

High-accuracy predictive modelling of biotreatment systems

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The biotreatment capability of gPROMS provides a rigorous and flexible approach to modelling activated sludge processes. An Advanced Model Solution (AMS) for the Bioreactor and the Clarifier is available in the gPROMS Bioreactor Library. These models can be used to model various activated sludge configurations or a standard activated sludge configuration can be selected from the Bioreactor Library. Kinetics parameters can be estimated and experiments designed within gPROMS. The models can be used for dynamic and steady-state simulation and the gPROMS model can be used to optimize both process design and operation.

Why gPROMS?

There are several software packages available for simulation of waste water treatment processes. So, why is gPROMS a better alternative? gPROMS offers a unique combination of modelling flexibility and power. Standard models are available from the Bioreactor Library for Bioreactors and Clarifiers. Common flowsheet combinations such as conventional activated sludge are also available. Unlike the typical software package, gPROMS allows the user to access the basic mathematical models describing the chemistry, thermodynamics, kinetics, mass transfer and all other defining equations. The user can substitute their own equations, amend the existing equations, or create an entirely new model that represents a specific proprietary unit. Unlike other “closed” models which are black boxes to the user, gPROMS allows you direct access to the model if desired, or you may use of the standard models without ever viewing a single equation.

A vital part of using gPROMS involves the Process Model Library (PML). The gPROMS PML is a collection of models of commonly used processing equipment and controls. gPROMS is designed to enable you to quickly construct process flowsheet models that are suitable for use in steady-state and dynamic simulation, parameter estimation and optimization studies. By simply dragging the units onto the flowsheet and dropping them at their desired location, a flowsheet may be easily assembled from the models in the Bioreactor Library, the PML or your own company library of proprietary models.

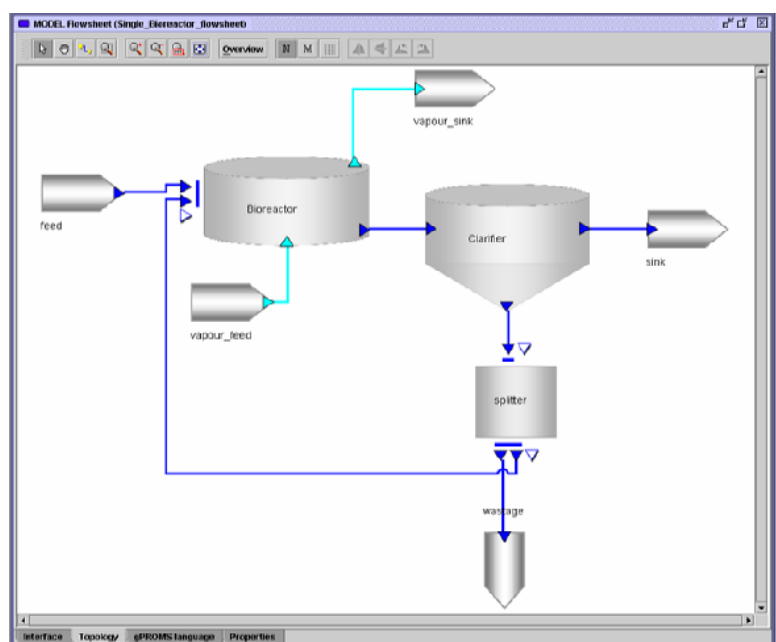


Fig. 1 gPROMS single-bioreactor flowsheet
The model company

Connections between units are also easily completed by the same drag-and-drop procedure. The gPROMS Bioreactor is significantly more rigorous in its treatment of the solution chemistry and the reaction kinetics. Because the model is based upon balanced heterotrophic and autotrophic reactions, the exact depletion and production can be determined for substrates and solution species such as CO₂, NH₃, O₂, N₂, HNO₃, HNO₂, HCl, sulphur and phosphorus compounds. Not only does this provide a mass balance at the atomic level, but it allows for computation of pH, oxygen solubility, free ammonia, undissociated nitrous acid, and free cations which may be toxic to the microorganisms. It also provides an accurate means of predicting inorganic solid formation (e.g., CaCO₃) and volatile organic compound (VOC) release.

The kinetics models originate with the ASM1 (2) and ASM3 (3) models, but many enhancements have been made including multiple substrates, self-inhibition and Han & Levenspiel inhibition, and sequential nitrification reactions. The standard kinetics models are described below, but specialized models are easily incorporated into the models.

