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SELECTION OF ONE-DIMENSIONAL SEDIMENTATION: MODELS FOR ON-LINE USE

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ABSTRACT

A comparative study of several recently proposed one-dimensional sedimentation models has been made. This has been achieved by fitting these models to steady-state and dynamic concentration profiles obtained in a down-scaled secondary decanter. The models were evaluated with several *a posteriori* model selection criteria. Since the purpose of the modelling task is to do on-line simulations, the calculation time was used as one of the selection criteria. Finally, the practical identifiability of the models for the available data sets was also investigated. It could be concluded that the model of Takács *et al.* (1991) gave the most reliable results.

KEYWORDS

Activated sludge; cross-validation; identifiability; model selection; one dimensional models; on-line measurements; settling.

NOMENCLATURE

a	Parameter in the Otterpohl model (m^3/kg)	SVI	Sludge volume index (ml/g)
D	Effective diffusivity (Hamilton model) (m^2/h)	v_S	Settling velocity (m/h)
f_l	Fraction micro flocs (-)	v_u	Underflow velocity (m/h)
f_{ns}	Non-settleable fraction (-)	v_0	Parameter in the Takács model (m/h)
f_0	Parameter in the Otterpohl model (-)	v	Parameter in the Takács model (m/h)
h_0	Height of the inlet (m)	$WSSQ$	Weighted residual sum of squares (-)
K_{hyd}	Parameter in the Dupont model (kg/m^3)	X	Concentration of activated sludge (kg/m^3)
K_{NO3}	Parameter in the Dupont model (kg/m^3)	X_{AT}	Influent concentration of the decanter (kg/m^3)
m	Number of layers (-)	X_{eff}	Effluent concentration (kg/m^3)
n	Parameter in the Vesilind model (m^3/kg)	X_F	Parameter in the Dupont model (kg/m^3)
n'	Parameter in the Cole model (-)	X_{hyd}	Parameter in the Dupont model (kg/m^3)
N	Number of data (-)	X_{min}	Minimum non-settleable concentration (kg/m^3)
p	Number of parameters (-)	X_{NO3}	Concentration of NO (kg/m^3)
Q	Flow rate (l/h)	$X_{NO3,M}$	Non-settleable concentration due to NO (kg/m^3)
R	Recycle ratio (-)	z	Length coordinate (m)
r_h	Settling parameter in the Takács model (m^3/kg)	α	Parameter in the Vesilind model (m/h)
r_p	Settling parameter in the Takács model (m^3/kg)	α'	Parameter in the Cole model (m^4/kg•h)
N_L	Limiting flux (kg/m^2•h)	Ω	Omega function of Härtel and Pöpel (-)

INTRODUCTION

The activated sludge process is the most widely used process for the purification of wastewater. Since it is a biological system, model parameters are highly time varying. Therefore, it is often desirable to perform an (adaptive) control to anticipate changes inherent in the process. An efficient control can also contribute in optimizing the performance of an existing plant and might allow us to avoid conservative design of new plants. The main bottleneck in controlling activated sludge plants is the lack of reliable on-line sensors (Vanrolleghem and Verstraete, 1993; Harremoës *et al.*, 1993). This deficiency is particularly striking for the secondary clarifier, which is nevertheless a very important process unit (STORA, 1981; Severin *et al.*, 1985; Billmeier, 1992). Hence, a lot of current research is focused on the development of reliable on-line sensors for the sedimentation process (Sekine *et al.*, 1989; Henze *et al.*, 1993; Reid and Nason, 1993; Watanabe *et al.*, 1994).

Figure 1 represents the scheme of a novel on-line sensor for the final settler based on image analysis of activated sludge samples taken from different heights of a model secondary clarifier (Grijspeerdt, 1993). This sensor provides, among others, a one-dimensional concentration profile of the settler as a function of time (the data points are distributed in time and space). To extract as much information as possible from these curves and to be able to predict the behaviour of the system for control purposes it is desirable to fit a mathematical model to this data (Van Impe *et al.*, 1992). Several sedimentation models for activated sludge have been developed. It was therefore necessary to make a preselection. In view of the specific nature of the data, one-dimensional models seemed the most appropriate for the task. The recently developed two-dimensional models (Krebs, 1991) are undoubtedly more accurate, but identification is very time-consuming and the model is difficult to verify.

