_A}{S_F + S_A + X_{ADS}}$
5 to 8	Heterotrophic growth on S_F	Substrate preference switch function	$\frac{S_F}{S_F + S_A + X_{ADS}}$
9 to12	Heterotrophic growth on X_{Ads}	Substrate preference switch function	$\frac{X_{Ads}}{S_F + S_A + X_{ADS}}$
3, 7, 11	Anoxic growth with S_{NH4}	Nitrate limitation	$\frac{S_{NO3}}{K_{NO3} + S_{NO3}}$
26, 29, 32	X_{PHA} lysis during (aerobic, anoxic, anaerobic) PAO decay	Ammonia and phosphate limitation (X_{PHA} is turned into X_{ENM}, which contains nitrogen and phosphorus. Ammonia and phosphate have thus to be consumed) Parameter $K_{PO4\text{-}lys}$ is introduced, the value of $K_{PO4\text{-}gro}$ is kept.	$\frac{S_{NH4}}{K_{NH4} + S_{NH4}} \cdot \frac{S_{PO4}}{K_{PO4-lys} + S_{PO4}}$
20 and 21	Aerobic growth of PAO, PO_4 limited	X_{PP} limitation (phosphorus source in case of PO_4 depletion)	$\frac{X_{PP}}{K_{PP} + X_{PP}}$

Gaps. In order to keep the continuity, N_2 as a state variable should be included in the Gujer Matrix for the processes 3, 4, 7, 8, 11, 12, 22, 23 and 27. As in ASM1 and New General, this variable is only useful to verify the model continuity but has no impact on model results.

As previously seen in the New General, a discontinuity for COD in processes 2, 4, 6, 8, 10, 12, 19, 21 and 23 is due to the use of NO_3^- as nitrogen source.

In the same way as in the New General, the authors suggest to lower the oxygen stoichiometric coefficient in aerobic processes (2, 6, 10, 19 and 21) and to increase the stoichiometric coefficient of substrate in anoxic processes (4, 8, 12 and 23). In contrast to the New General, some of the substrates contain a fraction of nitrogen and phosphorus (S_F for process 8 and X_{Ads} for process 12). The stoichiometric coefficients of S_{NH4} and S_{PO4} should be corrected to match the continuity.

Table 4-15. Gaps in stoichiometry of UCTPHO+ model publication (Hu *et al.*, 2007)

Process	Description	Gap	Corrected stoichiometry
3, 4, 7, 8, 11, 12	Anoxic growth of heterotrophs	S_{N2} variable missing	$(1-Y_{H2})/(i_{NOx,N2}*Y_{H2})$
22, 23	Anoxic growth of PolyP organisms	S_{N2} variable missing	$(1-Y_{PAO2})/ (i_{NOx,N2}*Y_{PAO2})$
27	Anoxic decay of PolyP organisms	S_{N2} variable missing	$\eta_{PAO}*(1-f_{XE.PAO}-f_{SI.PAO})$/iNOx,N2
2, 6, 10	Aerobic growth of heterotrophs on S_A / S_F / X_{ads} with S_{NO3}	Oxygen from consumed S_{NOx} not include in S_{O2}	$-(1-Y_{H1})/Y_{H1} -i_{COD\_NOx}*i_{NBM}$
19, 21	Aerobic growth of PolyP organisms on X_{PHA} with S_{NO3} without and with S_{PO4} limited	Oxygen from consumed S_{NOx} not include in S_{O2}	$-(1-Y_{PAO1})/Y_{PAO1} -i_{COD\_NOx}*i_{NBM}$
4	Anoxic growth of heterotrophs on S_A with S_{NO3}	Different yield of S_A consumption with S_{NOx}	$-1/Y_{H2}+i_{COD\_NOx}*i_{NBM}$
8	Anoxic growth of heterotrophs on S_F with S_{NO3}	Different yield of S_F consumption with S_{NO3}	$-1/Y_{H2}+i_{COD\_NOx}*i_{NBM}$
		S_{NH4} coefficient correction	$i_{NSF}*(1/Y_{H2}-i_{COD\_NOx}*i_{NBM})$
		S_{PO4} coefficient correction	$-i_{PBM}+i_{PSF}*(1/Y_{H2}-i_{COD\_NOx}*i_{NBM})$
12	Anoxic growth of heterotrophs on X_{Ads} with S_{NO3}	Different yield of X_{Ads} consumption with N_{O3}	$-1/Y_{H2}+i_{COD\_NOx}*i_{NBM}$
		S_{NH4} coefficient correction	$i_{NENM}*(1/Y_{H2}-i_{COD\_NOx}*i_{NBM})$
		S_{PO4} coefficient correction	$-i_{PBM}+i_{PENM}*(1/Y_{H2}-i_{COD\_NOx}*i_{NBM})$
23	Anoxic growth of PolyP organisms on X_{PHA} with S_{NO3}	Different yield of X_{PHA} consumption with S_{NO3}	$-1/Y_{PAO2}+i_{COD\_NOx}*i_{NBM}$

4.3.5 Conclusion

Several error sources can impact model quality. This chapter points out typing errors, inconsistencies and gaps in the publications of seven selected models. Table 4-16 synthesises the number of typing errors, gaps and inconsistencies found in each of the models verified. Some of the errors corrected in this chapter are mainly theoretical errors and will only have a minor impact on model results in typical conditions, but may have a significant impact in case of peculiar treatment conditions (e.g. near or outside model limits).

Table 4-16. Number of typing errors, gaps and inconsistencies found with the verification procedure

Model	Stœchiometry	Kinetic
ASM1	1	2
ASM2d	3	4
ASM3	0	0
ASM3+BioP	2	6
Barker & Dold	16	12
UCTPHO+	50	20
ASM2d+TUD	1	7

The number of errors found shows to what extent it is necessary to verify both a published model and the model implementation in simulators to avoid typing errors and inconsistencies. A simple spreadsheet, as presented in the attached file (see http://www.iwaponline.com/wst/06104/0898.xls), could be used for continuity checks. The evaluation of the kinetic rate expressions is only possible based on a detailed check of the individual expressions but should be carried out with great care. The attached spreadsheet provides corrected matrices with all stoichiometric coefficients for the discussed biokinetic models and gives an example of a proper continuity and kinetic rate expressions check.

Model verification is a time-consuming task that could be facilitated and automated by appropriate model editor tools as part of a simulator. Albeit model verification is facilitated with these tools, it remains that model users have to redo this work each time they implement a new model.

Additional material: http://www.iwaponline.com/wst/06104/0898.xls

4.4 Critical review of activated sludge modelling: State of process knowledge, modelling concepts and limitations

4.4.1 Introduction

Since ASM1 (Henze *et al.*, 1987), a dozen Activated Sludge Models (ASM) and even more extensions have been published. They have fixed some shortcomings of ASM1 and included new process insights. Nevertheless, ASM1 remains the most used model. Indeed, the results of an international survey among ASM users (Hauduc *et al.*, 2009) revealed that models are found too complex for 22% of the respondents, and that 24% of the model users do not trust their model. Furthermore, self training is the main source of knowledge for 78% of model users. Consequently, users are generally not mastering all published models to be able to choose the most suitable one for their modelling project, and ASM1 turns out too often be their first choice.

Since the first publication of ASM1 (Henze *et al.*, 1987), the biokinetic models are represented in a matrix format, named Gujer matrix or Petersen matrix (Takacs, 2005). Each row of this matrix stands for a process and each column for a state variable of the model. The stoichiometric coefficients, negative for consumed compounds and positive for produced ones, are stored in the cells at the intersection of the corresponding row and column. The process rates are listed in the rightmost column. This representation is very convenient, as it gathers complex models into a condensed form and facilitates their publication. It also allows seeing at once all state variables involved in a process, and all processes in which a state variable is involved. However, in case of large models such as ASM2d for example, it becomes difficult to "read" this matrix. Comeau and Takács (2008) proposed a schematic representation of ASM, in which each model is represented in a single scheme. This allows a global view of the model processes and their interactions, which is very helpful as a learning tool to understand the models. However, as processes are illustrated in different schematics and as stoichiometric and kinetic information are not represented, it is difficult to compare modelling concepts used by different models, and thus to compare models in detail.

This work aims at helping model users to better understand i) the model concepts used; ii) the differences between models and iii) the limits of the models. Seven published models have been chosen for this study: (1) ASM1 (Henze *et al.*, 2000a); (2) ASM2d

(Henze *et al.*, 2000b); (3) ASM3 (Gujer *et al.*, 2000); (4) ASM3+BioP (Rieger *et al.*, 2001); (5) ASM2d+TUD (Meijer, 2004); (6) Barker&Dold model (Barker and Dold, 1997); (7) UCTPHO+ (Hu *et al.*, 2007). Nine standard processes have been identified and will be discussed in separate sections of this chapter: Hydrolysis; Fermentation; Ordinary Heterotrophic Organisms (OHO) growth; Autotrophic Nitrifying Organisms (ANO) growth; OHO & ANO decay; Poly-hydroxyalkanoates (PHA) storage; Polyphosphates (polyP) storage; Phosphorus Accumulating Organisms (PAO) growth and PAO decay. For each standard process, a brief overview on the available biochemical knowledge is provided as basis for discussion of the modelling concepts. The major publications are cited for further reading. Then, the different modelling concepts used are compared through a new schematic representation of the stoichiometry and the kinetics. Finally, the consequences of the model simplifications are investigated to draw theoretical limits of the models. Alternative published models that cope with the studied model limits are cited. The final discussion synthetises the modelling concept diversity and the gray areas in theoretical knowledge, and discusses the model selection and existing model modifications.

4.4.2 Methods

4.4.2.1 Studied models

The seven published models have been chosen among the most used ones (Table 4-17). To keep the chapter readable, those references will not be repeated each time. Two of the seven models, ASM1 and ASM3, only consider carbon and nitrogen removal, whereas the others also consider biological phosphorus removal. UCTPHO+ is an update of the UCTPHO model (Wentzel *et al.*, 1992), and ASM2d+TUD is the last published version of the TUD (Technical University of Delft) metabolic model.

Table 4-17 indicates the complexity of the models through the number of processes, state variables, stoichiometric parameters, conversion coefficients and kinetic parameters they include. It can be deduced that complexity level differences come mainly from the PAO processes. However, the real complexity of the models stands in the number of parameters that should actually be calibrated. In this respect, the ASM2d+TUD metabolic model for phosphorus removal only has 3 independent stoichiometric parameters, and the simulation results seem to be sensitive to only one of

them, the P/O ratio (also called ATP per NADH ratio, δ) (Murnleitner *et al.*, 1997). Furthermore, some of the half-saturation coefficient are not "true" model coefficient in the sense that their value does not impact the simulation results, and are just used as switching function in case of component depletion (e.g. K_{NHx}).

A first step in the review was to check the published models for typos and continuity. Several errors were detected and corrected for continuity problems in the stoichiometry and inconsistencies in the kinetic rate expressions. The corrected model formulations (Hauduc *et al.*, 2010; paragraph 4.3) have been used in this chapter (full Gujer Matrices: http://www.iwaponline.com/wst/06104/0898.xls).

Table 4-17. List of studied activated sludge models

Models	Reference	Subs-trates	Nb of processes	Nb of state variables	Parameters												
					Total	conversion	Temperature adjustment	stoichiometry					kinetic				
								Hydrolysis	OHO	ANO	PAO	Biomass	Hydrolysis	OHO	ANO	PAO	Biomass
ASM1	Henze *et al.*, 2000a	CN	**8**	**13**	**26**	2	7	-	1	1	-	1	-	9	5	-	-
Barker&Dold	Barker and Dold, 1997	CNP	**36**	**19**	**81**	16	18	2	5	2	8	-	4	9	5	11	1
ASM2d	Henze *et al.*, 2000b	CNP	**21**	**19**	**74**	13	12	1	1	1	3	1	6	12	6	18	-
ASM3	Gujer *et al.*, 2000	CN	**12**	**13**	**46**	8	10	1	4	1	-	1	2	13	6	-	-
ASM3+BioP	Rieger *et al.*, 2001	CNP	**23**	**17**	**83**	15	13	1	4	1	5	1	2	13	7	21	-
UCTPHO+	Hu *et al.*, 2007	CNP	**35**	**16**	**67**	12	10	-	3	2	7	-	-	13	4	14	1
ASM2d+TUD	Meijer., 2004	CNP	**22**	**18**	**98**	16	15	1	2	2	12	-	6	12	6	26	-

N.B.: Chemical P precipitation not considered; kinetic parameters include temperature correction factors

4.4.2.2 Model processes

Nine standard processes have been identified for this study and are listed in Table 4-18. These "standard processes" involve mechanisms that only differ by the environmental conditions under which they take place. For instance, aerobic and anoxic OHO growth processes are combined into one OHO growth standard process.

Table 4-18 also synthesises the processes considered in each model. This work is limited to biological processes, and therefore chemical phosphorus precipitation is not discussed.

As OHO and ANO related processes of ASM2d+TUD are exactly the same as ASM2d, ASM2d+TUD will be studied only for BioP-related processes.

Table 4-18. List of processes and models considered

Processes types	ASM1	Barker & Dold	ASM2d	ASM3	ASM3+ BioP	UCTPHO+	ASM2d +TUD
Hydrolysis	X	X	X	X	X		X
Fermentation		X	X			X	X
OHO growth	X	X	X	X	X[1]	X[2]	X
ANO growth	X	X	X	X	X	X	X
OHO & ANO decay	X	X	X	X	X	X	X
PHA storage		X	X		X	X	X
PolyP storage		} X[3]	X		X	} X[3]	X
PAO growth			X		X		X
PAO decay		X	X		X	X	X

[1] Including storage of PHA in OHOs; [2] Including adsorption and hydrolysis; [3] Including polyP storage

4.4.2.3 A new schematic representation

A new schematic representation of the model processes is proposed to facilitate model concept comparison in a systematic and transparent way. For each process type, the standard processes that use the same modelling concept are represented on a single figure, and the standard processes that are different in terms of modelling concept are represented on separate figures.

The process is represented as a reaction with consumed components on the left of the figure and produced components on the right. Figure 4-3 shows the symbols used for the schematic representation:

- Models that consider the process are given by a coloured rectangle.
- The electron acceptor condition of the process is indicated by a yellow (aerobic), orange (anoxic) or red (anaerobic) spot, close to the corresponding model name.
- The included state variables are represented through both a shape and a colour: the shape indicates whether the variable is particulate, soluble or refers to an organism, and the colour indicates its composition in terms of COD (B for biodegradable, U for undegradable matter), nitrogen (N) or phosphorus (P). Undegradable nitrogen and phosphorus are not distinguished from biodegradable ones, since few models consider them. The state variable is indicated inside the shape, using the standardised notation from Corominas *et al.* (2010).
- The electron acceptor consumed in the process is represented in blue. For instance, depending on its usage, nitrate can be represented in blue (electron acceptor) or green (substrate).

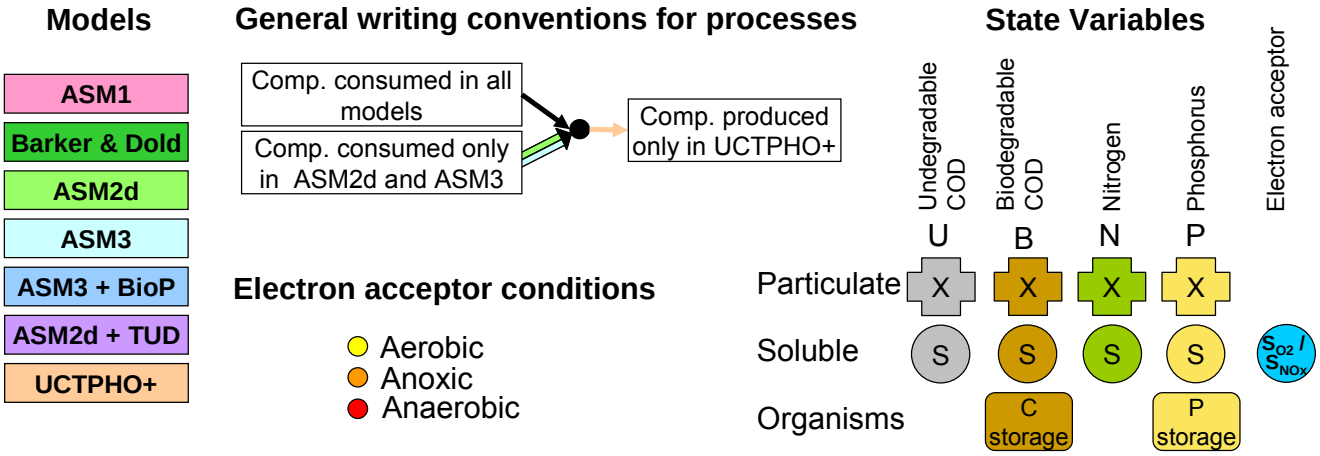


Figure 4-3**.** Symbols used for the schematic representation

To simplify the graphs, alkalinity and total suspended solids are not represented and only important stoichiometric coefficients (especially yields) are specified, as others can be calculated through continuity (Hauduc *et al.*, 2010).

In this process representation, the consumed and produced components of the reaction are linked by black arrows. In case state variables are not considered by all models, the arrow will not be black, but will have the models' colour.

The kinetic expression for the rate of reaction is also part of the concept and is therefore represented. This is also done in a condensed way by a standardised compact notation. Table 4-19 illustrates the different symbols used to keep the expression readable. The expressions of saturation and inhibition functions, which have the form of Monod expression, are simplified to M() or IM(), with the component concerned in parenthesis. The symbol $\langle\ \rangle$ is used to indicate optional or alternative terms depending on the model or the environmental condition (see Table 4-19 for examples).

4.4.2.4 Literature review on theoretical knowledge vs modelling concepts

The results are organised around the nine main processes listed in Table 4-18. For each process, the theoretical knowledge is first presented based on a brief literature review. Then the different concepts used in the models are analysed, supported by the schematic representation of the process. Different concepts are given different numbers (concept 1, concept 2…), whereas variations within the same concept are pointed out using letters (concept 1a, 1d…). Finally, model limitations in using particular concepts are listed.

Table 4-19. Symbols used for kinetic expressions: examples

Description	Notation	Symbol
Kinetic coefficients: maximum specific growth rate	μ_{OHO}	μ_{OHO}
Concentration of S_{NOx}	S_{NOx}	S_{NOx}
Monod function with S_B as substrate	$\frac{S_B}{K_{SB}+S_B}$	$M(S_B)$
Inhibition Monod function with S_{NOX} as electron acceptor	$\frac{K_{NOx}}{K_{NOx}+S_{NOx}}$	$IM(S_{NOx})$
Monod function with S_{PO4} as substrate, only used in models considering phosphorus removal	$\frac{S_{PO4}}{K_{PO4}+S_{PO4}}$	$\langle M(S_{PO4})\rangle$
Electron acceptor conditions (ex: OHO growth) (aerobic or anoxic conditions)		$\left\langle \begin{array}{c} M(S_{O2}) \\ \eta_{\mu OHO,Ax} M(S_{NOx}) \cdot IM(S_{O2x}) \end{array} \right\rangle$

N.B.: The symbol ⟨ ⟩ is used to indicate optional or alternative terms, one or none of the lines should be chosen.

4.4.3 Results

4.4.3.1 General modelling concepts

4.4.3.1.1 State variables

Some conceptual differences among the studied models come from the state variables used, as summarised in Table 4-20.

All studied models are COD-based. COD is the chosen organic material measure because it allows characterising the electron equivalents of organic substrates, biomasses and electron acceptors. Furthermore, COD is a conservative measure that enables mass balances to be calculated (Ekama and Marais, 1979; Henze *et al.*, 2000a).

Table 4-20. State variables used in the models and their composition in terms of COD (C), nitrogen (N) and phosphorus (P)

Description	Notation	Unit	ASM1 C N P	ASM2d C N P	ASM3 C N P	ASM3 + BioP C N P	Barker & Dold C N P	UCTPHO + C N P	ASM2d+TUD C N P
COD soluble									
Soluble biodegradable organics	S_B	g COD.m^{-3}							
Fermentable organic matter	S_F	g COD.m^{-3}							
Fermentation product (volatile fatty acids)	S_{VFA}	g COD.m^{-3}							
Soluble undegradable organics	S_U	g COD.m^{-3}							
Dissolved oxygen	S_{O2}	- g COD.m^{-3}							
COD particulate and colloidal									
Particulate and colloidal biodegradable organics	XC_B	g COD.m^{-3}							
Adsorbed slowly biodegradable substrate	X_{Ads}	g COD.m^{-3}							
Particulate undegradable organics	X_U	g COD.m^{-3}							
Particulate undegradable organics from influent	$X_{U,Inf}$	g COD.m^{-3}							
Particulate undegradable endogenous products	$X_{U,E}$	g COD.m^{-3}							
Nitrogen (N) and Phosphorus (P)									
Ammonium and ammonia nitrogen ($NH_4^+ + NH_3$)	S_{NHx}	g N.m^{-3}							
Nitrate and nitrite ($NO_3 + NO_2$)	S_{NOx}	g N.m^{-3}							
Dissolved nitrogen gas	S_{N2}	g N.m^{-3}							
Particulate and colloidal biodegradable organic N	$XC_{B,N}$	g N.m^{-3}							
Soluble biodegradable organic N	$S_{B,N}$	g N.m^{-3}							
Soluble undegradable organic N	$S_{U,N}$	g N.m^{-3}							
Soluble inorganic phosphate	S_{PO4}	g P.m^{-3}							
Biomass									
Ordinary heterotrophic organisms	X_{OHO}	g COD.m^{-3}							
Autotrophic nitrifying organisms (NH_4^+ to NO_3^-)	X_{ANO}	g COD.m^{-3}							
Phosphorus accumulating organisms	X_{PAO}	g COD.m^{-3}							
Internal cells products									
Storage compound in OHOs	$X_{OHO,Stor}$	g COD.m^{-3}							
Storage compound in PAOs	$X_{PAO,Stor}$	g COD.m^{-3}							
Stored poly-β-hydroxyalkanoates in PAOs	$X_{PAO,PHA}$	g COD.m^{-3}							
Stored glycogen in PAOs	$X_{PAO,Gly}$	g COD.m^{-3}							
Stored polyP in PAOs	$X_{PAO,PP}$	g P.m^{-3}							
Releasable stored polyP (Low molecular weight)	$X_{PAO,PP,Lo}$	g P.m^{-3}							
Non-releasable stored polyP (High mol. weight)	$X_{PAO,PP,Hi}$	g P.m^{-3}							
Other									
Alkalinity ($CaCO_3$)	S_{Alk}	mol $CaCO_3$.m^{-3}	X	X	X	X			X
Total suspended solids	X_{TSS}	g TSS.m^{-3}		X	X	X			X

4.4.3.1.2 Component-based / fraction-based models

In the ASM1 and the Barker & Dold model, organic nitrogen is considered in separate state variables (component-based model) and organic phosphorus is not considered. In these models nitrogen and phosphorus (Barker & Dold only) are, however, linked to biomass. In other models, nitrogen and phosphorus are linked to COD state variables (fraction-based models). The pros and cons for these two concepts as presented in Table 4-21.

Table 4-21. Pros and cons of component-based and fraction-based models

	Component-based model	**Fraction-based model**
pros	As variables are separated, the two hydrolysis processes are independent. It is thus easier to change parameters in case of variations in influent fractions.	Having linked variables limits the number of variables and processes. Furthermore it could be easier to understand the stoichiometry of process reactions by considering $C_xH_yO_zN_aP_b$ composition of the state variables.
cons	In the Barker & Dold model, organic phosphorus is not considered separately. Phosphorus is then always available in the form of PO_4^{3-}, without any delay due to hydrolysis, when released by biomass decay.	The substrate fraction is supposed to be homogeneous and constant in its composition. In reality different organic compounds with different fractions are coming in the influent. In this case this concept could induce a pitfall or the model complexity must be increased by considering more components.

4.4.3.1.3 Undegradable organics from influent and from biomass decay

ASM1, the Barker & Dold model and UCTPHO+ distinguish the influent undegradable organics, from those formed by biomass decay (or endogenous respiration). The latter fraction thus includes non-active biomass. Furthermore, this distinction allows a different nitrogen and phosphorus fraction content in soluble undegradable matter from influent and endogenous products, especially for the component-based models (ASM1 and Barker & Dold model, see above), increasing model flexibility.

4.4.3.1.4 N_2 considered as a state variable to close the nitrogen balance

To simplify the models, ASM1, the Barker & Dold model and UCTPHO+ do not consider dissolved dinitrogen gas (N_2) as a state variable. As a consequence, the continuity is not verified for these processes in terms of nitrogen and COD (Hauduc *et al.*, 2010). This state variable needs to be added to check the continuity of the model.

4.4.3.1.5 Total suspended solids (TSS) as a state variable

TSS is a combined variable in some models and a state variable in others, calculated from the linear combination of particulate state variables and from an assumed VSS/COD and VSS/TSS ratio to predict the sludge mass in the system. TSS is not considered in this study.

4.4.3.1.6 Alkalinity

A low alkalinity value (<50 g $CaCO_3.m^{-3}$ = 1 mol $CaCO_3.m^{-3}$) results in an unstable pH, which could cause nitrification inhibition and other process problems (Henze *et al.*, 2000a). Alkalinity is thus modelled to predict the risk of pH limitation.

As discussed previously (Hauduc *et al.*, 2010), alkalinity is not considered in the same way in all models:

- Alkalinity is not taken into account in the model at all (Barker & Dold model and UCTPHO+);
- Alkalinity is taken into account in the stoichiometry but does not limit the kinetic rates (ASM1);
- Alkalinity is taken into account in both stoichiometry and kinetic rates (ASM2d, ASM3, ASM3+BioP and ASM2d+TUD).

4.4.3.2 OHO and ANO processes

4.4.3.2.1 Hydrolysis of particulate substrate

4.4.3.2.1.1 Knowledge

A large fraction of wastewater substrate is particulate or colloidal, and is thus not directly available for biomass growth (Ekama and Marais, 1979; Morgenroth *et al.*, 2002). Hydrolysis is an extracellular biological reaction where hydrolytic enzymes

break down large organic molecules into smaller ones that can pass through the bacterial cell wall. A number of hydrolysis enzymes exist and seem to have a low specificity, thus enabling the breakdown of a large range of substrates. Hydrolytic enzyme synthesis is induced by bacteria when readily biodegradable substrate is not available (Morgenroth *et al.*, 2002). Hydrolytic enzymes seem to be bound to the floc and have a low turnover rate (hours to days) (Goel *et al.*, 1999).

Substrate. The diversity of substrates, hydrolytic enzymes and biological pathways make the hydrolysis process difficult to study. Experiments described in literature are mainly based on pure culture bacteria, with single or few substrates, providing results that can hardly be generalised.

Protozoa are also able to take up particulate substrate, and possibly release readily biodegradable substrate in the process, but this process and its importance in particulate substrate consumption is so far poorly described (Morgenroth *et al.*, 2002).

Electron acceptor conditions. Hydrolytic enzyme synthesis depends on the electron acceptor conditions (Goel *et al.*, 1999). However, their activity is not affected by the electron acceptor conditions (Goel *et al.*, 1999), which enables hydrolysis processes to continue under anoxic and anaerobic conditions.

4.4.3.2.1.2 Modelling

Morgenroth *et al.* (2002) distinguished five ways to model hydrolysis in the literature:

1. **Direct growth** on both soluble and particulate matter: bacteria are able to use both substrates but at a different rate
2. **Two biomass system:** particulate substrate is first adsorbed and then used by a specific type of organism, whereas soluble substrate is used by another type of organisms. This way to model hydrolysis is supported by experimental results (Ekama and Marais, 1979; Dold *et al.*, 1980; Frigon *et al.*, 2002).
3. **One step hydrolysis:** slowly biodegradable substrate is completely hydrolysed, then consumed by organisms.
4. **Parallel hydrolysis:** different types of particulate substrates are hydrolysed separately into soluble substrate (Orhon *et al.*, 1998). Larrea *et al.* (2002) considered the parallel hydrolysis of a particulate and a soluble slowly biodegradable substrate into S_B.

5. **Sequential hydrolysis:** different types of particulate substrates are considered where the largest substrate is first hydrolysed into a smaller one, and so on until soluble substrate is produced. This way of modelling hydrolysis is useful when intermediate hydrolysed substrate accumulation is observed. Nowak *et al.* (1999) introduced a very slowly biodegradable substrate fraction to model hydrolysis as a two stage process for long SRT systems.

In the models studied here, only two concepts are used (Table 4-22):

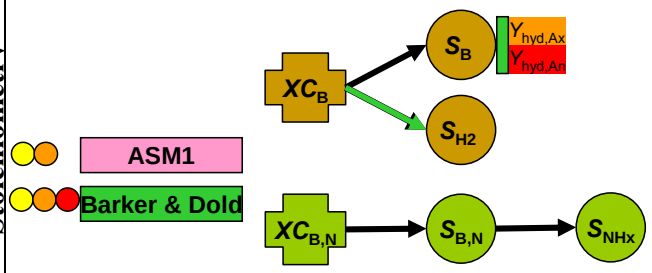
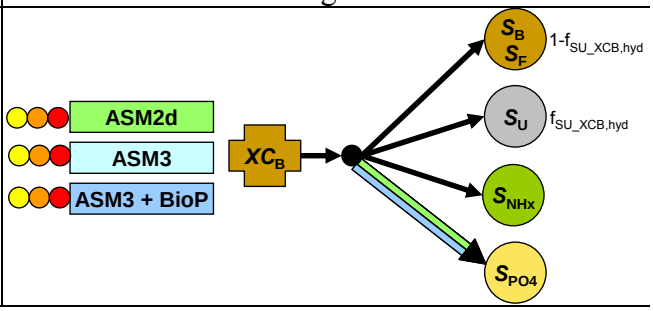
- The first concept is one step hydrolysis. The differences between the models concern the way the residues of the reaction and the nitrogen fractions are modelled:
  - Component-based model (ASM1, Barker & Dold);
  - Fraction-based model (ASM2d, ASM3, ASM3+BioP).
- The second concept used in UCTPHO+, is based on direct growth using adsorbed substrate. The hydrolysis is accounted for by a reduced growth rate for the use of this adsorbed substrate (see OHO growth process, Table 4-25). This way to model hydrolysis makes the hydrolysed substrate available for the organisms that produce hydrolysis enzymes, whereas in other modelling concepts the hydrolysed substrate is released into the bulk phase, in this way becoming available for all organisms, which will thus compete for it.

The hydrolysis process is in fact used to model all mechanisms that make slowly biodegradable substrate available for bacterial growth with a certain delay (chemical dissolution, mass transport, storage, etc.). Consequently, depending on the other processes considered in the model, the hydrolysis process does not have the same significance:

- Storage is considered as a separate process in ASM3 and ASM3+BioP, whereas it is not explicitly described in other models. However, storage and hydrolysis cannot be distinguished through respirometric methods (Goel *et al.*, 1999). Consequently, in ASM1, ASM2d, Barker & Dold and ASM2d+TUD, the storage is implicitly included in the hydrolysis process.
- Depending on the origin of the organic molecules, two types of hydrolysis reactions can be distinguished: hydrolysis of "primary substrate" that comes from the inffluent and hydrolysis of the matter produced by biomass metabolism

or decay, named "secondary substrate" (Morgenroth *et al.*, 2002). Consequently, models using the death-regeneration concept to model biomass decay (see paragraph 4.4.4.5.2) merge those two types of hydrolysis in a single process, whereas in case of the endogenous respiration concept, the hydrolysis of secondary substrate is modelled through biomass decay and endogenous respiration of storage compounds for maintenance processes (ASM3 and ASM3+BioP).

Table 4-22. Hydrolysis of particulate substrate

	Concept 1a: One step hydrolysis with organic N and C considered separately	**Concept 1b:** One step hydrolysis with N and P linked to organic matter
Stoichiometry		
Kinetics	**Organics:** ASM1: $q_{XCB\_SB,hyd} \cdot M\left(\frac{XC_B}{X_{OHO}}\right) \cdot \left\langle \frac{M(S_{O2})}{\eta_{qhyd,Ax} \cdot M(S_{NOx}) \cdot IM(S_{O2})} \right\rangle \cdot X_{OHO}$ Barker & Dold, ASM2d: $q_{XCB\_SB,hyd} \cdot M\left(\frac{XC_B}{X_{OHO}}\right) \cdot \left\langle \begin{matrix} M(S_{O2}) \\ \eta_{qhyd,Ax} \cdot M(S_{NOx}) \cdot IM(S_{O2}) \\ \eta_{qhyd,An} \cdot IM(S_{NOx}) \cdot IM(S_{O2}) \end{matrix} \right\rangle \cdot X_{OHO}$ ASM3, ASM3+BioP: $q_{XCB\_SB,hyd} \cdot M\left(\frac{XC_B}{X_{OHO}}\right) \cdot X_{OHO}$ **Particulate nitrogen hydrolysis:** $q_{XCB\_SB,hyd} \cdot M\left(\frac{XC_{B,N}}{X_{OHO}}\right) \cdot \left\langle \begin{matrix} M(S_{O2}) \\ \eta_{qhyd,Ax} \cdot M(S_{NOx}) \cdot IM(S_{O2}) \\ \eta_{qhyd,An} \cdot IM(S_{NOx}) \cdot IM(S_{O2}) \end{matrix} \right\rangle \cdot X_{OHO}$ **Ammonification:** ASM1: $q_{am} \cdot S_{B,N} \cdot X_{OHO}$ Barker & Dold: $q_{am} \cdot S_{B,N} \cdot (X_{OHO} + X_{PAO})$	

N.B.: in UCTPHO+, hydrolysis is considered simultaneously with growth. ASM2d+TUD is identical to ASM2d.
The symbol ‹ › is used to indicate optional or alternative terms, one or none of the lines should be chosen.

Electron acceptor conditions. The storage process and the utilisation of secondary substrate require an electron acceptor to produce energy. Models that implicitly merge these processes into the hydrolysis process (ASM1, ASM2d, Barker & Dold model, UCTPHO+ and ASM2d+TUD, see above), have then to take into account their electron

acceptor. Thus, the hydrolysis kinetic rates should depend on the electron acceptor. However, ASM1 does not consider hydrolysis under anaerobic conditions. As ASM3 and ASM3+BioP consider storage and hydrolysis separately, the electron acceptor is not rate limiting for hydrolysis.

The Barker & Dold model introduces a hydrolysis yield in anoxic and anaerobic conditions that allows modelling the experimentally observed "COD loss" (Barker and Dold, 1995). Although this observation is not explained so far, the "loss" may be considered to be due to H_2 gas formation (Kraemer *et al.*, 2008), and thus, a S_{H2} state variable has been added to the model to reach continuity (Hauduc *et al.*, 2010).

As UCTPHO+ modelled the hydrolysis process simultaneously with growth, anaerobic hydrolysis is not modelled.

Ammonification. In case of component-based models (ASM1, Barker & Dold), biodegradable organic nitrogen is produced by the hydrolysis process. To make this nitrogen available for organisms, ammonification has to be modelled.

4.4.3.2.1.3 Model limitations

Substrate. The concept of one step hydrolysis is used by all these models but one (UCTPHO+). This concept implies a simplification of the (primary) substrate into a single biodegradable particulate fraction. In case of peculiar influents with different particulate substrates behaviour or large colloidal fractions, it may be required to integrate other particulate fractions and to consider other hydrolysis concepts.

Electron acceptor conditions. Hydrolysis enzyme activity is independent of the electron acceptor. However, the hydrolysis process also covers other mechanisms that require an electron acceptor, such as degradation by protozoa and storage. In case of a large anaerobic zone, anaerobic hydrolysis should be considered, especially for BioP models to make substrate available for PHA storage.

Experimental parameters determination. Modelling hydrolysis and storage as two separated processes requires adequate experiments to independently determine the kinetic rates (Goel *et al.*, 1999).

4.4.3.2.2 Fermentation

4.4.3.2.2.1 Knowledge

Fermentation is a growth process under anaerobic conditions for OHOs. In absence of electron acceptor, the organic substrate catabolism reactions are partially blocked and the complete substrate oxidation is not possible. Under these conditions, organic substrate is catabolised into volatile fatty acids (VFA, e.g. acetate), which allows slow organisms growth.

4.4.3.2.2.2 Modelling

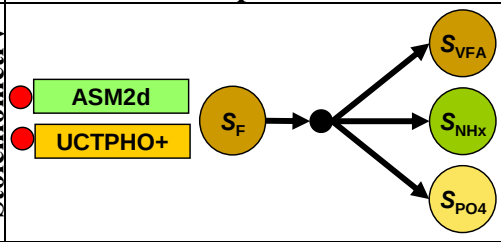
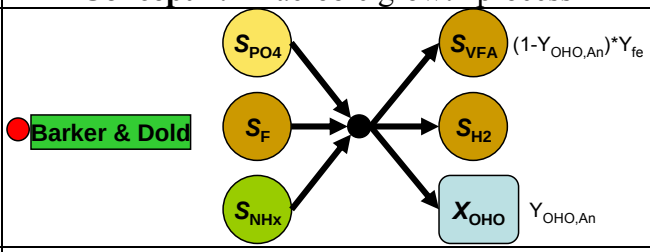
Two different concepts are used to model fermentation in the studied models:

- The first concept considers fermentation as a transformation (ASM2d, UCTPHO+)
- In the second concept fermentation is described as an anaerobic growth process.

The process kinetic rate always depends on the OHO concentration, which is the only biomass involved in this process.

Barker and Dold (1995) experimentally observed a COD "loss" during anaerobic processes, which they linked to fermentation, anaerobic hydrolysis and S_{VFA} sequestration. This phenomenon has been modelled by a S_{VFA} formation yield (Y_{fe}) in the fermentation process. The loss of (1-Y_{fe}) g COD.g S_{VFA}^{-1} may be considered to be due to H_2 gas formation (Kraemer *et al.*, 2008), and a S_{H2} state variable has thus been added to the model to reach continuity (Hauduc *et al.*, 2010).

Table 4-23. Fermentation

	Concept 1: Transformation	**Concept 2:** Anaerobic growth process
Stoichiometry		
Kinetics	ASM2d: $q_{SF\_VFA,Max} \cdot M(S_F) \cdot IM(S_{O2}) \cdot IM(S_{NOx}) \cdot X_{OHO}$ UCTPHO+: $q_{SF\_VFA,Max} \cdot S_F \cdot IM(S_{O2}) \cdot IM(S_{NOx}) \cdot X_{OHO}$	$q_{SF\_VFA,Max} \cdot M(S_F) \cdot M(S_{NHx}) \cdot M(S_{PO4}) \cdot IM(S_{O2}) \cdot IM(S_{NOx}) \cdot X_{OHO}$

N.B.: ASM2d+TUD is identical to ASM2d.

