user story

Automated statistical analysis and calibration of advanced process models – integrating MoDS with gPROMS

Model-based engineering can shorten and optimise process design and development. **gPROMS** is a language for advanced process modelling used worldwide and widely recognised as the next-generation standard for **process modelling**. Once model **parameterisation** has been implemented to a process, **sensitivity analysis** and model **calibration** have to be carried out to either validate the model or identify optimal operating conditions and design specifications. CMCL's Model Development Suite (**MoDS**) uses advanced and robust statistical analysis techniques to perform local, as well as global sensitivity analysis, automate optimal model parameter estimation and speed up computation by generating surrogates of the original models.

THE CHALLENGE

- Perform rapid analysis of sensitive and uncertain model parameters for computationally intensive processes, in the presence of interdependencies and model discontinuities

- Speed up process simulation and automate model calibration for any given system

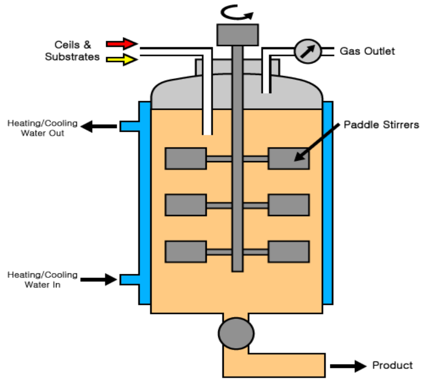


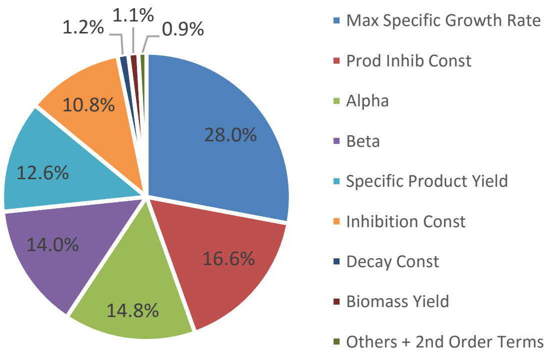
Figure 1: Representation of a fermenter with typical inputs and outputs.

SOLUTION – MoDS + gPROMS

gPROMS ModelBuilder, or another appropriate gPROMS family product, can be used to build or supply advanced and robust process models. These models can be exported and run within the gPROMS runtime object gO:RUN-xml. Via the gO:RUN-xml engine, MoDS can execute the exported "black-box" model, which does not require any modification.

When using the gO:Run-xml engine, an input xml file is created by the user and read by the gPROMS runtime object. MoDS is able to automatically write the input values into the xml file and perform advanced **statistical analysis** of the input and output spaces. Output files will be also created in the xml format by the runtime object for each set of values passed to it by MoDS. MoDS' flexibility in handling different types of input and output files, and its ability to run third party executables from any CAE tool or custom model, makes the integration with gPROMS-generated models straightforward.

The advanced input space sweeps performed by MoDS, for example using Sobol, Monte Carlo or other evaluators, is used to produce **surrogate models**, and also provide direct information on the outputs sensitivities and inputs uncertainty propagation. Single- or multi-objective **parameter identification** and **process optimisation** can be performed using MoDS on either the original or surrogate model.



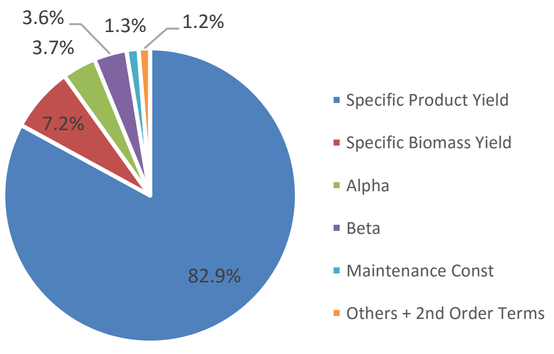


Figure 2: Sensitivity of fermentation product concentration and viable cell concentration to selected input values (Alpha and Beta are growth-related and non-growth-related product formation rates, i.e. $q_p = \alpha\mu + \beta$) for a fermenter.

RESULTS

The gPROMS model used here is taken from examples available in the gPROMS ModelBuilder installation package and simulates a fermenter, a representation of which is provided in **Figure 1**. The global sensitivity of fermentation product and viable cell concentrations to different input variables is presented in **Figure 2**. The optimal set of inputs required to achieve a specified product concentration target of 35 g/L is given in **Table 1**.

Table 1: Optimal input values computed using the Hooke-Jeeves algorithm for a target output of 35 g/L of fermentation product.