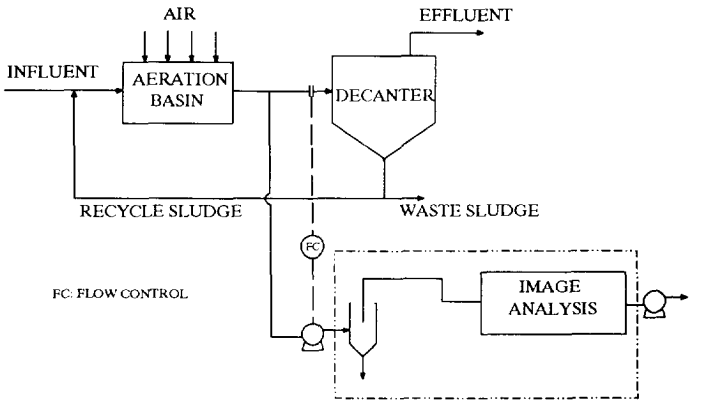

Fig. 1. Schematic overview of an on-line sensor for the sedimentation process (Grijspeerdt, 1993).

The study was organized as follows. To make a selection between the models, all were fitted to the data. Subsequently, the fit was evaluated based on different criteria which not only consider the model fit, but also the complexity of the model. This approach is the so-called *a posteriori* technique, in contrast with *a priori* methods, which select on the basis of certain parameter invariant characteristics of the models (Vanrolleghem *et al.*, 1994). At this point, the latter seems not to be usable in this case because the chosen models all predict more or less the same profile (Grijspeerdt, 1993). The necessity for on-line interpretation of the data imposes an additional constraint for model selection: the parameter estimation should proceed as fast as possible. Finally, practical identifiability of the models, i.e., can the parameters be given a unique value based on the available data, is at least as important as the above-mentioned criteria. Indeed, if the parameters are correlated, their physical meaning is limited.

MATHEMATICAL MODELS

Solid flux theory

All the models used for the study are based on the solid flux theory, as described by Kynch (1952). This theory says that the sedimentation velocity for a suspension varies only with the initial concentration in the regime of hindered settling. Based on this postulate, an analysis of continuous sedimentation can be performed (Marsili-Libelli, 1993). To conclude the mathematical description of sedimentation, it is necessary to propose a functional relationship between v_S and X. Several models can be found in the literature, but in practice the power model of Cole and the exponential model of Vesilind are most used (Cho *et al.*, 1993).

Power model:

$$v_S = \alpha' \cdot X^{-n'} \tag{1}$$

Exponential model:

$$v_S = \alpha \cdot e^{-n X} \tag{2}$$

Usually, the Vesilind model is considered to be more accurate (Smollen and Ekama, 1984). However, it has the disadvantage that numerical procedures are needed for further mathematical analysis.

Description of the models

The reader is referred to the literature for a detailed description of the models. In the following, a brief description of the models and their parameters is given. The same notation as in the original articles is used as much as possible.

Model of Laikari (1989)

This dynamic model divides the clarifier into m horizontal layers, which are all completely mixed. Laikari (1989) only regarded the zone below the inlet, but in this paper the model is extended for the whole clarifier. The model is constructed by considering the continuity equation for the sludge over each layer. If the limiting flux N_L is exceeded for a certain layer, the surplus of sludge in the layer is transferred to the layer just above. v_S is described by the power model, but α' is changed depending on the position of the sludge blanket, to model flocculation effects that are dependent of the height of sedimentation. The sedimentation tank is divided into four equal volumes where α' gets the value 1.3, 2.5, 3.3 or 3.9 m/h respectively, depending on the position of the sludge blanket. Laikari (1989) proposes the value 1.8 for the power coefficient n'.