4.4.3.2.2.3 Model limitations

ASM1 and ASM3 do not consider fermentation, consequently only one soluble substrate is considered (S_B). Fermentation is considered only in models with BioP, since PAOs only grow on fermentation products (S_{VFA}) and not on fermentable products (S_F). However, fermentation is not considered in ASM3+BioP: hydrolysis is considered as the rate-limiting step, so that the fermentation process rate is negligible. This could be a model limitation: hydrolysis should no longer be the rate-limiting step, e.g. in case of a peculiar influent (e.g. from agro-industries with high S_B concentration) or a specific plant configuration (e.g. with hydrolysis of return activated sludge).

All models except the Barker & Dold model neglect OHO formation during fermentation. Indeed, Ekama and Wentzel (1999) estimate the anaerobic growth yield at 0.10 g X_{OHO}.g S_B^{-1}. In case of large anaerobic zones, anaerobic growth may not be neglected.

4.4.3.2.3 Ordinary heterotrophic organisms (OHO) growth

4.4.3.2.3.1 Knowledge

Under aerobic or anoxic conditions OHOs use organic substrate as an energy and carbon source. The yield of biomass growth is the fraction of substrate that is used as a carbon source to produce biomass (Figure 2).

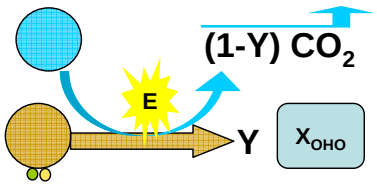


Figure 4-4. OHO use of organic substrate as carbon and energy source

Substrate. van Loosdrecht *et al.* (1997b) proposed the existence of two types of bacteria in terms of their capacity for substrate storage. Bacteria not capable of substrate storage will maximize their growth rate in periods with available substrate in order to be competitive, but will not be able to maintain their cell structure in case of long starvation periods. In case of a highly dynamic influent or in case of a process with a feast/famine cycle, bacteria capable of storing substrate will have a strong competitive

advantage due to their ability to maintain a low growth rate during starvation periods, which enables them to keep all their cell system viable (van Loosdrecht *et al.*, 1997b).

Stored compounds, e.g. poly-β-hydroxybutyrate (PHB), result from additional substrate that is taken up on top of the substrate requirement for direct growth (van Aalst-Van Leeuwen *et al.*, 1997). However, the nature of the storage compounds is still not well understood but seems to depend on the substrate used (Beccari *et al.*, 2002). As an example, propionate substrate would lead preferentially to poly-β-hydroxyvalerate (PHV) (Oehmen *et al.*, 2007).

The substrate uptake rate increases instantaneously when a high concentration occurs (up to the maximum rate), but the growth rate increases only slowly, and the extra substrate may be stored (van Aalst-Van Leeuwen *et al.*, 1997). Consequently, a high growth rate (e.g. at short SRT) will result in less storage (Beun *et al.*, 2002; van Loosdrecht and Heijnen, 2002). The growth rate on stored compounds is lower and limited by the storage product degradation process, which depends on its content of the biomass following a first order relationship (van Loosdrecht *et al.*, 1997b; Beun *et al.*, 2002).

Nutrients. Organism growth also requires nutrients such as nitrogen or phosphorus. The bacterial cell composition formula is generally considered to be $C_5H_7O_2N$ or $C_{60}H_{87}O_{23}N_{12}P$ (Comeau, 2008). This nutrient composition of biomass is important to take into account for process continuity and mass balance calculations.

In case of ammonia depletion, OHO seem able to use nitrate as nitrogen source. for instance, Wentzel *et al.* (1989) experimentally proved that when ammonia is depleted, PAOs consume nitrates for their growth with no modification of their kinetic behaviour.

Denitrification. Heterotrophic growth under anoxic condition requires oxidised form of nitrogen as electron acceptor: nitrate (NO_3^-), nitrite (NO_2^-), nitric oxide (NO) or nitrous oxide (N_2O). If denitrification is complete, these electron acceptors are reduced sequentially to nitrogen gas (N_2).

The need to use a different OHO yield under anoxic conditions ($Y_{OHO,Ax}$) to properly model the nitrate and COD consumptions was experimentally shown by several authors (Orhon *et al.*, 1996; Sozen *et al.*, 1998; Muller *et al.*, 2003). This phenomenon is due to

the smaller number of moles of electrons transferred through the electron transport chain to nitrate compared to oxygen, thus resulting in less ATP being produced (Muller *et al.*, 2003).

4.4.3.2.3.2 Modelling

The stoichiometry of OHO growth requires an organic substrate, an electron acceptor and nutrients. The modelling concepts differ in the substrates used, the nitrogen source and the use of different yields for aerobic and anoxic conditions (Table 4-25):

- The first concept considers direct growth of OHO on readily biodegradable substrate:
  - In concept 1a, NH_X is the only nitrogen source (ASM1, ASM2d),
  - In concept 1b, NO_X can be used as a nitrogen source in case of ammonia depletion (Barker & Dold, UCTPHO+). Additionally, UCTPHO+ considers adsorption of particulate substrate onto OHO biomass, followed by direct growth on the adsorbed substrate.
- The second concept first considers substrate storage and then OHO growth on storage compounds as unique carbon source (ASM3, ASM3+BioP).

The adsorption and storage processes are particularly useful in case of cyclic loading conditions. The kinetics of these processes are considered to depend on the ratio of adsorbed or stored substrate to biomass and are associated with a maximum adsorption/storage potential (Ekama and Marais, 1979). The kinetic expression for adsorption in the UCTPHO+ model is in agreement with this statement. However, ASM3 and ASM3+BioP only use a Monod expression for substrate uptake. The storage pool is thus not limited to a maximum storage potential.

Substrate: Several substrates are used depending on the models (Table 4-24):

- Readily biodegradable substrate (S_B) or fermentable substrate (S_F) are used by all models except ASM3 and ASM3+BioP.
- Volatile fatty acids (S_{VFA}) are considered in Bio-P models, except ASM3+BioP. For this substrate OHOs compete with PAOs.
- Adsorbed particulate substrate ($X_{OHO,Ads}$) is considered in UCTPHO+. This substrate has to be hydrolysed before use, which occurs simultaneously with growth. Modelling adsorption processes is a way to slow down OHO substrate

consumption and model the delay observed before growth occurs under some conditions (feed/starvation). This way to model hydrolysis is chosen by the UCT group to avoid the competition of organisms on hydrolysed substrate with the hydrolysis products being consumed directly by the organisms that produce hydrolysis enzymes (Wentzel *et al.*, 1992).

- Stored substrate ($X_{OHO,Stor}$) is the only usable substrate in ASM3 and ASM3+BioP. Direct growth on external substrate is not considered. This concept is needed in alternating feeding/starvation phases of the plant. It allows simulating the observed delay before OHO growth. The maximum storage capacity is 50% of the organisms mass in terms of COD (Ekama and Marais, 1979).

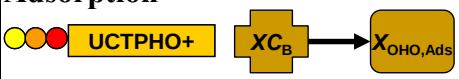
Nutrients. Barker & Dold and UCTPHO+ consider growth with NO_3 as nitrogen source in case of ammonia depletion. However, these models do not consider the fate of the oxygen contained in nitrate, which would be needed to maintain continuity of the COD balance.

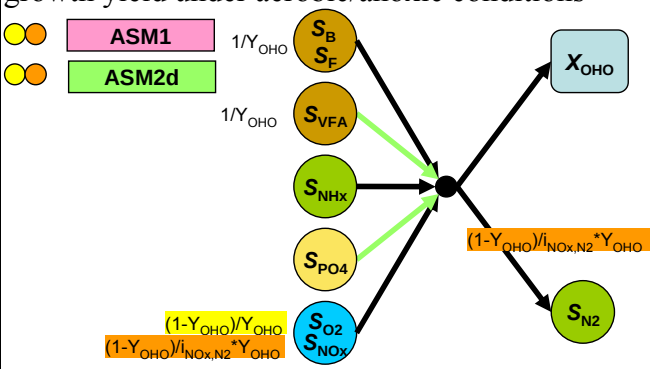
Denitrification. Denitrification is modelled as one step: nitrate is considered the only possible electron acceptor. The maximum anoxic growth rate is lower than under aerobic conditions, either because $\mu_{OHO,Max}$ is lower under anoxic conditions, or only a fraction of OHOs is able to denitrify. This is modelled through the reducing factor $\eta_{\mu OHO}$ <1 in all models. Furthermore, all models but two (ASM1 and ASM2d) use a lower anoxic growth yield (Table 4-24).

Table 4-24. Stoichiometry for OHO growth

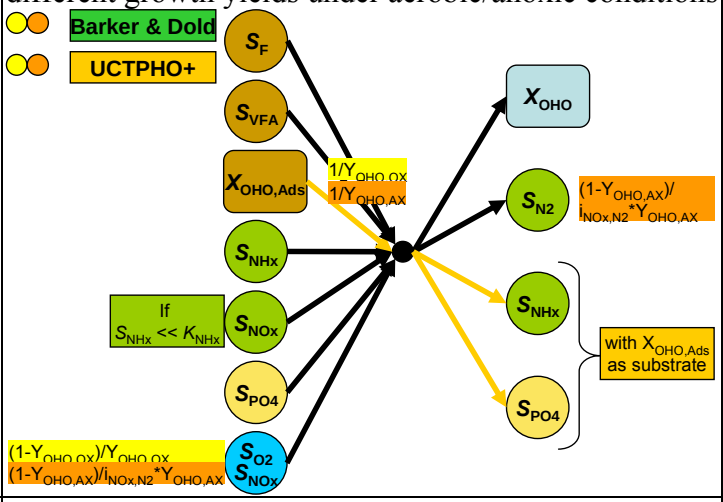
	Organic substrate				**Nitrogen source**		**Different anoxic growth yield**
Models	**S_{VFA}**	**S_F / S_B**	**X_{Ads}**	**X_{Stor}**	**S_{NHx}**	**S_{NOx}**	
ASM1		X			X		
Barker&Dold	X	X			X	X	X
ASM2d	X	X			X		
ASM3				X	X		X
ASM3+BioP				X	X		X
UCTPHO+	X	X	X		X	X	X
ASM2d+TUD	X	X			X		X

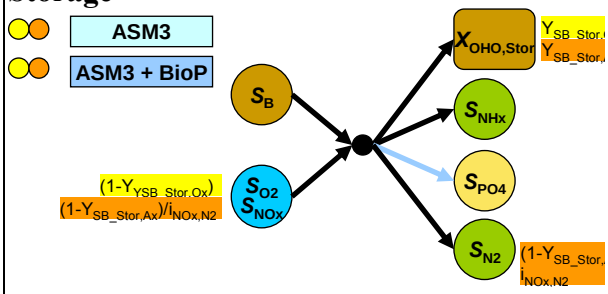
– Table 4-25. OHO growth process concepts

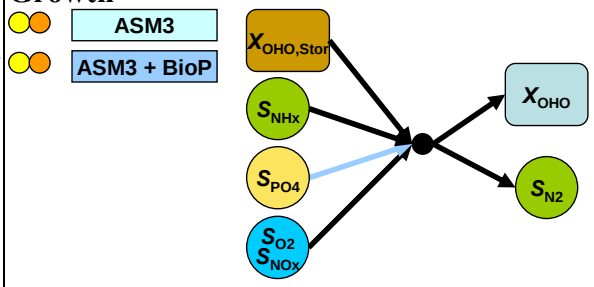
<table>
<tr><th></th><th>Concept 1: direct growth</th><th>Concept 2: storage then growth</th></tr>
<tr><td>Stoichiometry</td><td>
Adsorption


Growth
Concept 1a: S_{NHx} as unique nitrogen source and same growth yield under aerobic/anoxic conditions


S_{N2} has been added for continuity in ASM1

Concept 1b: S_{NHx} or S_{NOx} as nitrogen source and different growth yields under aerobic/anoxic conditions


</td><td>
Storage


Growth


</td></tr>
<tr><td>Kinetics</td><td>
Adsorption: $q_{XCB\_Ads} \cdot XC_B \left(f_{Ads\_OHO,Max} - \frac{X_{Ads}}{X_{OHO}} \right) \cdot X_{OHO}$

Growth:
$$\left\langle \begin{array}{l} \mu_{OHO,Max} \left[M(S_{Sub}) \frac{S_{Sub}}{\sum_i S_{Sub,i}} \right] \\ \mu_{Ads\_OHO,Max} \left[M\left(\frac{X_{Ads}}{X_{OHO}} \right) \frac{S_{Sub}}{\sum_i S_{Sub,i}} \right] \end{array} \right\rangle \cdot \left\langle \frac{M(S_{O2x})}{\eta_{\mu OHO,Ax} M(S_{NOx}) \cdot IM(S_{O2x})} \right\rangle \cdot \langle M(S_{PO4}) \rangle \cdot \left\langle \frac{M(S_{NHx})}{M(S_{NOx}) \cdot IM(S_{NHx})} \right\rangle \cdot X_{OHO}$$
With S_{Sub} the considered substrate (S_B, S_F or S_{VFA})
</td><td>
Storage:
$$q_{SB\_Stor} \cdot M(S_B) \cdot \left\langle \frac{M(S_{O2x})}{\eta_{\mu OHO,Ax} M(S_{NOx}) \cdot IM(S_{O2x})} \right\rangle \cdot X_{OHO}$$

Growth:
$$\mu_{OHO,Max} \cdot M\left(\frac{X_{OHO,Stor}}{X_{OHO}} \right) \cdot \left\langle \frac{M(S_{O2x})}{\eta_{\mu OHO,Ax} M(S_{NOx}) \cdot IM(S_{O2x})} \right\rangle \cdot \langle M(S_{PO4}) \rangle \cdot M(S_{NHx}) \cdot X_{OHO}$$
</td></tr>
</table>

4.4.3.2.3.3 Model limitations

Substrate. The substrate preference switching function avoids that the OHO specific growth rate increases above a maximum value if both substrates are present in high concentration (Henze *et al.*, 2000b) as two OHO growth processes run in parallel. The substrate preference switching function usually used in ASM models is in the form:

$$\left(\frac{S_{Sub}}{K_{SSub}+S_{Sub}}\right).\frac{S_{Sub}}{\sum_{i} S_{Sub,i}}$$

with S_{Sub} being the considered substrate.

However, this equation leads to wrong values in specific cases. For example, for n substrates, if all $S_{Sub,i}$=S/n, the sum of the substrate preference switching function is S/(n.K+S). This function leads to a value of one in case of S>>K, which is correct (maximum rate), but underpredicts the growth rate in case of S<<K (the function leads to S/(n.K) instead of S/K). An alternative mathematical description for substrate competition is proposed by Dudley *et al.* (2002):

$$\frac{S_{Sub}/K_{SSub}}{1+\sum_{i}\left(S_{Sub,i}/K_{SSub,i}\right)}$$

Adsorption and storage. The ASM3 growth on stored substrate is a simplified model that does not consider direct growth on soluble substrate and uses a different growth yield under feast or famine conditions. These simplifications lead to poor predictions in case of low SRT (<5 d) (van Loosdrecht and Heijnen, 2002), and long feast/famine cycles, which are conditions when growth rate and storage are not constant. Krishna and van Loosdrecht (1999), Karahan-Gül *et al.* (2003), Sin *et al.* (2005) and Guisasola *et al.* (2005) proposed ASM3 modifications considering parallel direct growth on soluble substrate and indirect growth on internally stored substrate.

Beccari *et al.* (2002) proposed a different modelling concept that includes first a biosorption step, in which substrate is absorbed by biomass without any transformation, contrary to the UCTPHO+ adsorption concept where substrate is adsorbed on the biomass. Then, the biosorbed substrate is used either for direct growth or is transformed into stored compound, which is later used for growth. This modelling concept allows a better description of the ammonia profile, because biosorption does not release the nitrogen content of the substrate into the mixed liquor.

Denitrification. In case of a large anoxic zone, using a single growth yield value for anoxic and aerobic processes (ASM1, ASM2d) could lead to an overestimation of the denitrification process in terms of biomass production, substrate consumption and nitrogen removal. The overprediction of substrate consumption could also have an effect on other processes such as P removal. A different anoxic growth yield should be added, but the model will then require a recalibration of the hydrolysis and storage processes to compensate the substrate consumption and maintain the experimentally observed denitrification rate (Muller *et al.*, 2003).

4.4.3.2.4 Autotrophic Nitrifying Organisms (ANO) growth

4.4.3.2.4.1 Knowledge

ANO oxidise ammonia to produce the required energy for carbon dioxide (CO_2) or bicarbonate ($CaCO_3$) uptake and growth. This oxidation of ammonia is named nitrification. It includes two steps that involve two distinct groups of autotrophic organisms: ammonia oxidisers and nitrite oxidisers (Figure 4-5). In the first step, nitritation, ammonia oxidisers produce energy required for their growth through ammonia oxidation into nitrite. Then, in the nitratation step, nitrite oxidisers convert nitrite into nitrate to produce energy. The first oxidation (nitritation) consumes alkalinity (Downing *et al.*, 1964).

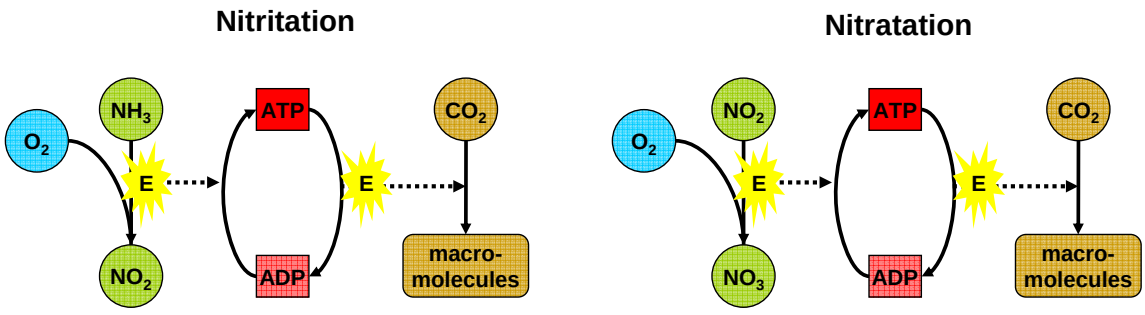


Figure 4-5. Simplified metabolism of autotrophic bacteria

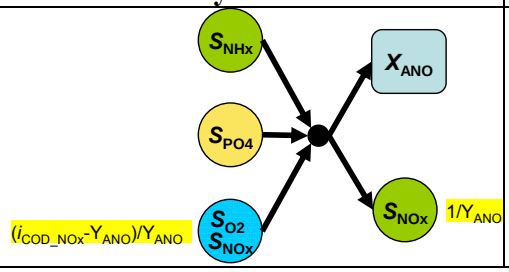
Because of a less efficient energy production pathway, autotrophic organisms have a lower growth rate and growth yield than OHOs. Furthermore, autotrophs, which are exclusively aerobic organisms, have a lower affinity for oxygen than heterotrophs. Therefore, to ensure good nitrification, it is necessary to provide sufficient dissolved oxygen to the activated sludge and to maintain a minimum SRT to avoid the wash out of nitrifiers (Downing *et al.*, 1964). Nitrification is also inhibited by a low pH and

sufficient alkalinity concentration (>50 g $CaCO_3$. m^{-3} = 1 mol $CaCO_3$ m^{-3}) has thus to be maintained to ensure a stable pH (Henze *et al.*, 2000a).

4.4.3.2.4.2 Modelling

Nitritation is normaly considered the limiting step in nitrification (Downing *et al.*, 1964). Consequently, nitrification is often modelled as a one step process, as in all studied models (Table 4-26), and initially proposed by Lijklema (1973).

Table 4-26. ANO growth process

Stoichiometry	Kinetics
ASM1 Barker & Dold ASM2d ASM3 ASM3 + BioP UCTPHO+ 	$\mu_{ANO,Max} \cdot M(S_{NHx}) \cdot \langle M(S_{PO4}) \rangle \cdot M(S_{O2}) \cdot X_{ANO}$

4.4.3.2.4.3 Model limitations

Multi-step nitrification/denitrification. The simplified concept of one-step nitrification is sufficient for most municipal wastewater systems.

However, the modelling project may require predicting nitrite accumulation or greenhouse gas emission, in the form of nitric and nitrous oxide. NO_2^- accumulation (partial nitrification) has actually been observed in specific situations such as (Sin *et al.*, 2008b; Kaelin *et al.*, 2009):

- unstable operation of municipal WWTP due to insufficient oxygen, low temperature, low sludge age and inhibitory compounds,
- high temperatures.

These modelling objectives cannot be reached with any of the studied models, which consider nitrification and denitrification as a single step. Consequently some models have been extended with two step nitrification (see 4.4.4.4.3) and denitrification, as reviewed by Sin *et al.* (2008b). A model with four step denitrification (NO_2^-, NO and N_2O as intermediates) and two step nitrification is also proposed by Hiatt and Grady (2008). Considerable attention to greenhouse gas production in wastewater treatment will certainly lead to much more detailed models of the nitrogen-related reactions.

Nitrification inhibition. Autotrophs are sensitive to inhibition (pH, nitrous acid, ammonia, chromium, nickel, copper, etc). Effects of some environmental conditions on activated sludge process are synthesised in Gujer (2010). Inhibitory effects are considered to be constant and are thus accounted for in the growth rate value (Henze *et al.*, 2000a). This can cause calibration problems in case of variability in the concentration of these compounds in the influent or in the treatment plant. To detect variability in influent inhibitors, some authors developed online respirometric methods to determine inhibition kinetics of nitrification (Nowak *et al.*, 1995; Kong *et al.*, 1996; Vanrolleghem *et al.*, 1996).

4.4.3.2.5 OHO and ANO decay

4.4.3.2.5.1 Knowledge

van Loosdrecht and Henze (1999) published a literature review on the theoretical knowledge regarding maintenance, endogenous respiration, lysis, decay and predation. Oxygen consumption linked to a loss of biomass was observed by various authors since the end of the 19th century. This phenomenon has been explained by the concept of "endogenous respiration" during which bacteria use their own storage pools of organic matter for maintenance purposes instead of using external substrate. Other experiments have shown accumulation of undegradable matter in the absence of substrate, leading to the cryptic growth (growth on dead bacteria) or the "death-regeneration" concepts (van Loosdrecht and Henze, 1999).

These concepts lump several mechanisms that result in oxygen consumption and biomass reduction (van Loosdrecht and Henze, 1999; Hao *et al.*, 2010):

- dormancy of bacteria: non-active state, which is seen as undegradable particulate.
- internal decay: consumption of internally stored compounds in case of starvation. This mechanism is not coupled to significant microorganism death.
- external decay: predation by protozoa, viral attack, and cell lysis (phages, etc). The cell walls may not be degraded by protozoa and phages, which results in unbiodegradable material production.

Several authors worked on the influence of the electron acceptor conditions on the OHO and ANO decay rate. Siegriest *et al*. (1999) showed a reduced anoxic and anaerobic

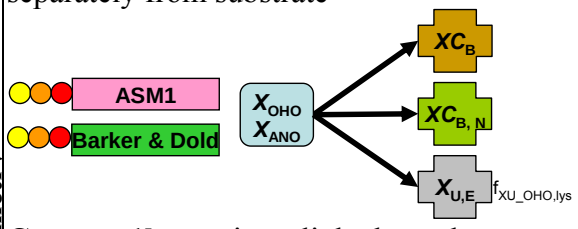
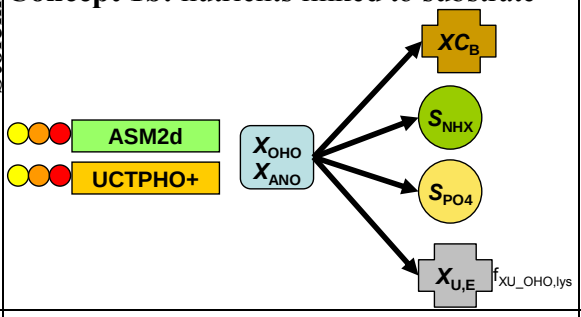
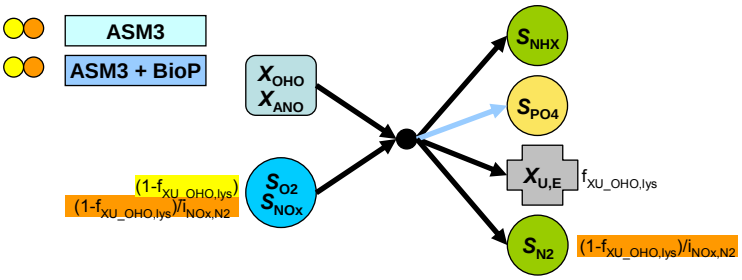
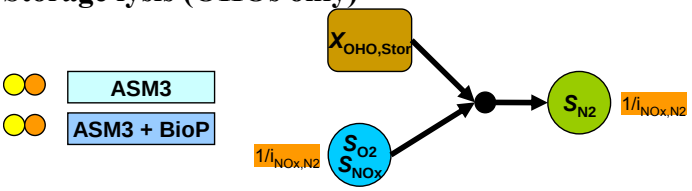
respiration of OHO compared to aerobic respiration. The nitrification activity was shown to be higher after keeping nitrifiers in batch reactors under anaerobic and anoxic conditions than nitrifiers kept under aerobic conditions, in absence of ammonia (Siegrist *et al.*, 1999). A 50% lower ANO decay rate under anaerobic and anoxic conditions was found compared to aerobic conditions.

4.4.3.2.5.2 Modelling

Two concepts are used (Table 4-27):

- Tthe death-regeneration concept. Two sub-concepts have to be distinguished :
  - Death-regeneration with component-based model (ASM1, Barker and Dold);
  - Death-regeneration with fraction-based model (ASM2d, UCTPHO+).
- The endogenous respiration concept (ASM3, ASM3+BioP).

Table 4-27. OHO and ANO decay process concepts

	Concept 1: Death-Regeneration concept	**Concept 2**: Endogenous respiration concept
Stoichiometry	**Concept 1a:** nutrients considered separately from substrate  **Concept 1b:** nutrients linked to substrate 	 **Storage lysis (OHOs only)** 
Kinetics	**Heterotrophs:** $b_{OHO} \cdot X_{OHO}$ **Autotrophs:** $b_{ANO} \cdot X_{ANO}$	**Heterotrophs:** $\left\langle \begin{matrix} m_{OHO,Ox} \cdot M(S_{O2}) \\ m_{OHO,Ax} \cdot M(S_{NOx}) \cdot IM(S_{O2}) \end{matrix} \right\rangle \cdot X_{OHO}$ **Storage lysis (OHOs only)** $\left\langle \begin{matrix} m_{Stor,Ox} \cdot M(S_{O2}) \\ m_{Stor,Ax} \cdot M(S_{NOx}) \cdot IM(S_{O2}) \end{matrix} \right\rangle \cdot X_{OHO,Stor}$ **Autotrophs:** $\left\langle \begin{matrix} m_{ANO,Ox} \cdot M(S_{O2}) \\ m_{ANO,Ax} \cdot M(S_{NOx}) \cdot IM(S_{O2}) \end{matrix} \right\rangle \cdot X_{ANO}$

N.B.: ASM2d+TUD is identical to ASM2d.
The symbol ‹ › is used to indicate optional or alternative terms, one or none of the lines should be chosen.

Death-regeneration concept. The biomass decay results in the release of a fraction (1-$f_{XU\_OHO,lys}$) of particulate substrate and a fraction $f_{XU\_OHO,lys}$ of undegradable material. The released particulate substrate will be hydrolysed, and then used again for OHO growth. Consequently, ANO biomass decay contributes to OHO growth.

This concept also allows modelling anaerobic decay, and modelling the high oxygen or nitrate demand observed after an anaerobic condition period (Warner *et al.*, 1986) would not be possible with the endogenous respiration concept. However, maintenance and endogenous respiration are neglected.

Endogenous respiration concept. This concept is closer to experimental observations (Gujer *et al.*, 2000). In this process energy is provided by the oxidation of the own biomass organic matter, which leads to undegradable matter and nutrients release. Models that consider a storage pool (ASM3, ASM3+BioP) have to consider storage degradation for maintenance: stored compounds are used to produce energy without biomass production. This process is similar to the maintenance concept of PAOs (see 4.4.5.4.2), and explains the fate of the OHO storage pool during OHO decay. This can be considered as endogenous respiration of the storage pool.

4.4.3.2.5.3 Model limitations

Biokinetic models using the endogenous respiration concept should have better identifiable parameters and should thus be easier to calibrate (Gernaey *et al.*, 2004). Indeed, the endogenous respiration concept parameters only influence the decay process of the considered organism, whereas the death-regeneration concept parameters influence the decay of the concerned organism (autotrophs and heterotrophs), hydrolysis and the growth processes of heterotrophs (substrate availability). Furthermore, the death-regeneration concept induces a higher biomass production rate, which has a general effect on all kinetic rate constants. Consequently, kinetic parameters are not directly comparable between models using the endogenous respiration concept or the corresponding death-regeneration concept as presented by Dold *et al.* (1980).

Electron acceptor conditions. The concept of endogenous respiration does not allow decay under anaerobic condition, since no electron acceptor for the respiration chain is available. The death-regeneration concept has been developed to cope with the anaerobic decay process in case the endogenous respiration concept is used and to keep the model as simple as possible (Dold *et al.*, 1980). However, ANO and OHO decay rates have been shown to be lower under anaerobic conditions (Siegrist *et al.*, 1999), and may thus be neglected, depending on the WWTP conditions. Inversely, none of the models consider the lower decay rates under anoxic and anaerobic conditions, which could cause an underprediction of biomasses; especially in case of long periods with unsuitable nitrification conditions (rain events, weekends, holidays, etc.) (Siegrist *et al.*, 1999).

Predation. Predation is explicitly modelled by Curds (1971), Lijklema (1973) and Moussa *et al.* (2005) considering a reduction of the active biomass through protozoa consumption. Not considering predation may lead to variable kinetic parameter values depending on the WWTP conditions.

The protozoa concentration is between 5% and 10% of the MLVSS according to Curds (1971). The protozoa population is composed of free-swimming, crawling and stalked ciliates. Curds (1971) considers free-swimming bacteria as their only prey, whereas Lijklema (1973) and Moussa *et al.* (2005) also take into account sludge floc organism consumption, with equal preference for different bacterial types.

4.4.3.3 Biological phosphorus removal

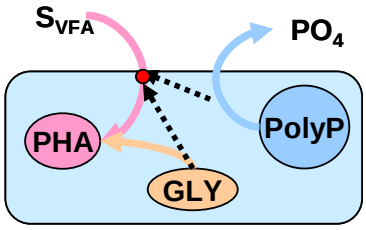
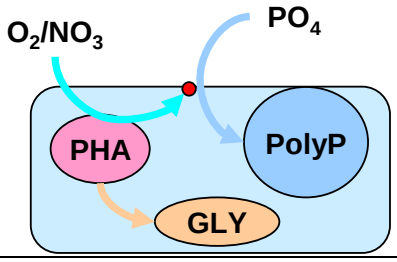
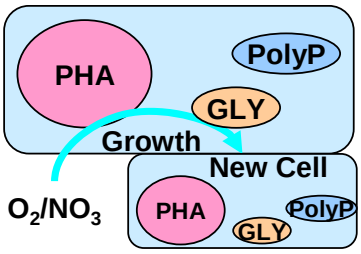
Phosphorous accumulating organisms (PAOs) have the ability to store carbon compounds as poly-β-hydroxyalkanoates (PHA) and glycogen, and phosphorus in the form of polyphosphates (polyP) in excess of normal metabolic requirements. This ability is used in wastewater treatment to biologically remove phosphorus, by stimulating PAO growth by a sequence of anaerobic and aerobic (or anoxic) conditions. PAO metabolism is usually described by 2 or 3 steps:

- substrate uptake (usually volatile fatty acids, S_{VFA}) and storage as PHA, typically under anaerobic conditions, associated with glycogen (ASM2D+TUD) and polyP consumption (all models);

- PolyP and glycogen storage pools restoration and PHA consumption under aerobic and anoxic conditions (modelled simultaneously with growth in the Barker and Dold and UCTPHO+ models);
- PAO growth associated to PHA consumption under aerobic and anoxic conditions.

Organic substrate uptake under anaerobic conditions provides PAOs a competitive advantage over OHOs. Furthermore, the anaerobic conditions enable the formation of S_{VFA} from fermentable substrate S_F. The simplified mechanisms of these steps are represented in Table 4-28.

Table 4-28. Simplified representation of phosphorus accumulating organisms growth

Anaerobic/Anoxic conditions	**Aerobic/Anoxic conditions**	
Substrate (S_{VFA}) uptake and storage in the form of PHA, thanks to the energy provided by glycogen and polyP breakdown, resulting in phosphate release	Storage pools restoration: phosphate uptake and glycogen formation	PAO growth, carbon and energy are provided by PHA storage pool oxidation
		

Metabolic model. To conceptualise EBPR, the Delft University of Technology (TUD) group introduced a metabolic model that considers cell internal reactions (Smolders *et al.*, 1994a; Smolders *et al.*, 1994b). The stoichiometry of anaerobic acetate uptake is dependent on the energetic (ATP) requirement for acetate uptake across the cell membrane (Y_{ATP_PHA}), which is dependent on the pH and expressed as a function of pH in ASM2d+TUD. The aerobic/anoxic stoichiometry is dependent on 3 metabolic yields: ATP formation per NADH (Y_{NADH_ATP}), biomass production per ATP (Y_{ATP_X}) and NADH requirement for PO_4 transport across the cell membreane (Y_{NADH_P}) (Smolders *et al.*, 1994a; Smolders *et al.*, 1994b). The cell internal concentrations of metabolites (NADH, acetyl-CoA, ATP, etc.) are considered to be in steady state conditions. Consequently, these components are not modelled, and only the overall stoichiometric reaction is formulated. The resulting model has a similar structure to the other ones.

4.4.3.3.1 PHA storage

4.4.3.3.1.1 Knowledge

Under anaerobic conditions, in the presence of substrate, PAO store PHA. Figure 4-6 illustrates the main biochemical steps of PHA storage. Enzyme formation that allows anaerobic substrate uptake seems to be induced by alternating aerobic/anaerobic conditions (Mino *et al.*, 1998). Some experiments (Comeau *et al.*, 1987; Wentzel *et al.*, 1989; Brdjanovic *et al.*, 1998a) indicated that PAOs can also store PHA under anoxic or even aerobic conditions, if sufficient substrate is available.

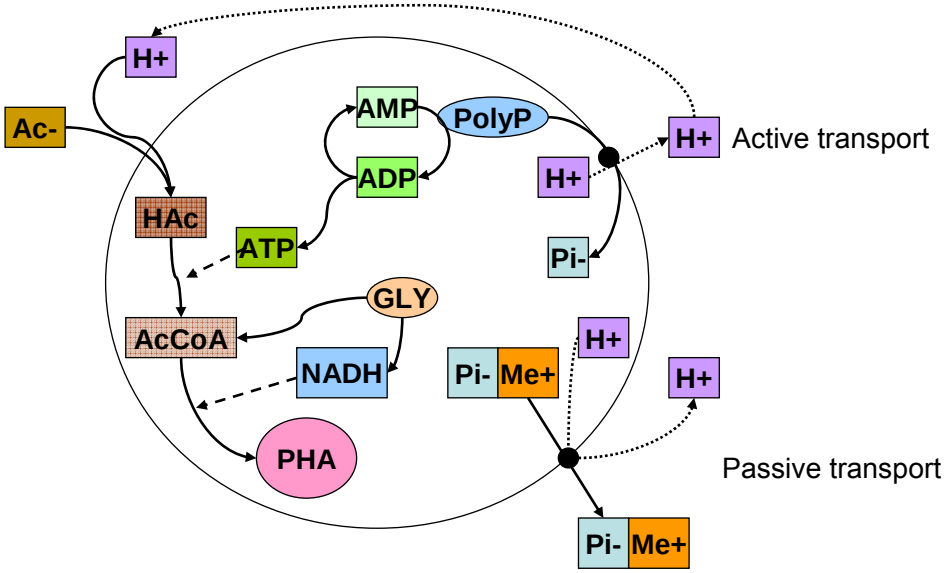


Figure 4-6. PHA storage: biochemistry details (adapted from Wentzel *et al.*, 2008).

PHA storage. The storage of PHA from S_{VFA} requires mainly 3 reactions (Wentzel *et al.*, 2008):

- Active transport across the cell membrane for substrate uptake using energy from glycogen (ASM2d+TUD) and polyP breakdown
- Transformation of substrate into acetyl-CoA, the PHA precursor, using energy from glycogen (ASM2d+TUD) and polyP breakdown
- Conversion of acetyl-coA into PHA using reducing power (NADH) provided by glycogen conversion

Energy source. VFAs are transported in the undissociated form (associated to a proton), which causes dissipation of the membrane proton motive force. PolyP breakdown and phosphate release associated to proton ions allow the re-establishment of the proton

motive force (Comeau *et al.*, 1986). This phosphate release is also concomitant with Mg^{2+} and K^{+} release, which serve as counter-ions for stabilisation of the polyP chain (Wentzel *et al.*, 1986).

This polyP breakdown also provides the required energy to metabolise substrate into acetyl-CoA (Comeau *et al.*, 1986). Indeed, polyP breakdown allows phosphorylation of AMP into ADP and then ATP thanks to the AMP-phosphotransferase enzyme (Wentzel *et al.*, 1992).

Reducing power. Two theories for NADH production were developed: the "Comeau-Wentzel model" and the "Mino model" (Jenkins and Tandoi, 1991; Wentzel *et al.*, 1992).

- The "Comeau-Wentzel model" hypothesises that NADH is provided by the anaerobic oxidation of acetate through the TCA (Tricarboxylic acid cycle) cycle.
- The "Mino model" considers that the NADH is provided by glycolysis under anaerobic conditions, turning stored glycogen into pyruvate and then into acetyl-CoA and CO_2 (Mino *et al.*, 1998; Oehmen *et al.*, 2007). This reaction also provides energy.

The Mino model theory is supported by several experimental evidences, but the TCA cycle seems to effectively supply part of the reducing power for PHA formation under certain conditions, such as low temperature or an insufficient quantity of stored glycogen (Mino *et al.*, 1998; Zhou *et al.*, 2010). Oehmen *et al.* (2007) hypothesise that either metabolic pathway is used by a specific microbial group of PAOs, or that PAOs are able to use different metabolic pathways depending on their internal or external conditions.

PolyP storage pool. Mino *et al.* (1985) and Wentzel *et al.* (1989) observed that not all the stored polyP can be degraded. They hypothesised that two different polyP molecular weights exist: short polyP chains have low molecular weight and can be released, whereas long polyP chains cannot. However, no experimental evidence has supported this hypothesis so far. Glycogen limitation, however, has been shown to result in the incomplete degradation of polyP (Brdjanovic *et al.*, 1998c). Such a limitation may occur at a low pH (less than 7.3) in the presence of an excess of VFAs.