Among the unique capabilities included in gPROMS are Optimal Experiment Design and Parameter Estimation. Once the process model has been assembled, the user can design the experiments which will optimally provide the data necessary to regress model parameters. The advanced Optimal Experiment Design algorithm in gPROMS makes experimental trial-and-error procedures passé, eliminating the time and expense of performing experiments which do not provide the data necessary to develop model parameters. Furthermore, once the experiments have been completed, the resulting data can be entered in the same process model and gPROMS will perform a Parameter Estimation to complete the process model or an individual Bioreactor model.

The process model, having been assembled and model parameters developed, it can be executed in either dynamic or steady-state mode. It is particularly helpful to perform a Dynamic Optimization on the process to determine optimum design and operating conditions without the need for a trial-and-error approach. Design optimization might include

- reactor and clarifier sizing
- process type and layout (CAS, SFAS, ...)
- air injection points
- number of bioreactors

The Mixed Integer Optimization capability of gPROMS allows one to optimize the integral number of bioreactors and location of air injection points and bioreactors. Operating conditions which might be optimized include

- pH control and reagent usage
- effluent quality
- wastage volume/SRT
- step-feed distribution
- air flow
- inorganic solid formation
- VOC release

The gPROMS model can be used to predict process response to

- start-up and shutdown
- upsets and shock loads

- control setpoint change
- operator action

gPROMS is a full-feature modelling and simulation tool which allows the user to model waste water treatment in the same modelling environment as used in all other parts of the process facility. New process operations such as a membrane bioreactor can be added by the user or the PSE technical and consulting staff. The open nature of gPROMS makes the modelling capabilities practically unlimited.

The gPROMS models are fully CAPE-OPEN. Once developed, they can be transported to other CAPE-OPEN software packages such as Excel, CFD software, ASPEN™, Simulink®, etc.

The bioreactor model

The work of McCarty (1) provides the link between the biological oxidation of organic and inorganic substrates and balanced chemical reactions. This allows the gPROMS AMS Bioreactor to account for all mass and energy without any simplifying assumptions since the substrates and microorganisms are represented in molecular form during growth and decay.

McCarty also discusses rate relationships, maximum utilization and yield. He does not, however, consider the combination of several reaction types and rate expressions in the model. The ASM models, Grady and others (2,3,4,5,6) provide more detail in describing the kinetics models and their interdependence. They include not only growth and decay constants, but also switching functions and other factors relevant to specific reaction types. The IWA ASM1 and ASM3 models (2,3) are the basis for the areas of heterotrophic aerobic, heterotrophic anoxic and autotrophic aerobic reactions. Implementation of heterotrophic anaerobic reactions and multiple substrate reactions are included in the gPROMS model. Further developments beyond the basic IWA models include multiple decay reactions (aerobic and anoxic), Andrews self-inhibition, Arrhenius temperature-dependent reaction constants, carbonate switching functions, Han & Levenspiel inhibition functions and sequential Nitrification reactions ($\text{NH}_3 \rightarrow \text{NO}_2 \rightarrow \text{NO}_3$).

McCarty's chemistry and ASM kinetics, however, are only as good as the thermodynamic equilibrium model which determines the conditions of each phase. Since gPROMS is a fully CAPE-OPEN system, you can select your own thermodynamics model to compute solution chemistry. This could be Multiflash, OLI Electrolyte model, or any other thermodynamic/database interface which is CAPE-OPEN compliant. gPROMS is capable of taking full advantage of accurate solution chemistry in determination of pH, temperature, ionic strength and liquid concentrations which greatly affect growth and decay rates. The buildup of free cations which may be toxic (e.g., copper and iron) can be accurately predicted. The evolution or disappearance of carbonates, nitrates, sulfates and amino compounds is easily monitored as well as the effects of these species on solution pH. Accurate vapor-liquid equilibrium conditions are also very important in determining stripping and volatilization of VOCs or reaction products. Prediction of free ammonia concentration and undissociated nitrous acid is necessary to compute the

