WEST, a general tool for dynamic modelling and simulation (e.g. biodegradation processes)

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INTRODUCTION

- Mechanistic models can be used to improve our understanding of biological processes (e.g. biodegradation).
- These models often consist of differential equations which cannot be solved by many available software tools.
- A tool is needed to easily handle these kind of equations.

WEST:

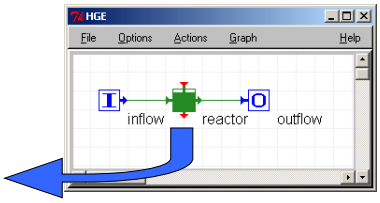
Set of algebraic and differential equations

Ex. Single Monod:

$$\frac{dS}{dt} = -\left(\mu_{max} \cdot \frac{S}{K_S + S}\right)\frac{X}{Y} + \frac{Q}{V}(S_{in} - S)$$

$$\frac{dX}{dt} = -\left(\mu_{max} \cdot \frac{S}{K_S + S}\right) \cdot X + \frac{Q}{V}(X_{in} - X)$$

WEST Modelling Environment



MSL (user friendly modelling language):

```
DERIV(state.S,independent.t) = - ( parameters.mumax * state.S / ( parameters.Ks +
state.S )) * state.X / parameters.Y + state.Q / state.V * (state.Sin - state.S);

DERIV(state.X,independent.t) = - ( parameters.mumax * state.S / ( parameters.Ks +
state.S )) * state.X + state.Q / state.V * (state.Xin - state.X);
```

Parser (transform MSL code to C++)

C++

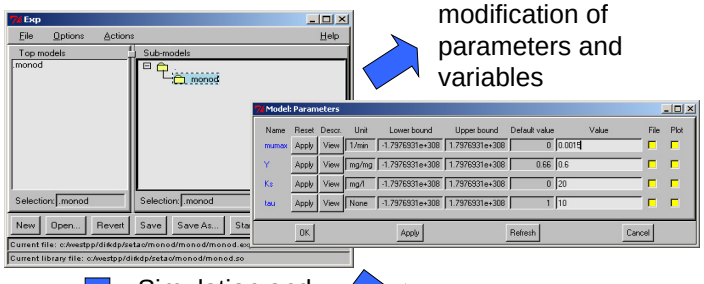
Compiler

Object library (dll)

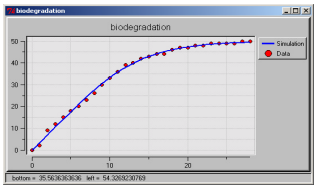
Automatic process, no user interaction required ! (Vangheluwe, 2000)

WEST Experimentation Environment

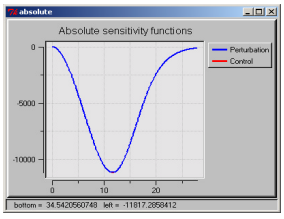
Easy navigation and modification of parameters and variables



Simulation and Optimisation



Sensitivity Analysis



Reference:

Vangheluwe, H.L. (2000). Multi-Formalism Modelling and Simulation. DSc Thesis, Faculty of Sciences. Ghent University. Ghent.

Applications:

Finding an alternative for the 10-day window criterion through kinetic information obtained by modelling

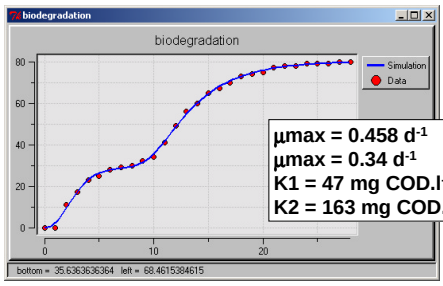
Mechanistic models
- Single Monod
- Double Monod

↓ Parameters have physical meaning

Non-mechanistic models
- First order
- Gompertz
- Chapman

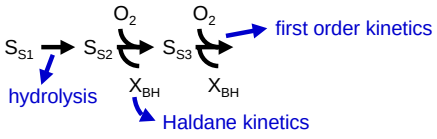
↓ Parameters have **no** physical meaning

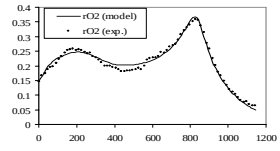
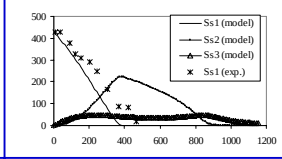
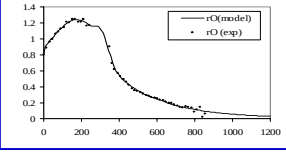
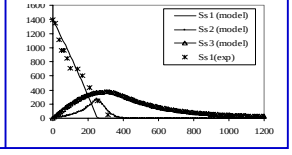
Example: Double-Monod mechanistic model fitted to biodegradation data (OECD 301F)



Modelling of activated sludge acclimisation to a non-ionic surfactant

- SBR (Sequencing Batch Reactor) using non-acclimatised sludge
- non-ionic surfactant as sole carbon source
- Implemented model based on three sequentially degraded fractions:



	Simulated and measured respiration rates	Simulated COD fractions and measurements
SBR cycle 1		
SBR cycle 5		

Other applications

- Wastewater treatment
- River quality modelling
- Compartmental models (e.g. for chemical fate in species & environment)

TAKE HOME MESSAGE

- WEST is a powerfull tool for solving differential equations often present in mechanistic models describing biological and chemical systems.
- WEST has different experiment types like: simulation, optimisation, sensitivity analysis, ...
- WEST helps understanding and opens up new perspectives for the investigation of biological and chemical processes.