Substrate. Other substrates than acetate can be used by PAOs (Oehmen *et al.*, 2007) such as carboxylic acids, sugars and amino acids (Mino *et al.*, 1998). However, most experiments have been carried out on enriched cultures with acetate, which is usually considered as the unique substrate source in order to simplify the models (Mino *et al.*, 1998).

pH dependency. The energy requirements for S_{VFA} uptake have been observed to increase with pH, leading to an increased phosphorus release to S_{VFA} uptake ratio. This is interpreted as a higher energy required for maintaining the proton motive force for S_{VFA} transport (Mino *et al.*, 1998).

Competition with GAOs. PAOs have to compete with GAOs (glycogen accumulating non-polyP organisms) for the VFAs under anaerobic conditions. Indeed, GAOs store acetate as PHA under anaerobic conditions without using polyP reserves. GAOs use this PHA as carbon and energy source for aerobic/anoxic growth and glycogen production. Their glycogen storage is used both as energy and reducing power source for anaerobic substrate uptake (Mino *et al.*, 1998). Therefore, GAOs are able to store more glycogen than PAOs (Sudiana *et al.*, 1999).

However, this competition seems to highly depend on external factors such as carbon source, pH, temperature, sludge age, dissolved oxygen concentration and inhibitory compounds (Meijer, 2004; Oehmen *et al.*, 2007). Lopez-Vazquez *et al.* (2009) concluded that GAOs are favoured by higher temperatures and lower pH.

4.4.3.3.1.2 Modelling

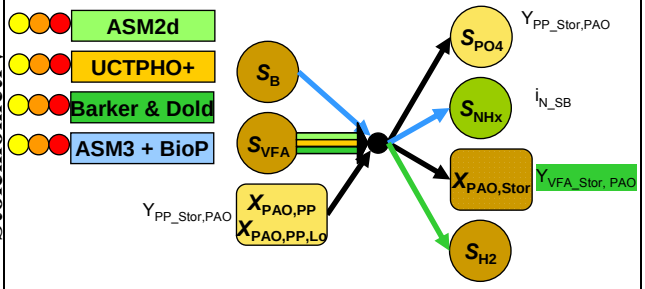
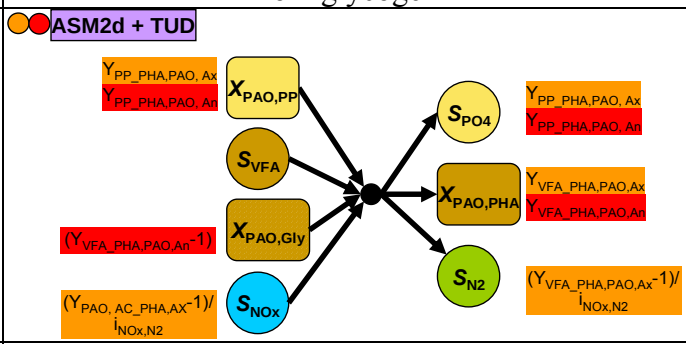
The concepts vary in terms of substrate used (S_B or S_{VFA}) and in terms of source of energy (Table 4-29):

- In the first concept, energy for storage is provided by polyP breakdown, and reducing power production is not considered (ASM2d, UCTPHO+, Barker & Dold, ASM3+BioP).
- In the second concept that only concerns ASM2d+TUD, energy is provided by polyP breakdown and glycogen degradation, while reducing power is also generated through glycolysis.

PHA storage. In the first concept glycogen storage is not distinguished from PHA storage. Consequently, the storage pool for these models is named $X_{PAO,Stor}$ (Corominas *et al.*, 2010).

Energy source. In the Barker & Dold model an additional observed need of energy is recognised in the form of a PHA formation yield. This causes a "COD loss", suggested to be due to H_2 formation (see 4.4.4.2.2).

Table 4-29: PHA storage process concept

	Concept 1: Energy from polyP, reducing power neglected	**Concept 2:** Energy from polyP, reducing power from glycogen
Stoichiometry		
Kinetics	Barker & Dold, UCTPHO+: $q_{PAO,VFA\_Stor} \cdot M(S_{VFA}) \cdot M(X_{PAO,PP}) \cdot X_{PAO}$ ASM2d, ASM3 +BioP: $q_{PAO,VFA\_Stor} \cdot \left\langle \frac{M(S_{VFA})}{M(S_B)} \right\rangle \cdot M(X_{PAO,PP}/X_{PAO}) \cdot X_{PAO}$	$\left\langle \frac{q_{PAO,VFA\_PHA,An} \cdot IM(S_{O2}) \cdot IM(S_{NOx})}{q_{PAO,VFA\_PHA,Ax} \cdot IM(S_{O2}) \cdot M(S_{NOx})} \right\rangle \cdot M(S_{VFA}) \cdot M(X_{PAO,Gly}) \cdot M(X_{PAO,PP}) \cdot X_{PAO}$

Reducing power. In the first concept the redox balance in the cell is neglected. In the second concept, NADH production comes from glycogen hydrolysis under anaerobic conditions; and under anoxic conditions NOx utilisation as electron acceptor in the oxidative phosphorylation pathway stimulates the TCA cycle that produces NADH.

Substrate. For all models except ASM3+BioP, S_{VFA} is the unique PAO substrate. For ASM3+BioP, S_B is used as unique substrate for both PAOs and OHOs. Indeed, fermentation is neglected since hydrolysis is considered to be the rate limiting step. PAOs are then in competition with OHOs for substrate uptake under aerobic and anoxic conditions.

PolyP storage pools. The Barker & Dold model considers two types of polyP: low and high molecular weight fractions. Only polyP with low molecular weight can be released during the PHA storage process.

pH dependency. In ASM2d+TUD the anaerobic yield for S_{VFA} uptake is a function of pH.

Kinetics. The kinetic rate expression for PHA storage does not depend on the electron acceptor in the first concept (energy from polyP only), but does in the second one.

The rate is limited by the polyP concentration in Barker & Dold, UCTPHO+ and ASM2d+TUD and by the polyP storage pool filling ratio for ASM2d and ASM3+BioP.

4.4.3.3.1.3 Model limitations

Reducing power. In cases in which glycogen is depleted, the substrate storage may stop (Brdjanovic *et al.*, 1998c), and models using the first concept that neglects glycogen storage would overpredict substrate storage. However, depending on the PAO sub-group or on their internal or external conditions, some PAOs seem to be able to use another pathway for reducing power formation through the TCA cycle, without using glycogen storage (Oehmen *et al.*, 2007). Further research is needed on this topic.

Substrate. In ASM3+BioP, S_B is used as substrate with the hypothesis that hydrolysis is the rate-limiting step. PHA storage will be overestimated should fermentation become the rate limiting step, because less substrate will be available for PAOs.

PolyP storage pool. The Barker & Dold model considers polyP with high molecular weight as state variable, based on the observation of Wentzel *et al.* (1989) and Mino *et al.* (1985) that a quantity of polyP always remains despite PHA storage being stopped. However, glycogen can also be limiting the substrate uptake process (Brdjanovic *et al.*, 1998c; Mino *et al.*, 1998). As glycogen was not considered by Mino *et al.* (1985), their observation might in fact be due to glycogen depletion.

Competition with GAOs. In some cases phosphorus removal deterioration has been reported. Those cases are often related to growth of GAOs (Mino *et al.*, 1998). GAOs should then be included in a comprehensive model (Oehmen *et al.*, 2010).

4.4.3.3.2 PolyP storage

4.4.3.3.2.1 Knowledge

In the presence of an electron acceptor and the absence of an available carbon source, PAOs will restore their polyP and glycogen storage pools, a metabolism that provides them an ecological advantage over OHOs (Mino *et al.*, 1998).

PAOs have a high affinity for PO_4 (0.1 g $P.m^{-3}$) and are able to store up to 12% of their dry weight as polyP (against 1 to 3% for OHOs) (van Loosdrecht *et al.*, 1997a). The polyP polymer storage granules were first observed by Buchan (1983), and are called volutins. Their ability to store polyP makes the PAOs very efficient in terms of phosphorus removal.

Energy source. PHA oxidation allows the establishment of a proton motive force, which allows phosphorus uptake and ATP formation through ATP-ase. ATP is then used to form polyphosphates (Comeau *et al.*, 1986).

Denitrification. PAOs are also capable of simultaneous denitrification and phosphorus uptake under anoxic conditions, using either their stored PHA, or if available, S_{VFA}. However, the phosphorus uptake efficiency is lower with nitrate as electron acceptor, and thus more stored carbon is consumed compared to aerobic conditions (Barker and Dold, 1996).

Glycogen storage. Glycogen is formed from PHA oxidation under aerobic and anoxic conditions (Oehmen *et al.*, 2007).

4.4.3.3.2.2 Modelling

Models differ in the source of energy for polyP storage and in the overall concept for energy utilisation (Table 4-30):

- the first concept independently considers growth and polyP storage processes (ASM2d and ASM3+BioP). Consequently, PHA oxidation is the result of phosphate uptake and growth.
- in the second concept storage pool restoration and growth are coupled. A part of the energy provided by PHA oxidation is allocated to each process.

- UCTPHO+ and the Barker & Dold model include the polyP storage process in an overall growth process (described in the PAO growth paragraph). This concept is consequently close to the second one.

Energy source. The polyP storage process is linked to the growth process as they use both the same source of energy. In concept 1, the polyP storage is considered independently of PAO growth. Conversely, in concept 2 (ASM2d+TUD) polyP and glycogen storage pools restoration are coupled to PAO growth. Therefore, energy production for polyP storage has been represented mathematically as PAO biomass oxidation. However, this process has to be considered to take place in parallel with glycogen storage and PAO growth to make sense (Meijer, 2004).

Denitrification. Under anoxic conditions, only a fraction (η) of PAOs are able to denitrify. In concept 1, the same amount of PHA is used under aerobic or anoxic conditions, whereas in concept 2 more energy is required under anoxic conditions to store the same amount of polyP, because the energy production efficiency is lower with nitrate than with oxygen (Mino *et al.*, 1998).

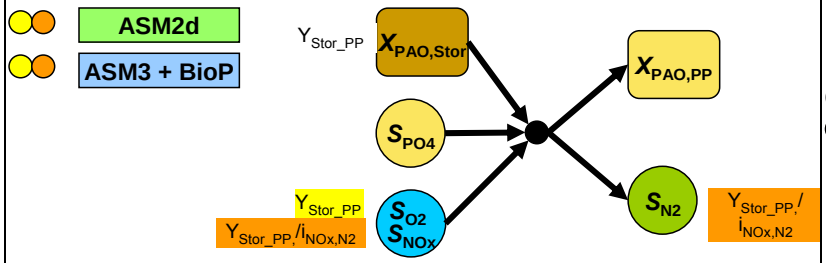
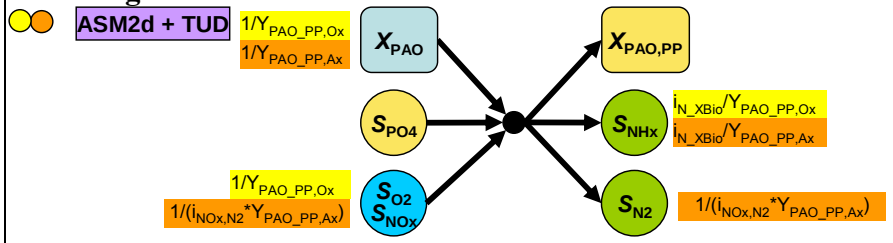
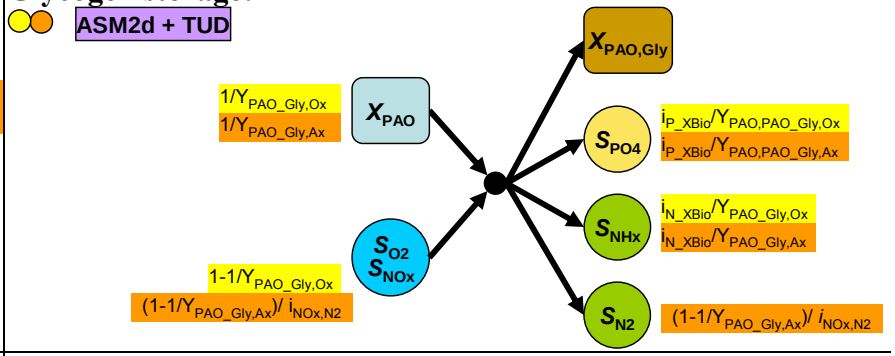
Glycogen storage. Glycogen storage is considered only in the ASM2d+TUD metabolic model and is modelled as a result of PAO biomass oxidation in the same way as described above.

Kinetics. When PAOs reach their maximum polyP storage potential, the phosphorus uptake is stopped.

4.4.3.3.2.3 Model limitations

Energy source. The stoichiometry of polyP uptake and PAO growth processes in ASM2d and ASM3+BioP models are described as independent. However, experimental results show that oxidation of stored organic compounds (i.e. PHA) provides the energy for both PAO growth and polyP storage (Wentzel *et al.*, 1989). Therefore, ASM2d+TUD links both yields to energy production, whereas Barker & Dold and UCTPHO+ model PAO growth and polyP storage as a single process. This will impact the identifiability of the model parameters, which will make calibration more difficult in ASM2d and ASM3+BioP.

Table 4-30: PolyP storage process concept

	Concept 1 Uncoupled processes	**Concept 2** Coupled processes (metabolic model)
Stoichiometry		**PP storage:**  **Glycogen storage:** 
Kinetics	$$q_{PAO,PO4\_PP} \cdot \left\langle \frac{M(S_{O2})}{\eta_{qPAO,Ax} \cdot IM(S_{O2}) \cdot M(S_{NOx})} \right\rangle \cdot M(S_{PO4}) \cdot M(X_{PAO,PHA}) \cdot M(f_{PP\_PAO,Max} - X_{PAO,PP} / X_{PAO}) \cdot X_{PAO}$$	**PP storage:** $$q_{PAO,PO4\_PP} \cdot \left\langle \frac{M(S_{O2})}{\eta_{qPAO,Ax} \cdot IM(S_{O2}) \cdot M(S_{NOx})} \right\rangle \cdot [X_{PAO} / X_{PAO,PP}] \cdot M(S_{PO4}) \cdot M(X_{PAO,PHA}) \cdot M(f_{PP\_PAO,Max} - X_{PAO,PP} / X_{PAO}) \cdot X_{PAO}$$ **Glycogen storage:** $$q_{Gly} \cdot \left\langle \frac{M(S_{O2})}{\eta_{qPAO,Ax} \cdot IM(S_{O2}) \cdot M(S_{NOx})} \right\rangle \cdot [X_{PAO,PHA} / X_{PAO,Gly}] \cdot M(X_{PAO,PHA}) \cdot M(f_{Gly\_PAO,Max} - X_{PAO,Gly} / X_{PAO}) \cdot X_{PAO}$$

NB: PolyP storage in the Barker & Dold and UCTPHO+ models are considered simultaneously with growth.
The symbol ‹ › is used to indicate optional or alternative terms, one or none of the lines should be chosen.

Denitrification. ASM2d and ASM3+BioP consider a constant yield for aerobic and anoxic processes, which is in contradiction with Barker and Dold's (1996) observations. In the same way as for OHO anoxic growth (4.4.4.3.3), using a single yield for polyP formation and PHA consumption under aerobic and anoxic conditions will lead to an overestimation of polyP storage and PAO denitrification.

Glycogen storage. The model limitations occurring when glycogen storage or GAOs are neglected are discussed in paragraph 4.4.5.1.3 since they relate to anaerobic substrate uptake differences.

Phosphate precipitation. Under certain conditions, such as high pH (>7.5) and high Ca^{2+} or metals concentration, chemical precipitation of phosphorus (e.g. calcium phosphate) cannot be neglected in comparison with the BioP removal process. Phosphate precipitation is favoured by high local phosphate concentrations in anaerobic tanks due to phosphate release by PAOs. Under these conditions, a biologically induced phosphorus precipitation process should be considered to correctly predict the phosphorus removal (Maurer and Gujer, 1998; Maurer and Boller, 1999).

In case of chemical phosphorus removal (by adding e.g. iron, aluminium or calcium salts) a chemical precipitation model needs to be added

4.4.3.3.3 PAO growth

4.4.3.3.3.1 Knowledge

The carbon source and energy for PAO growth are provided by PHA oxidation (Comeau *et al.*, 1986).

PAOs have to compete with GAOs for substrate uptake under anaerobic conditions in order to form the PHA that is oxidised under aerobic/anoxic conditions. To be competitive, the first priority of PAOs is to resupply their storage pools. However, this cyclic storage and consumption of storage pools leads to energy wastage. Consequently, PAOs have a growth yield that is 13% lower than that of OHOs growing on the same substrate (Mino *et al.*, 1998).

Substrate. When S_{VFA} are present under aerobic conditions, Comeau *et al.* (1987) and Wentzel *et al.* (1989) observed both a direct growth of PAO on S_{VFA} and storage of S_{VFA} linked to phosphate release.

Nutrient source. Wentzel *et al.* (1989) observed the ability of PAO organisms to use nitrate as nitrogen source in case of ammonia depletion, with no modification of their kinetic behaviour. In case PO_4 becomes limiting, Wentzel *et al.* (1989) observed that growth continued and hypothesised that PAO can use their cell internal polyP storage as phosphorus source.

Denitrification. Some PAOs are able to use nitrate as an electron acceptor to oxidise stored carbon (Wentzel *et al.*, 1989). Experiments using different methods (molecular tools, chemical analysis, etc) have been carried out to determine whether denitrifying PAOs are distinct from non-denitrifying PAOs, but no consensus has been reached so far (Oehmen *et al.*, 2007). Recent studies show even more complex behaviour of PAO biomasses with some sub-groups capable to use only nitrites and sub-groups capable to use both nitrates and nitrites (Oehmen *et al.*, 2010). However, growth yields depend on the electron acceptor because energy production efficiency is lower with nitrate than with oxygen (Mino *et al.*, 1998).

Kinetics. Brdjanovic *et al.* (1998b) showed that PAO growth does not depend on the SRT, but on the PHA conversion rate and on the PHA storage capacity, provided that a sufficient minimum SRT is attained.

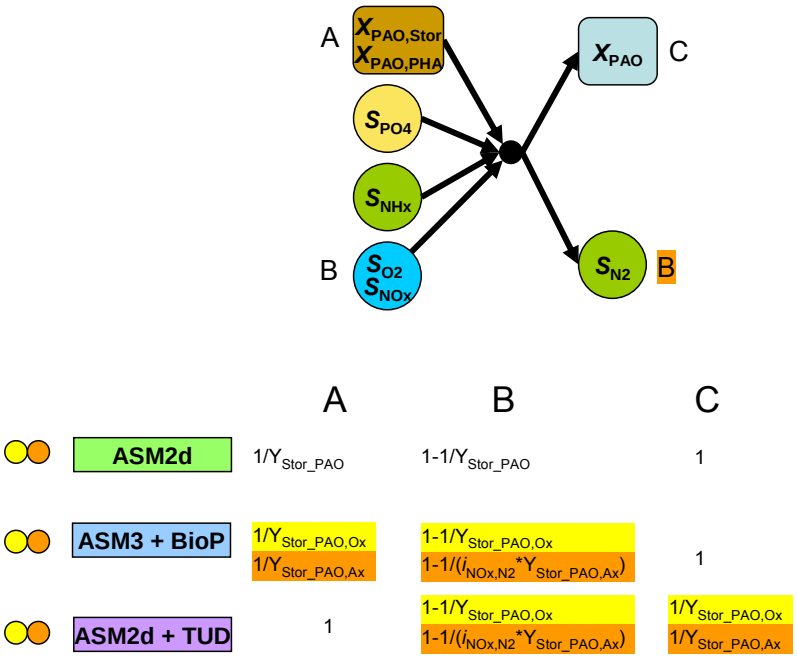
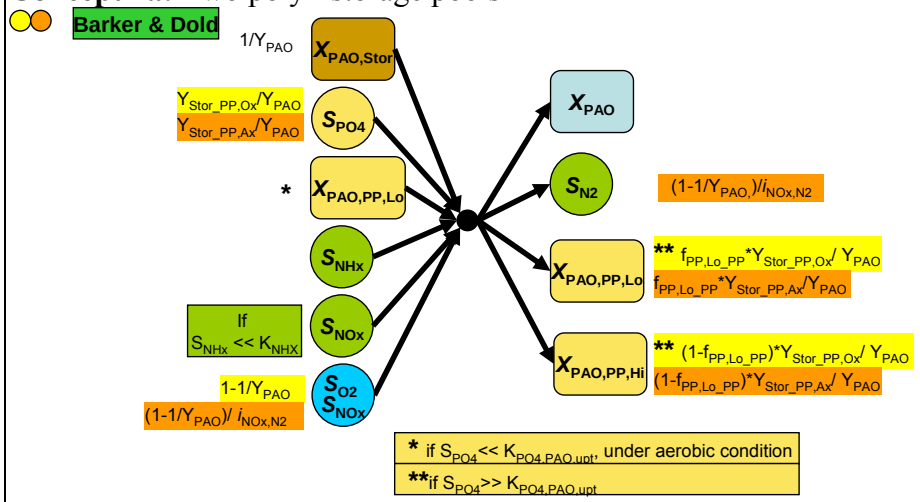
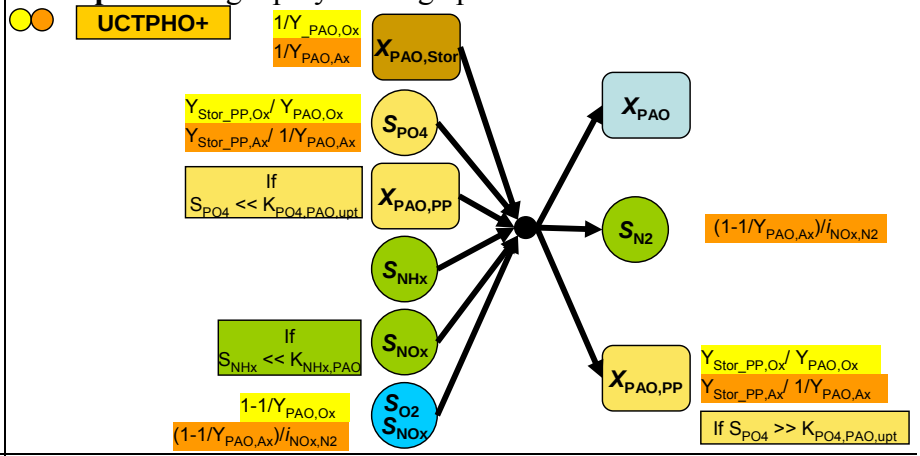
4.4.3.3.3.2 Modelling

Two main concepts are used in the seven published models (Table 4-31):

- In the first concept PAO growth is similar to OHO growth and the process is separated from polyP storage (ASM2d, ASM3+BioP, ASM2d+TUD).
- In the second concept, followed by UCTPHO+ and Barker & Dold, phosphate uptake is simultaneous to growth: PAOs take up phosphate as nutrient for growth and store it as energy source. Barker & Dold consider two polyP storage pools (low and high molecular weight), whereas UCTPHO+ considers a single polyP storage pool.

Substrate. All models consider PHA as the only carbon source for PAO growth.

Table 4-31. PAO growth

	Concept 1: PAO growth	**Concept 2:** Simultaneous growth and polyP storage
Stoichiometry		**Concept 2a:** Two polyP storage pools  **Concept 2b:** Single polyP storage pools 
Kinetics	ASM2d, ASM3+BioP: $\mu_{PAO,Max} \cdot \left\langle \frac{M(S_{O2})}{\eta_{\mu PAO} \cdot IM(S_{O2}) \cdot M(S_{NOx})} \right\rangle \cdot M\left(\frac{X_{PAO,Stor}}{X_{PAO}}\right) \cdot M(S_{NHx}) \cdot M(S_{PO4}) \cdot X_{PAO}$ ASM2d+TUD: $q_{PHA\_PAO} \cdot \left\langle \frac{M(S_{O2})}{\eta_{\mu PAO} \cdot IM(S_{O2}) \cdot M(S_{NOx})} \right\rangle \cdot M\left(\frac{X_{PAO,PHA}}{X_{PAO}}\right) \cdot M(S_{NHx}) \cdot M(S_{PO4}) \cdot X_{PAO}$	$\left\langle \frac{\mu_{PAO,Max}}{\mu_{PAO,Max,Plim}} \right\rangle \cdot \left\langle \frac{M(S_{O2})}{\eta_{\mu PAO} \cdot IM(S_{O2}) \cdot M(S_{NOx})} \right\rangle \cdot M(X_{PAO,Stor} / X_{PAO}) \cdot$ $\left\langle \frac{M(S_{NHx})}{IM(S_{NHx}) \cdot M(S_{NOx})} \right\rangle \cdot \left\langle \frac{M(S_{PO4})}{IM(S_{PO4}) \cdot M(X_{PAO,PP})} \right\rangle \cdot X_{PAO}$

Nutrient source. In the UCTPHO+ and Barker & Dold models, nitrate can be used as nitrogen source in the case of ammonia depletion. In the case of phosphate depletion, PAOs will use their polyP storage as phosphorus source. In the Barker & Dold model, only the polyP storage compound with low molecular weight ($X_{PAO,PP,Lo}$) can be used.

The Barker & Dold model does not consider potential NH_X or PO_4 depletion during anoxic PAO growth, because it was considered unlikely to have ammonia or phosphate depletion in an anoxic tank (Barker and Dold, 1997).

Denitrification. PAO denitrification is considered in all studied BioP models. As a simplification, all models consider a single homogenous population, with a fraction η capable of denitrification. This way to model PAO denitrification has been successfully applied in several models, whereas the concept of two PAO populations leads systematically to the dominance of the aerobic PAOs (Hu *et al.*, 2007). **Erreur ! Référence non valide pour un signet.** indicates whether the models use a different growth or polyP storage yield in aerobic and anoxic conditions.

Kinetics. All the models except ASM2d+TUD use the same kinetic growth concept as OHO, based on a maximum growth rate ($\mu_{PAO,Max}$). ASM2d+TUD bases the PAO growth on the consumption rate of PHA (q_{PHA_PAO}). This is consistent with the stoichiometric coefficients that are normalised to PHA, and the storage pool restoration concept (4.4.5.2.2).

Table 4-32. Synthesis of anoxic and aerobic yields used by each model

Models	Aerobic / anoxic growth yield	Aerobic / anoxic polyP storage yield
Barker & Dold	Same	Different
ASM2d	Same	Same
ASM3+BioP	Different	Same
UCTPHO+	Different	Different
ASM2d+TUD	Different	Different

4.4.3.3.3.3 Model limitations

The Barker & Dold model considers polyP with a high molecular weight. As already discussed in paragraph 4.4.5.1.3., this distinction may have been introduced to cope with glycogen depletion conditions that stopped substrate uptake.

Substrate. Should S_{VFA} be present under aerobic conditions, the studied models may lead to erroneous results. Indeed, the studied models consider that PAOs can only grow on organic stored compound whereas it seems that PAOs can grow directly on S_{VFA} substrate (Wentzel *et al.*, 1989). PAOs are then in competition with OHOs under aerobic and anoxic conditions for S_{VFA} uptake. This direct growth has been neglected because it was considered unlikely (and undesirable) that S_{VFA} remain available under aerobic conditions.

Nutrient source. For a WWTP with a high nitrification efficiency and/or a high phosphorus removal, the aerobic tank may be limited in ammonia and/or phosphorus. However, PAOs seem able to use nitrate and stored phosphorus as nutrients. Consequently, ASM2d, ASM3+BioP and ASM2d+TUD may lead to an underprediction of PAO growth under ammonia and/or phosphorus depletion.

Denitrification. Potential consequences in using single aerobic and anoxic yields are discussed in paragraph 4.4.5.2.3.

4.4.3.3.4 PAO decay

4.4.3.3.4.1 Knowledge

PAOs organisms have the ability to store energy in the form of carbon (glycogen, PHA) or polyphosphates. These stored compounds make it essential to distinguish decay and maintenance in endogenous processes.

Decay is defined as the loss of biomass weight or activity due to internal cell factors or external factors, such as environmental conditions, viruses or predation (Lopez *et al.*, 2006; Hao *et al.*, 2010). Endogenous mass loss has been observed to be very low for PAOs compared to non-PAOs (Wentzel *et al.*, 1989). Also, Hao *et al* (2009) found that the rate of cell death is far lower than the activity decay (i.e. reduction in specific activity rates). With all their storage polymers, PAOs “die” very slowly, and maintenance seems to be the main endogenous process. Furthermore, experiments show that the PAOs' decay rate is higher under aerobic conditions, and is negligible under anoxic and anaerobic conditions (Siegrist *et al.*, 1999; Lu *et al.*, 2007). However, it should be noted that lab-scale results of decay rates do not consider the impact of external factors (e.g. environmental conditions, viruses, predation) on biomass.

Maintenance is defined as the production of the amount of energy required to maintain essential life conditions in the cell, such as cell motility, maintenance of ion gradients, turnover of cell material (e.g. proteins, RNA) and transport of material (Lopez *et al.*, 2006; Hao *et al.*, 2010). In the case of endogenous processes, this energy is provided by internal storage sources. For OHO and ANO, maintenance is considered as negligible and is considered part of the decay process in all models, except for OHO decay in ASM3 and ASM3+BioP models, which also consider a storage pool. The source of maintenance energy depends on the environmental conditions:

- Under aerobic conditions, PAOs use PHA, then glycogen (Brdjanovic *et al.*, 1998a; Lopez *et al.*, 2006; Lu *et al.*, 2007), but seem not able to use polyP for energy production (Lu *et al.*, 2007)
- Under anoxic conditions, PAOs use first PHA, which is rapidly depleted (Lopez *et al.*, 2006), then glycogen and polyP (Lu *et al.*, 2007). Experiments by Wentzel *et al.* (1989) showed the so-called secondary P-release during endogenous mass loss, due to polyP use.
- Under anaerobic conditions, PAOs use glycogen then polyP for maintenance (Lopez *et al.*, 2006; Lu *et al.*, 2007).

4.4.3.3.4.2 Modelling

Death-regeneration vs endogenous respiration. PAO decay is modelled according to the death-regeneration exclusively (ASM2d), endogenous respiration exclusively (ASM3+BioP, ASM2d+TUD), or as a mix of the two concepts (Barker & Dold, UCTPHO+). The death-regeneration concept is used only when PAOs are not able to use the available electron acceptor. Table 4-33 synthesises the concepts used in each model, depending on the electron acceptor conditions. The schematic representation of PAO decay and maintenance is shown in Table 4-34.

Table 4-33. Synthesis of decay concept used in each model, depending on the electron acceptor condition

Models	Death-regeneration concept	Endogenous respiration concept
Barker & Dold		X
ASM2d	X	
ASM3+BioP		X
UCTPHO+	Anoxic (fraction 1-η) Anaerobic	Aerobic Anoxic (fraction η)
ASM2d+TUD		X

Table 4-34: PAO decay process concepts

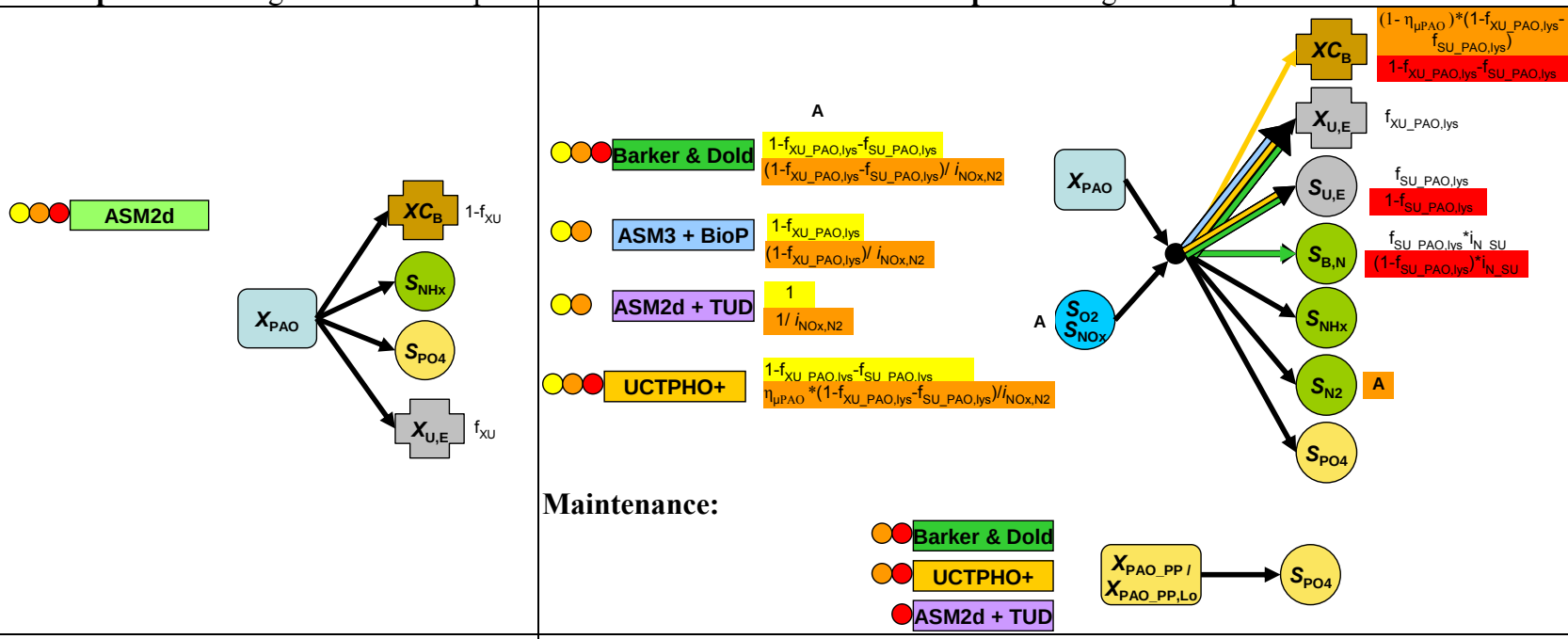
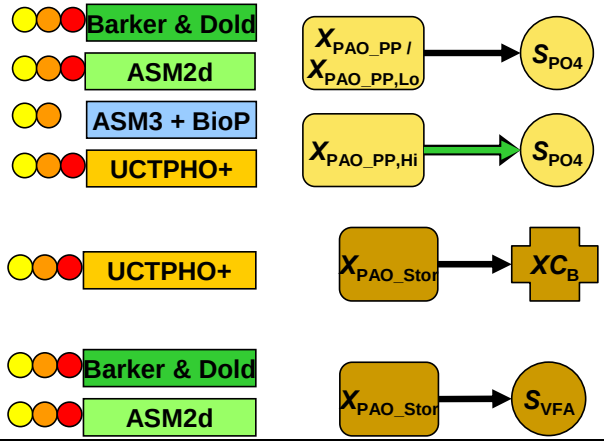
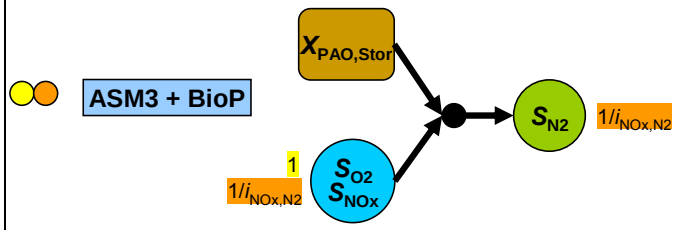
	Concept 1: Death-regeneration concept	**Concept 2:** Endogenous respiration
Stoichiometry	
Kinetics	$b_{PAO} \cdot X_{PAO}$	**Decay:** Barker & Dold, UCTPHO+: $m_{PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ IM(S_{O2}) \cdot M(S_{NOx}) \\ IM(S_{O2}) \cdot IM(S_{NOx}) \end{matrix} \right\rangle \cdot X_{PAO}$ ASM3+BioP: $m_{PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ \eta_{mPAO} \cdot IM(S_{O2}) \cdot M(S_{NOx}) \end{matrix} \right\rangle \cdot X_{PAO}$ ASM2d+TUD: $\left\langle \begin{matrix} m_{PAO,Ox} \cdot M(S_{O2}) \\ m_{PAO,Ax} \cdot IM(S_{O2}) \cdot M(S_{NOx}) \end{matrix} \right\rangle \cdot X_{PAO}$ **Maintenance:** Barker & Dold: $b_{PP\_PO4} \cdot IM(S_{O2}) \cdot M(X_{PAO,PP,Lo}) \cdot X_{PAO}$ ASM2d+TUD: $m_{PAO,An} \cdot IM(S_{O2}) \cdot IM(S_{NOx}) \cdot M(X_{PAO,PP}) \cdot X_{PAO}$ UCTPHO+: $b_{PP\_PO4} \cdot \left\langle \begin{matrix} (1-\eta_{\mu PAO}) \cdot IM(S_{O2}) \cdot M(S_{NOx}) \\ IM(S_{O2}) \cdot IM(S_{NOx}) \end{matrix} \right\rangle \cdot M(X_{PAO,PP}) \cdot X_{PAO}$

Table 4-35: PAO storage pools release/consumption during lysis

	Concept 1: Stored compounds are released	**Concept 2:** Stored compounds are consumed
Stoichiometry	**PolyP lysis:**  	
Kinetics	**PolyP lysis:** Barker & Dold, UCTPHO+: $m_{PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ IM(S_{O2}) \cdot M(S_{NOx}) \\ IM(S_{O2}) \cdot IM(S_{NOx}) \end{matrix} \right\rangle \cdot \left\langle \begin{matrix} X_{PAO,PP,Lo} / X_{PAO} \\ X_{PAO,PP,Hi} / X_{PAO} \end{matrix} \right\rangle \cdot X_{PAO}$ ASM2d: $b_{PP\_PAO} \cdot X_{PAO,PP}$ ASM3+BioP: $b_{PP\_PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ \eta_{bPP\_PAO} \cdot IM(S_{O2}) \cdot M(S_{NOx}) \end{matrix} \right\rangle \cdot X_{PAO,PP}$ **PHA lysis:** Barker & Dold: $m_{PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ IM(S_{O2}) \cdot M(S_{NOx}) \\ IM(S_{O2}) \cdot IM(S_{NOx}) \end{matrix} \right\rangle \cdot \frac{X_{PAO,Stor}}{X_{PAO}} \cdot X_{PAO}$ ASM2d: $b_{Stor\_PAO} \cdot X_{PAO,Stor}$ UCTPHO+: $m_{PAO} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ IM(S_{O2}) \cdot M(S_{NOx}) \\ IM(S_{O2}) \cdot IM(S_{NOx}) \end{matrix} \right\rangle \cdot M(S_{NHx}) \cdot M(S_{PO4}) \cdot \frac{X_{PAO,Stor}}{X_{PAO}} \cdot X_{PAO}$	$m_{PAO,Stor} \cdot \left\langle \begin{matrix} M(S_{O2}) \\ \eta_{mPAO,Stor} \cdot IM(S_{O2}) \cdot M(S_{NOx}) \end{matrix} \right\rangle \cdot X_{PAO,Stor}$

Electron acceptor conditions: In the Barker & Dold and UCTPHO+ models the maximum PAO decay rate is independent of the electron acceptor conditions, whereas two different decay rates are used under aerobic and anoxic conditions in the ASM2d+TUD model, and a reduction factor η_{mPAO} is used in ASM3+BioP.