Model of Takács *et al.* (1991)

This model is based on the same principles as the Laikari model: the clarifier is divided into horizontal layers and the mass balance is calculated for each layer. The novelty of this model is the fact that an expression is proposed for v_S which is valid for both the thickening and the clarification zones. In the upper layers, v_S can be related to X through a double exponential function due to the operational constraints of the clarifiers (Patry and Takács, 1992). This generalized settling velocity model contains five parameters (Table 1). The incoming flux in a certain layer is determined as the minimum of the flux in the layer just above and the flux in the layer itself. If X is lower than a threshold value (Takács *et al.* (1991) suggested a value of 3 kg/m^3), this condition does not hold, because it is assumed that no hindered settling occurs.

Table 1. Model parameters as found by Takács *et al.* (1991) for a specific case.Model of Otterpohl and Freund (1992)

v_0	v_0'	r_p	r_h	f_{ns}
8.9	6.25	5.7	0.36	$1.23 \cdot 10^{-3}$

Model of Otterpohl and Freund (1992)

This model continues the work of Härtel and Pöpel (1992) for the thickening of activated sludge. The settling flux is multiplied with a correcting Ω-function to describe transition and compression effects. Ω is dependent of SVI, h_0, X_{AT} and the position in the clarifier. Otterpohl and Freund (1992) partition the sludge flocs into micro and macro flocs, with the limit between the two at 10 Nm. The fraction of micro flocs can be calculated from X_{AT} with eq. (3):

$$f_l = f_0 \cdot e^{-a X_{AT}} \tag{3}$$

The settling velocity of the micro flocs is considered constant at 0.01 m/h. The macro flocs settle according to a modified Vesilind law:

$$v_S = (17.4 \cdot e^{-0,00581 \cdot SVI} + 3.931) e^{-(-0.9834 \cdot e^{-0.00581 \cdot SVI} + 1.043)X} \tag{4}$$

The model equations are constructed analogously as in Takács *et al.* (1991), but twice as many equations are needed for the same number of layers. Although this model is quite complicated, there are only a limited number of parameters. Suggested values for these are 0.04 for f_0 and 0.78 m^3/kg for a. The most important parameter is undoubtedly the *SVI*, which can be determined experimentally or by model fitting.

Combination of Takács and Otterpohl model

It was suspected that the Takács model was not really accurate for the simulation of the compression zone. So for this study, a model was constructed that consisted of the Takács model combined with the Ω-function as used in the Otterpohl model. It was believed that this correcting function could give better results.

Model of Dupont and Henze (1992)

In this model, v_S is modelled according to Vesilind. The clarifier is divided into horizontal layers. Similar to the method of Laikari (1989), the limiting flux is calculated for each layer and compared with the applied flux. Because it is not possible to obtain an analytical solution for N_L, this needs to be done numerically. Dupont and Henze (1992) do not mention the numerical method used, but in this study a combined Newton-Raphson-bisection method was used (Press *et al.*, 1992).

A model is proposed to relate the effluent concentration X_{eff} with X_{AT}, derived from empirical observation and conceptual ideas. Based on the influent characteristics of the clarifier, a non-settleable concentration can be derived:

$$X_F = X_{\min} + X_{NO_3,M} \frac{X_{NO_3}}{K_{NO_3} + X_{NO_3}} + X_{hyd} \frac{X_{AT} \cdot SVI \frac{Q(1+r)}{A}}{K_{hyd} + X_{AT} \cdot SVI \frac{Q(1+r)}{A}} \tag{5}$$

This expression collects the sludge that will not settle due to denitrification, hydraulic load and the sludge characteristics. X_F goes through all the layers above the inlet, to model the hydraulic retention time. Proposed parameter values can be found in Table 2.