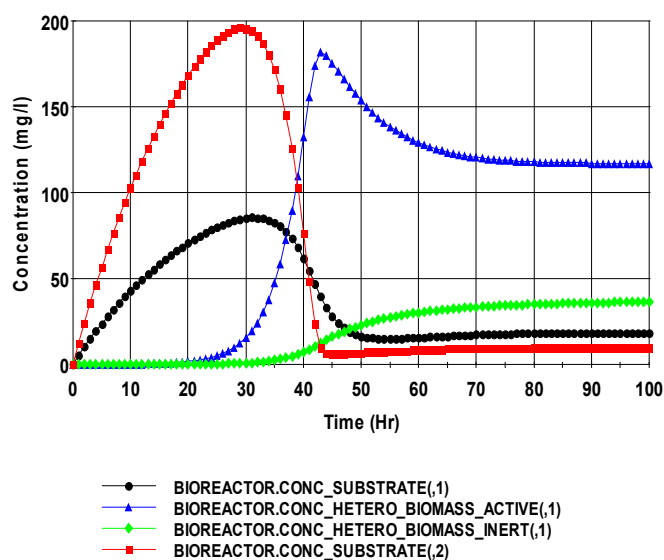


Fig. 2 Bioreactor start up
(Plot generated by gPROMS)

reaction rates for Nitrification reactions. gPROMS offers the opportunity of using outside thermodynamic packages with the specialized models developed by the user.

Using AMS biotreatment models

Substrate specification may be by specific molecule (e.g., phenol) or may be characterized as a "lumped" substrate in which the molecular weight, ThOD (COD), total organic carbon and/or total organic nitrogen are known. By specifying the stoichiometric quantities of C, H, O, N, Cl, S, and P, a statistical substrate molecule can be built using stoichiometric coefficients that need not be integers (e.g., $C_{5.2}H_{11.7}O_{1.2}N_{0.5}$). Multiple substrate cases may include both types simultaneously, allowing the user to identify all of the known molecules individually and lump the remainder.

The gPROMS Excel Bioreactor interface automatically derives the Synthesis, Energy and Decay stoichiometric relationships which may be heterotrophic and/or autotrophic. Heterotrophic reactions for each substrate include aerobic, anoxic and anaerobic reactions, while autotrophic reactions are aerobic. Reactions are characterized by such bioreaction constants as maximum specific growth rate, decay rate, half-saturation constants, yield coefficients, Andrews self-inhibition coefficients and Han & Levenspiel inhibition coefficients.

One of the most powerful capabilities of gPROMS is Parameter Estimation and Design of Optimal Experiments. These capabilities give the user unique opportunities to complete the biotreatment model by designing the experiments necessary to estimate parameters without leaving the gPROMS environment. Trial-and-error is eliminated providing the necessary model parameters at a minimum of computing and experimental expense.

Biotreatment process models

The basic Unit in a biotreatment process is the Bioreactor. The gPROMS Bioreactor is based upon a single CSTR model. Many configurations are possible such as multiple bioreactors, in series or parallel, intermediate feeds, step feeds, recirculation, process control loops including pH neutralization and oxygen saturation. Also available is a clarifier unit operation with or without suspended solids.

The Conventional Activated Sludge Process (CAS) shown here is available as a standard model in the gPROMS Bioreactor Library.

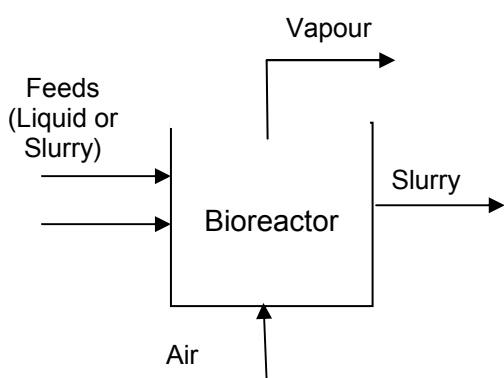


Fig. 3 Single gPROMS bioreactor

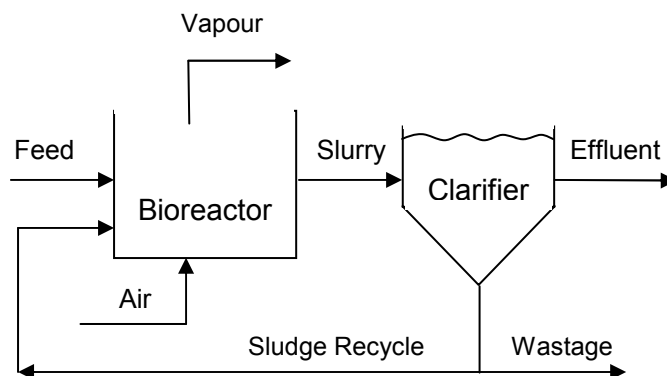


Fig. 4 Conventional Activated Sludge

An example of a process employing several of these capabilities is the Sequential Activated Sludge process with pH control on the anoxic bioreactor (shown below).