Undegradable particulate matter production. Only ASM2d+TUD does not consider undegradable particulate matter production in the PAO decay process, because it is considered that insufficient experimental proof was available to evaluate this released material (Meijer, 2004).

Maintenance. This process is applied in the Barker & Dold, UCTPHO+ and ASM2d+TUD models. It consists exclusively in the cleavage of polyP to produce energy. The Barker & Dold and UCTPHO+ models also include a polyP storage lysis, but it is not associated to energy production.

PAO storage pools lysis. The fate of PAO storage pools (PHA, glycogen, polyP) has to be modelled to ensure that the storage products decay together with the biomass (ASM2d, ASM3+BioP, Barker & Dold, UCTPHO+) (Table 4-35). In these lysis processes, storage compounds are usually released in the bulk phase into their initial form (VFAs for PHA and phosphate for polyP). However, UCTPHO+ considers that PHA is released as particulate biodegradable substrate. In ASM3+BioP, decay of PHA storage is associated with electron acceptor consumption and leads to total PHA oxidation.

Some models consider that the polyP storage pool lysis process does not produce energy, contrary to the maintenance process, and is considered to occur at the same rate as the biomass decay. The stoichiometry is however identical to the maintenance process. Table 4-36 synthesises the models that consider maintenance and/or polyP storage pool lysis.

Table 4-36. Synthesis of polyP storage pool fate associated with PAO decay

Models	**Maintenance by polyP cleavage**	**Lysis of polyP storage pool**
Barker & Dold	X	X
ASM2d		X
ASM3+BioP		X
UCTPHO+	X	X
ASM2d+TUD	X	

ASM2d+TUD uses a maintenance concept and thus, the lysis of the storage pools do not appear directly, but is modelled with the aerobic and anoxic maintenance through PAO consumption.

4.4.3.3.4.3 Model limitations

Death-regeneration vs endogenous respiration. The limits highlighted for OHO and ANO decay processes (paragraph 4.4.4.5.3) also hold for the PAO decay process. In the death-regeneration concept, the released carbon (XC_B) from PAO biomass would first benefit OHOs (after hydrolysis).

Electron acceptor conditions. The Barker & Dold and UCTPHO+ models consider the same decay rate under all electron acceptor condition. However, experimental results have shown that the anoxic and anaerobic decay may be neglected. The Barker and Dold and UCTPHO+ models will thus lead to an overestimation of the PAO decay, and to an underestimation of the biological phosphorus removal. Supressing the anoxic and anaerobic decay of PAO processes will solve the problem and simplify the model.

Maintenance. Only three models consider maintenance (Barker & Dold, UCTPHO+ and ASM2d+TUD), whereas maintenance seems to to be the main endogenous process for PAOs. Furthermore, only polyP is considered as a source of maintenance energy in these models, while experiments indicated the important role of PHA and glycogen at the beginning of the maintenance process, polyP being cleaved only after PHA and glycogen depletion.

It should also be noted that aerobic maintenance is not considered explicitly. The maintenance energy needed is thus included in the aerobic growth process. This simplification could lead to an inadequate PAO biomass estimation in case of famine conditions (e.g.: due to industrial activities interruption during the weekend).

PAO storage pools lysis. In UCTPHO+, PHA storage is lysed into XC_B, which will benefit OHOs' growth first.

4.4.4 Discussion

4.4.4.1 Diversity of modelling concepts

ASM models have been proposed to be mechanistic models that try to represent the microbiological reality of activated sludge ecology through several simplified process descriptions. For the processes presented above no general consensus exists among modellers. Two main reasons can be mentioned:

- The biological mechanisms are not yet fully understood and the models reflect the different hypotheses that were formulated.
- The mechanisms are too complex and models use different simplifications to reach the same agreement with measured data. However, this is at the expense of a clear mechanistic meaning of the models, and may limit the extrapolation potential of the models.

Table 4-37 synthesises all the modelling concepts used in the seven studied models, for each standard process. Only the ANO growth process is modelled identically in all considered models.

4.4.4.2 Model selection

When starting a new project, model users should carefully select the model to use to reach the objectives. Their model choice should include the following considerations:

- **Adequate for the objectives**: able to answer the stated questions, in terms of nutrients and biomasses considered (e.g.: modelling phosphorus removal, impact of GAO, etc.),
- **Adequate for the modelling conditions**: the WWTP model should not be used beyond the models' limits; i.e. the simplification hypotheses should be verified (e.g. nitritation is the limiting step in nitrification process). Table 4-37 summarises the main theoretical limitations highlighted in this study through comparison of theoretical knowledge statements and modelling concepts,
- **Simplicity of the model**: The simplest model that allows reaching the objectives and can handle the conditions of the modelling study should be chosen. The simplest model is defined as the model with the lowest number of parameters to calibrate,

Table 4-37. Synthesis of modelling concepts for each of the standard processes

	Concept 1	Concept 2
Hydrolysis	**One step hydrolysis** *Component-based model:* ASM1, Barker & Dold *Fraction-based model:* ASM2d, ASM3, ASM3+BioP	**Direct growth on particulate substrate** UCTPHO+
Fermentation	**Transformation** ASM2d, UCTPHO+, ASM2d+TUD	**Anaerobic growth process** Barker & Dold
OHO Growth	**Direct growth on substrate** *NH_X as only nitrogen source:* ASM1, ASM2d *NH_X/NO_X as nitrogen source:* Barker & Dold, UCTPHO+	**Storage – Growth** ASM3, ASM3+BioP
ANO Growth	**One-step nitrification** ASM1, Barker & Dold, UCTPHO+, ASM2d, ASM3, ASM3+BioP	
OHO & ANO decay	**Death-regeneration** *Component-based model:* ASM1, Barker & Dold *Fraction-based model:* ASM2d, UCTPHO+	**Endogenous respiration** ASM3, ASM3+BioP
PHA storage	**Energy from polyP, reducing power neglected** ASM2d, ASM3+BioP, UCTPHO+, Barker & Dold	**Energy from polyP, reducing power from glycogen** ASM2d+TUD
PolyP storage	**Uncoupled processes** ASM2d, ASM3+BioP	**Coupled processes** ASM2d+TUD
PAO growth	**Growth** ASM2d, ASM3+BioP, ASM2d+TUD	**Simultaneous growth and polyP storage :** Barker & Dold, UCTPHO+
PAO decay	**Death-regeneration** ASM2d	**Endogenous respiration** UCTPHO+, Barker & Dold, ASM2d+TUD, ASM3+BioP **Maintenance** Barker & Dold, ASM2d+TUD, UCTPHO+
PAO storage pool lysis	**PolyP lysis** Barker & Dold, ASM3+BioP, UCTPHO+ **PHA lysis** UCTPHO+, Barker & Dold, ASM2d	**Respiration of stored compounds** ASM3+BioP

- **Experience with the model**: when the model user already masters one or several models, he/she should prefer one of these models, if they are adequate for the objectives and the modelling conditions, even if a simpler model exists. Indeed, his/her experience with the model will facilitate the calibration step and the use of the model.

4.4.4.3 Increased knowledge needed

The review of biochemical knowledge on biological processes and the comparison with the modelling concepts allow pointing out some research needs:

- Hydrolysis mechanisms are not yet well understood, especially in mixed-culture and mixed-substrate conditions (Morgenroth *et al.*, 2002),
- Protozoa seem to be involved in the hydrolysis process and in the biomass decay processes, but their role and importance are barely known,
- The factors that govern the competition between PAOs and GAOs are not yet fully understood,
- The diversity of the PAOs and especially the sub-groups involving different metabolic mechanisms under different electron acceptor conditions (reducing power formation without using glycogen, denitrification) should be better known,
- The transfer of lab-scale results to full-scale often seems difficult. Indeed, lab-scale experiments are often carried out on pure cultures with pure substrates. Consequently, the phenomena observed do not take into account biomass interactions, protozoa presence or environmental conditions, such as inhibitors in the influent. The parameters determined under these conditions are then difficult to generalise.
- Methods to experimentally determine parameter values are insufficiently developed.

These gray areas on the biological processes behaviour knowledge lead to the use of simplifications (e.g. lumped processes, such as decay) in the models or the definition of hypotheses without mastering or even acknowledging the associated model error.

4.4.4.4 Existing model modifications

Once the model chosen, the user may have to include some modifications, either to reach the modelling objective (e.g. including multi-step nitrification and denitrification)

or to cope with environmental conditions (e.g. modifying yields and kinetics depending on the electron acceptor), as underlined through this chapter for each process in the paragraphs "model limitations". When modifying an existing model, the user should be particularly careful on the following points:

- The stoichiometric continuity and the kinetic consistency should be carefully checked using the methods of Hauduc *et al.* (2010), to ensure the mathematical accuracy of the model.

- As model processes often merge different mechanisms for simplification, the significance of other processes and parameters may change when adding (explicitly defined) or modifying some processes. For example, adding a storage process for OHO will lead to a different meaning of the hydrolysis process, and will lower the hydrolysis parameters (see discussion in paragraph 4.4.4.1.2). Consequently, model users should be very careful in using default model parameters in modified models.

Table 4-38. Synthesis of theoretical limitations of models for each standard process

	State variables / Substrate	**Nutrients**	**Aerobic conditions**	**Anoxic conditions**	**Anaerobic conditions**	**Simplified mechanisms**
Hydrolysis	XC_B as only particulate fraction	ammonification for component-based models (**ASM1** and **Barker & Dold**)			**ASM1** and **UCTPHO+** do not take anaerobic hydrolysis into account	chemical dissolution, mass transport, storage (except **ASM3**, **ASM3 +BioP**)
Fermentation					**ASM2d** and **UCTPHO+** neglect anaerobic biomass production	neglected in **ASM3+BioP**
OHO Growth		- P not limiting in **ASM1** and **ASM3** - NO_X as N source in **UCTPHO+**, **Barker & Dold**	**ASM3** does not consider direct growth on S_B	- Constant yield for **ASM1**, **ASM2d** - **ASM3** does not consider direct growth on S_B		one-step denitrification
ANO Growth						one-step nitrification
OHO & ANO decay	death-regeneration makes substrate available only for OHOs				Endogenous respiration concept (**ASM3**, **ASM3+BioP**) does not consider anaerobic decay	dormancy, maintenance, predation
PHA storage	glycogen neglected					competition with GAOs
PolyP storage	two polyP storage pools in **Barker & Dold**			constant yield for **ASM2d** and **ASM3+BioP**		biologically induced phosphate precipitation
PAO growth		NO_X as N source and polyP as P source only in **UCTPHO+**, **Barker & Dold**	direct growth on S_{VFA} not considered	constant yield for **ASM2d** and **Barker & Dold**		
PAO decay			Aerobic maintenace is not considered		**ASM3+BioP** does not model anaerobic decay, nor anaerobic maintenance	PHA and glycogen utilisation for maintenance are not considered
PAO storage pool lysis	**UCTPHO+** releases PHA in the form of XC_B		**ASM3+BioP** consumes electron acceptor	**ASM3+BioP** consumes electron acceptor		Storage pool lysis is not modelled in **ASM2d+TUD**

4.4.5 Conclusion

Activated sludge models have been published based on theoretical knowledge of process mechanisms. Seven of the most widely used models have been theoretically compared in terms of their underlying modelling concepts. A schematic representation has been developed to allow representing modelling concepts for each standard process in a few figures.

First, this representation will help model users to better understand modelling concepts and model differences. This representation is complementary to the model representation developed by Comeau and Takács (2008) that allows a global view of the model processes.

Secondly, this representation allows determining the main conceptual differences between models (modelling schools), that highlights their main models theoretical limits, among which:

- Component-based models (more flexible) versus fraction-based models (less complex),
- Constant yields or different yields (depending on the electron acceptor) impacting the biomass production and the electron acceptor consumption,
- Fermentation modelled as transformation or as anaerobic growth process impacting the biomass production in case of large anaerobic zones,
- Direct growth or growth on stored substrate will depend on the loading conditions (cyclic),
- Death-regeneration is simpler and adequate under anaerobic conditions, while endogenous respiration is closer to reality and applicable for secondary substrate use,
- Modelling glycogen adds model complexity but also completeness and
- Simultaneous PAO growth and polyP storage accurately represent the interactions between metabolic mechanisms.

These differences and limitations should be taken into account when selecting a model in a modelling project.

4.5 Conclusion

This chapter critically reviewed seven popular models. First, to cope with the different notations used for the different models models, a standardised notation has been developed in collaboration with model users and developers. The correspondances with original notation can be found for the studied models in a spreadsheet (http://www.iwaponline.com/wst/06104/0912.xls). This uniformed language will help model users to understand new models and to communicate on them.

A systematic procedure for model verification has been set up and applied to the studied models. The tools to check stoichiometric continuity and kinetic consistency are provided in a spreadsheet (http://www.iwaponline.com/wst/06104/0898.xls). Through this procedure, a number of typing errors, gaps and inconsistencies in the stoichiometry and kinetics have been pointed out. Some common errors are highlighted:

- rounding the conversion coefficients instead of using exact values (e.g.: i_{NOx_N2}=-2.86 g COD.g N^{-1} inste ad of i_{NOx_N2}=-40/14 g COD.g N^{-1}),
- using a different temperature adjustement equation,
- considering alkalinity limitation not in the appropriate processes,
- missing the substrate preference functions in case of several possible substrates,
- considering "COD loss", as in Barker & Dold model and UCTPHO+.

The corrected matrices for the discussed biokinetic models are provided in the same spreadsheet. Some of these errors are mainly theoretical errors and will only have a minor impact on model results in typical conditions, but may have a significant impact in case of peculiar treatment conditions. This strongly shows the necessity for model users to check the models they develop, implement or use.

Finally, the modelling concepts were compared on the basis of a schematic representation and on a review of the theoretical biochemistry knowledge. Nine standard processes have been discussed in this way:

- Hydrolysis;
- Fermentation;
- Ordinary Heterotrophic Organisms (OHO) growth;

- Autotrophic Nitrifying Organisms (ANO) growth;
- OHO & ANO decay;
- Poly-hydroxyalkanoates (PHA) storage;
- Polyphosphates (polyP) storage;
- Phosphorus Accumulating Organisms (PAO) growth and
- PAO decay.

This comparison allows pointing out the theoretical limits of the models studied, especially depending on the electron acceptor conditions, the substrate and nutrients considered and the mechanism simplifications. It also helps model users and especially engineers to understand the theoretical bases of the models, the modelling concepts and the differences between the models. Moreover, knowledge gaps in microbiology and biochemistry are pointed out.

This work should be considered as a toolbox by new model users, which allows them to better understand models. Applying these procedures and the schematic representation to their own models will help them to better understand the theoretical basis of their model, its structure and the significance of the parameters. This knowledge will provide them with better judgement in the calibration step and in the use of their model. Model developers should also benefit from this work by developing error-free and easily understandable models for the modelling community. It also provides them with graphical tools to communicate about their model. To facilitate and spread the use of these tools, software developers are playing an important role. Indeed, using these procedures is time consuming, especially for engineers and consultants. Modelling software should then provide models in both their original and standardised notation, and tools to automatically check the stoichiometry and the kinetics of the models.

CHAPITRE 5 Towards a default parameter set

L'objectif de ce chapitre était de mettre au point une méthodologie visant à établir un jeu de paramètres par défaut. Le jeu de paramètres par défaut pourra être utilisé comme point de départ à l'étape de calage du modèle, ou comme approximation dans le cas où les données nécessaires au calage ne sont pas disponibles.

i. Calage multi-jeux de données

Le jeu de paramètres par défaut devra permettre de simuler de façon adéquate des jeux de données représentatifs de conditions de fonctionnement variés. Il est donc envisagé d'obtenir ce jeu de paramètres par calage simultané de plusieurs jeux de données. La Figure 5-1 décrit la démarche utilisée pour le développement de cette méthodologie en vue de l'obtention d'un jeu de paramètres par défaut. Une procédure de calage automatisée est d'abord mise en place afin de pouvoir caler les différents jeux de paramètres de façon objective, sans intervention de l'utilisateur. Cependant, cette procédure nécessite la définition de critères de qualité, qui permettent de spécifier l'arrêt de la procédure de calage. Une revue de littérature de ces critères est donc également menée. Ces deux étapes sont détaillées dans les paragraphes suivants.

ii. Calage automatisé des paramètres

Cette procédure doit permettre de passer outre les problèmes de non-linéarité des modèles de type ASM, ayant pour conséquence l'existence de minimums locaux dans la fonction objectif de calage. De plus, les critères de qualité des modèles n'étant que peu utilisés dans le domaine du traitement des eaux usées, la procédure ne doit pas être dépendante du choix de ces critères.

La procédure développée par Sin *et al.* (2008a) a été choisie comme base de travail. Cette procédure repose sur l'échantillonnage par hypercube latin de jeux de paramètres qui sont ensuite simulés un à un. Le choix du meilleur jeu de paramètres est réalisé après les simulations, et ce choix peut être modifié en fonction des critères de qualité choisis. Les principales étapes de cette procédure, les données d'entrée nécessaires et les logiciels utilisés sont présentés sur la Figure 5-2.

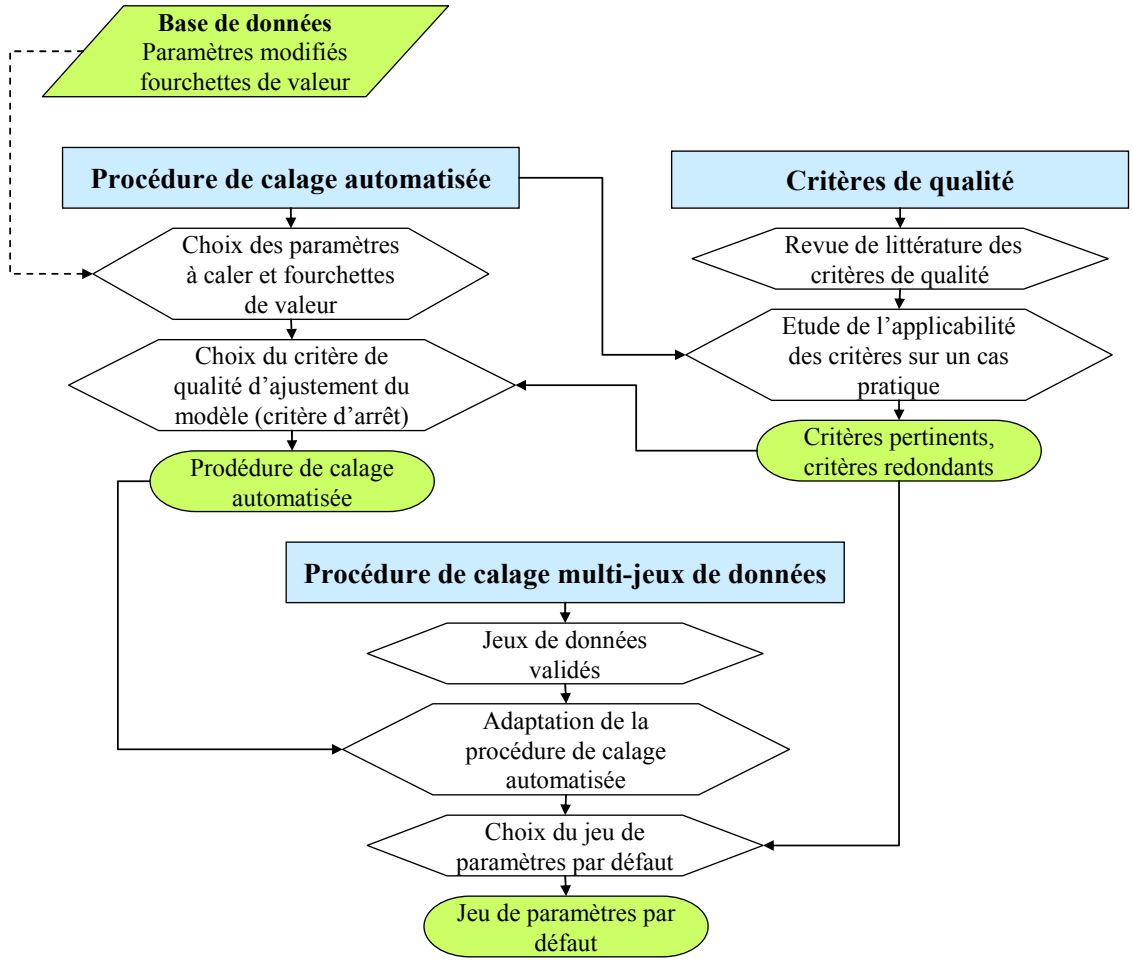


Figure 5-1. Démarche utilisée pour le développement d'une méthodologie d'obtention de jeux de paramètres par défaut

L'échantillonnage par hypercube latin est effectué dans les fourchettes de valeurs obtenues précédemment (paragraphe 3.2), qui sont utilisées comme connaissances *a priori*.

Une fois calculés, les critères de qualité sont analysés successivement, afin de reconstituer les étapes traditionnelles de calage, qui assurent l'obtention de jeux de paramètres cohérents. Ainsi, la production de boues et la décantation vont d'abord être analysées, puis la nitrification, la dénitrification et éventuellement la déphosphatation biologique, en fonction du modèle considéré. Les jeux de paramètres fournissant des résultats aberrants pour chacune des variables correspondantes sont exclus. Puis, les jeux de paramètres encore en lice sont analysés sur la base d'un critère multi-variables et multi-objectifs pour déterminer le meilleur jeu de paramètres.

Pour chaque étape, des outils ont été développés. Ils apparaissent sur la Figure 5-2 qui récapitule la procédure générale. L'échantillonnage par hypercube latin est réalisé grâce au logiciel R (http://www.r-project.org/). La configuration de la station d'épuration est implémentée dans le logiciel de simulation WEST (Vanhooren *et al.*, 2003). Les simulations sont ensuite réalisées de façon automatisées dans Tornado (Claeys *et al.*, 2006), le cœur de calcul de WEST. L'adaptation des fichiers de simulation aux différents jeux de paramètres est effectuée par une macro Visual Basic for Application dans MS Excel. Enfin, les critères de qualité sont calculés automatiquement par l'application BlueM.Opt (Bach *et al.*, 2009), et fournissent l'ensemble des critères de qualité dans une base de données MS Access.

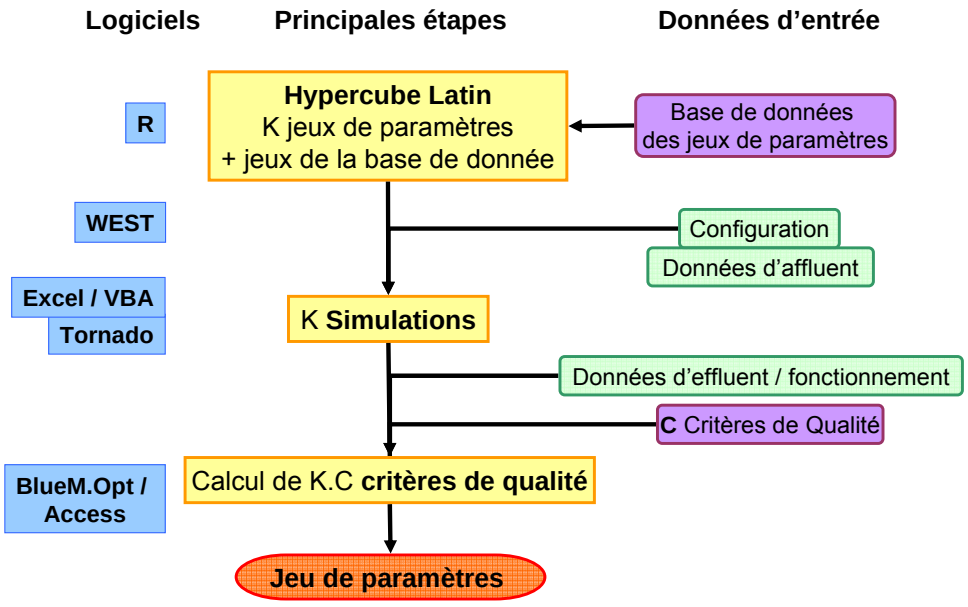


Figure 5-2. Procédure de calage automatisé

iii. Critères de qualité des modèles

Le calage des modèles de type ASM est un problème multivarié : le modèle doit simuler plusieurs variables d'intérêt (multi-variables), et doit pouvoir reproduire, selon les objectifs du projet de modélisation, notamment la moyenne, les pics de pollution, les valeurs maximum (multi-objectifs). Les critères de qualité des modèles sont largement utilisés en sciences de l'environnement, notamment comme critère d'arrêt des procédures de calage. Cependant, ce sont en général des critères univariés. Peu d'applications ont été trouvées dans le domaine des eaux usées pour les critères de qualité quantitatifs (Dochain and Vanrolleghem, 2001; Petersen *et al.*, 2002a; Ahnert *et al.*, 2007; Sin *et al.*, 2008a).

Une revue de littérature sur les critères a donc alors été effectuée, incluant des exemples dans plusieurs domaines des sciences de l'environnement, et notamment l'hydrologie. Les critères graphiques, utilisés principalement dans le domaine des eaux usées, sont d'abord présentés. Puis, l'ensemble des critères quantitatifs univariés recensés sont décrits. Ils ont été regroupés en neufs schémas, sur lesquels peuvent être appliqués une partition des données, des transformations logarithmiques, exponentielles ou puissances, pour accentuer le poids des erreurs faibles ou importantes, en fonction des objectifs de l'étude. Les neufs types de critères sont les suivants :

- Statistiques descriptives
- Statistiques sur des évènements uniques
- Propriétés de la distribution des erreurs
- Critères simples sur les erreurs
- Critères relatifs sur les erreurs par rapport aux données observés
- Critères sur la somme totale des erreurs rapportée à la somme totale des observations
- Concordance entre les distributions des données observées et prédites
- Comparaison des erreurs avec un modèle de référence
- Comparaison de modèles

Une réflexion est également menée sur la construction d'un critère global, intégrant la prise en compte de différents objectifs d'ajustement du modèle et différentes variables d'intérêt.

La procédure d'obtention des jeux de paramètres par défaut proposée est en cours de test. Elle permettra dans un premier temps de préciser les points clés de la procédure (nombre de simulations, critères de qualité), puis elle pourra être utilisée pour définir les jeux de paramètres par défaut des modèles publiés, moyennant l'obtention de jeux de données validés et représentatifs de conditions de fonctionnement variées.

5.1 Introduction

The objective of model calibration is to adjust any model parameters until simulation results match an observed set of data. This step is seen by activated sludge modellers as time-consuming and source of pitfalls (see paragraph 2.1).

ASM type models are non-linear multivariate models and their parameters are more or less correlated, depending on the experimental measurements performed (Von Sperling, 1993). This causes parameter identifiability problems: several sets of parameters can achieve the same goodness-of-fit of the model (Dochain and Vanrolleghem, 2001). Therefore, calibration procedures are generally performed with a subset of the whole set of parameters: only a subset of parameters is estimated, the other parameters being fixed to "default values". The subset of parameters to be calibrated can be determined either relying on expert knowledge or by sensitivity analysis (Ruano *et al.*, 2007). Furthermore, the non-linearity of the ASM-type models may cause the existence of local minima, i.e. there are regions inside the parameter range where a minimum exists, which is not the minimum of the whole parameter range. Depending on the initial parameter values, a model user may stop his/her calibration procedure in such local minimum.

As a consequence, the initial parameter set used in the calibration step and the default values chosen for the non-identifiable parameters have a significant influence on the model performance. However, such a "default parameter set" exists only for ASM1 (Henze *et al.*, 2000a). Other model publications proposed a parameter set as "an example", which is specifically recommended not to be used as a default parameter set. These values are nevertheless widely used as "default" (see paragraph 3.2).

The objective of this work was therefore to set up a methodology to get default parameter sets for each activated sludge model under study. This default parameter set should suit a large range of environmental and process conditions, and should thus rely on numerous datasets. To reach this main objective, a calibration procedure that allows calibration of several datasets simultaneously is set up. As presented in Figure 5-3, such procedure first requires an automated calibration procedure to objectively calibrate a

model to a number of datasets. Secondly, objective functions are needed to assess the goodness-of-fit of the model and to stop the calibration procedure after convergence.

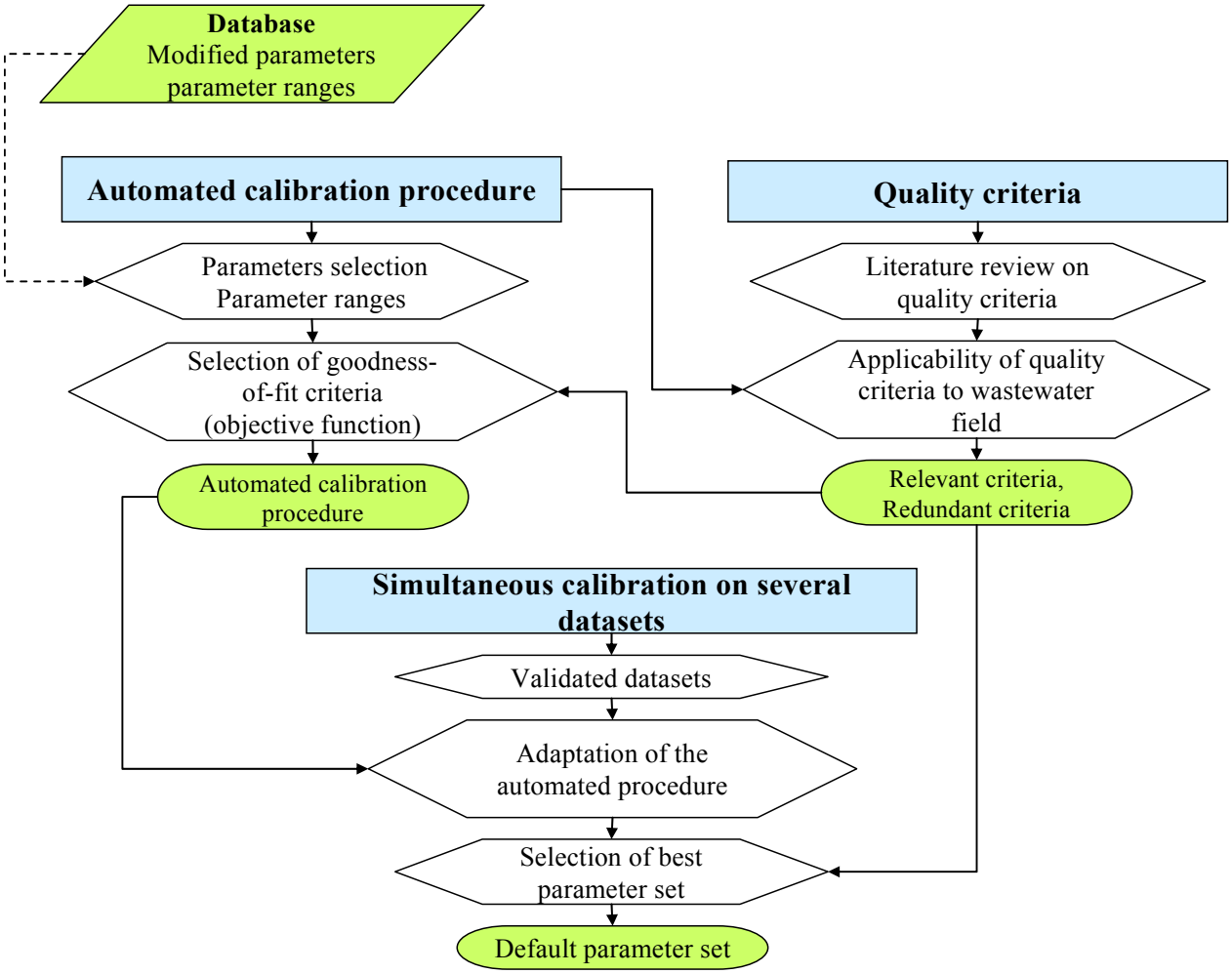


Figure 5-3. Framework for the developpement of a methodology to get default parameter sets

The general procedure for simultaneous calibration on several datasets will be presented first. Then, the automated calibration procedure will be described in more details. Finally, goodness-of-fit criteria used in environmental sciences have been reviewed and tested for their applicability in the wastewater treatment field.

5.2 Simultaneous calibration on several datasets

To be reliable, default parameter sets should suit a large range of environmental and process conditions, and should thus be based on numerous datasets. To get a default

parameter set for each model under study, a procedure is proposed and presented on Figure 5-4 and explained below.

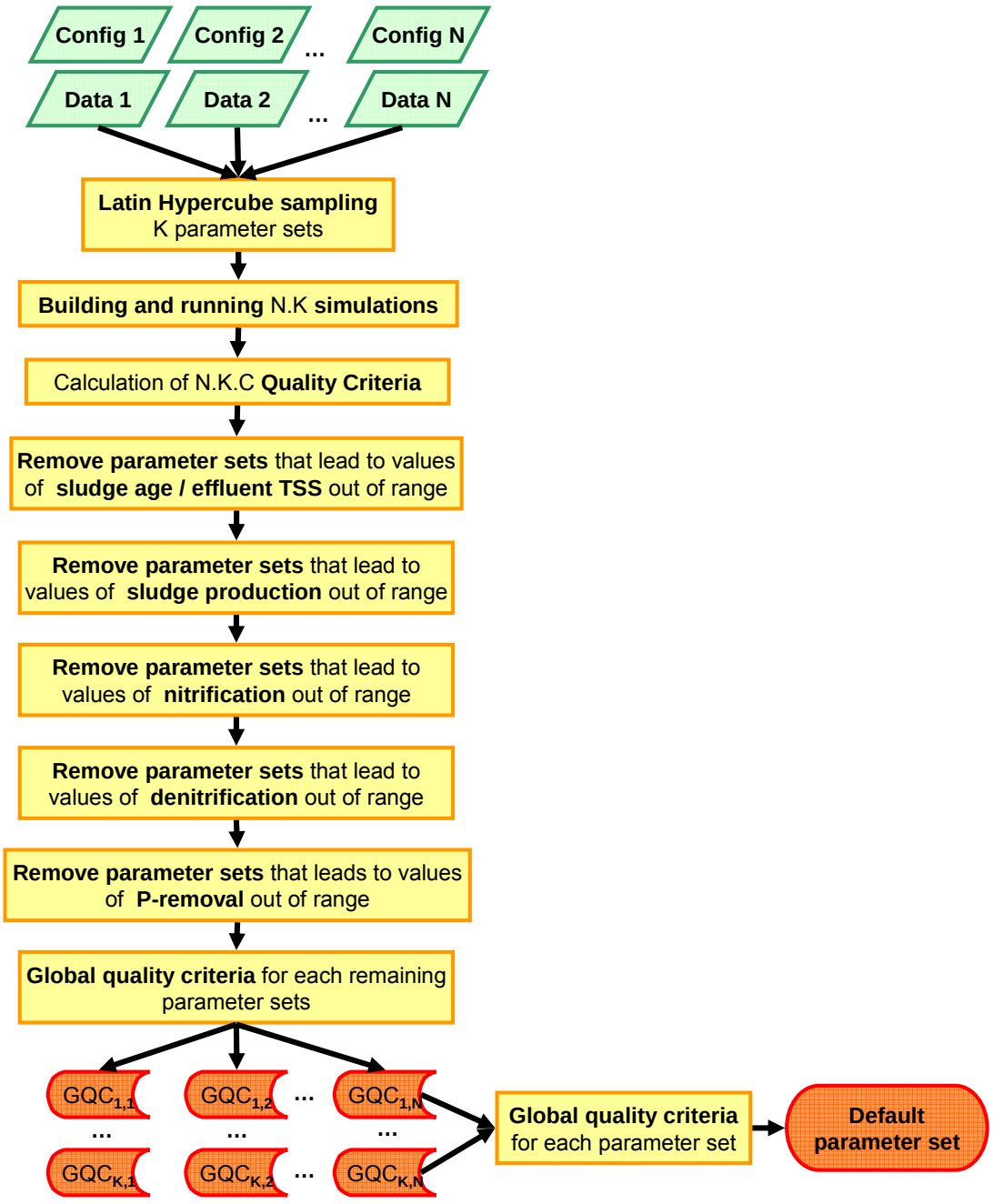


Figure 5-4. Procedure to obtain a default parameter set of a particular model

This procedure should be seen as a tool to be used by modelling experts to get model default parameter sets, and should normally be used only once, or to update the default values when new data is available.

5.2.1 Calibration method

The Monte Carlo method was selected as a suitable method for simultaneous calibration of several datasets. This method, already used by Sin *et al.* (2008a), is based on the random sampling of a pool of parameter sets in parameter space. Then, each dataset is modelled with each parameter set. To apply this method, two items have to be specified: how to sample the parameter sets, and how to select the best parameter set.

In addition to biokinetic model parameters, influent characterics are among the dominating factors influencing model predictions (Roeleveld and van Loosdrecht, 2002). Whereas the main influent concentrations are generally measured (COD, MES, NH_4, TKN, P_{Tot}, PO_4), variable fractions are not always determined, or determined with large uncertainties (Roeleveld and van Loosdrecht, 2002; Gillot and Choubert, 2010). Therefore, the influent fractions should be considered in the calibration procedure.

The prior knowledge on the parameter values distribution acquired in paragraph 3.2 will be used to sample the parameter sets. To optimise the distribution of the parameter sample in parameter space, the Latin Hypercube sampling method was selected. This method is presented in further details in paragraph 5.3.1.2.2 and its application to the automated procedure is described in paragraph 5.3.3.1.

5.2.2 Quality criteria calculations

The simulation outputs have now to be analysed to determine the parameter set which fits the observations "best". To be independent of the user, this analysis should be objective, reproducible and automated.

The objective functions are metrics used during calibration to evaluate the capacity of the parameter set to provide a model with adequate quality, which means with an objective function below a predefined threshold. Such goodness-of-fit criteria are commonly used in environmental sciences, but not often used in the wastewater field. Their use in environmental sciences will be reviewed and discussed in paragraph 5.4.

5.2.3 Removal of non-sense parameter sets

Usually the calibration procedure is carried on in steps, as presented for example in Hulsbeek *et al.* (2002). First, the settling parameters and the sludge production are

adjusted because they determine the sludge age and the sludge concentration, and consequently the ability of the biomass to consume nutrients. Then, nitrification, denitrification and biological phosphorous removal are calibrated successively.

This calibration by steps can be transposed to the automated calibration procedure in the analysis of the Monte Carlo simulation results by analysing the quality criteria of variables of interest successively. For each variable, the parameter sets that lead to simulated values out of range will be excluded from the pool of parameter sets. Consequently the pool will be reduced at each step.

At the end, a pool of possible parameter sets will remain. The selection of the best parameter set is a multivariate problem that should take into account the fit to different variables of interest (multi-variable problem), but also the modelling focal point (mean peak's timing, peak's magnitude or typical diurnal, weekly or seasonal variations … = multi-objective problem). To objectively select the parameter set and consider the number of datasets, parameter sets, variables and objectives, this selection of the best parameter set should be automated. The following paragraph discusses a method to procede to the selection of the best parameter set.