Table 2. Suggested parameter values for the model of Dupont and Henze (1992)

X_{min}	$X_{NO3,M}$	K_{NO3}	X_{hyd}	K_{hyd}	α	n
$5 \cdot 10^{-3}$	$25 \cdot 10^{-3}$	$12 \cdot 10^{-3}$	$25 \cdot 10^{-3}$	$6.25 \cdot 10^{-2}$	5.71	0.37

Model of Hamilton *et al.* (1992)

This model starts from the following partial differential equation:

$$\frac{\partial X}{\partial t} = -\frac{\partial S_g}{\partial z} + v_u \frac{\partial X}{\partial z} + D \frac{\partial^2 X}{\partial z^2} \tag{6}$$

The addition of an effective diffusion term provides for extra mixing (Levenspiel, 1984) and a more smooth concentration profile. The model is constructed in the same way as the other models: the mass balance equation is discretized by dividing the settler into a number of horizontal layers. v_S is described by the Vesilind model. Suggested model parameters are 15.4 m/h for α, 0.416 m^3/kg for n and 0.54 m^2/h for D.

MATERIALS AND METHODS

The concentration profiles were determined using a model secondary clarifier, able to simulate full-scale behaviour (Grijspeerdt, 1993). A schematic overview of this decanter with the relevant dimensions is given in Figure 2. A stirrer is installed to prevent wall effects. Sludge samples were collected at different heights with a telescopic tube. In the neighbourhood of the sludge blanket, more samples were taken. The sludge concentration of the samples was determined using an image analysis system (Digithurst, UK) coupled with a stereo microscope (magnification of 50x) according to Grijspeerdt (1993). This method has the advantage of combining fast measurements (±five minutes) with acceptable errors (±10%). Because the data were not evenly distributed in space, the models were adapted by considering non-equal layer volumes.

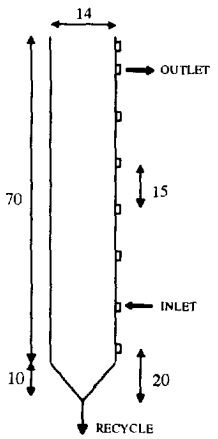

Fig. 2. Scheme of the lab scale decanter. Dimensions are given in cm.

The models were integrated with an embedded Runge-Kutta algorithm (Press *et al.*, 1992). Parameters were estimated by minimizing the residual sum of squared errors (*WSSQ*) weighted by the variance (with X as independent variable) by using Brent's modification of Powell's direction set algorithm (Powell, 1964; Brent, 1973). Several conventional *a posteriori* model selection criteria were evaluated (Ljung, 1987; Vanrolleghem *et al.*, 1994). These criteria take one of the following two forms:

$$\frac{WSSQ}{N}[1+\beta(N,p)] \tag{7}$$

$$N.\log\left(\frac{WSSQ}{N}\right)+\gamma(N,p) \tag{8}$$

For both cases, the first term decreases for a better fit while the second term penalizes overparametrized models. Hence, a compromise is sought between fit and complexity. Different authors have presented several functional forms for ß and γ. The two best known are the Final Prediction Error (*FPE*), with ß $(N, p) = 2\ p/(N\text{-}p)$, and Aikake's Information Criterion (*AIC*), with $\gamma(N, p) = 2\ p$. Another criterion is the Baysian Information Criterion (*BIC*) that uses $\gamma(N, p) = p \cdot \log(N)$. The last criterion evaluated in this study is *LILC*, where $\gamma(N, p) = p \cdot \log(\log(N))$.

The identifications were done on a 486/66 MHz PC. The CPU times needed were collected and served as an additional criterion. The identifiability problem was addressed by considering the rank of the Fisher information matrix, which is the inverse of the covariance matrix. It is known that if this matrix is not full rank, the parameters are not identifiable for the given data set (Ljung, 1987).

STEADY-STATE EXPERIMENTS

Ten concentration profile data sets were collected using the method described above. For all these sets, ten different heights were sampled under steady state conditions. The sludge used was collected from the wastewater treatment plant of the Maria Midellares Hospital of Gent. This sludge had an *SVI* ranging from 100 to 150 ml/g. Steady state is not easy to obtain with biological systems, but it was supposed that after 24 h of the same conditions the decanter was operating under steady state. The influent flow rate Q was varied between 7.5 and 14.7 l/h, the recycle ratio R between 0.41 and 1.12 and X_{AT} between 3.9 and 6.6 kg/m^3. A typical concentration profile, together with the simulated curves can be found in Figures 3 and 4.