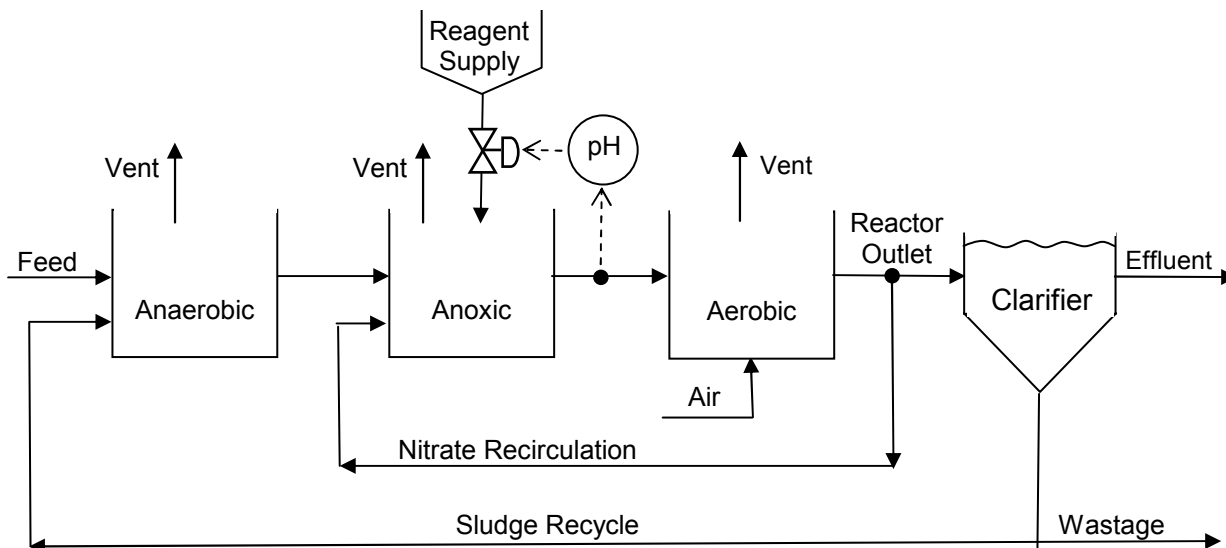


Fig. 5 Sequential Activated Sludge

Depending upon the bioreaction constants and the solution concentrations, different reactions may dominate in the bioreactor. For example, increased aeration will increase the aerobic reactions, both heterotrophic and autotrophic. While the growth portions of these reactions produce biomass, the energy portions utilize oxygen to oxidize the carbon-containing substrate (heterotrophic) and ammonia (autotrophic). When autotrophic reactions occur (nitrification) nitrates are produced. When nitrates are present anoxic reactions (denitrification) increase, removing nitrates and producing nitrogen gas which can have a stripping effect on the solution. When aeration is not employed, anoxic reactions can still occur if an external source of nitrate is provided, such as another aerated reactor. When neither aeration nor nitrates are provided, anaerobic reactions often dominate. The interdependence of multiple reactions and concentrations are accounted for automatically and accurately in the Bioreactor model.

The user can control the type of reaction environment desired by changing the air flow, nitrate flow, recycle flow, bioreaction constants or numerous other process specifications. Multiple bioreactors in series, with different reaction environments, can effectively model a sequential biotreatment process. Such a process may use anaerobic, anoxic and aerobic conditions in series to remove degradable substances efficiently.

Execution of the biotreatment model

gPROMS may be run in dynamic or steady-state mode. The feed to biotreatment processes is often scheduled and sometimes erratic, making dynamic simulation a necessity to assure continuous operation of the process. Considering the frequency of feed stream changes, including upsets and shock loads, the process is susceptible to microorganism death from starvation, toxic species concentrations or pH swings. The process effluent can produce undegraded organics in the liquid or vaporization of volatile organics if the process is not prepared to sustain the upsets. The gPROMS model gives you the opportunity to monitor the process conditions which would occur as a result potential upsets.

Furthermore, gPROMS allows for dynamic optimization of the process design and operation. This includes design issues such as bioreactor and clarifier sizing, process types and layout (CAS, SFAS, etc.), air injection points, and number of bioreactors. Mixed Integer Optimization is an effective means of optimizing the number of bioreactors or air injection points. Operating conditions are also easily optimized including pH control and reagent usage, effluent quality, wastage volume/SRT, step-feed distribution, air flow, inorganic solid formation and VOC release.

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