

# Advanced Process Modelling for Biotreatment processes

*“The power and flexibility of the gPROMS® environment and the expert ModelCare® consulting support have allowed us to develop a state-of-the-art model for a complex process with minimum time and effort”*

– **Steve Pietsch**

Senior Research Associate  
BP Chemicals



Wastewater treatment processes are used to degrade industrial and municipal organic waste and render it innocuous by converting it to water, CO<sub>2</sub> and disposable sludge.

A key challenge in operation of such processes is response to upsets. By its very nature, at end of production processes, the waste treatment system is subject to wide variation in feed rates and composition. Because of the dynamics of microbial population growth, difficulties in operation can translate into downtime in the upstream processes with potential significant losses in production.

The dynamics of such processes which give rise to operational difficulties are difficult to predict without rigorous modelling of the chemistry and kinetics.

Detailed dynamic modelling can be used during both the process design phase and afterwards to predict the process response and then optimise equipment and process control schemes.

## The PSE solution

PSE's Advanced Process Models for Biotreatment, implemented in PSE's state-of-the-art gPROMS process modelling package, are designed specifically to address these challenges. The models consider rigorous chemistry, thermodynamics and kinetics simultaneously in order to provide accurate prediction of performance.

*“The models consider rigorous chemistry, thermodynamics and kinetics simultaneously, for both steady-state and dynamics”*

gPROMS provides modelling power suitable for both steady-state and dynamic analysis of the reaction and separation aspects of the system. It includes many unique and powerful features not found in other water treatment software:

- **Automatic generation** of all stoichiometrically-balanced heterotrophic and autotrophic **reactions** from definition of the substrate(s) alone (via MS Excel).
- **Estimation of parameters for biochemical kinetics** for various reactions from experimental data, including a full statistical significance analysis of the quality of these estimates.

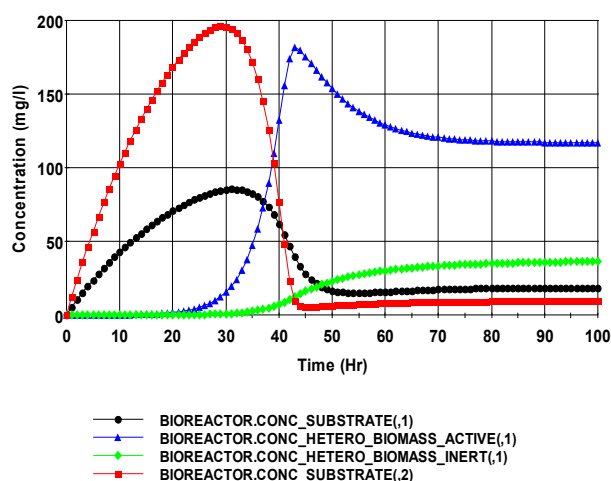
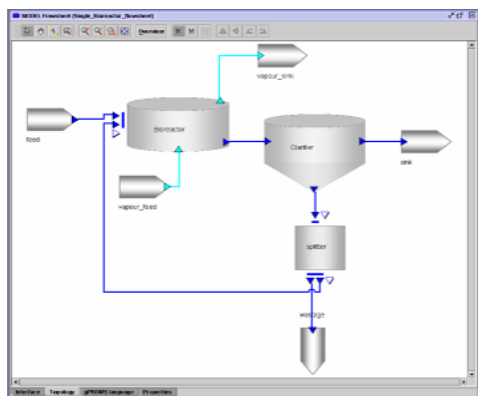
- **Design of optimal experiments** to determine these parameters, aimed at producing the maximum amount of information for parameter estimation and model discrimination from the minimum possible number of experiments.
- **Dynamic and steady-state simulation** of process operation allows you to investigate a wide range of static and dynamic effects.
- **Rigorous mathematical optimisation** to establish optimal designs of treatment units and their control systems, and to derive optimal steady-state and/or dynamic operating procedures while satisfying all important constraints.
- **Model library.** The Bioreactor Library provides standard models, including Bioreactors, Clarifiers and common flowsheet combinations such as those used for conventional activated sludge.
- **Open models.** Unlike other “black box” models, gPROMS allows you to inspect and modify the mathematics describing the chemistry, thermodynamics, kinetics, mass transfer and all other defining equations.
- **Choice of physical property** methods, including the OLI Electrolyte package, Multiflash and any Cape-Open package such as Aspen Properties Plus™.
- **Customisation.** Users can substitute their own equations, amend the existing equations, or create an entirely new model for a specific proprietary unit.

PSE's Biotreatment Advanced Process Models help give definitive answers to **complex questions**:

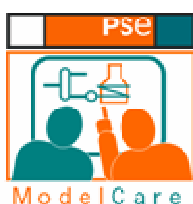
- What is the complete atomic accountability for up to fifty degradable substrates including exact nutrient usage, CO<sub>2</sub> generation, inorganic solid formation and tracking of VOCs?
- What is the optimum pH control scheme to minimise reagent usage and promote microbial growth?
- How will the process respond to startup, shutdown and shock loads?
- How will I optimise the number of bioreactors, their size and the oxygen injection points?

## Biotreatment example

The single-bioreactor process (shown in the gPROMS flowsheet diagram) was executed for a two-substrate process feed. The plot below shows the dynamic behaviour of the bioreactor startup.



## PSE ModelCare



PSE's **ModelCare** consulting service can provide expert assistance in constructing sophisticated models of any type of process. We can also assist in formally validating these against data, and advise on any experiments required. ModelCare is specifically designed to help you or your specialists to implement robust, detailed models in the minimum of time, while ensuring a handover of custom modelling know-how to your organisation.