MODEL SELECTION

The six models were fitted to the ten data sets using the previously mentioned procedure. Ten layers were used for all the models. Typical results are summarized in Figures 3 and 4. It is striking that all models have difficulties with the simulation of the thickening zone, which is indeed a phenomenon very difficult to model (Anderson and Hanson, 1972). Besides this, the fit is remarkably good. Table 3 summarizes the mean value of the criteria for all the experiments. After examination of the results it is clear that only two models are left in the running: the model of Takács *et al.* (1991) and the model of Hamilton *et al.* (1992). Therefore, only the results for these models were represented in Figures 5 and 6. Figure 5 shows the values of the *FPE* for all the experiments. The other criteria revealed the same trends (data not shown). Figure 6 represents the CPU-times needed for the minimization. Table 4 summarizes the findings of the identifiability test.

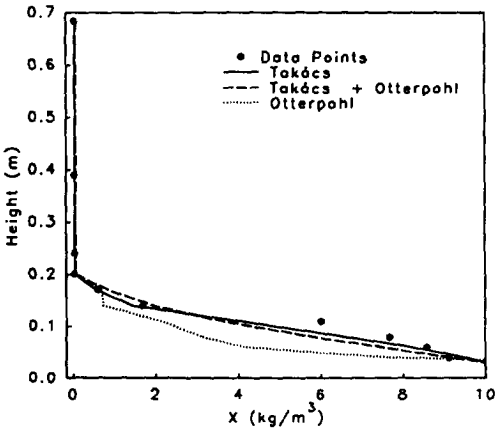

Fig. 3. Simulation results for the Takács and Otterpohl models and the combination of both.

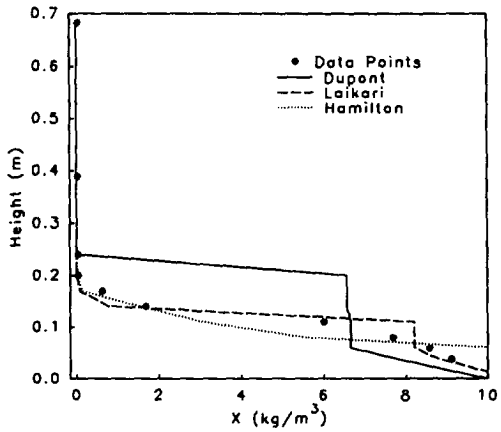

Fig. 4. Simulation results for the Dupont, Laikari and Hamilton models.

Table 3. The mean value for the different criteria for all the experiments (N=10)

Model	*WSSQ*	*FPE*	*AIC*	*BIC*	*LILC*
Takács	330	99	23	18	13
Takács+Otterpohl	1155	462	32	29	33
Otterpohl	2554	596	31	26	24
Dupont	325	617	44	29	31
Laikari	1000	400	34	24	22
Hamilton	528	98	21	17	14

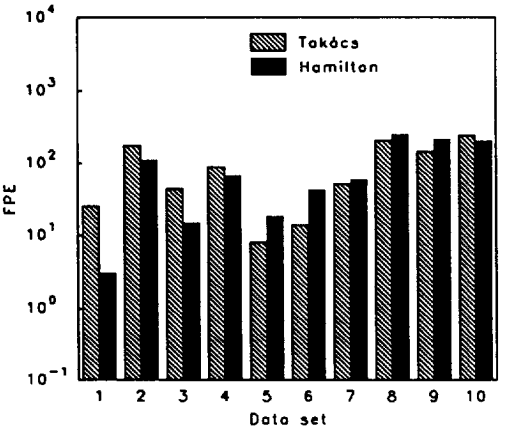

Fig. 5. Evolution of AIC for the Takács and Hamilton models.

