Available online at www.sciencedirect.com

ScienceDirect

Procedia Social and Behavioral Sciences 2 (2010) 7678–7679a

Procedia
Social and Behavioral Sciences

Sixth International Conference on Sensitivity Analysis of Model Output

A computer-aided framework for systematic model development, analysis and identification in innovative product-process engineering

Martina Heitzig[a], Gürkan Sin[a], Peter Glarborg[a], Rafiqul Gani[a,*]

[a]*Department of Chemical and Biochemical Engineering, Technical University of Denmark, Soltofts Plads, 2800 Kgs. Lyngby, Denmark*

Abstract

A computer-aided modelling framework for developing, analyzing, identifying and applying models in chemical and biochemical product-process design has been developed. The modelling framework incorporates generalized approaches for solving different modelling problems in a systematic way and at the same time connects the required support and tools.

Keywords: Modelling framework, model identification, sensitivity analysis, uncertainty analysis, reaction kinetics

1. Main text

Models and computer-aided methods are playing roles of increasing importance in design and analysis of chemicals/bio-chemicals based products and the processes that manufacture them. The process of developing the required models for these tasks is of decisive importance while these models are and in future will become more and more challenging, complex and can be on multiple time and/or length scales. The development of these models is time-consuming, expertise-demanding and cost-intensive. This motivates the development of a framework which is able to assist the user in the development of models for a wide range of applications in chemical engineering.

Sensitivity and uncertainty analysis are essential elements of any model development process in chemical and biochemical engineering in order to evaluate the credibility of model predictions and to be able to compare the quality of different models. Uncertainties that need to be considered in the later application of the model, for example in process design, originate to a great extend from the model and the modelling process itself. They are caused by the fact that the model equations always must contain certain simplifications and assumptions. Another source of uncertainty in the model output is caused by the uncertainties in the model parameters which originate from inaccuracies with experimental data (e.g. measurement errors) and the parameter identification process itself. Uncertainty analysis will not eliminate the uncertainties in the input, but certainly it will help to quantify to what extent they impact the quality of decision making. Sensitivity analysis likewise plays an important role in the model

* Corresponding author. Tel.: +45-45-25-2882; fax: +45-45-93-2906.
E-mail address: rag@kt.dtu.dk.

doi:10.1016/j.sbspro.2010.05.175

development because it quantifies the sensitivity of the model output to different model parameters and allows a parameter significance ranking. It can be used for example with identifiability analysis to reveal which parameter subsets are actually identifiable by the available experimental data.

The goal here is to systematize the modelling process by providing the work-flow and data-flow for different modelling problems in a user-friendly modelling framework and combining the required tools, database connections and know-how at each step of the modelling process and thus increasing its efficiency. The user can then select from the different problem types offered in the framework: model development, simulation, identification and design. These problem types can be combined according to the user needs. The modelling tool needs to provide a single and a multiscale mode for each of the problem types since multiscale modelling requires a number of extra features.

In this contribution, the work-flow for the single-scale model development and subsequent identification is being presented. For each step it will be shown what features the modelling tool offers to support the modeller. The proposed work-flow is shown in Figure 1. The modelling tool provides a user-friendly interface programmed in visual c++.

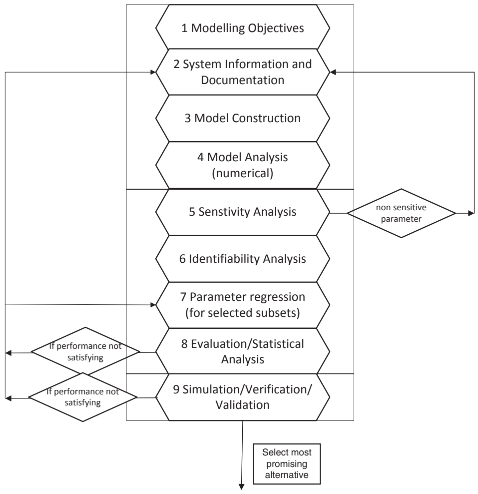

Figure 1 Work-flow for general model development and parameter regression

The first two steps are mainly opportunities for systematic model documentation to ease the later re-use of the model. In step 3 the model equations are constructed. Here, the user will provide the model equations in a text-format and the modelling tool is able to translate these inputs so that the user does not need to perform any programming work. The next step is the model analysis. The user can specify the types of the different variables. The tool performs a degree of freedom analysis and shows the incidence matrix of the problem. If the user desires the tool will automatically find the optimal order of the equations for the later solution of the model. The next step would be the sensitivity analysis. So far the tool supports Morris screening as well as local differential sensitivity analysis. The results are shown in tables, plots and in a parameter significance ranking. In step 6 the user can pick the parameters selected for identification based on the results of the sensitivity analysis and conduct an identifiability analysis. Afterwards, the parameter regression can be performed and in a last step the quality of the regression is summarized and evaluated. Herein, also the confidence intervals of the parameters are determined and an uncertainty analysis can be performed in order to evaluate the impact of uncertainties in the parameters on the model output. Finally, it is good practice to validate the model performance applying independent experimental data.

The developed models can be applied by solving them directly in the modelling tool since it contains solvers that are able to solve ordinary differential equations, partial differential equations, algebraic equations and combinations of these different equation types. During model application, for example for a design problem, the tools for uncertainty and sensitivity analysis can be applied. The difference with respect to the model development and identification is that the model parameters are fixed now and instead the design variables are the perturbed variables. The modelling tool is only one part of the integrated computer aided system (ICAS) which combines various tools. Consequently, the developed models can for example be applied in an integrated process simulator. The tool and methodology is presented and an exemplary case study. The case study elaborates on the application of sensitivity and uncertainty analysis in the field of chemical engineering.