Input variable	Optimal value
Max Specific Growth Rate	0.47 1/hr
Saturation Const	1.25 g/L
Inhibition Const	21.7 g/L
Product Inhibition Const	46.3 g/L
Alpha	2.34
Beta	0.21 1/hr
Specific Biomass Yield	0.36
Specific Product Yield	0.49
Maintenance Const	0.10 1/hr
Decay Const	0.01 1/hr

Variables' dependencies are represented in **Figure 3**. In this figure a screenshot of MoDS' outputs shows, for example, the relation between the fermentation product concentration and a selection of input variables, such as maximum specific growth rate, saturation constant, etc. (second raw of the diagram). The global sensitivities (performed on a total of 55 first and second order inputs), the correlations presented in **Figure 3** and the optimal parameters listed in **Table 1** were calculated on a 3.40 GHz multi-core work station in approximately 8 minutes using 1000 Sobol points.

SUMMARY

• First-principles models are written in gPROMS and then integrated with MoDS to perform advanced statistical analysis and produce fast-response surrogate models

• Global sensitivity studies and uncertainty propagation analysis are performed on the process model

• Single- and multi-objective optimisation routines are used in MoDS for model calibration and process optimisation

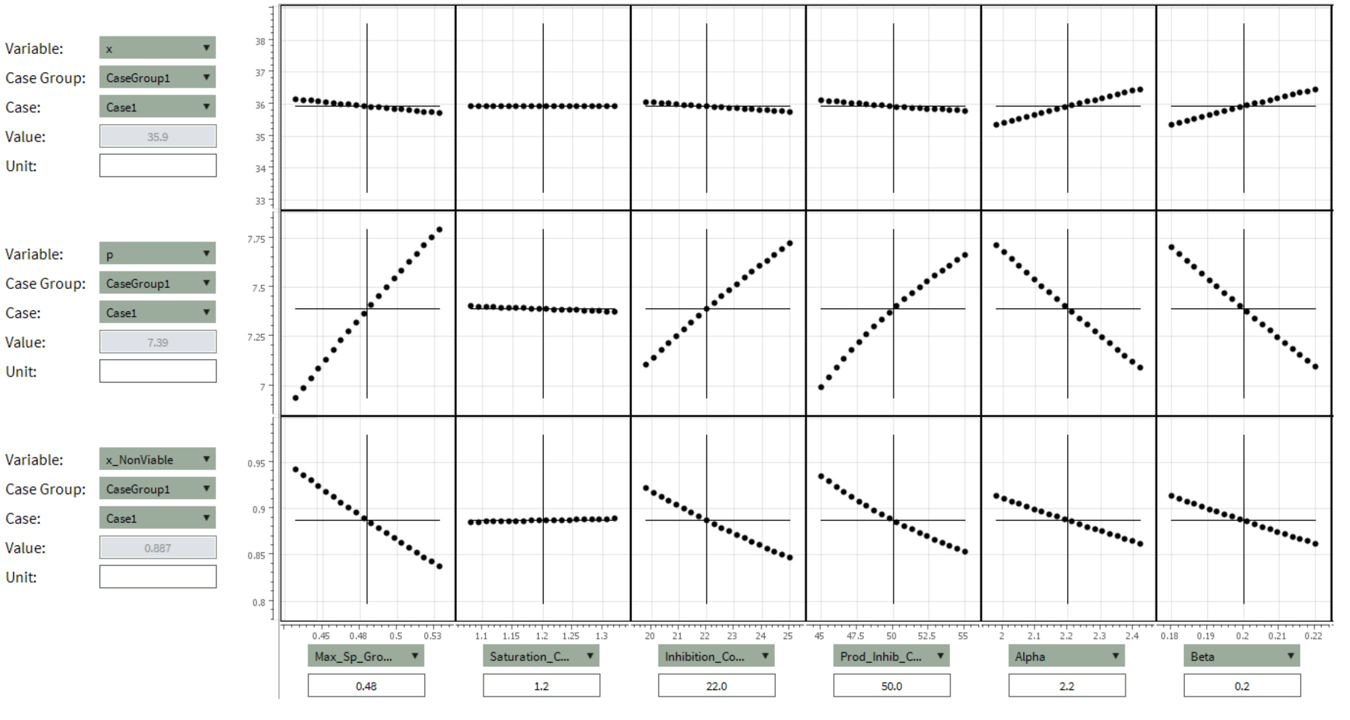


Figure 3: MoDS screenshot showing dependencies of output variables from parameter and input variables (all interchangeable with possibility to define different input values) for a fermenter.

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