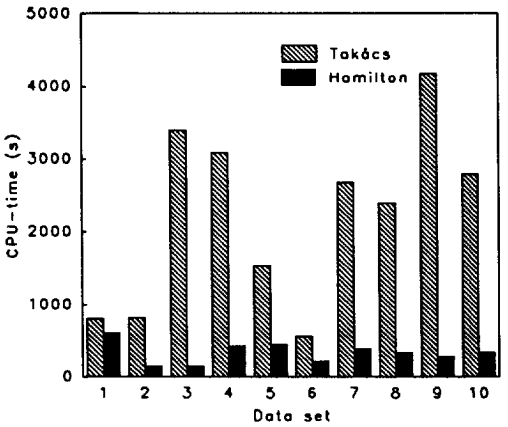

Figure 6. Evolution of the CPU time for the Takács and Hamlton models.

Table 4. The practical identifiability for the different models. (+ is identifiable; - is unidentifiable)

Data set → / Model ↓	1	2	3	4	5	6	7	8	9	10
Takács	-	+	-	+	+	+	+	+	+	+
Takács + Otterpohl	-	+	-	-	+	+	+	-	+	-
Otterpohl	+	-	-	+	+	-	+	-	-	-
Dupont	-	-	-	+	-	-	+	-	-	+
Laikari	-	-	+	+	+	+	+	+	+	+
Hamilton	+	-	+	+	+	+	+	+	+	+

It has to be remarked that in general the Takács model gives better fits in terms of absolute values of the WRSSQ. The Hamilton-model is favoured because only three parameters have to be estimated versus five for the Takács model.

Considering the identifiability problem, it is clear from Table 4 that these two models also give acceptable results here. It is worthwhile to mention that the simulation results with the Hamilton model are very sensitive to the effective diffusivity D. In one way, this is an advantage for the identification process, but

offers certain dangers in terms of physical interpretation. Evaluation of the CPU times points to the Hamilton-model as best, which could be expected since it has only three parameters. However, the time needed for the identification of the Takács model is still within acceptable limits for on-line purposes.

CROSS-VALIDATION

Because it can be expected that a model will perform well on the data set to which it was fitted, it was decided to do an additional cross-validation on the two remaining models. Cross-validation is a pragmatic *a posteriori* approach where two (or more) models are evaluated for their ability to fit to fresh data (Ljung, 1987). The procedure used here was to fit the two models to two subsequent steady state data sets. Because the parameters must be (short-term) invariant, they should remain constant. If this is not the case, it can be concluded that the model structure is not adequate and changes in operational conditions are compensated by changes in parameter values. Naturally, such behaviour is unwanted for physical models.

Table 5. Parameter values for the cross-validation experiments

Model →	Takács					Hamilton		
Data set ↓	v_0	v_0'	r_p	r_h	f_{ns}	α	n	D
1	5.87	3.60	0.43	0.96	0.099	2.60	0.29	$2.0 \cdot 10^{-1}$
	5.87	3.60	0.42	0.97	0.098	2.56	0.17	$1.1 \cdot 10^{-1}$
2	4.12	2.51	0.53	1.01	0.16	5.20	0.54	$6.9 \cdot 10^{-3}$
	4.23	2.88	0.58	0.99	0.19	2.67	0.44	$6.8 \cdot 10^{-2}$
3	5.56	3.16	0.57	2.23	0.41	3.38	0.46	$9.0 \cdot 10^{-3}$
	5.12	3.20	0.53	2.00	0.36	2.82	0.63	$1.5 \cdot 10^{-2}$

The cross-validation procedure was carried out three times, each time using two data sets. Q was varied from 5.6 to 8.3, 6.9 to 8.6 and 8.7 to 7.9 l/h, and R from 0.6 to 0.4, 0.8 to 0.5 and 0.8 to 0.6 respectively. Because the biological process is inherently time-varying in the parameters, not more than two data sets were used, so the parameter values could be expected to be constant during the limited time span of the experiment. The identification results for this experiment are summarized in Table 5. It is clear that the Hamilton model did not pass this test, since the diffusivity D changes drastically, up to a factor ten. These results point strongly to the use of the Takács model, where the parameters remained fairly constant.