5.2.4 Determining the best parameter set

The aim of this step is to determine a single parameter set that allows representing several datasets at a time. The procedure above provides several quality criteria for each simulation (parameter set) and each dataset. A method is thus required to synthesise the information provided by all these quality criteria to determine which parameter set is best.

This is a multi-objective problem that will lead to a compromise regarding the parameter set: the improvement of some quality criteria with a parameter value could be compensated by the deterioration of other quality criteria. In these cases Pareto fronts are used to determine the set of possible solutions, which are defined as all parameter sets for which the modification of any parameter value will deteriorate at least one of the quality criteria (Yapo *et al.*, 1998). However this method is subjective and cannot be automated. Furthermore, in this work the quality criteria have to be synthesised for two stages: first for each simulation and then for each parameter set. Thus, aggregate quality

criteria may be more suitable. The design of a global quality criterion will be discussed in further details in 5.4.2.7.

The default parameter set should allow reaching on average an acceptable goodness-of-fit for all datasets. To determine the default parameter set, a global quality criterion is then calculated for each dataset and each parameter set. Figure 5-5 illustrates the case of two different parameter sets (θ_k, k=1 to 2) that have been used to simulate 5 datasets (i= 1 to 5). For each dataset and each parameter set, a global quality criteria $GQC_{k,i}$ is calculated (in purple in Figure 5-5).

Then, for each parameter set, a single global quality criterion GQC is computed based on linear combination of individual global quality criteria $GQC_{k,I}$ (in red in Figure 5-5). However, not all data sets have the same quality. In order to not influence the parameter set by a case with low quality data, datasets should not all have the same weight in this decision. To deal with this, the Fisher Information Matrix could be used. It is the inverse of the parameter estimation error covariance matrix, and summarises the information content of a dataset (Dochain and Vanrolleghem, 2001). This matrix could be used to assign different weights to each data set in the objective function for parameter estimation.

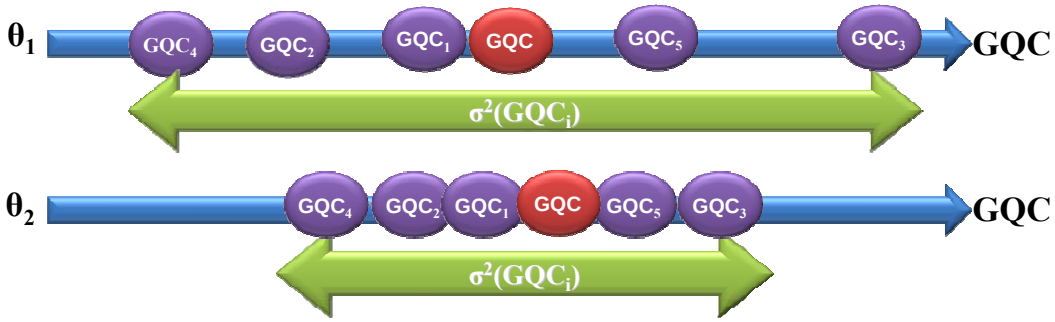


Figure 5-5 : Method to choose the best parameter set: lowest global criteria GQC and lowest variance between individual criteria (GQC_i)

The selection of the best parameter set should be based on the compromise between two characteristics of the parameter set:

- the lowest global quality criterion value (GQC),
- the lowest variance between individual quality criteria ($\sigma^2(GQC_i)$), to ensure that all the datasets are equally well modelled.

Consequently, on the example on Figure 5-5, the parameter set θ_2 is preferred.

5.3 An automated calibration procedure

Four activated sludge calibration protocols have been published so far: BIOMATH (Vanrolleghem *et al.*, 2003), STOWA (Hulsbeek *et al.*, 2002), HSG (Langergraber *et al.*, 2004) and WERF (Melcer *et al.*, 2003). These current calibration procedures are based on manual trial and error approaches (except for BIOMATH protocol) and rely heavily on subjective judgments of the user. As a consequence, the procedures are not repeatable: two modellers will find a different set of calibrated parameters based on their own experience for the same modelling project.

The purpose of this step is to establish a repeatable and automated procedure, in which the user does not intervene. Sin *et al.* (2008a) already developed such procedure for recalibration of an existing model. The goal is to adapt this procedure for simultaneously calibrating a single parameter set on a number of datasets and to integrate the prior knowledge on parameter values from the database analysis (see paragraph 3.2). First, the theory on existing optimisation algorithms is briefly discussed to highlight their weaknesses and strengths that lead to the choice of the Monte Carlo optimisation method. The approach to adapt the Monte Carlo method to the prior knowledge on parameters acquired in CHAPITRE 3 and to integrate the method to an automated procedure is then presented.

5.3.1 Optimisation algorithms

5.3.1.1 Local algorithms

An optimisation algorithm achieves an iterative estimation of the parameter set so as to converge to a minimum, i.e. the set of parameters that minimises the objective function describing the goodness-of-fit of the model to the observed dataset. Local minimisation algorithms are generally used by simulation software for model calibration. These algorithms are based on finding the direction of the minimum, by analyzing the slope of the objective function around the current parameter value at each step (gradient method, Newton, Levenberg-Marquardt, Rosenbrock…). In the case of complex nonlinear models, local minima may exist. Figure 5-6 illustrates the notion of local and global minima in the case of a one parameter optimisation and for three different initial conditions. Depending on the initial conditions, the algorithm will converge to the local

minimum (A and B) or to the global minimum (C). Some local minimisation algorithms, such as the Simplex method, developed by Nelder and Mead, or the method of Brent (Praxis), include a random aspect, which make them more robust against local minima (Dochain and Vanrolleghem, 2001). However, these methods still remain sensitive to the initial parameter values. These methods would be efficient in case default parameter values close to the optimum are available. As a consequence, these optimisation algorithms are not suited for the present case, where the goal is to determine such default values.

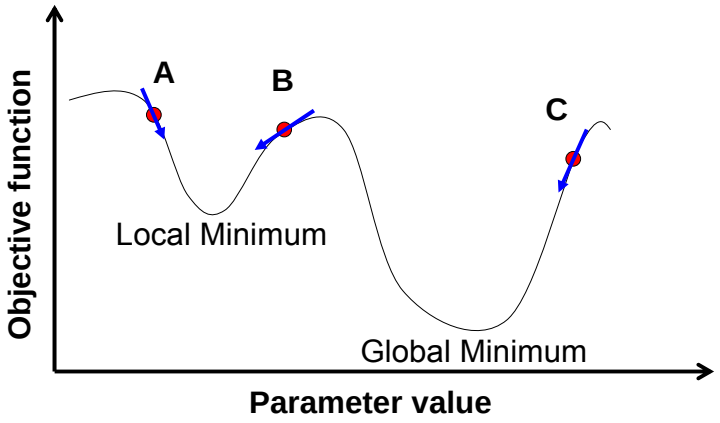


Figure 5-6. Local minimum and global minimum notions: illustration of the consequence of the initial choice of a parameter value (A, B or C) in local minimisation algorithms (only the initial condition C will reach the global minimum) (after Dochain and Vanrolleghem, 2001)

5.3.1.2 Global algorithms

Global minimisation algorithms have been developed to overcome the limits of local minimisation algorithms. These algorithms are either based on gridding the parameter space, or using randomised methods to have a large sampling of the parameter space (Dochain and Vanrolleghem, 2001).

5.3.1.2.1 Genetic algorithms

Genetic or evolutionary algorithms, based on the imitation of biological natural selection, are particularly efficient. In these algorithms, an initial population is sampled randomly and will evolve at each step (generation) by crossing the best parameter sets of the former step. These algorithms are used for calibration of hydrologic and water quality models (Zhang *et al.*, 2010), but only one application was found so far for ASM

type models (Kim *et al.*, 2000). Furthermore, genetic algorithms require the definition of an objective function to determine "the best" parameter sets at each step. So far, model quality criteria are rarely reported in the wastewater field (Petersen *et al.*, 2002a; Ahnert *et al.*, 2007; Sin *et al.*, 2008a). Contrary to genetic algorithms for which the result depends on the definition of the objective function, gridding methods allow analysing the sampled parameter sets afterwards, and are thus preferred to genetic algorithms for this work.

5.3.1.2.2 Griding methods

The gridding methods consist of evaluating combinations of parameter values determined on a grid drawn on the parameters space.

An example of a uniform grid is represented on Figure 5-7 a) for n=9 samples and two parameters: Y_{OHO} (0.558-0.737 g X_{OHO}.g XC_B^{-1}) and $K_{SB,OHO}$ (9-22 g S_F.m^{-3}). This sampling method will only test a small number of parameter values (in the example on Figure 5-7 a), only 3 different values per parameter).

The Monte Carlo method is a probabilistic random sampling procedure used to explore the parameter space. It is illustrated on Figure 5-7 b) for uniform sampling. This sampling method allows exploring a maximum number of parameter values in parameter space. However, some part of parameter space may be under-sampled, such as the lower part on Figure 5-7 b. This problem can be overcome by increasing the number of samples or by using the Latin hypercube sampling method (LHS), which allows optimising the coverage of the parameter space.

The Latin hypercube sampling method is based on the division of the parameter space in equal probability areas of 1/n, with n the number of samples. In case of uniform sampling of two parameters (Figure 5-7 c), a grid of n^2 equal intervals is drawn. Each interval will be represented only once in the set of samples (one square per column and per row on Figure 5-7 c), and the parameter values are randomly chosen in these intervals.

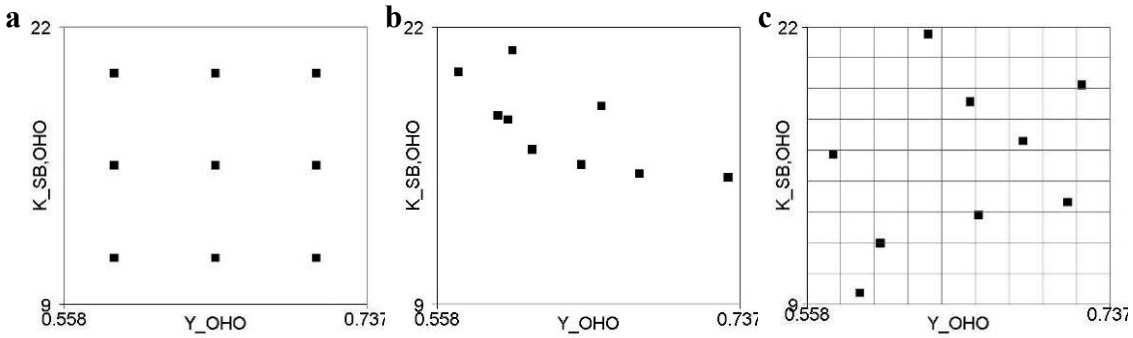


Figure 5-7. Sampling for gridding methods (n=9): a) full uniform grid; b) random (Monte Carlo) and c) Latin hypercube sampling

Monte Carlo optimisation with a Latin hypercube sampling method has been recently used by Sin *et al.* (2008a) to automatically calibrate the ASM2d model. These authors developed an automated re-calibration procedure in 4 steps: i) selection of the parameter subset, ii) definition of parameter space (parameter ranges and distribution), iii) sampling and running simulation, and i) evaluation of the simulation results, choice of the parameter set that fits the model most accurately. These steps are summarised on Figure 5-8.

This automated calibration procedure is used in this study as well, but it is adapted to fulfil the different objectives. The different steps are discussed in the next paragraphs.

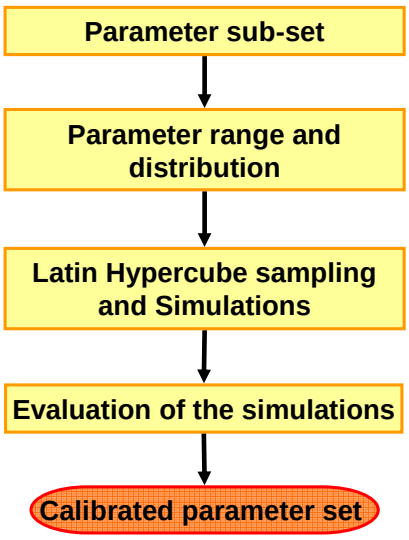


Figure 5-8. Automated calibration procedure from Sin *et al.* (2008a)

5.3.2 Parameter subset selection and parameter ranges definitions

5.3.2.1 Parameters identifiability

The first step of the procedure is to define the parameter subset to be calibrated. Indeed, the activated sludge models are high-order non-linear systems that include a large number of state variables and parameters. It results in non-identifiable models, meaning that several parameter sets can reach a same level of model fitting. The lack of identifiability of parameters can either be structural, which means inherent of the model and the experimental set-up, or practical, due to insufficient data quality or quantity (Dochain and Vanrolleghem, 2001). Few structural identifiability studies of ASM type model have been published so far (Dochain *et al.*, 1995; Julien *et al.*, 2000; Petersen *et al.*, 2002b; Zhang *et al.*, 2010). All of them seem to focus on ASM1 and ASM2d. Practical identifiablity studies are usually based on local sensitivity analysis (Weijers *et al.*, 1996; Brun *et al.*, 2002; Ruano *et al.*, 2007), which quantifies the magnitude of the model results' dependency on the parameter values, around a particular parameter set. Other methods, termed "global" sensitivity analysis, involve Monte Carlo simulations and are carried out on the entire parameter space (Von Sperling, 1993; Sin *et al.*, 2011).

Several modelling protocols have been published, advising calibration of parameter subsets and providing parameter value ranges (see paragraph 3.2). However, as stated above, the practical identifiability of the model depends mostly on the quality and quantity of available data. Consequently, the identifiable parameters may vary from one WWTP to another. In that respect, Ruano *et al.* (2007) compared subsets based on expert knowledge and subsets defined by sensitivity analysis, and proved that expert-based subsets are either too large or not large enough. Considering the high computational demand of a sensitivity analysis, Ruano *et al.* (2007) propose a combination of the two approaches.

5.3.2.2 Prior knowledge on parameter subsets and ranges

The results extracted from the database of practical modelling projects presented in chapter 3, provide the state of expert knowledge on ASM1 and ASM2d models. For these models, parameters that have been changed in most of the studies and the ranges they have been varied in were determined. These results will be used as prior knowledge in the automated calibration procedure. So far the database analysis didn't

allow determining correlations of parameters or their statistical distribution. When sufficient results will be available, these correlations and distribution could be integrated in the Latin hypercube sampling procedure (Helton and Davis, 2003). Parameters that are determined experimentally in specific studies could also be integrated, either by fixing these parameters to the values determined experimentally, or by taking into account the uncertainty on the measurement as the parameter range.

However, in the case of determining a default parameter set, the parameter values usually considered as fixed to a default value in the database should also be questioned. Consequently, all parameters will be included in the Monte Carlo analysis performed here. Furthermore, applying the Monte Carlo method on the complete parameter set allows performing a general sensitivity analysis as described by Sin *et al*. (2011).

5.3.3 General frame of the automated calibration procedure

The proposed calibration procedure is summarised on Figure 5-9. The main steps and software required at each step are specified. The practical implementation of the procedure is discussed in more details in the following paragraphs.

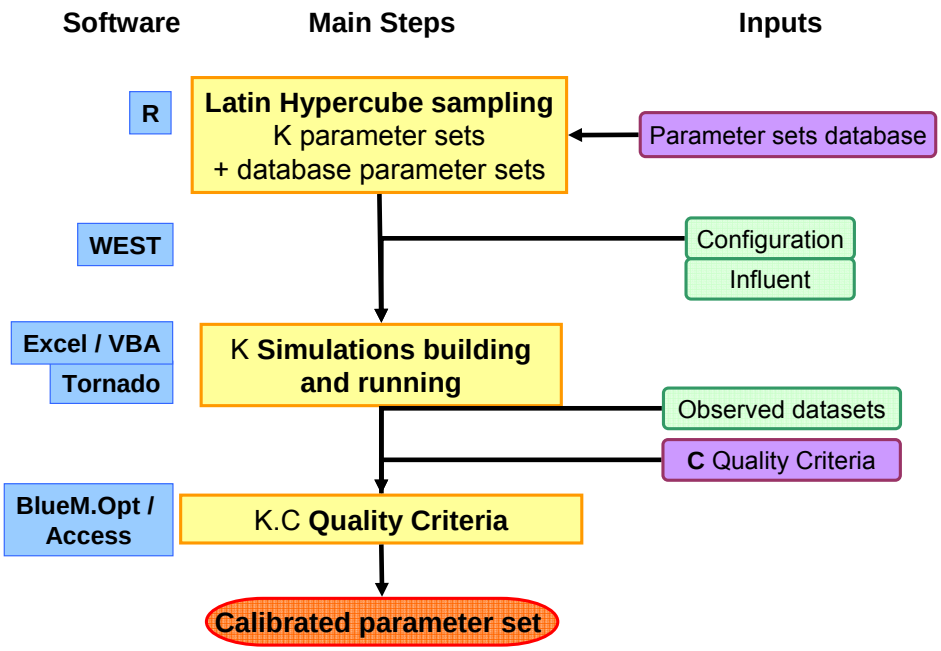


Figure 5-9. General frame of the automated calibration procedure

5.3.3.1 Latin hypercube sampling

The practical knowledge synthesised with the database analysis (see paragraph 3.2) is used to determine the parameter ranges. To eliminate the outliers of the database, the parameters space is defined between the 25th and 75th quartiles determined in paragraph 3.2. To start with, the parameter ranges will be enlarged by 10% to ensure that the sampling ranges cover a sufficiently wide parameter space. As no knowledge is available on the parameter distribution, a uniform law is assumed for the sampling. The parameters that are not changed from their default value in the database will be sampled in a range ± 10% the default value. The value of 10% is arbitrarily chosen at this stage, but could be revised after testing the procedure and analysing the first results.

In addition to Latin hypercube sampled parameter sets, all particular parameter sets included in the database concerning the model to be calibrated will be included as well. The performance of these parameter sets will be confronted with the Latin hypercube samples.

With respect to the influent fractionation, the proposed procedure has to be flexible enough so that it can be adapted for simultaneous calibration of multiple datasets (see paragraph 5.2.1). However, the fractionation depends on the sewage collection characteristics (geographical location, length of sewer system, etc…). Consequently, the fractionation uncertainty should be considered for each dataset and independent from the parameters sampling.

To keep a total COD fraction of 100%, one fraction should be chosen as the residual of the other fractions. Among the COD fractions, the unbiodegradable particulate fraction has a big influence on sludge production and soluble biodegradable fractions influence the denitrification and BioP processes. The soluble undegradable fraction is usually quite small and thus has little flexibility to absorb the variability of the other fractions. Consequently, the slowly biodegradable substrate is chosen to be the residual of the other fractions. For the ASM1 and Barker & Dold models, the soluble organic nitrogen fractionation is chosen to vary, whereas particulate organic nitrogen fractionation is the residual, to keep a total nitrogen fraction of 100%. A range of ±20% of variability on the initial fractionation is chosen arbitrarily, but could be revised after testing the procedure and analysing the first results.

The Latin hypercube sampling is performed with the function *randomLHS* of the R software (http://www.r-project.org/). The results are saved in a text file, containing one row per parameter set.

5.3.3.2 Simulation building and running

The simulation software used is WEST (Vanhooren *et al.*, 2003), marketed by the company MOSTforWATER (Kortrijk, Belgium). The configuration is first implemented in WEST2009, for its simplicity in use. However, WEST2009 does not allow to automatically run multiple simulations with varying parameter sets. Therefore, the simulations are carried out directly in Tornado (Claeys *et al.*, 2006), the generic kernel of WEST, through which all the functionality of WEST is accessible from the command line.

Each simulation requires its own experimental file which is automatically created through a macro in Excel Visual Basic for Applications. This macro is well documented and easily adaptable for other projects.

Each simulation parameter set may lead to a different steady-state condition. The influent files are thus modified to start with about 3 sludge ages steady-state influent before the dynamic influent data. All dynamic simulations are then run from their steady-state condition.

5.3.3.3 Quality criteria calculation

The simulation outputs have to be analysed to determine the parameter set which gives the best fit between simulated and observed data. To be independent of the user, this analysis should be objective, reproducible and automated. The following paragraph investigates the current practice in goodness-of-fit criteria for the environmental sciences and the possibility to use these quality criteria as objective functions in automated calibration procedures.

The quality criteria presented in paragraph 5.4.2 are automatically calculated by the software BlueM.Opt (Bach *et al.*, 2009) from the simulation output files and the reference file (which contains the observation measurements). The quality criteria are subsequently stored in an Access database.

5.3.3.4 Selection of the best parameter set

As described in paragraph 5.2.3, the selection of the parameter sets is carried out in two steps. First, the fit to the variables of interest for settling, sludge production, nitrification, denitrification and P-removal are successively analysed. For each variable, the parameter sets leading to non-sense values are excluded. Second, global quality criteria are computed for the remaining parameter sets to determine the best parameter set.

5.3.3.5 Test of the procedure: a French municipal WWTP case study

To test the procedure, an actual WWTP modelling project has been performed. The WWTP under investigation is located in France and receives exclusively municipal sewage from 250 000 Population Equivalents. It is configured in two parallel lanes that operate under similar conditions, each lane containing a plug-flow tank with a predenitrification zone. Aeration is controlled by a timer. Chemical phosphate removal is carried out with addition of aluminium. The SRT is 27 days long and the HRT 8.8 hours.

The simulation period chosen consists of 84 consecutive days, from February 15 to May 9 2009. This period was chosen because in that period the added aluminium quantity is known, allowing calulation of the chemical sludge production by phosphorous precipitation. The first half-part of this period had a typical behaviour. However, on day 47, all aerators broke down for 3 days. Then from day 50 to 67 the aerators were running permanently. These operating conditions provide dynamic conditions that are interesting to model.

5.3.3.5.1 Implementation of the configuration

The configuration was first implemented in WEST2009. Both lines were modelled as a single one with double volumes. Considering the U-shape of the aerobic tank, it was represented by an anoxic tank and three aerobic tanks, each with the same volume. It is supposed that there is no sludge accumulation in the secondary settler, and consequently a point-settler model is chosen The target variables (TSS in the biological reactors, effluent COD, TSS, TKN, NH_4^+-N and NO_3^--N) were sampled in the output through a modelled flow-proportional sampler so as to directly obtain flow-proportional daily

averages as model output. The configuration of the wastewater treatment plant is presented in Figure 5-10.

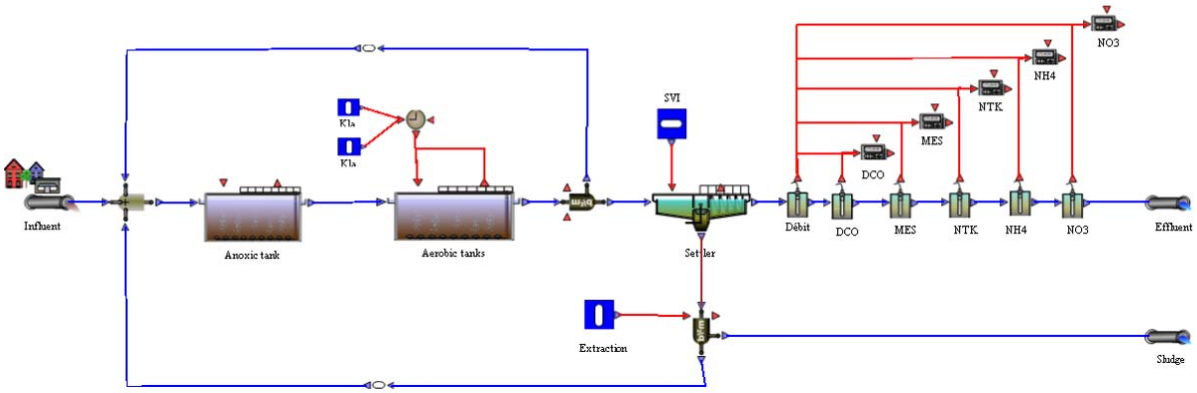


Figure 5-10. Layout of the WWTP in WEST

A first simulation was carried out with a modified ASM1, using Cemagref's default parameters (Choubert *et al.*, 2005; Marquot, 2006) (Table 5-1). This modified ASM1 includes a different heterotrophic growth yield under anoxic conditions (see paragraph 3.2). The ASM1 model code in WEST 2009 was thus adapted to include this modification.

The fraction of non-settleable particulates was fixed to 0.003 to approximately fit the effluent TSS concentration. The fractionation of the influent was roughly adjusted during a pre-calibration step to (visually) fit the sludge production and the mean effluent output data (Table 5-1).

5.3.3.5.2 Parameter sets sampling

To test the procedure, 5000 parameter sets were sampled through Latin hypercube sampling, in the R software, following the procedure specified in paragraph 5.3.2. The parameter ranges used are summarised in Table 5-1.

As stated in paragraph 5.3.2.2, fractionation has a strong impact on WWTP simulations. Therefore, it was also included in the Latin hypercube sampling. To keep a total COD fraction of 100%, XC_B was chosen to be the residual of the other fractions. A range of ±20% around the initial fractionation was chosen. Under these variations, XC_B varied from 41% to 73%.

The simulation files and the influent files were then built following the procedure presented in paragraph 5.3.3.2. The changes in parameter values may lead to steady-state conditions that are very different from the initial conditions obtained with Cemagref's default parameter set. Therefore, to ensure correct initial steady-state conditions for the 84 days of dynamic simulation, 100 days (about 3 SRT) were first simulated with pseudo steady-state conditions (alternating aeration periods, constant influent).

Table 5-1. Cemagref ASM1 default parameter set at 20°C (Choubert *et al.*, 2005; Marquot, 2006) and fractionation used in the modelling project, ASM1 parameter range values from percentiles 25%-75% of database results (Hauduc *et al.*, in press) enlarged by 10% and fractionation ranges ±20% of initial fractionation.

Kinetic parameters			
Parameter*	**Initial**	**Range**	**Unit**
$q_{XCB\_SB,hyd}$	3	1.98 - 3.3	g XC_B.g X_{OHO}^{-1}.d^{-1}
$K_{XCB,hyd}$	0.03	0.018 - 0.187	g XC_B.g X_{OHO}^{-1}
$\eta_{qhyd,Ax}$	0.4	0.36 - 0.55	-
$\mu_{OHO,Max}$	6	5.13 - 6.6	d^{-1}
$\eta_{\mu OHO,Ax}$	0.8	0.72 - 0.88	-
b_{OHO}	0.62	0.549 - 0.682	d^{-1}
$K_{O2,OHO}$	0.05	0.045 - 0.22	g S_{O2}.m^{-3}
$K_{SB,OHO}$	20	9 - 22	g S_B.m^{-3}
K_{NOx}	0.1	0.09 - 0.55	g S_{NOx}.m^{-3}
$\mu_{ANO,Max}$	0.8	0.594 - 0.99	d^{-1}
b_{ANO}	0.17	0.072 - 0.187	d^{-1}
q_{am}	0.08	0.063 - 0.088	m^3.g $X_{CB,N}^{-1}$.d^{-1}
K_{NHx}	0.1	0.675 - 1.1	g S_{NHx}.m^{-3}
$K_{O2,ANO}$	0.2	0.18 - 0.825	g S_{O2}.m^{-3}
$\theta_{KXCB,hyd}$	1		-
$\theta_{\mu OHO,Max}$	1.072		-
$\theta_{\mu ANO,Max}$	1.059		-
θ_{bOHO}	1.029		-
θ_{bANO}	1.027		-
$\theta_{qXCB\_SB,hyd}$	1.072		-
θ_{qam}	1.072		-

Stoichiometric parameters			
Parameter*	**Initial**	**Range**	**Unit**
$Y_{OHO,Ox}$	0.67	0.558 - 0.737	g X_{OHO}.g XC_B^{-1}
$Y_{OHO,Ax}$	0.54	0.496 - 0.594	g X_{OHO}.g XC_B^{-1}
Y_{ANO}	0.24	0.216 - 0.264	g X_{ANO}.g S_{NOx}^{-1}
$f_{XU\_Bio,lys}$	0.08	0.072 - 0.11	g X_U.g X_{Bio}^{-1}
Composition parameters			
i_{N_XBio}	0.086	0.0711 - 0.0946	g N.g X_{Bio}^{-1}
i_{N_XUE}	0.06	0.054 - 0.066	g N.g X_{UE}^{-1}
Settling parameters			
f_{ns}	0.003	0.001-0.005	-
Fractionation			From
S_U	7%	5.6-8.4%	DCO
S_B	25%	20-30%	DCO
$X_{U,Inf}$	8%	6.4-9.6%	DCO
X_{OHO}	8%	6.4-9.6%	DCO
XC_B	52%		DCO
S_{NHx}	100%		NH4
$S_{B,N}$	22%	17.6-26.4%	Norg
$S_{U,N}$	0%		Norg
$XC_{B,N}$	78%		Norg

* Standardised notation from Corominas *et al.* (2010)

5.3.3.5.3 Overview of the results

Simulated and target variables (TSS in biological reactors, effluent COD, TSS, TKN, NH_4^+-N and NO_3^--N) are presented in Figure 5-11 for the 5000 simulation runs. These graphs show the dependency of the model response to changes in the parameter set, compared to the observed values represented by the thick line.

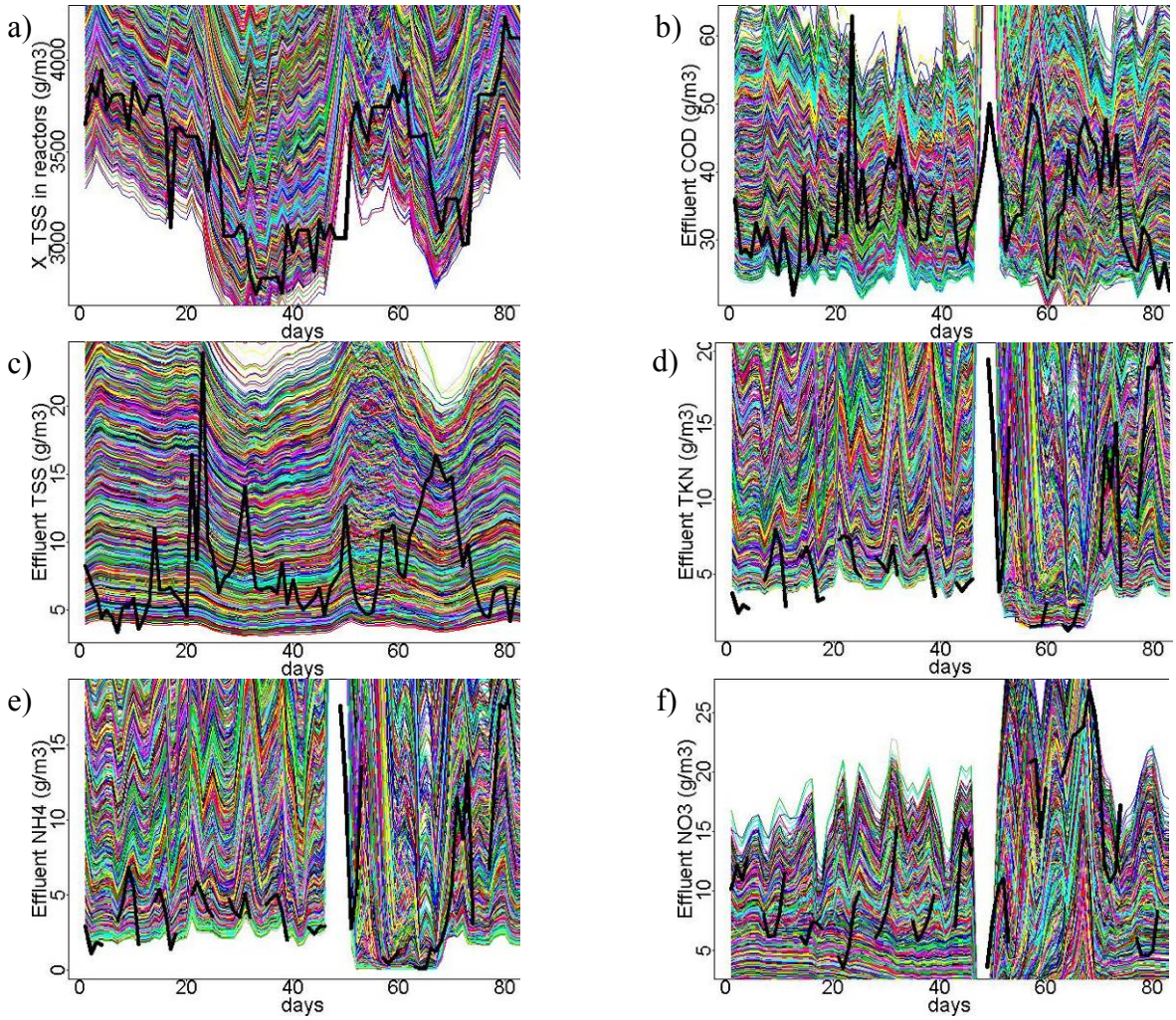


Figure 5-11. Results of the 5000 simulations for a) TSS in the biological reactors, b) Effluent DCO, c) Effluent TSS, d) Effluent TKN, e) Effluent NH_4^+ and f) Effluent NO_3^-. Bold lines correspond to the observed values. On day 47 all aerators broke down for 3 days, then from day 50 to 67 the aerators were running permanently.

This case study shows that the procedure and especially the files exchange between softwares were correctly set up. The 5000 simulation results have now to be analysed to evaluate the quality of each simulation and choose an appropriate parameter set for the model.

5.4 Quality criteria for wastewater treatment plant modelling: review and applicability of quality criteria from environmental sciences

The study of the database of practical modelling applications (chapter 3) shows that it is difficult to objectively assess the model prediction accuracy of published modelling projects. Most of the time in wastewater treatment applications, at best a graphical comparison of time series plots of part of the observations with the model predictions is provided. The conclusion on the fit of the model to observation data is then drawn on visual criteria and generally concerns only the calibration step, omitting the validation step. Although this qualitative evaluation is useful, it does not allow an objective assessment of the quality of the calibration parameter set, and thus cannot be used in the case of an automatic calibration procedure as presented in paragraph 5.3. An objective assessment is required as well when, for instance, comparing different model results.

Bennett *et al.* (2010) reviewed the tools for performance evaluation of environmental models comparing different quantitative methods: data division methods, the direct comparison method, residual methods, transformation methods, spatial methods, multi-criteria methods and diagnostic based evaluation methods. The direct comparison and residual methods based on graphical or mathematical comparisons of predicted and observed values are widely used in hydrology (Dawson *et al.*, 2007). In the wastewater field, quantitative criteria are rarely calculated (Petersen *et al.*, 2002a; Ahnert *et al.*, 2007; Sin *et al.*, 2008a). A review is presented in Dochain and Vanrolleghem (2001).

In the framework of the development of an automated calibration procedure, the direct comparison and residual methods seem particularly suited given their objectivity and their simplicity of calculation (in simple spreadsheets, and an automated calculation can be easily coded). The aim of this study is to investigate the possibility to use these methods more generally for model accuracy evaluation in the wastewater field. These goodness-of-fit measures could then be used for (Dawson *et al.*, 2007):

- Calibrating model parameters
- Evaluating how well the data is captured by the model
- Determining the extrapolation power and the uncertainty on predictions;
- Comparing the results of different modelling studies.

First, a literature review provides a list of graphical and quantitative quality criteria that have been used in a number of water-related disciplines (WWT, river hydrology, urban hydrology, climate sciences, environmental sciences…). In these disciplines a single variable of interest is usually considered (flow), the criteria are thus mostly univariate. However, in the wastewater treatment field, several variables are usually taken into account simultaneously in a model calibration exercice (sludge production, TSS, COD, nitrate and nitrogen at the effluent …). A methodology to investigate the use of these criteria in the wastewater field is then proposed and it is discussed how to consider this multivariable nature of the problem in the criteria.

5.4.1 Graphical methods

Graphical methods are widely used for model calibration. Some possible graphs were presented on a real case study example. The modelled outputs are obtained with an ASM1 simulation using the Cemagref default parameter set (Choubert *et al.*, 2005; Marquot, 2006).

A Time-series graph represents the time-series of observed (O_i) and modelled data (P_i) for a particular variable in the same figure (Legates and McCabe Jr, 1999). This graph allows a visual appreciation of the goodness-of-fit of the model for a particular variable. Consequently, one graph per variable of interest has to be drawn. Figure 5-12 shows that the model does not capture the dynamics of the first 45 days and overestimates the average. After day 45, the dynamics are well captured, with an underestimation between day 45 and day 55. Finally, from day 55 to 80 a time lag and an overestimation can be observed.

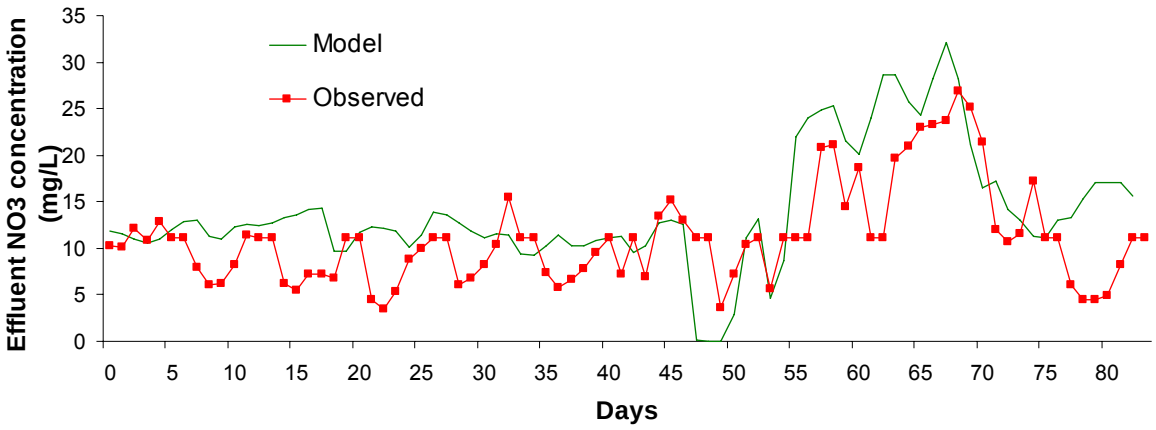


Figure 5-12. Time-series of observed (O_i) and predicted data (P_i)

The plot of residuals indicates the magnitudes of errors along the time-series. Figure 5-13 plots the residuals and relative residuals for the chosen example. It can be noticed that the errors are not systematic (either all positive or all negative values), but generally indicate an overestimation and are quite large (up to 300% of percentage error). Furthermore, the errors seem to be autocorrelated, because the residuals are not randomly distributed but present sequences with the same signs (Dochain and Vanrolleghem, 2001). This means that some behaviour is not included in the model, due to simplifications in the mechanisms or concepts modelled.

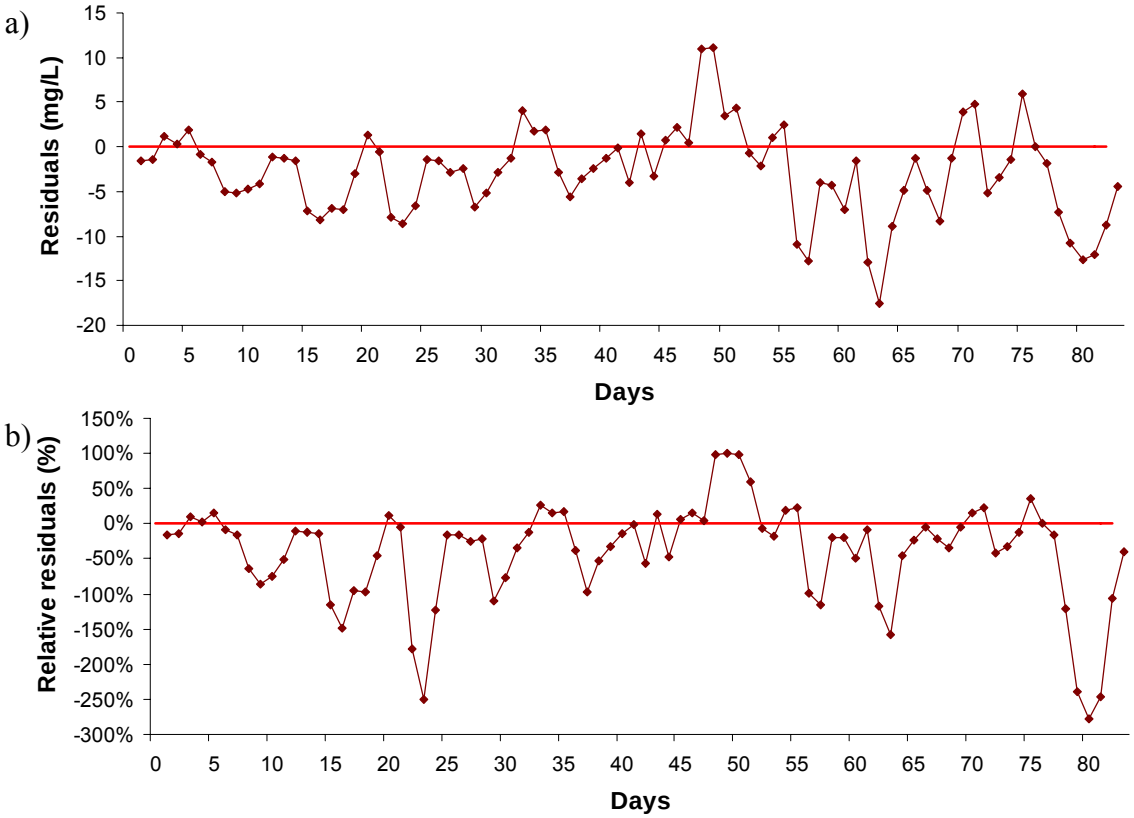


Figure 5-13. Plot of a) residuals (O_i-P_i) and b) relative residuals (O_i-P_i)/O_i

The scatter-plot (also termed Q-Q plot in some disciplines) confronts the observed data with the predicted data (Legates and McCabe Jr, 1999). For a perfect model the dots should be around the line with unitary slope and zero intercept (P_i=O_i). The regression line P=aO+b provides information on systematic (b) and value-dependant errors (a). In this case (Figure 5-14) the values in the scatter-plot are quite widely spread, which agrees with the large errors found on Figure 5-13.

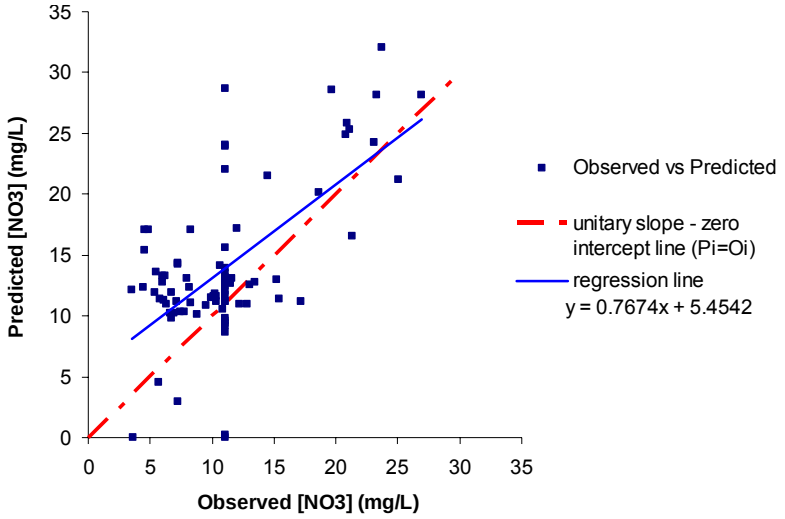


Figure 5-14. Scatter-plot of observed versus predicted data

Box-plots (Modarres, 2009) represent the distribution of values in the observed and modelled dataset. A box-plot of observed and model datasets allows to easily compare minimum, first quartile (25%), median, third quartile (75%) and maximum values. It can be seen from Figure 5-15 that the distribution of predicted data is wider and has a higher average, which indicates a tendency of over-prediction of the model. This is confirmed by the box-plot of residuals (CREM, 2009), which indicates a majority of negative residuals.

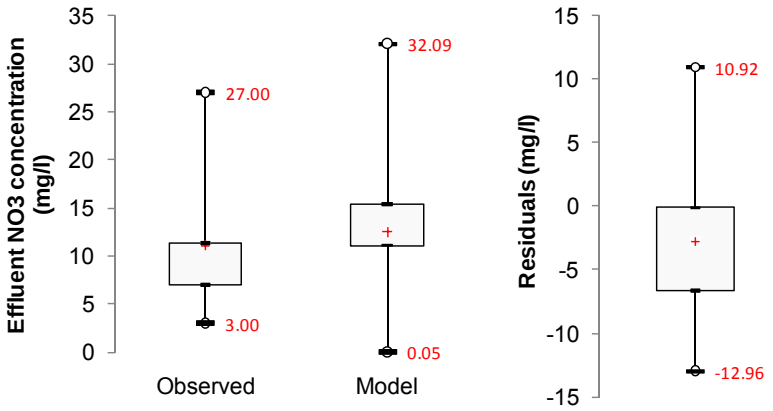


Figure 5-15. Box-plots of observed and model data and Box-plot of residuals

5.4.2 List of quantitative quality criteria used in environmental sciences

The graphical methods presented above are widely used in model calibration as they are simple and visual. However, the analysis of these graphs is subjective and cannot be carried out automatically or with a large number of tested parameter sets. Therefore, quantitative quality criteria used in the environmental sciences are reviewed. These quality criteria are based on the comparison of observed and predicted data with the aim of quantifying the differences observed with graphical methods.

Dawson *et al.* (2007) have listed a number of quality criteria for hydrological modelling and provide an on-line tool, Hydrotest, to calculate the goodness-of-fit criteria (https://co-public.lboro.ac.uk/cocwd/HydroTest/index.html). Most of these quality criteria are included in this review.

First, the general methods to compare datasets are presented, and then the quality criteria are presented following a classification inspired by Dawson *et al.* (2007). The following notation is used:

O: observed data

P: predicted data

n: number of data

p: number of model parameters

5.4.2.1 General methods to compare observed and predicted data

Depending on the modelling objectives, the goodness-of-fit of a model can be defined as the capability of the model to capture one or several characteristics of the observed data: mean, peak's timing, peak's magnitude or typical periodical variations (diurnal, weekly, seasonal…). Thus, to characterise the goodness-of-fit of the model, different quality criteria can be used. These criteria vary in the way they are computed from the observed and predicted data:

- Criteria can be **normalized to n**, the number of data, which allows comparing results of different size of datasets;
- **Absolute criteria** are expressed in the same units as the variables of interest;

- **Relative criteria** (divided by observed or predicted variance) are interesting because they are dimensionless (unit-free); the criteria obtained for different variables can thus be compared;
- **Comparison of residuals obtained with simplistic models** are used in several goodness-of-fit criteria to define the improvement of using the model compared to a simplistic model ("no knowledge"), such as a model defined as the mean of the observed values or the last observed value. The simplistic model can also be describing the typical variations (e.g. daily mean time-series calculated from historical yearly time-series), or the seasonal mean value (Legates and McCabe Jr, 1999).

Other arithmetic operations can be applied to emphasise small or large errors:

- Partition the dataset according to different measurement magnitudes (e.g.: low/intermediate/high flows) and compute the quality criteria on each of these subsets (Perrin *et al.*, 2006; Moriasi *et al.*, 2007),
- to **emphasise small errors or low magnitude values**: a power transformation of the data errors or values with an exponent lower than 1 (square root…) or a logarithmic transformation will give more importance to smaller errors or lower magnitude values,
- to **emphasise high errors or high magnitudes values**: a power transformation of the data with an exponent larger than 1 or an exponential transformation will provide higher importance to larger errors or high magnitude values,
- to **avoid error compensation**: absolute values and even power values will avoid compensation of negative and positive errors when summing them.

These arithmetic operations are used to modify the basic criteria to extract the information one wants, given a certain objective, as e.g. more importance towards errors at low magnitude, maximum errors or errors on peaks. It is important to note that all criteria given are based on sums. Consequently, in case of non-homogeneous time-step the criteria will emphasise the errors on more frequently sampled periods. If this is not desired, a solution to overcome this problem is to use weighted criteria inversely proportional to frequency (an isolated point will have a higher weight) (Willmott *et al.*, 1985).

The reviewed papers are listed in Table 5-7 and the criteria used in each of them are indicated.

5.4.2.2 Statistical criteria of observed and modelled time series

5.4.2.2.1 Descriptive statistics

Descriptive statistics are calculated for observed and predicted data and compared:

- Minimum value $min(\{O\})$ and $min(\{P\})$
- Maximum value $max(\{O\})$ and $max(\{P\})$
- Mean value
- Median value
- Variance, Standard deviation
- Skewness of the distribution (with y either O or P, and s() the standard deviation):

$$G_1 = \frac{n}{(n-1)(n-2)} \sum_{i=1}^{n} \left(\frac{y_i - \bar{y}}{s(y)} \right)^3$$

- Kurtosis (peakedness of the distribution):

$$G_2 = \frac{(n+1)n}{(n-1)(n-2)(n-3)} \sum_{i=1}^{n} \left(\frac{y_i - \bar{y}}{s(y)} \right)^4 - 3\frac{(n-1)^2}{(n-2)(n-3)} - 3$$

5.4.2.2.2 Single event statistics

In case modelling objectives require the simulation of dynamic events accurately (e.g.: handle storm flows, toxic peaks), criteria are needed to characterise the goodness-of-fit of the model for this event. The following criteria aim at characterising the difference between the maximum observed and the maximum modelled value:

- **PDIFF** Peak difference; values from -∞ to +∞; optimum value: minimum (Gupta *et al.*, 1998)

Equation: $$PDIFF = max(\{O\}) - max(\{P\})$$

- **PEP** Percent error in peak; values from -∞ to +∞; optimum value: minimum (Dawson *et al.*, 2007)

Equation: $$PEP = \frac{max(O_i) - max(P_i)}{max(O_i)} \times 100$$

These citeria evaluate how well the highest modelled value matches the highest observed value in percent. However, it does not take into account whether the max(O_i) and max(P_i) occur at the same time-step i. Consequently, in case of multiple events on the same time-series, first the single events must be extracted from the whole time series to have less chance to mix up with peaks from another event.

5.4.2.3 Statistical criteria of residual error between observed and modelled datasets

5.4.2.3.1 Correlation and distribution of residuals

An interesting criterion is the **number of sign changes** (NSC) (Gupta *et al.*, 1998), which counts the number of times the residual (O_i-P_i) sign change. The minimum value is zero and the maximum n. A value close to zero indicates a systematic error (over-estimating or under-estimating model) but a more consistent model. A value close to n indicates a random error. The criterion does not indicate the magnitude of the errors.

The **Number of runs test** (Dochain and Vanrolleghem, 2001) is a similar criterion. The number of runs R is the number of consecutive sequences of sign changes (negative-positive value). The expected value for R is n/2. A test of normality is then performed:

$\frac{R - n/2}{\sqrt{n/2}}$ is compared to the normal distribution $N(0,1)$ with a confidence level α. The error distribution follows a normal law if the computed value is below $u_{(1-\alpha/2)}$, the quantile (1-α/2) of the normal distribution.

The **autocorrelation of residuals** (lag-one and others) characterises how well the model takes into account all the information included in the observed dataset (e.g.Dochain and Vanrolleghem, 2001; Neumann and Gujer, 2008). This criterion is calculated for each time-lag τ, to provide information on the correlation of the error at any time t_k with the error at time t_k-τ. The autocorrelation of residuals is expressed as follows, with the error $\varepsilon=O_i-P_i$:

$$r_\varepsilon(\tau) = \frac{\sum_{k=\tau}^{N-\tau} \varepsilon(t_k - \tau).\varepsilon(t_k)}{\sum_{k=\tau}^{N-\tau} \varepsilon^2(t_k)}$$

5.4.2.3.2 Absolute criteria

The absolute criteria are based on the sum of residuals (difference between observed and predicted data), generally normalized to the number of data, n. The criteria are typically in the form expressed as follows, with γ a power, or in a similar form:

Equation: $$E_\gamma = \frac{1}{n}\sum_{i=1}^{n}\left(O_i - P_i\right)^\gamma$$

These criteria should in general be as close as possible to zero. Different variations on the theme, following the principles presented in 5.4.2.1, can be found in literature and are presented in Table 5-2.

Table 5-2. Absolute criteria

	Criteria	Equation	Min	Max	Optimum
1	**ME, Bias**=E_1 Mean error	$ME = \frac{1}{n}\sum_{i=1}^{n}\left(O_i - P_i\right)$	-∞	+∞	0
2	**MAE**=E'_1 Mean absolute error (' : abs)	$MAE = \frac{1}{n}\sum_{i=1}^{n}\left\|O_i - P_i\right\|$	0	+∞	0
3	**AME**=E_∞ Absolute Maximum Error	$AME = max\left(\left\|O_i - P_i\right\|\right)$	0	+∞	0
4	**MSE**=E_2 Mean Square Error	$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(O_i - P_i\right)^2$	0	+∞	0
5	**MSSE**=$E(sorted)_2$ (j pairs) Mean Square Sorted Errors	$MSSE = \frac{1}{n}\sum_{j=1}^{n}\left(O_j - P_j\right)^2$	0	+∞	0
6	**MSLE**=$E(\ln)_2$ Mean Square Logarithm Error	$MSLE = \frac{1}{n}\sum_{i=1}^{n}\left(ln\,O_i - ln P_i\right)^2$	0	+∞	0
7	**MSDE**=$E(deriv)_2$ Mean Square Derivative Error	$MSDE = \frac{1}{n-1}\sum_{i=1}^{n}\left(\left(O_i - O_{i-1}\right) - \left(P_i - P_{i-1}\right)\right)^2$	0	+∞	0

The mean of residuals (ME, γ=1) (1) allows highlighting the existence of systematic bias, i.e. characteristic of a model leading to systematic over- or under-prediction (Power, 1993). However, with this criterion errors can compensate each other, so no information on the magnitude of the errors is obtained.

The mean absolute error (MAE) (2) indicates the average magnitude of the model error (accuracy) (Willmott *et al.*, 1985). Taking the absolute value avoids error compensation, but does not indicate the direction of the deviation.

The absolute maximum error (AME, γ=∞) (3) indicates the maximum error of the model (Gupta *et al.*, 1998). This criterion is very sensitive to outliers.

The mean square error (MSE, γ=2) (4) avoids error compensations and emphasises high errors (Willmott *et al.*, 1985).

The mean square error of sorted errors (MSSE) (5) is calculated based on sorted observed and predicted data (van Griensven and Bauwens, 2003). Observations and predictions are sorted independently one from the other. The sorted series are then compared (comparison of their cumulative distributions) and it is evaluated wether the model reproduces the same distribution as the observed data.

The mean square logarithm error (MSLE) (6) is the sum of the squares of the differences of the natural logarithm of the predicted and observed value (Dawson *et al.*, 2009). It emphasises low magnitude errors.

The mean square derivative error (MSDE) (7) is the square of the differences of predicted and observed variations between two time steps (Dawson *et al.*, 2009). This criterion penalizes noisy time series and series with timing error; it thus allows evaluating the peak's timing.

The root mean square error (RMSE) is an absolute criterion that is often used (Willmott *et al.*, 1985). It indicates the overall agreement between predicted and observed data. The values can range from 0 to +∞, the smaller the value the better the quality of the model.

The *square* allows avoiding error compensation and emphasises larger errors. The *root* provides a criterion in actual units. Consequently, this quality criterion can be compared to the MAE to provide information on the prominence of outliers in the dataset.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(O_i - P_i)^2}{n}}$$

To put even more emphasis on the larger errors, the fourth root mean quadruples error could be used (Dawson *et al.*, 2007):

$$R4MS4E = \sqrt[4]{\frac{\sum_{n}^{i=1}(O_i - P_i)^4}{n}}$$

Willmott *et al.* (1985) propose distinguishing between the systematic and unsystematic part of the error by conducting an ordinary least squares regression between observed

and predicted data P=aO+b. This straight line (solid blue line on Figure 5-16) represents the systematic error, which is (partly) constant if b≠0 and value dependent if a≠1. If the model only has systematic errors, all the values would be on this line, and a predicted model value on this line would be: $\hat{P}_i = aO_i + b$.

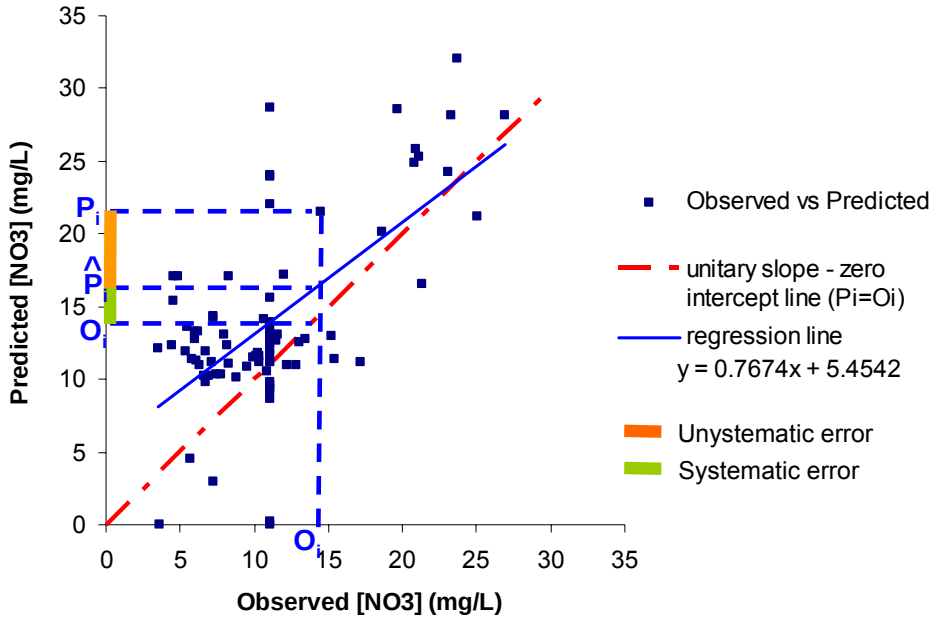


Figure 5-16. Representation of systematic and unsystematic errors on effluent nitrate concentrations

The RMSEs is then calculated as the sum, for each time step, of the difference between the observed value (O_i) and the corresponding predicted model value on this line ($\hat{P}_i$). This error is represented in green on Figure 5-16. The unsystematic error (RMSEu) is then the difference between the predicted model values ($\hat{P}_i$) and the model values (P_i) (in orange on Figure 5-16), which represents the noise of the model. The equations of these criteria are given hereafter and are represented on Figure 5-16. It should be noticed that $RMSE^2 = RMSEs^2 + RMSEu^2$.

Systematic RMSE: $RMSEs = \sqrt{\frac{\sum_{i=1}^{n}\left(O_i - \hat{P}_i\right)^2}{n}}$ unsystematic RMSE: $RMSEu = \sqrt{\frac{\sum_{i=1}^{n}\left(\hat{P}_i - P_i\right)^2}{n}}$

5.4.2.3.3 Relative criteria

The relative criteria are based on the sum of some function of the residuals (difference between observed and predicted data), generally normalized by the number of data, n, as well as by either the observation or the prediction. This is desired to obtain a unit-free criterion that allows comparison of criteria calculated on different value magnitudes (e.g. different periods, dry and wet weather conditions, variables of interest, events or modelling projects).

Relative error to observed or predicted value at same time step

At each time step, the error is related to the corresponding observed or predicted value. The general equation can be expressed as follows, with γ a power:

Equation:
$$RE_{\gamma} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{O_i - P_i}{O_i}\right)^{\gamma}$$

A low value of this criterion signifies a good agreement between observation and prediction. Different variations of the same theme, following the principles presented in 5.4.2.1, can be found in literature and are presented in Table 5-3.

The mean percentage error (MPE) (1) (Power, 1993) and mean relative error (MRE) (2) (Dawson *et al.*, 2007) provide the average relative model error. However, negative and positive errors can compensate for each other.

The mean absolute relative error (MARE) (3) is similar to the previous criteria, but avoids the compensation of errors (Petersen *et al.*, 2002a). An alternative criterion is the median of the absolute relative error (MdARE) (4) expressed in percentage (Dawson *et al.*, 2007). This criterion is less affected by outliers and the errors distribution form.

The mean square relative error (MSRE) (5) avoids compensation of errors and emphasises larger relative errors (Dawson *et al.*, 2007).

The mean absolute percent error (MAPE) (6) used by Power (1993) and Elliott *et al.* (2000) is close to MARE. However, the errors are relative to the predicted values instead of the observed values. Consequently, the under-predicted values are penalised (for a similar error). This is an interesting criterion for situations in which one wants to determine a risk to reach concentration limits.

Table 5-3. Relative error criteria

	Criteria	Equation	Min	Max	Optimum
1	**MPE**=100.RE_1 Mean percent error	$MPE = \frac{100}{n}\sum_{i=1}^{n}\left(\frac{O_i - P_i}{O_i}\right)$	-∞	+∞	0
2	**MRE**=RE_1 Mean relative error	$MRE = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{O_i - P_i}{O_i}\right)$	-∞	+∞	0
3	**MARE**=RE'$_1$ Mean absolute relative error	$MARE = \frac{1}{n}\sum_{i=1}^{n}\frac{\lvert O_i - P_i\rvert}{O_i}$	0	+∞	0
4	**MdAPE** median absolute error percentage	$MdAPE = Median\left(\left\lvert\frac{O_i - P_i}{O_i}\right\rvert \times 100\right)$	0	+∞	0
5	**MSRE**=RE_2 Mean square relative error	$MSRE = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{O_i - P_i}{O_i}\right)^2$	0	+∞	0
6	**MAPE** Mean absolute percent error	$MAPE = \frac{100}{n}\sum_{i=1}^{n}\frac{\lvert O_i - P_i\rvert}{\lvert P_i\rvert}$	0	+∞	0

Total error relative to the total of observed values

For the following parameters, the sum of errors is related to the sum of observed values, without any correspondence in time-step. The general equation can be expressed as follows, with γ a power:

Equation: $$TRE_\gamma = \frac{\sum_{i=1}^{n}(O_i - P_i)^\gamma}{\sum_{i=1}^{n}O_i^\gamma}$$

Following the principles presented in 5.4.2.1, different variations of the same theme can be found in literature and are presented in Table 5-4.

The percent bias (PBIAS) (1) (Dawson *et al.*, 2007) and relative volume error (RVE) (2) are the sum of errors related to the sum of observed values, expressed as relative value or in percentage. These criteria measure an overall adequacy, but the errors can be compensated.

The relative mean absolute error (RMAE) (3) is the sum of absolute errors related to the sum of observed data (Elliott *et al.*, 2000). The difference with the previous criteria is that errors are not compensated.

Theil's inequality coefficient (U) (4) used by Power (1993) and Elliott *et al.* (2000) is the mean square error divided by the sum of observed data. This criterion avoids error compensation and emphasises larger errors.

Table 5-4. Total relative error criteria

	Criteria	Equation	Min	Max	Optimum
1	**PBIAS** =TRE_1.100 Percent Bias	$PBIAS_\gamma = 100 \cdot \frac{\sum_{i=1}^{n}(O_i - P_i)}{\sum_{i=1}^{n} O_i^\gamma}$	-∞	+∞	0
2	**RVE**= TRE_1 Relative volume error	$RVE = \frac{\sum_{i=1}^{n}(O_i - P_i)}{\sum_{i=1}^{n} O_i}$	-∞	+∞	0
3	**RMAE**= TRE'/100 Relative mean absolute error	$RMAE = \frac{\sum_{i=1}^{n}\lvert O_i - P_i\rvert}{\sum_{i=1}^{n} O_i}$	0	+∞	0
4	**Theil's coefficient =** TRE_2/100 Theil's inequality coefficient	$U^2 = \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n} O_i^2}$	0	+∞	0

5.4.2.4 Agreement between observed and modelled datasets

Some criteria are not based on error comparison, but on a comparison between cumulative predicted and observed data. These criteria originate in hydrology and aim at verifying whether the total water volume has been reproduced by summing the flows. In the wastewater field these criteria can be relevant for influent and effluent pollutant loads by summing the fluxes.

van Griensven and Bauwens (2003) use the Total Mass Controller (TMC) criterion as an objective function. This criterion compares the cumulative predicted and observed values. This criterion is in the range 0 to +∞, with an optimum value of 0.

$$TMC = 100 \cdot \left| \frac{\sum_{i=1}^{n} O_i}{\sum_{i=1}^{n} P_i} - 1 \right|$$

Perrin *et al.* (2001) use the *balance criterion* to measure the ability of the model to reproduce the same cumulative as observed. The difference between the inversed fractions penalises larger differences between observed and modelled cumulative values. This criterion is in the range -∞ to 1, with an optimum value of 1.

$$BalanceCriterion = 1 - \left| \sqrt{\frac{\sum_{i=1}^{n} P_i}{\sum_{i=1}^{n} O_i}} - \sqrt{\frac{\sum_{i=1}^{n} O_i}{\sum_{i=1}^{n} P_i}} \right|$$

5.4.2.5 Comparison of residuals with reference values

These criteria compare the residuals with residuals obtained with a reference and simplistic ("no knowledge") model $\widetilde{P}$, such as a model describing the mean value ($\widetilde{P}_i = \overline{O}$) or the previous value ($\widetilde{P}_i = O_{i-1}$).

The general equation can be expressed as follows, with γ and α as powers:

$$CE_{\alpha,\gamma} = 1 - \frac{\sum_{i=1}^{n} \left(O_i^{\alpha} - P_i^{\alpha} \right)^{\gamma}}{\sum_{i=1}^{n} \left(O_i^{\alpha} - \widetilde{P}_i^{\alpha} \right)^{\gamma}}$$

Different variations along this theme, following the principles presented in paragraph 5.4.2.1, can be found in literature and are presented in Table 5-5.

The first criterion is the Nash-Sutcliffe ($CE_{1,2}$) criterion (1), a widely used criterion in hydrology. The values range is between -∞ and 1. A value of zero means that the model is not better than the "no knowledge" model, which is characterised by the mean value of observations. This criterion is sensitive to extreme values.

The second criterion $CE_{1/2,2}$ (2) is close to the Nash-Sutcliff criterion, but it is calculated from the root values, which emphasises low magnitudes.

In the same way the third criterion $CE_{ln,2}$ (3) is calculated from the value logarithms, which emphasises very low magnitudes (Perrin *et al.*, 2001).

The *relative absolute error* (RAE) (4) compares the sum of absolute residuals to the residuals of the no *knowledge model* (mean of observed values) (Legates and McCabe Jr, 1999). This criterion does not allow error compensation.

Table 5-5. Coefficient of efficiency criteria

	Criteria	Equation	Min	Max	Optimum
1	Nash-Sutcliffe **$CE_{1,2}$**	$CE = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \overline{O})^2}$	-∞	1	1
2	**$CE_{1/2,2}$**	$CE_{1/2,2} = 1 - \frac{\sum_{i=1}^{n}(\sqrt{O_i} - \sqrt{P_i})^2}{\sum_{i=1}^{n}(\sqrt{O_i} - \overline{\sqrt{O}})^2}$	-∞	1	1
3	**$CE_{ln,2}$**	$CE_{ln,2} = 1 - \frac{\sum_{i=1}^{n}(ln(O_i) - ln(P_i))^2}{\sum_{i=1}^{n}(ln(O_i) - \overline{ln(O)})^2}$	-∞	1	1
4	**RAE**=CE1,abs Relative Absolute Error	$RAE = \frac{\sum_{i=1}^{n}\lvert O_i - P_i\rvert}{\sum_{i=1}^{n}\lvert O_i - \overline{O}\rvert}$	0	+∞	0
5	**RSR** RMSE-observation standard deviation ratio	$RSR = \frac{\sqrt{\sum_{i=1}^{n}(O_i - P_i)^2}}{\sqrt{\sum_{i=1}^{n}(O_i - \overline{O})^2}}$	0	+∞	0
6	**IA** index of agreement	$IA = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(\lvert P_i - \overline{O}\rvert + \lvert O_i - \overline{O}\rvert)^2}$	0	1	1
7	**PI** coefficient of persistance	$PI = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - O_{i-1})^2}$	-∞	1	1
8	**J** Janus coefficient	$J = \frac{\frac{1}{n\_val}\sum_{i=1}^{n\_val}(O_{k,i} - P_k(t_i,\theta))^2}{\frac{1}{n\_cal}\sum_{i=1}^{n\_cal}(O_{k,i} - P_k(t_i,\theta))^2}$	0	+∞	1

The RMSE-observation standard deviation ratio (RSR) (5) is the RMSE of the predicted data divided by the RMSE of the no knowledge model (mean of observed values) (Moriasi *et al.*, 2007). It is a scaled criterion that emphasises larger errors and can be, as for MAE and RMSE, compared to the RAE to indicate the influence of larger errors.

The *index of agreement* (IA) (6) is the ratio of the sum of squared errors (SSE) and the largest potential error with respect to the mean of observed values (Willmott *et al.*, 1985). This parameter is sensitive to the model mean and to the peak values, and is insensitive to low magnitude values.

The *coefficient of persistence* (PI) (7) is close to the Nash-Sutcliffe criterion, but the simplistic model used is the last observed value instead of the mean of observed values (Moriasi *et al.*, 2007).

The *Janus coefficient* (8) evaluates the robustness of the model and indicates the change in model accuracy between the calibration step (estimation) and the validation step (prediction) (Power, 1993). It is calculated as the ratio of the root mean square error (RMSE) obtained on the validation dataset and on the calibration dataset. A Janus coefficient equal to one means that the model has the same performance in validation and in calibration. A high coefficient could indicate a change in the model's structure or that the model has been over-fitted and is not robust against the change of conditions. However, this coefficient does not indicate a good predictive performance per se, because the ratio of a poor calibration to a poor validation RMSE could also lead to a value close to 1.

The Chi-square (χ^2) criterion (Dochain and Vanrolleghem, 2001) allows comparing the variability of the residuals with the measurement errors. It is composed by the sum of the squares of the residuals divided by the standard deviation of the measurements (σ). The result is then compared to the χ^2 distribution for n-p degrees of freedom. The calculated value should be as close as possible to the value from the theoretical distribution to indicate that model errors are close to the measurement errors. If a calculated value is below the theoretical value, it means that the model is more accurate than the data, and indicates an over-fitting of the model. Conversely, if the value is significantly above the theoretical value, it means the model is not able to describe part of the dynamics observed.

$$\chi^2 = \sum_{i=1}^{n} \frac{(O_i - P_i)^2}{\sigma^2(O_i)} \qquad \text{with } \sigma^2(O_i) = \frac{1}{n}\sum_{i=1}^{n}\left(O_i - \overline{O}\right)^2$$

5.4.2.6 Comparison of models (model selection)

Some criteria are used to compare models of different complexity, by balancing the improvement in fitting the observations with the increase in model complexity.

The **Akaike Information Criterion** (AIC) is a weighted measure of an error that penalises complex models. Non-negative error criteria (named Quality Criteria, QC, in the AIC equation) that do not have an upper bound can be used, typically the RMSE is used (Dawson *et al.*, 2007). The AIC decreases proportionally with the quality criteria (favours low errors). Inversely, AIC increases with the number of model parameters (p) (penalises complex models). The values are between 0 and +∞, with an optimum at the minimum value.

Equation: $$AIC = n \times ln(QC) + 2 \times p$$

The **Bayesian information criterion** (BIC) is similar to AIC, but should be more efficient to determine the best model (Dochain and Vanrolleghem, 2001) as it penalises complexity more than AIC does. This criterion has values between 0 and +∞, with an optimum at minimum value.

Equation: $$BIC = n \times ln(QC) + p \times ln(n)$$

The **F-Test** compares the RMSE of two models: model I and a more complex model J ($p_J > p_I$) (Dochain and Vanrolleghem, 2001). It assesses whether the model J is significantly better than model I, taking into account the increase of complexity. This criterion is compared to the $F_\alpha(p_J-p_I, n-p_J)$-distribution with α the confidence level and (p_J-p_I, $n-p_J$) degrees of freedom. The improvement obtained when using model J over model I is deemed to be significant when $F > F_\alpha(p_J-p_I, n-p_J)$.

Equation: $$F = \frac{(RMSE_I - RMSE_J)/(p_J - p_I)}{RMSE_J/(n - p_J)}$$

5.4.2.7 Multi-objective problem

All criteria presented above are calculated for single variables. However, a WWTP study typically involves several output variables to which the model is fitted, depending on the model objectives: O_2 consumption, sludge production, NH_4, N_{Tot} or PO_4 effluent concentration… Furthermore, these variables are not always sampled at the same frequency and measurements may be correlated (e.g. NH_4 ant N_{Tot}).

As discussed in paragraph 5.4.2.1, the quality criteria should be chosen depending on the modelling objectives. Consequently, the calibration and goodness-of-fit assessment of a typical wastewater treatment plant model calibration requires a "multi-variable, multi-objective" criterion. As an example, Table 5-6 lists twelve typical modelling objectives that are defined by the Good Modelling Practice Task Group for design, operation and training. For each of these objectives, the required measurements and calibration of the model are indicated.

Aggregate quality criteria are already used in different studies and are based on the sum of normalised quality criteria. To take several measured variables into account, Brun *et al.* (2002) and Sin *et al.* (2008a) normalised the sum of squared errors by the mean of the measurement and the standard error of the measurement respectively. Dochain and Vanrolleghem (2001) show how this weighting method is generalised for correlated variables by using the covariance matrix of the measurement errors of the different variables. This matrix is used to assign different weights to each variable in the least square objective function for parameter estimation.This means that the multicriteria problem is turned into a single criterion one. To sum several quality criteria, van Griensven and Bauwens (2003) first normalise all chosen criteria between 0 and 1, and then sum them with an identical weight (Global Optimisatioon Criterion). Emphasis can be put on certain criterion/measurements by changing these weights.

Table 5-6 Typical modelling objectives and their required measurements and calibration from the GMP-TG Application matrix (https://iwa-gmp-tg.cemagref.fr/)

		Objectives	Measurements					Calibration			
			O2 cons-umption	Sludge production	NH_4	N_{Tot}	P_{Tot}	Mean *	Dynamic simulation	Max value 95% time	Model error
Design	1	Calculate Sludge Production		X				M			
	2	Design Aeration System	X					D	X		
	3	Develop a Process Configuration for Nitrogen Removal			X	X		A/M		X	
	4	Develop a Process Configuration for Phosphorus Removal					X	A/M		X	
	5	Assess Plant Capacity for Nitrogen Removal			X	X		A/M		X	
	6	Design a Treatment System to Meet Peak Effluent Nitrogen Limits			X	X		I	X	X	X
Operation	7	Optimise Aeration Control	X		X			H	X		
	8	Test Effect of Taking Tanks Out of Service			X	X	X	M	X	X	
	9	Use Model to Develop Sludge Wastage Strategy		X	X		X	W/D	X	X	
	10	Develop A Strategy to Handle Storm Flows		X	X	X	X	H	X	X	X
Training	11	Develop a General Model for Process Understanding									
	12	Develop a Site Specific Model for Operator Training	X	X	X	X	X	M	X	X	

*A: Annual; M: Monthly; W: Weekly; D: Daily; H: Hourly; I: Instantaneous value

Table 5-7. List of articles studied and corresponding quality criteria used.

(Field: WW: Wastewater; RH: River hydrology; ES: environmental sciences; CS: climate sciences. X: used criteria, CE= Criterion of Efficiency, $CE_{1,2}$=Nash-Sutcliffe criterion)

	Field	Graphical Methods	Descriptive statistics	Distribution of residuals	Single event statistics	Absolute criteria	Relative criteria to time-step	Relative criteria to cumulative values	Observed vs predicted agreement	Comparison with reference model	Models comparison	Multivariate criteria
Ahnert *et al.* (2007)	WW	time-series Scatterplot Residuals	Mean Median Variance							$CE_{1,2}$; RAE IA_2		
Corominas, *et al.* (2011)	WW					ME; MAE				J		
Dawson *et al.* (2007)	RH		Mean; Median Variance Skewness, kurtosis	autocorrelation NSC	PDIFF PEP	ME ; MAE ; AME RMSE R4MS4E	MRE; MARE MSRE MdAPE	PBIAS		$CE_{1,2}$ RAE IA_2 ; PI	AIC BIC	
Dawson *et al.* (2009)	RH					MSLE; MSDE				J; IRMSE		
Dochain and Vanrolleghem (2001)	WW	time-series Scatterplot Residuals		Autocorrelation Nb of runs		MAE; MASE; AME				X^2	AIC ; BIC F-Test	X
Elliott *et al.* (2000)	O	time-series				ME ; MAE; MSE RMSE	MPE MAPE	RMAE U (Theil)		$CE_{1,2}$		
CREM (2009)		Box-plot				ME ; MAE; MSE	MPE					
Gupta *et al.* (1998)	RH			Autocorrelation NSC	PDIFF	ME ; MAE ; AME				$CE_{1,2}$		
Legatesand McCabe. (1999)	RH	time-series Scatterplot	Mean Variance			MAE				$CE_{1,2}$; RAE IA_2 ; IA_{abs}		
Modarres (2009)	RH	Box-plot			PDIFF PEP	MAE ; AME RMSE; R4MS4E	MRE; MARE MSRE	PBIAS		$CE_{1,2}$; RAE IA_2 ; PI		X
Moriasi *et al.* (2007)	RH	time-series				MAE; MSE RMSE		PBIAS		$CE_{1,2}$, RSR ; IA_2; IA_{abs} ; PI		
Nash and Sutcliffe (1970)	RH									$CE_{1,2}$		
Perrin *et al.* (2001)	RH								Balance criteria	$CE_{1,2}$; $CE_{1/2,2}$ $CE_{ln,2}$		
Petersen *et al.* (2002a)	WW						MARE					
Power (1993)	ES			autocorrelation		ME ; MAE RMSE	MPE, MAPE	U (Theil)		J		
Reichert (2009)	ES										AIC ; BIC	
Sin *et al.* (2008a)	WW					MAE; MSE, RMSE				J		X
van Griensven and Bauwens (2003)	UH					MSE MSSE			TMC			X
Wagener and Kollat (2007)	RH					RMSE						
Willmott *et al.* (1985)	CS					MAE, MSE, RMSE RMSEs; RMSEu				IA_2 IA_{abs}		X
Yapo *et al.* (1998)	RH					MSE, RMSE						X

5.4.2.8 Conclusion on quantitative criteria review

A large number of model quality criteria that are applied in the environmental sciences have been reviewed. These criteria allow pointing out different model adjustment types (mean, typical periodical variations (diurnal, weekly, seasonal…), peaks, peaks timing…). Moreover, model prediction accuracy assessment can be the basis for model uncertainty evaluation. Belia *et al.* (2009) identify 4 main sources of uncertainty: i) inputs, ii) model structure, iii) model parameters and iv) implementation of models in software packages. The presented quality criteria allow characterizing the overall uncertainty including model structure, parameters and coding uncertainty, provided the input data are accurate. Indeed, the majority of the quality criteria are based on the hypothesis that the observed values are accurate, except for the χ^2 estimation.