DYNAMIC EXPERIMENTS

Four dynamic concentration profiles were collected by measuring the concentration profile in the decanter as a function of height and time after a disturbance of an initial steady-state. The sludge used (the *SVI* ranged from 75-130) was obtained from a pilot plant treating synthetic wastewater. This disturbance was achieved by imposing a step change in Q and/or R. The parameter estimation was restricted to the Takács and Hamilton models, in view of the results obtained after the steady state analysis. The same *a posteriori* procedure was used for the comparison of the two models. A typical model fitting result for the Takács model is presented in Figure 7, from which it can be seen that the model simulates satisfactorily the transient behaviour. The *FPE* and *CPU* values are summarized in Figures 8 and 9. In contrast to the steady-state results, it is clear that the Takács-model gives better results with respect to the fitting of the data. This confirms that the Takács model possesses a higher flexibility to describe the behavior under the changing conditions imposed by the dynamic experiments. However, the calculation times are substantially higher than for the Hamilton-model, a clear disadvantage for on-line purposes. Practical identifiability was good for both models. No cross-validation was done in this case, due to the constraints imposed by the time-consuming nature of the experiments.

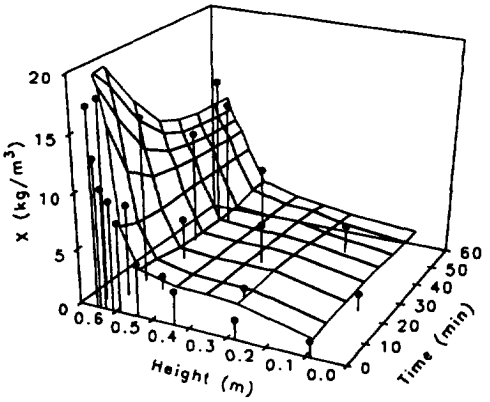

Figure 7. Simulated profile (Takács model) and experimental points for a dynamic experiment.

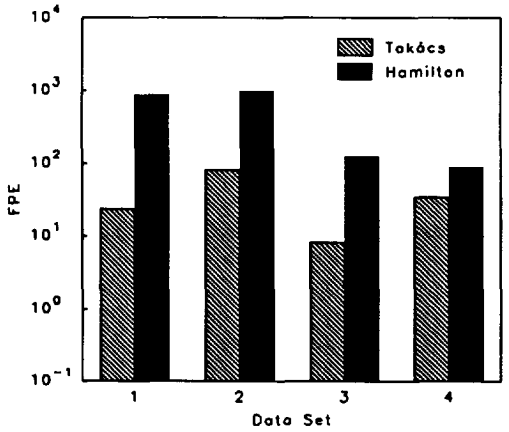

Figure 8. The FPE criterion for the dynamic experiment

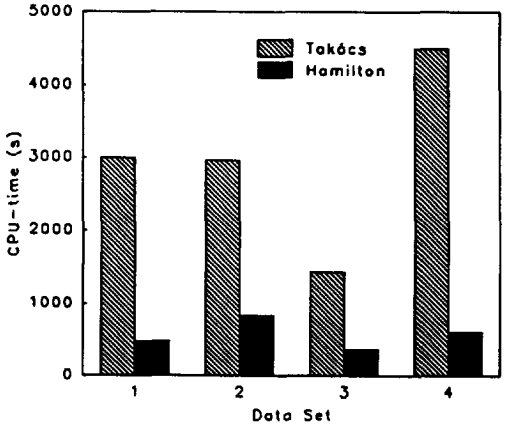

Figure 9. The CPU times needed for the parameter estimation based on dynamic measures.

CONCLUSION

It can be concluded that the Takács model is the most reliable to fit the data, both for steady state and dynamic conditions. The main disadvantage of this model is the relatively long calculation time required for convergence. Future research should focus on the long-term behaviour of the model, i.e., the variability of the parameters as a function of time, and their relation to the settling properties of different sludges. To minimize computing time, adaptive minimization schemes should be investigated.

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