The calculation of these criteria on a single model does not provide information on why model predictions deviate from measured data, i.e., which of the uncertainty sources is contributing how much. However, the uncertainty sources can be investigated through several methods:

- Comparing simulation with different ASM-type models that use different modelling concepts will provide insights on the effect of model structure uncertainty,

- Comparing simulations with different parameter sets, e.g. by Monte Carlo simulation, will provide insights on the effects of model parameter uncertainties.

- Using different simulation softwares or independent implementations will provide insights on model implementation uncertainty (Copp *et al.*, 2008).

These criteria are widely used in environmental sciences, especially in hydrology, but only few of the criteria reviewed above have been used in the field of wastewater treatment. Indeed, hydrological models usually consider only one variable (flow), whereas many more variables of interest are considered in the wastewater treatment field. This makes the statistics on ASM models much more complicated. Hence, the presented criteria should be tested to select the more suitable criteria for this application field and try to provide guidance to what is a good criterion value.

5.5 Conclusion

In this chapter a methodology to get a default parameter set is developped. These default parameter sets should provide a good first approximation of any case study (or under definite conditions) model, and could then be used as initial values in model calibration step. This methodology is not yet fully tested and applied. Great care has been taken to keep this methodology independent on the model used and to keep it easily usable by other teams.

The procedure consisting of simultaneously calibration on multiple datasets to get default parameter sets requires a large number of datasets. These datasets should be representative of a large variety of wastewater treatment conditions to ensure that the default parameter set obtained can be used to initiate the calibration of a new system.

First, an automated calibration procedure is developed. It relies mainly on the procedure already published in Sin *et al.* (Sin *et al.*, 2008a), but also integrates the prior knowledge extracted in chapter 3. Tools have been developed to automate the procedure, based on WEST software for the simulation. These tools, which were validated on a case study, are flexible and well documented to be easily reusable and adapted to other aims.

Second, the automated calibration procedure heavily relies on quality criteria, which influence the choice of the calibrated parameter set. So far, such quality criteria are not often used in the wastewater treatment field. A synthesis of quality criteria applied in environmental sciences was carried out and nine main criteria types could be distinguished:

- Descriptive statistics
- Single event statistics
- Residuals distribution properties
- Absolute criteria from residuals
- Residuals relative to observed values
- Total residuals relative to total observed values
- Agreement between observed and modelled distribution data
- Comparison of residuals with reference values

- Comparison with other models

All the presented criteria are based on variations on these nine themes, by using data transformations such as partition of the dataset, powers, logarithms or exponential transformation, in order to emphasise small or large errors. Depending on the objectives of the modelling project, one can choose the variables to predict and which kind of fit is required, as e.g. to represent the mean, the total flux, peaks, peaks timing…

However, all these criteria are univariate criteria, whereas the ASM type models' calibration is a multivariate (multi-variables, multi-objectives) problem. Consequently, to automate the calibration procedure and to make it objective, the relevant univariate criteria for the relevant variables have to be aggregated in a single goodness-of-fit criterion. Such global quality criteria facilitate comparison of the fitting of simulations with different parameter sets on an observed dataset.

Work is under way to apply these quality criteria on a wastewater treatment modelling case study to determine the more relevant criteria and the uncorrelated criteria. This study is ongoing and involves also researchers from the urban drainage field, who struggle with the same problem. These quality criteria could be used to communicate about the goodness-of-fit of models, and to compare different models applied on a single case study or different model studies.

CHAPITRE 6 Conclusion

Les outils de modélisation sont utilisés de plus en plus systématiquement dans le domaine du traitement des eaux résiduaires. Or, une prise de décision basée sur des résultats obtenus à l'aide de modèles non adaptés pourrait avoir un impact négatif sur la conception, le dimensionnement et/ou l'optimisation de l'installation de traitement. Il est donc nécessaire de garantir la qualité de ces projets par une utilisation adéquate des outils à disposition.

L'objectif principal du travail présenté était de développer et de fournir aux utilisateurs de modèles biocinétiques de boues activées les éléments requis pour faciliter et optimiser deux des principales étapes de l'utilisation de ces modèles : (i) la sélection du modèle adéquat, permettant de répondre aux objectifs du projet, et (ii) l'étape de calage des modèles. Le travail est axé sur l'analyse de sept modèles publiés : (1) ASM1 (Henze *et al.*, 2000a); (2) ASM2d (Henze *et al.*, 2000b); (3) ASM3 (Gujer *et al.*, 2000); (4) ASM3+BioP (Rieger *et al.*, 2001); (5) ASM2d+TUD (Meijer, 2004); (6) Barker & Dold model (Barker and Dold, 1997); (7) UCTPHO+ (Hu *et al.*, 2007).

Ces travaux ont été réalisés en lien avec le groupe de travail de l'IWA "Good Modelling Practice" (TG-GMP), dont l'objectif est d'élaborer une procédure de bonnes pratiques en matière de modélisation des boues activées.

Etat de l'utilisation pratique des modèles

La première étape du travail présenté a été de synthétiser les réponses à un premier questionnaire mis en place par le TG-GMP, afin de mieux connaitre le profil des utilisateurs des modèles, leurs attentes et leurs difficultés face à la modélisation des stations à boues activées. L'analyse des 96 réponses obtenues a montré que l'utilisation de la modélisation était différente en Amérique du Nord et en Europe. En Amérique du Nord, les modélisateurs sont généralement employés par des bureaux d'étude pour réaliser des projets de dimensionnement d'installations. En Europe, la modélisation relève encore largement du domaine de la recherche, à des fins d'optimisation (dynamique) de procédés. La modélisation est un outil de l'ingénieur, mais très peu de formations sont disponibles en traitement des eaux résiduaires. Les résultats ont

également affirmé la nécessité d'élaborer des procédures standardisées pour mener à bien les deux étapes - indispensables à tout projet de modélisation - qui forment les deux axes principaux de cette thèse : le choix du modèle et son calage.

Analyse des connaissances théoriques de modélisation

Une évaluation théorique des modèles a été menée dans le but de faciliter leur compréhension et donc de faciliter le choix du modèle approprié au projet de modélisation. La mise en place d'une notation standardisée a apporté un langage commun qui facilite la communication sur les modèles et leur compréhension. Un tableau de correspondance entre la notation d'origine et la nouvelle notation pour chacun des modèles analysés est disponible en ligne (http://www.iwaponline.com/wst/06104/0912.xls)

Une procédure systématique a été développée pour vérifier la continuité des réactions stœchiométriques et des équations cinétiques du modèle. Les outils mis en place sont regroupés dans une feuille de calcul, également disponible en ligne (http://www.iwaponline.com/wst/06104/0898.xls). L'application de cette méthode aux modèles étudiés a permis de déceler plusieurs erreurs de frappe, oublis et incohérences dans les publications d'origine, et notamment des erreurs récurrentes suivantes:

- l'utilisation de valeurs arrondies (par exemple : i_{NOx_N2}=-2.86 g COD.g N^{-1} au lieu de i_{NOx_N2}=-40/14 g COD.g N^{-1}),
- l'utilisation inappropriée ou l'oubli de l'alcalinité comme paramètre limitant dans certains processus,
- l'omission des fonctions interrupteur de préférence pour le substrat dans le cas où différents substrats sont disponibles,
- l'utilisation du concept de "perte de DCO" dans les modèles Barker & Dold et UCTPHO+.

Enfin, une représentation graphique des modèles par processus a été proposée et constitue un outil de communication sur les modèles pour faciliter leur compréhension. L'application de cette représentation aux modèles étudiés a permis de les comparer et de mettre en évidence différents concepts théoriques de modélisation des processus. Neufs processus ont été distingués et étudiés individuellement :

- L'hydrolyse
- La fermentation
- La croissance des OHO
- La croissance des ANO
- Le décès des OHO et ANO
- Le stockage des PHA
- Le stockage des polyphosphates
- La croissance des PAO
- Le décès des PAO

La mise en parallèle de ces concepts avec les connaissances théoriques sur les mécanismes de croissance de la biomasse met en avant les limites théoriques à l'utilisation des modèles, notamment en cas de zones importantes de traitement en anoxie et/ou en anaérobie, en fonction des substrats et nutriments considérés et des simplifications utilisés pour les concepts. En fonction des conditions de traitement de la station d'épuration, ces limites théoriques sont donc autant d'arguments à prendre en compte pour le choix du modèle adéquat au projet de modélisation.

Analyse des connaissances pratiques de modélisation

Une base de données rassemblant divers projets de modélisation a été constituée. Cette base de données synthétise les réponses à un second questionnaire mis en place avec le TG-GMP et intègre des projets de modélisation publiés. L'analyse de cette base de données indique les paramètres le plus souvent modifiés lors du calage et fournit les fourchettes de valeur dans lesquelles les paramètres varient pour les modèles ASM1 et ASM2d.

Pour l'**ASM1**, 6 paramètres ont été mis en exergue :

- le rendement hétérotrophe Y_{OHO}, pour lequel la structure du modèle doit être modifiée pour inclure des valeurs différentes en aérobiose et en anoxie,
- le taux de croissance maximum et le taux de décès des autotrophes ($\mu_{ANO,Max}$, b_{ANO},) qui sont des paramètres corrélés. En utilisant une valeur plus élevée pour b_{ANO} (0.17 d^{-1} à 20°C) la valeur de $\mu_{ANO,Max}$ serait fixée (0.8 d^{-1} à 20°C) quel que soit l'âge des boues considéré.

- les constantes de demi-saturation $K_{SB,OHO}$, $K_{NOx,OHO}$, et $K_{NHx,ANO}$, dependent des conditions environnementales et sont fortement variables d'une station d'épuration à l'autre.

En ce qui concerne l'**ASM2d** les paramètres les plus modifiés sont:

- les taux maximum de croissance hétérotrophe et autotrophe, $\mu_{OHO,Max}$ et $\mu_{ANO,Max}$,
- les constantes d'absorption des AGV et des polyphosphates, q_{PAO,VFA_Stor} et $q_{PAO,PO4\_PP}$, ce qui pourrait indiquer un problème dans la structure du modèle de déphosphatation biologique,
- le taux de maintenance des PAO et la lyse des stockages internes, m_{PAO}, b_{PP_PO4} et b_{Stor_VFA},
- la constante de demi-saturation des autotrophes pour l'ammonium $K_{NHx,ANO}$.

Le nombre et la qualité des données synthétisées n'ont pas permis de tirer des conclusions sur les lois de distribution des paramètres, les corrélations entre les paramètres et avec les conditions de traitement. Les résultats obtenus sont néanmoins d'une grande utilité lors de l'étape de calage, puisqu'ils indiquent selon les pratiques actuelles, quels sont les paramètres à modifier, les valeurs typiques, et les fourchettes de valeur à utiliser comme guide pour le calage. Les ratios typiques, notamment concernant les caractéristiques de l'affluent, obtenus à l'aide du questionnaire peuvent également être très utiles lors de l'étape de validation et réconciliation des données.

Développement d'une méthodologie d'obtention de jeux de paramètres par défaut

En dernier lieu, une réflexion a été engagée sur le développement d'une méthodologie permettant l'obtention d'un jeu de paramètres par défaut pour chacun des modèles. Ces jeux de paramètres par défaut pourraient être utilisés comme point de départ à l'étape de calage du modèle, ou comme approximation dans le cas où les données nécessaires au calage ne sont pas disponibles.

Dans l'objectif de mise en place d'une telle méthodologie, une procédure de calage automatisée a d'abord été élaborée sur la base de simulations par méthode de Monte Carlo. Cette procédure intègre les connaissances préalablement acquises sur les paramètres lors de l'analyse de la base de données, à savoir les paramètres susceptibles d'être modifiés et leurs fourchettes de valeurs. Les outils développés pour cette

procédure ont été validés sur un exemple. Ils sont par ailleurs bien documentés et peuvent être facilement adaptés à diverses utilisations.

Le critère de choix du jeu de paramètres représentant le mieux les données observées s'est révélé stratégique. Une synthèse des critères de qualité des modèles utilisés en sciences de l'environnement a été réalisée. L'ensemble des critères décrits sont des variations autour de neufs schémas, en appliquant une partition des données, des transformations logarithmiques, exponentielles ou puissances, pour accentuer le poids des erreurs faibles ou importantes, en fonction des objectifs de l'étude. Les neufs types de critères sont les suivants:

- Statistiques descriptives
- Statistiques sur des évènements uniques
- Propriétés de la distribution des erreurs
- Critères simples sur les erreurs
- Critères relatifs sur les erreurs rapportées aux données observés
- Critères sur la somme totale des erreurs rapportée à la somme totale des observations
- Concordance entre les distributions des données observées et prédites
- Comparaison des erreurs avec un modèle de référence
- Comparaison de modèles

L'ensemble des critères présentés sont univariés, c'est-à-dire qu'ils ne considèrent qu'une variable et un seul objectif. Or, le calage des modèles de type ASM est un problème multivarié : le modèle doit simuler plusieurs variables d'intérêt (multi-variables), et doit pouvoir reproduire, selon les objectifs du projet de modélisation, notamment la moyenne, les pics de pollution, les valeurs maximum (multi-objectifs). Une réflexion a également été initiée sur la construction d'un critère global de qualité intégrant la prise en compte de différents objectifs d'ajustement du modèle et différentes variables d'intérêt.

Perspectives

Les résultats de ce travail de thèse font émerger de nouvelles perspectives de recherche :

1. La **base de données** mise en place doit pouvoir être mise à disposition des utilisateurs de modèles. Les utilisateurs de modèles devraient aussi pouvoir avoir la possibilité d'intégrer à cette base de données leurs propres résultats, permettant ainsi de l'enrichir. Une base de données incluant un nombre plus important de résultats permettrait une analyse plus approfondie, notamment des lois de distribution des paramètres, des corrélations entre les valeurs des paramètres, et des corrélations entre les valeurs des paramètres et les conditions de traitement.

2. L'analyse des **critères de qualité** des modèles devrait fournir un outil à la fois de décision pour l'étape de calage du modèle et d'évaluation de la qualité du modèle et des incertitudes liées. Ces critères permettront également de communiquer plus clairement sur les résultats de projets de modélisation, notamment lors de leur publication dans des revues scientifiques, mais aussi de comparer les résultats obtenus avec différents modèles sur le même jeu de données.
   Le calcul de l'ensemble de ces critères sur un cas d'étude de modélisation de station d'épuration permettra de déceler les critères pertinents pour ce domaine, et mettra en évidence les critères redondants. Des fourchettes de valeurs pourront être déterminées pour les critères choisis.

3. La méthodologie pour l'obtention d'un jeu de paramètres par défaut pourra également être utilisée pour tester la sensibilité du jeu de paramètres par défaut à la variation des conditions environnementales des jeux de données et des questions posées. Cette étude permettrait de définir s'il est raisonnable de proposer un jeu de paramètre par défaut "universel" ou s'il est préférable de proposer des jeux de paramètres par défaut différents en fonction des conditions environnementales et des objectifs d'étude (type de station d'épuration, réseau d'égouts, climat…).

4. La procédure de calage automatisée proposée, par son objectivité et sa répétabilité, est un outil utile pour répondre à des questions sur le choix du modèle et le calage :
   - Evaluer les modèles : les différents modèles étudiés peuvent être calés sur le même jeu de données. Il sera alors possible de conclure si tous les modèles permettent d'atteindre le même niveau d'ajustement aux observations.

- Définir si les différents modèles calés sur un même jeu de données réagissent de la même façon aux variations de conditions environnementales et apportent la même réponse à une question posée. (Exemples de questions: conséquences sur le traitement de la station, d'un orage, d'une augmentation saisonnière ou permanente de la population, d'une panne sur une pompe ou sur l'aération…)
- Evaluer l'impact de la quantité (planification d'expérience) et de la qualité (étape de validation et réconciliation des données) des données disponible pour l'étape de calage sur la qualité du modèle calé et sur les résultats de simulation.

5. L'ensemble de ces connaissances pourrait être synthétisé dans un arbre de décision, qui guiderait l'utilisateur dans le choix du modèle adéquat à son projet. Les clés d'entrées de l'arbre pourraient par exemple inclure les conditions environnementales de la station d'épuration et les objectifs de l'étude.

6. La modélisation d'une station d'épuration dans sa globalité nécessite l'utilisation de modèles pour chacun de ces procédés utilisés en traitement des eaux résiduaires et notamment les procédés de traitement des boues de stations (digesteurs, méthaniseurs…). Pour éviter la multiplication de ces modèles et les problèmes liés à l'interface entre les modèles, des modèles uniques ont été développés. Ainsi le "supermodel" (Jones and Takacs, 2004) regroupe en une seule matrice de Gujer l'ensemble des réactions des modèles de tous les procédés à modéliser. Une autre approche, le "plant-wide modelling" par Grau *et al.* (2007), envisage la construction d'un modèle pour chaque cas de station d'épuration, en additionnant telles des briques, les seules réactions nécessaires à la modélisation de la station. Il serait donc envisageable de choisir non seulement les processus à modéliser, mais également les concepts à utiliser en fonction des conditions environnementales et des objectifs du projet. Le choix des concepts pourra être facilité par la représentation graphique développée au CHAPITRE 4. De nouvelles problématiques émergent alors pour le calage de tels modèles, à savoir si certains processus/concepts sont liés entre eux (et ne peuvent pas être choisis indépendamment), et l'impact du choix indépendant des différents concepts sur la signification et les valeurs des paramètres (par exemple: l'hydrolyse de l'ASM1 et de l'ASM3 n'incluent pas les mêmes phénomènes).

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ANNEXE 1. Tableau de correspondance notation originale – Notation standardisée

Models references: see below N.B.: see below				ASM1	ASM2d	ASM3	ASM3 + Bio-P	Barker & Dold	UCTPHO+	ASM2d + TUD
Description	Parameter	NB	Units	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
COD soluble										
Soluble biodegradable organics	S_B		g COD.m^{-3}	S_S		S_S	S_S			
Fermentable organic matter	S_F		g COD.m^{-3}		S_F			S_{BSC}	S_F	S_F
Fermentation product (Volatil Fatty Acids)	S_{VFA}		g COD.m^{-3}		S_A			S_{BSA}	S_A	S_A
Soluble undegradable organics	S_U		g COD.m^{-3}	S_I	S_I	S_I	S_I	S_{US}	S_I	S_I
Dissolved oxygen	S_{O2}		- g COD.m^{-3}	S_O	S_{O2}	S_O	S_O	S_O	S_{O2}	S_O
COD particulate and colloidal										
Particulate biodegradable organics	XC_B		g COD.m^{-3}	X_S	X_S	X_S	X_S	S_{ENM}	X_{ENM}	X_S
Adsorbed slowly biodegradable substrate	X_{Ads}		g COD.m^{-3}						X_{ADS}	
Particulate undegradable organics	X_U		g COD.m^{-3}		X_I	X_I	X_I			X_I
Particulate undegradable organics from the influent	$X_{U,Inf}$		g COD.m^{-3}	X_I				S_{UP}	X_I	
Particulate undegradable endogenous products	$X_{U,E}$		g COD.m^{-3}	X_P				Z_E	X_E	
Nitrogen (N)										
Ammonium and ammonia nitrogen (NH_4 + NH_3)	S_{NHx}		g N.m^{-3}	S_{NH}	S_{NH4}	S_{NH}	S_{NH}	N_{H3}	S_{NH4}	S_{NH}
Nitrate and nitrite (NO_3 + NO_2) (considered to be NO_3 only for stoichiometry)	S_{NOx}		g N.m^{-3}	S_{NO}	S_{NO3}	S_{NO}	S_{NO}	N_{O3}	S_{NO3}	S_{NO}
Dissolved nitrogen gas	S_{N2}		g N.m^{-3}		S_{N2}	S_{N2}	S_{N2}			S_{N2}
Particulate biodegradable organic N	$XC_{B,N}$		g N.m^{-3}	X_{ND}				N_{BP}		
Soluble biodegradable organic N	$S_{B,N}$		g N.m^{-3}	S_{ND}				N_{BS}		
Soluble inert organic N	$S_{U,N}$		g N.m^{-3}					N_{US}		
Phosphorus (P)										
Soluble inorganic phosphorus	S_{PO4}		g P.m^{-3}		S_{PO4}		S_{PO4}	P_{O4}	S_{PO4}	S_{PO}
Biomass										
Ordinary heterotrophic organisms	X_{OHO}		g COD.m^{-3}	$X_{B,H}$	X_H	X_H	X_H	Z_H	X_H	X_H
Autotrophic nitrifying organisms (NH4 to NO3-)	X_{ANO}		g COD.m^{-3}	$X_{B,A}$	X_{AUT}	X_A	X_A	Z_A	X_{NIT}	X_A
Phosphorus accumulating organisms	X_{PAO}		g COD.m^{-3}		X_{PAO}		X_{PAO}	Z_P	X_{PAO}	X_{PAO}
Organisms (biomass)	X_{Bio}		g COD.m^{-3}							
Internal cells products										
Storage compound in OHOs	$X_{OHO,Stor}$		g COD.m^{-3}			X_{STO}	X_{STO}			
Storage compound in PAOs	$X_{PAO,Stor}$		g COD.m^{-3}		X_{PHA}		X_{PHA}	S_{PHB}	X_{PHA}	

Models references: see below N.B.: see below				ASM1	ASM2d	ASM3	ASM3 + Bio-P	Barker & Dold	UCTPHO+	ASM2d + TUD
Description	Parameter	NB	Units	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
Stored poly-β-hydroxyalkanoate in PAOs	$X_{PAO,PHA}$		g COD.m^{-3}							X_{PHA}
Stored glycogen in PAOs	$X_{PAO,Gly}$		g COD.m^{-3}							X_{GLY}
Stored polyphosphates in PAOs	$X_{PAO,PP}$		g P.m^{-3}		X_{PP}		X_{PP}		X_{PP}	X_{PP}
Releasable stored polyphosphates in PAOs (Low molecular weight)	$X_{PAO,PP,Lo}$		g P.m^{-3}					P_{PP-LO}		
Non-releasable stored polyphosphates in PAOs (High molecular weight)	$X_{PAO,PP,Hi}$		g P.m^{-3}					P_{PP-HI}		
Inorganics										
Metal hydroxide compounds	X_{MeOH}		g TSS.m^{-3}		X_{MeOH}					
Metal phosphate compounds	X_{MeP}		g TSS.m^{-3}		X_{MeP}					
Alkalinity (HCO_3^-)	S_{Alk}		mol HCO_3^-.m^{-3}	S_{ALK}	S_{ALK}	S_{ALK}	S_{HCO}			S_{HCO}
TSS										
Total suspended solids	X_{TSS}		g TSS.m^{-3}		X_{TSS}	X_{SS}	X_{SS}			X_{TSS}
Stoichiometry										
Hydrolysis										
Fraction of inert COD generated in hydrolysis	$f_{SU\_XCB,hyd}$		g S_U.g XC_B^{-1}		f_{SI}	f_{SI}	f_{SI}			f_{SI}
Hydrolysis efficiency factor (anoxic)	$Y_{hyd,Ax}$		g S_F.g XC_B^{-1}					E_{ANOX}		
Hydrolysis efficiency factor (anaerobic)	$Y_{hyd,An}$		g S_F.g XC_B^{-1}					E_{ANA}		
Biomass										
Fraction of X_U generated in biomass decay	$f_{XU\_Bio,lys}$	*1*	g X_U.g X_{Bio}^{-1}	f_p	f_{XI}	f_{Xi}	f_{XI}			
Heterotrophic organisms										
Yield for X_{OHO} growth	Y_{OHO}		g X_{OHO}.g S_B^{-1}	Y_H	Y_H					Y_H
Yield for X_{OHO} growth (Aerobic)	$Y_{OHO,Ox}$		g X_{OHO}.g S_B^{-1}					$Y_{H,AER}$	Y_{H1}	
Yield for X_{OHO} growth (Anoxic)	$Y_{OHO,Ax}$		g X_{OHO}.g S_B^{-1}					$Y_{H,ANOX}$	Y_{H2}	
Yield for X_{OHO} growth (Anaerobic)	$Y_{OHO,An}$		g X_{OHO}.g S_B^{-1}					$Y_{H,ANA}$		
Yield for X_{OHO} growth per $X_{OHO,Stor}$ (Aerobic)	$Y_{Stor\_OHO,Ox}$		g X_{OHO}.g X_{Stor}^{-1}			$Y_{H,O2}$	$Y_{H,O2}$			
Yield for X_{OHO} growth per $X_{OHO,Stor}$ (Anoxic)	$Y_{Stor\_OHO,Ax}$		g X_{OHO}.g X_{Stor}^{-1}			$Y_{H,NOX}$	$Y_{H,NO}$			
Yield for $X_{OHO,Stor}$ formation per S_B (Aerobic)	$Y_{SB\_Stor,Ox}$		g X_{Stor}.g S_B^{-1}			$Y_{STO,O2}$	$Y_{STO,O2}$			
Yield for $X_{OHO,Stor}$ formation per S_B (Anoxic)	$Y_{SB\_Stor,Ax}$		g X_{Stor}.g S_B^{-1}			$Y_{STO,NOX}$	$Y_{STO,NO}$			
Fraction of X_U generated in heterotrophic biomass decay	$f_{XU\_OHO,lys}$	*1*	g X_U.g X_{OHO}^{-1}					$f_{EP,H}$	f_{XE-H}	$f_{XI,H}$
Yield for fermentation	Y_{fe}		g S_{VFA}.g S_B^{-1}					Y_{AC}		

Models references: see below N.B.: see below				ASM1	ASM2d	ASM3	ASM3 + Bio-P	Barker & Dold	UCTPHO+	ASM2d + TUD
Description	Parameter	NB	Units	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
Phosphorus accumulating organisms (PAO)										
Yield for X_{PAO} growth per $X_{PAO,Stor}$	Y_{PAO}		g X_{PAO}.g X_{Stor}^{-1}		Y_{PAO}			Y_P		
Yield for X_{PAO} growth per $X_{PAO,PHA}$ or $X_{PAO,Stor}$ (Aerobic)	$Y_{PAO,Ox}$		g X_{PAO}.g X_{PHA}^{-1} or g X_{PAO}.g X_{Stor}^{-1}				$Y_{PAO,O2}$		Y_{PAO1}	
Yield for X_{PAO} growth per $X_{PAO,PHA}$ or $X_{PAO,Stor}$ (Anoxic)	$Y_{PAO,Ax}$		g X_{PAO}.g X_{PHA}^{-1} or g X_{PAO}.g X_{Stor}^{-1}				$Y_{PAO,NO}$		Y_{PAO2}	
Yield for consumption of $X_{PAO,PHA}$ per X_{PAO} formation (Aerobic)	$Y_{PHA\_PAO,Ox}$		g X_{PHA}.g X_{PAO}^{-1}							Y_{PHA}^{O}
Yield for consumption of $X_{PAO,PHA}$ per X_{PAO} formation (Anoxic)	$Y_{PHA\_PAO,Ax}$		g X_{PHA}.g X_{PAO}^{-1}							Y_{PHA}^{NO}
Yield for $X_{PAO,PP}$ storage (S_{PO4} uptake) per $X_{PAO,Stor}$ utilized	Y_{Stor_PP}	2	g X_{PP}.g X_{Stor}^{-1}		$1/Y_{PHA}$		$1/Y_{PHA}$			
Yield for $X_{PAO,PP}$ storage (S_{PO4} uptake) per $X_{PAO,Stor}$ utilized (Aerobic)	$Y_{Stor\_PP,Ox}$		g X_{PP}.g X_{Stor}^{-1}					$f_{P,UPT1}$	Y_{PP1}	
Yield for $X_{PAO,PP}$ storage (S_{PO4} uptake) per $X_{PAO,Stor}$ utilized (Anoxic)	$Y_{Stor\_PP,Ax}$		g X_{PP}.g X_{Stor}^{-1}					$f_{P,UPT2}$	Y_{PP2}	
Yield for $X_{PAO,PP}$ formation per X_{PAO} (Anoxic)	$Y_{PAO\_PP,Ax}$		g X_{PP}.g X_{PAO}^{-1}							Y_{PP}^{NO}
Yield for $X_{PAO,PP}$ formation per X_{PAO} (Aerobic)	$Y_{PAO\_PP,Ox}$		g X_{PP}.g X_{PAO}^{-1}							Y_{PP}^{O}
Yield for $X_{PAO,Stor}$ storage per S_{VFA}	$Y_{VFA\_Stor,PAO}$		g X_{Stor}.g S_{VFA}^{-1}					Y_{PHB}		
Yield for $X_{PAO,PHA}$ storage per S_{VFA} (Anoxic)	$Y_{VFA\_PHA,PAO,Ax}$		g X_{PHA}.g S_{VFA}^{-1}							Y_{SA}^{NO}
Yield for $X_{PAO,PHA}$ storage per S_{VFA} (Anaerobic)	$Y_{VFA\_PHA,PAO,An}$		g X_{PHA}.g S_{VFA}^{-1}							Y_{SA}^{AN}
Yield for $X_{PAO,PP}$ requirement (S_{PO4} release) per $X_{PAO,Stor}$ stored (S_{VFA} utilized)	$Y_{PP\_Stor,PAO}$	3	g X_{PP}.g X_{Stor}^{-1} or g X_{PO4}.g S_{VFA}^{-1}		Y_{PO4}		Y_{PO4}	$f_{P,REL}$	Y_{PO4}	
Yield for $X_{PAO,PP}$ requirement (S_{PO4} release) per $X_{PAO,PHA}$ stored (S_{VFA} utilized) (Anoxic	$Y_{PP\_PHA,PAO,Ax}$	3	g X_{PP}.g X_{Stor}^{-1} or g X_{PO4}.g S_{VFA}^{-1}							Y_{PO}^{NO}
Yield for $X_{PAO,PP}$ requirement (S_{PO4} release) per $X_{PAO,PHA}$ stored (S_{VFA} utilized) (Anaerc	$Y_{PP\_PHA,PAO,An}$	3	g X_{PP}.g X_{Stor}^{-1} or g X_{PO4}.g S_{VFA}^{-1}							Y_{PO}^{AN}
Fraction of $X_{PAO,PP}$ that can be released	f_{PP,Lo_PP}		g $X_{PP,Lo}$.g X_{PP}^{-1}					f_{PP}		
Yield for formation of $X_{PAO,Gly}$ (Anoxic)	$Y_{PAO\_Gly,Ax}$	6	g X_{Gly}.g X_{PAO}^{-1}							Y_{GLY}^{NO}
Yield for formation of $X_{PAO,Gly}$ (Aerobic)	$Y_{PAO\_Gly,Ox}$	6	g X_{Gly}.g X_{PAO}^{-1}							Y_{GLY}^{O}
Fraction of X_U generated in X_{PAO} decay	$f_{XU\_PAO,lys}$	1	g X_U.g X_{PAO}^{-1}					$f_{EP,P}$	$f_{XE\text{-}PAO}$	
Fraction of S_U generated in X_{PAO} decay	$f_{SU\_PAO,lys}$	1	g X_U.g X_{PAO}^{-1}				f_{SI}	$f_{ES,P}$	$f_{SI\text{-}PAO}$	
ATP produced per NADH or P/O ratio	Y_{NADH_ATP}		mol ATP.mol $NADH^{-1}$							δ
Observed biomass ratio TOC over COD	i_{TOC_COD}		g C.g COD^{-1}							α
Autotrophic organisms										
Yield of X_{ANO} growth per S_{NOx}	Y_{ANO}		g X_{AUT}.g S_{NOx}^{-1}	Y_A	Y_A	Y_A	Y_{AUT}	Y_A	Y_{NIT}	Y_A
Fraction of X_U generated in X_{ANO} decay	$f_{XU\_ANO,lys}$		g X_U.g X_{ANO}^{-1}					$f_{EP,A}$	$f_{XE\text{-}NIT}$	$f_{XI,A}$
Precipitation										
X_{MeOH} requirement per S_{PO4} utilized	$f_{MeOH\_PO4,MW}$		g X_{MeOH}. g S_{PO4}^{-1}							
X_{MeP} formation per S_{PO4} utilized	$f_{MeP\_PO4,MW}$		g X_{MeP}. g S_{PO4}^{-1}							

Models references: see below N.B.: see below				ASM1	ASM2d	ASM3	ASM3 + Bio-P	Barker & Dold	UCTPHO+	ASM2d + TUD
Description	Parameter	NB	Units	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
Nitrogen										
N content of S_B	i_{N_SB}		g N.g S_B^{-1}			$i_{N,SS}$	$i_{N,SS}$			
N content of S_F	i_{N_SF}		g N.g S_F^{-1}		$i_{N,SF}$				i_{NSF}	$i_{N,SF}$
N content of S_U	i_{N_SU}		g N.g S_U^{-1}		$i_{N,SI}$	$i_{N,SI}$	$i_{N,SI}$	$f_{N,SEP}$	i_{NSI}	$i_{N,SI}$
N content of X_U	i_{N_XU}		g N.g X_U^{-1}		$i_{N,XI}$	$i_{N,XI}$	$i_{N,XI}$		i_{NXI}	$i_{N,XI}$
N content of XC_B	i_{N_XCB}		g N.g XC_B^{-1}		$i_{N,XS}$	$i_{N,XS}$	$i_{N,XS}$		i_{NENM}	$i_{N,XS}$
N content of biomass (X_{OHO}, X_{PAO}, X_{ANO})	i_{N_XBio}		g N.g X_{Bio}^{-1}	i_{XB}	$i_{N,BM}$	$i_{N,BM}$	$i_{N,BM}$		i_{NBM}	$i_{N,BM}$
N content of products from biomass	i_{N_XUE}		g N.g X_{UE}^{-1}	i_{XE}					i_{NXE}	
N content of X_{OHO}	i_{N_OHO}		g N.g X_{OHO}^{-1}					$f_{N,ZH}$		
N content of products from X_{OHO}	$i_{N\_XUE,OHO}$	*1*	g N.g X_{UE}^{-1}					$f_{N,ZEH}$		
N content of X_{PAO}	i_{N_PAO}		g N.g X_{PAO}^{-1}					$f_{N,ZP}$		
N content of products from X_{PAO}	$i_{N\_XUE,PAO}$	*1*	g N.g X_{UE}^{-1}					$f_{N,ZEP}$		
N content of X_{ANO}	i_{N_ANO}		g N.g X_{ANO}^{-1}					$f_{N,ZA}$		
N content of products from X_{ANO}	$i_{N\_XUE,ANO}$	*1*	g N.g X_{UE}^{-1}					$f_{N,ZEA}$		
Phosphorus										
P content of S_B	i_{P_SB}		g P.g S_B^{-1}				$i_{P,SS}$			
P content of S_F	i_{P_SF}		g P.g S_F^{-1}		$i_{P,SF}$				i_{PSF}	$i_{P,SF}$
P content of S_U	i_{P_SU}		g P.g S_U^{-1}		$i_{P,SI}$		$i_{P,SI}$		i_{PSI}	$i_{P,SI}$
P content of X_U	i_{P_XU}		g P.g X_U^{-1}		$i_{P,XI}$		$i_{P,XI}$		i_{PXI}	$i_{P,XI}$
P content of XC_B	i_{P_XCB}		g P.g X_B^{-1}		$i_{P,XS}$		$i_{P,XS}$		i_{PENM}	$i_{P,XS}$
P content of biomass (X_{OHO}, X_{PAO}, X_{ANO})	i_{P_XBio}		g P.g X_{Bio}^{-1}		$i_{P,BM}$		$i_{P,BM}$		i_{PBM}	$i_{P,BM}$
P content of products from biomass	i_{P_XUE}		g P.g X_{UE}^{-1}						i_{PXE}	
P content of X_{OHO}	i_{P_OHO}		g P.g X_{OHO}^{-1}					$f_{P,ZH}$		
P content of products from X_{OHO}	$i_{P\_XUE,OHO}$	*1*	g P.g X_{UE}^{-1}					$f_{P,ZEH}$		
P content of X_{PAO}	i_{P_PAO}		g P.g X_{PAO}^{-1}					$f_{P,ZP}$		
P content of products from X_{PAO}	$i_{P\_XUE,PAO}$	*1*	g P.g X_{UE}^{-1}					$f_{P,ZEP}$		
P content of X_{ANO}	i_{P_ANO}		g P.g X_{ANO}^{-1}					$f_{P,ZA}$		
P content of products from X_{ANO}	$i_{P\_XUE,ANO}$	*1*	g P.g X_{UE}^{-1}					$f_{P,ZEA}$		
Conversion factor for X_{MeP} (FePO4) in P	i_{P_MeP}		g P.g X_{MeP}^{-1}							

Models references: see below N.B.: see below				ASM1	ASM2d	ASM3	ASM3 + Bio-P	Barker & Dold	UCTPHO+	ASM2d + TUD
Description	Parameter	NB	Units	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
TSS										
Conversion factor X_U in TSS	i_{TSS_XU}		g TSS.g X_U^{-1}		$i_{TSS,XI}$	$i_{SS,XI}$	$i_{TSS,XI}$			$i_{TSS,XI}$
Conversion factor XC_B in TSS	i_{TSS_XCB}		g TSS.g XC_B^{-1}		$i_{TSS,XS}$	$i_{SS,XS}$	$i_{TSS,XS}$			$i_{TSS,XS}$
Conversion factor $X_{OHO,Stor}$ in TSS	$i_{TSS\_XOHO,Stor}$		g TSS.g X_{Stor}^{-1}			$i_{SS,STO}$	$i_{TSS,XSTO}$			
Conversion factor $X_{PAO,PHA}$ in TSS	$i_{TSS\_XPAO,PHA}$		g TSS.g X_{PHA}^{-1}		$i_{TSS,XPHA}$					$i_{TSS,PHA}$
Conversion factor biomass in TSS	i_{TSS_XBio}		g TSS.g X_{Bio}^{-1}		$i_{TSS,BM}$	$i_{SS,BM}$	$i_{TSS,BM}$			$i_{TSS,BM}$
Conversion factor $X_{PAO,PP}$ in TSS	$i_{TSS\_XPAO,PP}$		g TSS.g X_{PP}^{-1}		$i_{TSS,XPP}$		$i_{TSS,XPP}$			$i_{TSS,PP}$
Conversion factor $X_{PAO,Gly}$ in TSS	$i_{TSS\_XPAO,Gly}$		g TSS.g X_{Gly}^{-1}							$i_{TSS,GLY}$
Ratio COD/VSS (OHO)	i_{VSS_OHO}		g X_{OHO}.g VSS^{-1}					$f_{CV,H}$		
Ratio COD/VSS (ANO)	i_{VSS_ANO}		g X_{ANO}.g VSS^{-1}					$f_{CV,A}$		
Ratio COD/VSS (PAO)	i_{VSS_PAO}		g X_{PAO}.g VSS^{-1}					$f_{CV,P}$		
COD										
Conversion factor for NO_3 reduction to N_2	$i_{NOx,N2}$		g COD.g N^{-1}							
Conversion factor for NO_3 in COD	i_{COD_NOx}		g COD.g N^{-1}							
Conversion factor for N_2 in COD	i_{COD_N2}		g COD.g N^{-1}							
Conversion factor for H_2 in COD	i_{COD_H2}		g COD.g H^{-1}							
Charge										
Conversion factor for S_{VFA} (CH_3COO^-) in charge	i_{Charge_VFA}		Charge.g COD^{-1}							
Conversion factor for NH_x in charge	i_{Charge_NHx}		Charge.g N^{-1}							
Conversion factor for NO_3 in charge	i_{Charge_NOx}		Charge.g N^{-1}							
Conversion factor for PO_4 in charge	i_{Charge_PO4}		Charge.g P^{-1}							
Conversion factor for $X_{PAO,PP}$ $(K_{0.33}Mg_{0.33}PO_3)_n$ in charge	$i_{Charge\_XPAO,PP}$		Charge.g P^{-1}							
Kinetics										
Hydrolysis										
Maximum specific hydrolysis rate	$q_{XCB\_SB,hyd}$	5	g XC_B.g X_{OHO}^{-1}.d^{-1}	k_h	K_h	k_H	k_H	K_H		k_h
Half-saturation coefficient for XC_B/X_{OHO}	$K_{XCB,hyd}$		g XC_B.g X_{OHO}^{-1}	K_X	K_x	K_X	K_X	K_X		K_X
Correction factor for hydrolysis under anoxic conditions	$n_{qhyd,Ax}$		-	η_h	η_{NO3}			$\eta_{S,ANOX}$		η_{NO}
Correction factor for hydrolysis under anaerobic conditions	$n_{qhyd,An}$		-		η_{fe}			$\eta_{S,ANA}$		η_{fe}
Half-saturation/inhibition coefficient for S_{O2}	$K_{O2,hyd}$		g S_{O2}.m^{-3}		K_{O2}					K_O
Half-saturation/inhibition coefficient for S_{NOx}	$K_{NOx,hyd}$		g N.m^{-3}		K_{NO3}					K_{NO}

Models references: see below N.B.: see below				ASM1	ASM2d	ASM3	ASM3 + Bio-P	Barker & Dold	UCTPHO+	ASM2d + TUD
Description	Parameter	NB	Units	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
Biomass										
Half-saturation coefficient for S_{PO4} as nutrient	$K_{PO4,Bio,gro}$		g S_{PO4}.m^{-3}					$K_{LP,GRO}$	$K_{PO4-gro}$	
Heterotrophic organisms										
Rate constant for $X_{OHO,Stor}$ storage	q_{SB_Stor}	5,7	g XC_B.g X_{OHO}^{-1}.d^{-1}			k_{STO}	k_{STO}			
Rate constant for X_{Ads} adsorption	q_{XCB_Ads}	5,7	g X_{Ads}.g XC_B^{-1}.d^{-1}						K_{ADS}	
Maximum growth rate of X_{OHO}	$\mu_{OHO,Max}$		d^{-1}	μ_H	μ_H	μ_H	μ_H	μ_H	μ_H	μ_H
Reduction factor for anoxic growth of X_{OHO}	$n_{\mu OHO,Ax}$		-	η_g	η_{NO3}	η_{NOX}	$\eta_{NO,H}$	η_{gro}	η_H	η_{NO}
Maximum growth rate of X_{OHO} on X_{Ads} (hydrolysis + growth)	$\mu_{Ads\_OHO,Max}$		d^{-1}						K_{MP}	
Maximum adsorption on X_{OHO} (X_{Ads}/X_{OHO} ratio)	$f_{Ads\_OHO,Max}$		g X_{Ads}.g X_{OHO}^{-1}						f_{MA}	
Rate constant for fermentation / Maximum specific fermentation growth rate	$q_{SF\_VFA,Max}$	4,7	g S_F.g X_{OHO}^{-1}.d^{-1}		q_{fe}			K_C	K_{FE}	q_{fe}
Half-saturation coefficient for S_B	$K_{SB,OHO}$	5	g S_B.m^{-3}	K_s		K_S	$K_{SS,H}$			
Half-saturation coefficient for S_F	$K_{SF,OHO}$	5	g S_F.m^{-3}		K_F			$K_{S,H}$	K_F	K_F
Half-saturation coefficient for S_{VFA}	$K_{VFA,OHO}$	5	g S_{VFA}.m^{-3}		K_A			$K_{S,H}$	K_A	K_{Ac}
Half-saturation coefficient $X_{OHO,Stor}$/X_{OHO}	K_{Stor_OHO}		g X_{Stor}.g X_{OHO}^{-1}			K_{STO}	$K_{STO,H}$			
Half-saturation coefficient for hydrolysis/growth on X_{Ads}	K_{Ads_OHO}		g X_{Ads}.g X_{OHO}^{-1}						K_{SP}	
Decay rate for X_{OHO}	b_{OHO}		d^{-1}	b_H	b_H			b_H	b_H	b_H
Endogenous respiration rate of X_{OHO}	m_{OHO}		d^{-1}				b_H			
Reduction factor for Anoxic endogenous respiration of OHO	$n_{mOHO,Ax}$		-				$\eta_{NO,end,H}$			
Endogenous respiration rate of X_{OHO} (Aerobic)	$m_{OHO,Ox}$		d^{-1}			$b_{H,O2}$				
Endogenous respiration rate of X_{OHO} (Anoxic)	$m_{OHO,Ax}$		d^{-1}			$b_{H,NOX}$				
Endogenous respiration rate of $X_{OHO,Stor}$	$m_{OHO,Stor}$		d^{-1}				b_{Stor}			
Endogenous respiration rate of $X_{OHO,Stor}$ (Aerobic)	$m_{Stor,Ox}$		d^{-1}			$b_{STO,O2}$				
Endogenous respiration rate of $X_{OHO,Stor}$ (Anoxic)	$m_{Stor,Ax}$		d^{-1}			$b_{STO,NOX}$				
Half-saturation coefficient for fermentation of S_F	$K_{SF,fe}$		g S_F.m^{-3}		K_{fe}			$K_{S,ANA}$		K_{fe}
Half-saturation coefficient for S_{O2}	$K_{O2,OHO}$		g S_{O2}.m^{-3}	$K_{O,H}$	K_{O2}	K_{O2}	$K_{O,H}$	$K_{O,HET}$	K_{OH}	K_O
Half-saturation coefficient for S_{NOx}	$K_{NOx,OHO}$	5	g S_{NOx}.m^{-3}	K_{NO}	K_{NO3}	K_{NOX}	$K_{NO,H}$	K_{NO}	K_{NO3}	K_{NO}
Half-saturation coefficient for S_{NHx}	$K_{NHx,OHO}$		g S_{NHx}.m^{-3}		K_{NH4}	K_{NH4}	$K_{NH,H}$	K_{NA}	K_{NH4}	K_N
Half-saturation coefficient for S_{PO4}	$K_{PO4,OHO}$		g S_{PO4}.m^{-3}		K_P		$K_{PO4,H}$			K_P
Half-saturation coefficient for S_{Alk}	$K_{Alk,OHO}$		mol HCO_3^-.m^{-3}		K_{ALK}	K_{ALK}	$K_{HCO,H}$			K_{HCO}

Models references: see below N.B.: see below				ASM1	ASM2d	ASM3	ASM3 + Bio-P	Barker & Dold	UCTPHO+	ASM2d + TUD
Description	Parameter	NB	Units	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
Phosphorus accumulating organisms (PAO)										
Rate constant for S_{VFA} uptake rate ($X_{PAO,Stor}$ storage)	q_{PAO,VFA_Stor}	5	$g\ X_{Stor}.g\ X_{PAO}^{-1}.d^{-1}$		q_{PHA}			K_P	q_{PHA}	
Rate constant for S_B uptake rate ($X_{PAO,Stor}$ storage)	q_{PAO,SB_Stor}	5	$g\ X_{Stor}.g\ X_{PAO}^{-1}.d^{-1}$				q_{PHA}			
Rate constant for S_{VFA} uptake rate ($X_{PAO,PHA}$ storage) (anaerobic)	$q_{PAO,VFA\_PHA,An}$	5	$g\ X_{PHA}.g\ X_{PAO}^{-1}.d^{-1}$							q_{Ac}
Rate constant for S_{VFA} uptake rate ($X_{PAO,PHA}$ storage) (anoxic)	$q_{PAO,VFA\_PHA,Ax}$	5	$g\ X_{PHA}.g\ X_{PAO}^{-1}.d^{-1}$							q_{Ac}^{NO}
Rate constant for storage of $X_{PAO,PP}$	$q_{PAO,PO4\_PP}$	5	$g\ X_{PP}.g\ X_{PAO}^{-1}.d^{-1}$		q_{PP}		q_{PP}			k_{PP}
Reduction factor for K_{O2} for $X_{PAO,PP}$ formation	n_{KO2}		-							g_{PP}
Reduction factor for K_{NOx} for $X_{PAO,PP}$ formation	n_{KNOx}		-							g_{PP}
Maximum ratio of $X_{PAO,PP}/X_{PAO}$	$f_{PP\_PAO,Max}$		$g\ X_{PP}.g\ X_{PAO}^{-1}$		K_{MAX}		$K_{max,PAO}$			f_{PP}^{max}
Half-saturation coefficient for $X_{PAO,PP}/X_{PAO}$	K_{S,fPP_PAO}		$g\ X_{PP}.g\ X_{PAO}^{-1}$		K_{PP}		$K_{PP,PAO}$			
Half-Inhibition coefficient for $X_{PAO,PP}/X_{PAO}$	K_{I,fPP_PAO}		$g\ X_{PP}.g\ X_{PAO}^{-1}$		K_{iPP}		$K_{iPP,PAO}$			K_{fPP}
Rate constant for formation of $X_{PAO,Gly}$	q_{Gly}		$g\ X_{Gly}.g\ X_{PAO}^{-1}.d^{-1}$							k_{GLY}
Maximum ratio of $X_{PAO,Gly}/X_{PAO}$	$f_{Gly\_PAO,Max}$		$g\ X_{Gly}.g\ X_{PAO}^{-1}.d^{-1}$							f_{GLY}^{max}
Half-saturation coefficient for $X_{PAO,Gly}/X_{PAO}$	K_{fGly_PAO}		$g\ X_{Gly}.g\ X_{PAO}^{-1}$							K_{fGLY}
Maximum growth rate of X_{PAO}	$\mu_{PAO,Max}$		d^{-1}		μ_{PAO}		μ_{PAO}	μ_{P1}	μ_{PAO1}	
Maximum growth rate of X_{PAO} (when P is limiting)	$\mu_{PAO,Max,Plim}$		d^{-1}					μ_{P2}	μ_{PAO2}	
Reduction factor for anoxic growth of X_{PAO}	$n_{\mu PAO}$		-		η_{NO3}		$\eta_{NO,PAO}$	η_p	η_{PAO}	
Half-saturation coefficient for $X_{PAO,PHA}/X_{PAO}$	K_{fPHA_PAO}		$g\ X_{PHA}.g\ X_{PAO}^{-1}$							K_{fPHA}
Half-saturation coefficient for $X_{PAO,Stor}/X_{PAO}$	K_{fStor_PAO}		$g\ X_{Stor}.g\ X_{PAO}^{-1}$		K_{PHA}		K_{PHA}	K_{SP1}	K_{PHA1}	
Half-saturation coefficient for $X_{PAOStor}/X_{PAO}$ (P limit)	$K_{fStor\_PAO,Plim}$		$g\ X_{Stor}.g\ X_{PAO}^{-1}$					K_{SP2}	K_{PHA2}	
Rate for $X_{PAO,PHA}$ consumption (X_{PAO} growth)	q_{PHA_PAO}	6	$g\ X_{PHA}.g\ X_{PAO}^{-1}.d^{-1}$							k_{PHA}
Reduction factor for denitrifying processes	n_{qPAO}		-							η_{NO}
Observed oxygen consumption for maintenance	$m_{PAO,O2}$		$g\ S_{O2}.g\ X_{PAO}^{-1}.d^{-1}$							m_{OC}
Decay rate for X_{PAO}	b_{PAO}		d^{-1}		b_{PAO}					
Endogenous respiration rate of X_{PAO}	m_{PAO}		d^{-1}				b_{PAO}	b_P	b_{PAO}	
Reduction factor for anoxic endogenous respiration of X_{PAO}	n_{mPAO}		-				$\eta_{NO,end,PAO}$			
Maintenance rate for X_{PAO} (Aerobic)	$m_{PAO,Ox}$		d^{-1}							m_O
Maintenance rate for X_{PAO} (Anoxic)	$m_{PAO,Ax}$		d^{-1}							m_{NO}
Maintenance rate for X_{PAO} (Anaerobic)	$m_{PAO,An}$		$g\ P.g\ X_{PAO}^{-1}.d^{-1}$							m_{AN}

Models references: see below N.B.: see below				ASM1	ASM2d	ASM3	ASM3 + Bio-P	Barker & Dold	UCTPHO+	ASM2d + TUD
Description	Parameter	NB	Units	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
Rate constant for Lysis of $X_{PAO,PP}$	b_{PP_PO4}		d^{-1}		b_{PP}		b_{PP}	b_{PP}	b_{PP}	
Reduction factor for anoxic lysis of $X_{PAO,PP}$	n_{bPP_PO4}		-				$\eta_{NO,lys,PP}$			
Rate constant for respiration of $X_{PAO,Stor}$	b_{Stor_VFA}		d^{-1}		b_{PHA}					
Rate constant for respiration of $X_{PAO,Stor}$	$m_{PAO,Stor}$		d^{-1}				b_{PHA}			
Reduction factor for anoxic respiration of $X_{PAO,Stor}$	$n_{mPAO,Stor}$		-				$\eta_{NO,resp,PHA}$			
Half-saturation coefficient for S_B	$K_{SB,PAO}$		$g\ S_B.m^{-3}$				$K_{SS,PAO}$			
Half-saturation coefficient for S_{VFA}	$K_{VFA,PAO}$		$g\ S_{VFA}.m^{-3}$		K_A			K_{SSEQ}	K_{AC}	K_{Ac}
Half-saturation coefficient for S_{O2}	$K_{O2,PAO}$		$g\ S_{O2}.m^{-3}$		K_{O2}		$K_{O,PAO}$		K_{OH}	K_O
Half-saturation coefficient for S_{NOx}	$K_{NOx,PAO}$		$g\ S_{NOx}.m^{-3}$		K_{NO3}		$K_{NO,PAO}$		K_{NO3}	K_{NO}
Half-saturation coefficient for S_{NHx}	$K_{NHx,PAO}$		$g\ S_{NHx}.m^{-3}$		K_{NH4}		$K_{NH,PAO}$		K_{NH4}	K_N
Half-saturation coefficient for S_{PO4} uptake ($X_{PAO,PP}$ storage)	$K_{PO4,PAO,stor}$		$g\ S_{PO4}.m^{-3}$		K_{PS}		$K_{PO4,PP}$	$K_{LP,UPT}$	$K_{PO4\text{-}up}$	K_{PO}
Half-saturation coefficient for S_{PO4} as nutrient (X_{PAO} growth)	$K_{PO4,PAO,gro}$		$g\ S_{PO4}.m^{-3}$		K_P		$K_{PO4,PAO}$			K_P
Half-saturation coefficient for $X_{PAO,PP}$	$K_{PP,PAO}$		$g\ X_{PP}.m^{-3}$					K_{XP}	K_{PP}	K_{PP}
Half-saturation coefficient for $X_{PAO,PHA}$	$K_{PHA,PAO}$		$g\ X_{PHA}.m^{-3}$							K_{PHA}
Half-saturation coefficient for $X_{PAO,Gly}$	$K_{Gly,PAO}$		$g\ X_{Gly}.m^{-3}$							K_{GLY}
Half-saturation coefficient for S_{Alk}	$K_{Alk,PAO}$		$mol\ HCO_3^-.m^{-3}$		K_{ALK}		$K_{HCO,PAO}$			K_{HCO}
Autotrophic organisms										
Maximum growth rate of X_{ANO}	$\mu_{ANO,Max}$		d^{-1}	μ_A	μ_{AUT}	μ_A	μ_A	μ_A	μ_{NIT}	μ_A
Decay rate for X_{ANO}	b_{ANO}		d^{-1}	b_A	b_{AUT}			b_A	b_{NIT}	b_A
Endogenous respiration rate for X_{ANO}	m_{ANO}		d^{-1}				b_A			
Reduction factor for anoxic endogenous respiration of X_{ANO}	n_{mANO}		-				$\eta_{NO,end,A}$			
Endogenous respiration rate for X_{ANO} (Aerobic)	$m_{ANO,Ox}$		d^{-1}			$b_{A,O2}$				
Endogenous respiration rate for X_{ANO} (Anoxic)	$m_{ANO,Ax}$		d^{-1}			$b_{A,NOX}$				
Rate constant for ammonification	q_{am}		$m^3.g\ XC_{B,N}^{-1}.d^{-1}$	k_a				K_R		
Half-saturation coefficient for S_{O2}	$K_{O2,ANO}$		$g\ S_{O2}.m^{-3}$	$K_{O,A}$	K_{O2}	$K_{A,O2}$	$K_{O,A}$	$K_{O,AUT}$	K_{ON}	$K_{A,O}$
Half-saturation coefficient for S_{NHx}	$K_{NHx,ANO}$		$g\ S_{NHx}.m^{-3}$	K_{NH}	K_{NH4}	$K_{A,NH4}$	$K_{NH,A}$	K_{NH}	K_{NH4}	K_{NH}
Half-saturation coefficient for S_{PO4}	$K_{PO4,ANO}$		$g\ S_{PO4}.m^{-3}$		K_P		$K_{PO4,A}$			K_P
Half-saturation coefficient for S_{Alk}	$K_{Alk,ANO}$		$mol\ HCO_3^-.m^{-3}$		K_{ALK}	$K_{A,ALK}$	$K_{HCO,A}$			K_{HCO}

Models references: see below N.B.: see below				ASM1	ASM2d	ASM3	ASM3 + Bio-P	Barker & Dold	UCTPHO+	ASM2d + TUD
Description	Parameter	NB	Units	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
Precipitation										
Rate constant for P precipitation	$q_{P,pre}$		$m^3.g\ Fe(OH)_3^{-1}.d^{-1}$		k_{PRE}					
Rate constant for redissolution	$q_{P,red}$		d^{-1}		k_{RED}					
Half-saturation coefficient for alkalinity	$K_{Alk,pre}$		$mol\ HCO3^-.m^{-3}$		K_{ALK}					

N.B.
1. The organism type can be skipped in models where no differences is made between those parameters (ASM1, ASM2d, ASM3 and ASM3+Bio-P)
2. To have consistent units between models for the same parameter and to keep the notation simple, it was chosen to use the inverse of the parameter Y_{PHA} for ASM2d and ASM3+Bio-P
3. The units g X_{PP}/g X_{PHA} or g X_{PO4}/g S_A (in ASM2d+TUD) are equivalent since there is no yield between X_{PP} and X_{PO4}, and between X_{PHA} and S_A in other models than ASM2d+TUD
4. zero or first order kinetics / first order kinetic for UCTPHO+ (no S_F/(K_fe + S_F) term)
5. If a parameter name is used for different organisms, the name of the organism should appear. Otherwise, it can be ommitted.
6. If the organism name appear twice (as organism name and as reactant_product) it is possible to simplify and just keep the reactant_product part
7. If the reactant_product subscript is self explaining, the specification of the process can be ommitted.

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ANNEXE 2. Liste des articles intégrés dans la base de données

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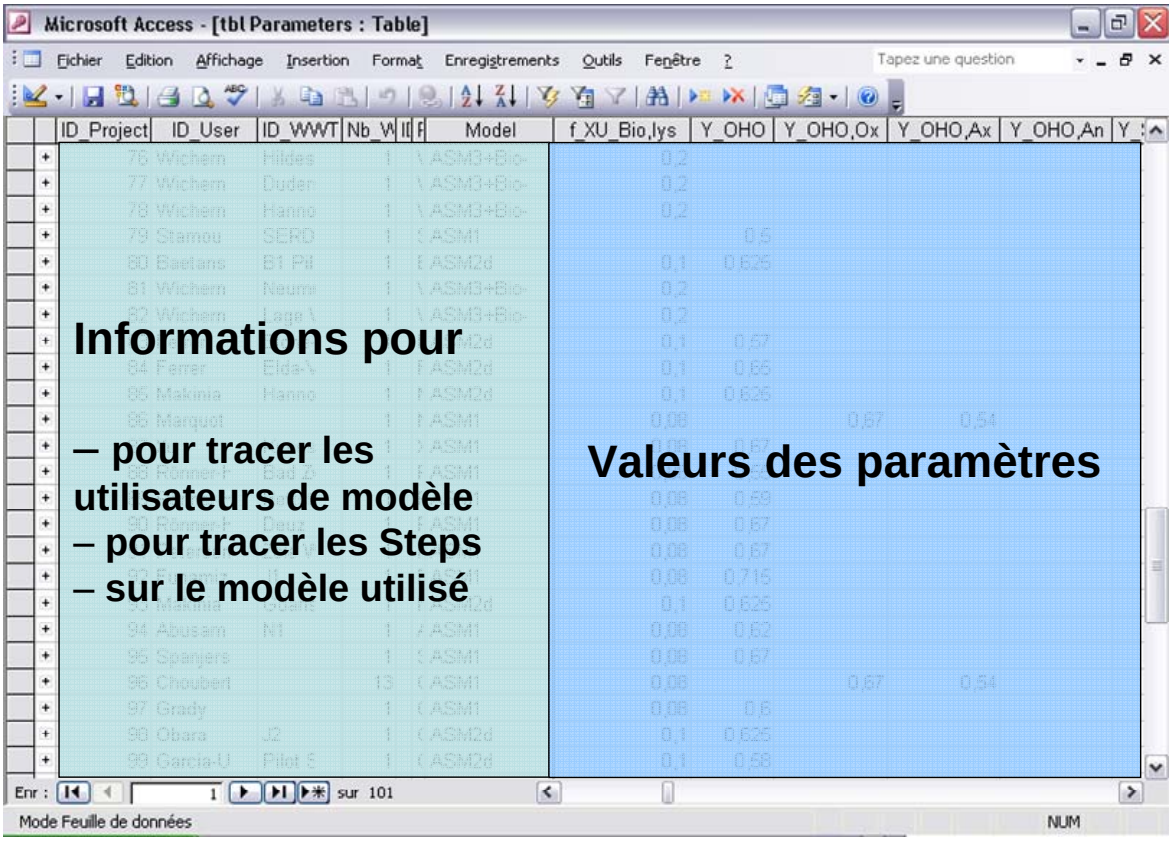
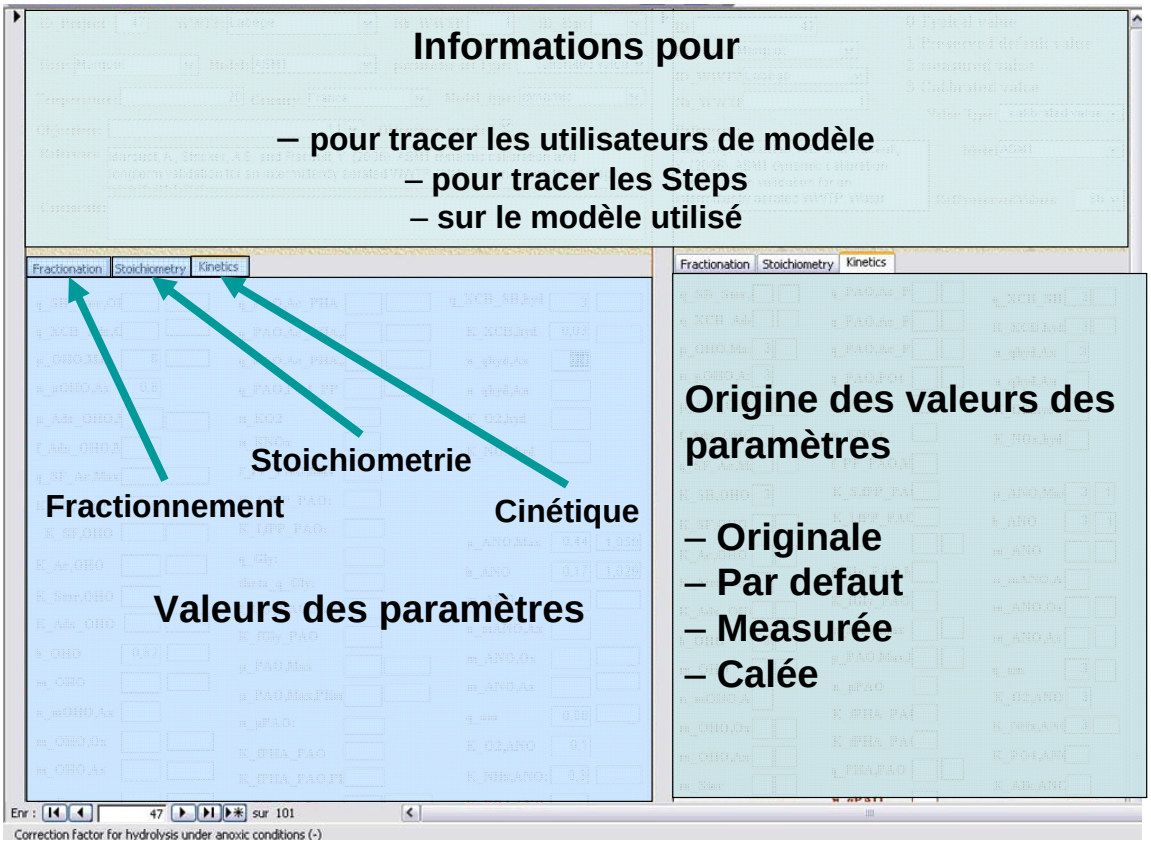
ANNEXE 3. Apparence de la base de données

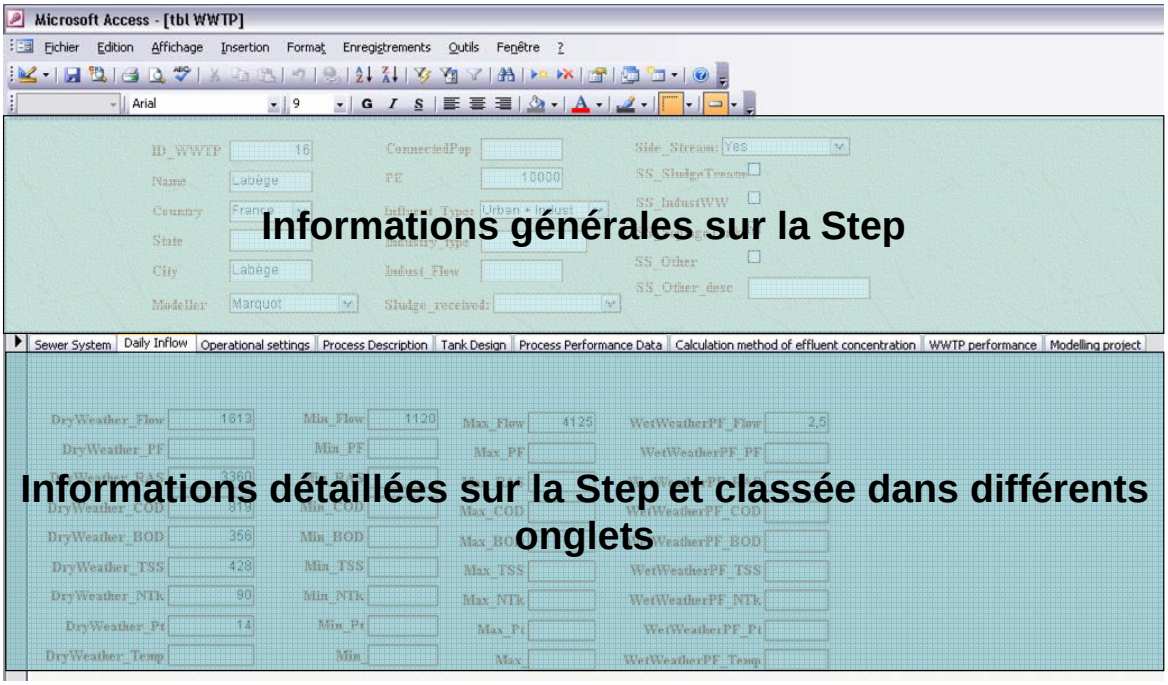
Aperçu de la table de données :



Formulaire des jeux de paramètres :



Formulaire des caractéristiques de la station d'épuration :



ANNEXE 4. Résultats de la base de données pour l'ASM3, ASM3+BioP et Barker & Dold model

ASM3

Data description. The database contains 5 parameter sets for ASM3, of which 1 is a "proposed new default parameter sets", and 3 are "optimised parameter sets". The modelling studies were exclusively carried out in the North of Europe (Belgium, Finland, Germany) on full scale WWTP. Table 6-1 synthesises the main results for ASM3 and is structured as.

Table 6-1. Synthesis of database results for ASM3 model, only modified parameters are given

Parameter*	Unit	Original parameter set		Proposed new default parameter set	Optimised parameter sets					
Parameter sets		Notation	Value (k)	l	n	Modif >50%	Median	Perc. 25%	Perc. 75%	V (%)
Stoichiometric parameters										
$Y_{Stor\_OHO,Ox}$	g X_{OHO}.g X_{Stor}^{-1}	$Y_{H,O2}$	**0.85**	0.8	5		0.80	0.80	0.80	0
$Y_{Stor\_OHO,Ax}$	g X_{OHO}.g X_{Stor}^{-1}	$Y_{H,NOX}$	**0.8**	0.7	5		0.70	0.70	0.70	0
$Y_{SB\_Stor,Ox}$	g X_{Stor}.g S_B^{-1}	$Y_{STO,O2}$	**0.63**	0.8	5		0.80	0.63	0.80	21
$Y_{SB\_Stor,Ax}$	g X_{Stor}.g S_B^{-1}	$Y_{STO,NOX}$	**0.54**	0.65	5		0.65	0.54	0.65	17
Conversion coefficient										
i_{N_XU}	g N.g X_U^{-1}	$i_{N,XI}$	**0.02**	0.04	5		0.040	0.035	0.040	13
i_{N_XCB}	g N.g X_{CB}^{-1}	$i_{N,XS}$	/ **0.04**	0.03	5		0.030	0.030	0.030	0
Kinetic parameters										
Hydrolysis										
$q_{XCB\_SB,hyd}$	g X_{CB}.g X_{OHO}^{-1}.d^{-1}	k_H	**3**	9	5		9.0	3.0	9.0	67
q_{SB_Stor}	g X_{CB}.g X_{OHO}^{-1}.d^{-1}	k_{STO}	**0.1**		5		12.0	10.0	12.0	17
Ordinary Heterotrophic Organisms										
$\mu_{OHO,Max}$	d^{-1}	μ_H	**2**	3	5		3.0	2.0	3.0	33
$\eta_{\mu OHO,Ax}$	-	η_{NOX}	/ **0.6**	0.5	5		0.50	0.50	0.60	20
$K_{SB,OHO}$	g S_B.m^{-3}	K_S	**2**	10	5		10.0	2.0	10.0	80
K_{Stor_OHO}	g X_{Stor}.g X_{OHO}^{-1}	K_{STO}	/ **1**	0.1	5		0.10	0.10	0.10	0
$m_{OHO,Ox}$	d^{-1}	$b_{H,O2}$	**0.2**	0.3	5		0.30	0.20	0.30	33
$m_{OHO,Ax}$	d^{-1}	$b_{H,,NOX}$	**0.1**	0.15	5		0.15	0.10	0.15	33
$m_{Stor,Ox}$	d^{-1}	$b_{STO,O2}$	**0.2**	0.3	5		0.30	0.20	0.30	33
$m_{Stor,Ax}$	d^{-1}	$b_{STO,NOX}$	**0.1**	0.15	5		0.15	0.10	0.15	33
$K_{O2,OHO}$	g S_{O2}.m^{-3}	K_{O2}	**0.2**		5		0.200	0.200	0.500	150
Autotrophic Nitrifying Organisms										
$\mu_{ANO,Max}$	d^{-1}	μ_A	**1**	1.3	5	X	1.00	1.00	1.30	30
$m_{ANO,Ox}$	d^{-1}	$b_{A,O2}$	**0.15**	0.2	5		0.20	0.15	0.20	25
$m_{ANO,Ax}$	d^{-1}	$b_{A,NOX}$	**0.05**	0.1	5		0.10	0.05	0.10	50
$K_{NHx,ANO}$	g S_{NHx}.m^{-3}	$K_{A,NH4}$	**1**	1.4	5		1.40	1.00	1.40	29

k: Gujer *et al.* (2000); l: Koch *et al.* (2000). Please refer to the appendix for the parameter definitions. *Standardised notation from Corominas *et al.* (2010) is used. n: number of parameter values in the database.

ASM3+BioP

Data description. The database contains 9 parameter sets for ASM3+BioP, 1 original parameter set and 8 "optimised parameter sets". The modelling studies were exclusively carried out in Germany. Half of them were carried out on full scale WWTP.

Table 6-2. Synthesis of database results for ASM3+BioP model, only modified parameters are mentioned

Parameter*	Unit	Original notation	Original parameter set	Optimised parameter sets					
Parameter sets			m	n	Modif >50%	Median	Perc. 25%	Perc. 75%	V (%)
Kinetic parameters									
Ordinary Heterotrophic Organisms									
$\eta_{mOHO,Ax}$	-	$\eta_{NO,end,H}$	**0.33**	9		0.33	0.33	0.50	52
$K_{O2,OHO}$	g $S_{O2}.m^{-3}$	$K_{O,H}$	**0.2**	9		0.200	0.200	0.500	150
Phosphorus Accumulating Organisms									
$q_{PAO,PO4\_PP}$	g $X_{PP}.g\ X_{PAO}^{-1}.d^{-1}$	q_{PP}	**1.5**	9	X	1.50	1.50	2.30	53
$f_{PP\_PAO,Max}$	g $X_{PP}.g\ X_{PAO}^{-1}$	$K_{max,PAO}$	**0.2**	9	X	1.00	0.24	1.00	76
Autotrophic Nitrifying Organisms									
$\mu_{ANO,Max}$	d^{-1}	μ_A	**0.9 - 1.8**	9	X	1.20	1.10	1.60	42
$K_{O2,ANO}$	g $S_{O2}.m^{-3}$	$K_{O,A}$	**0.5**	9	X	0.18	0.13	0.50	206

m: Rieger *et al.* (2001). Please refer to the appendix for the parameter definitions.
*Standardised notation from Corominas *et al.* (2010) is used. n: number of parameter values in the database.

Barker & Dold model

The database contains 6 parameter sets for the Barker & Dold model, of which 1 is "proposed new default parameter sets" and 4 are "optimised parameter sets". Two of the modelling studies were carried out in North-America, one in Africa and one in Oceania. The modelling studies mainly concern full scale WWTP with domestic influent (3).

Table 6-3. Synthesis of database results for Barker & Dold model, only modified parameters are mentioned

Parameter*	Unit	Original parameter set		Proposed new default parameter set	n	Optimised parameter sets				
Parameter sets		Notation	Value (n)	o		Modif >50%	Median	Perc. 25%	Perc. 75%	V (%)
Conversion coefficient										
i_{N_SU}	g N.g S_U^{-1}	$f_{N,SEP}$	**0.07**	0.034	5		0.070	0.034	0.070	51
i_{N_OHO}	g N.g X_{OHO}^{-1}	$f_{N,ZH}$	**0.07**		6	X	0.069	0.068	0.070	3
$i_{N\_XUE,OHO}$	g N.g X_{UE}^{-1}	$f_{N,ZEH}$	**0.07**	0.034	6		0.069	0.034	0.070	52
$i_{N\_XUE,PAO}$	g N.g X_{UE}^{-1}	$f_{N,ZEP}$	**0.07**	0.034	6		0.070	0.034	0.070	51
$i_{N\_XUE,ANO}$	g N.g X_{UE}^{-1}	$f_{N,ZEA}$	**0.07**	0.034	6		0.068	0.034	0.068	50
Kinetic parameters										
Ordinary Heterotrophic Organisms										
$\eta_{\mu OHO,Ax}$	-	η_{gro}	**0.37**		6		0.37	0.37	0.50	35
$K_{O2,OHO}$	g $S_{O2}.m^{-3}$	$K_{O,HET}$	**0.002**	0.05	6		0.002	0.002	0.050	2400
Phosphorus Accumulating Organisms										
$K_{PP,PAO}$	g $X_{PP}.m^{-3}$	K_{XP}	**0.05**	0.01	6	X	0.010	0.010	0.010	0
Autotrophic Nitrifying Organisms										
$\mu_{ANO,Max}$	d^{-1}	μ_A	**0.6**	0.9	6	X	0.73	0.60	0.90	41
b_{ANO}	d^{-1}	b_A	**0.04**	0.17	6	X	0.08	0.04	0.17	163
$K_{O2,ANO}$	g $S_{O2}.m^{-3}$	$K_{O,AUT}$	**0.5**	0.25	6		0.50	0.25	0.50	50
$K_{NHx,ANO}$	g $S_{NHx}.m^{-3}$	K_{NH}	**1**	0.5	6		1.00	0.50	1.00	50

n: Barker & Dold (1997); o: Questionnaire (based on >100 modelling project studies)
*Standardised notation from Corominas *et al.* (2010) is used. n: number of parameter values in the database.
Please refer to the appendix for the parameter definitions.

ANNEXE 5. Analyse des jeux de paramètres de la base de données par les boites à moustache : exemple de l'ASM1