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Computer-Aided Multiscale Modelling for Chemical Process Engineering

Ricardo Morales-Rodríguez, Rafiqul Gani*

*CAPEC, Department of Chemical engineering Technical University of Denmark, DK-2800 Lyngby, Denmark, *rag@kt.dtu.dk*

Abstract

Chemical processes are generally modeled through monoscale approaches, which, while not adequate, satisfy a useful role in product-process design. In this case, use of a multi-dimensional and multi-scale model-based approach has importance in product-process development. A computer-aided framework for model generation, analysis, solution and implementation is necessary for the development and application of the desired model-based approach for product-centric process design/analysis. This goal is achieved through the combination of a system for model development (ModDev), and a modelling tool (MoT) for model translation, analysis and solution. The integration of ModDev, MoT and ICAS or any other external software or process simulator (using COM-Objects) permits the generation of different models and/or process configurations for purposes of simulation, design and analysis. Consequently, it is possible to reduce time and human resources in the development and solution of models.

Keywords

Multiscale modelling, MoT, ModDev, COM-Object, CAPE-OPEN.

1. Introduction

The development of special materials and/or chemical products as well as a broad variety of scientific and engineering problems, requires models covering a wide spectrum of partial and temporal scales. Traditionally, chemical processes have been modeled through monoscale approaches, which, while not adequate, nevertheless satisfied a useful role in product-process design. Product-centric process design integrates aspects of product evaluation into the process design problem. In this case, use of multi-dimension and multi-scale model-based approach is beneficial in product-process development and it basically consists of a mathematical model that represents a complex problem divided into a family of subproblems that exists at different scales and that can be organized along various scales depending on the system and on the intended use of the model [1].

A flexible computer-aided framework for model generation, analysis, solution and implementation will allow the development and application of the desired model-based approach for product-centric process design/analysis. This can be achieved through the integration of a model generating system (ModDev), and a modelling tool (MoT) for model translation, analysis and solution. The combination of ModDev, MoT and ICAS [2] or any other simulators or external software (through standard interface like CAPE-OPEN or special interfaces) permits that different models and/or process configurations can be simulated very easily and quickly, reducing time and human resources for model development and solution with almost zero programming effort. Also, this framework gives the possibility for producing customized simulators for a particular process.

The objective of this paper is to present the modelling framework, and through it, the synergy between ModDev and MoT; together with new modelling features such as multiscale modelling and models needed for specific product-centric process design that are usually not found in commercial simulators (for example, fuel cells, thin-film evaporators). The paper will highlight the application of the modelling framework to generate model equations using ModDev and model analysis/solution through MoT for different non-trivial modelling tasks. The examples will also highlight the development of personalized simulators with models generated through ModDev-MoT and using EXCEL as the simulator executive through COM-Object.

2. Computer-Aided Process Modelling Framework

Nowadays, Computer-Aided Process Modelling Frameworks which have become an important tool in the development and solution of process and product engineering can be classified as: generic modelling languages and domain-oriented modelling languages. Process modelling languages (PML) could be classified inside of domain-oriented modelling languages [3]. PML should be provided with varying level of granularity (multiscale modelling) concepts to enhance the accuracy and prediction of the behaviour of some process that have to be solved including multiscale phenomena. Multiscale is an essential pre-requisite for making full use of advances in scientific understanding within engineering applications of practical interest. Chemical engineers are turning to multiscale modelling to extend traditional modelling approaches into new application areas and to achieve higher levels of detail and accuracy. There is, however, little advice available on the best strategy to use in constructing a multiscale model [4]. Consequently, Computer-Aided Framework including a Multiscale approach is usually not available, and it is therefore necessary to assist in the development of these types of models. Furthermore, multiscale approach facilitates the discovery and manufacture of complex products [5]. The challenges and opportunities for multiscale modelling for chemical process are open and partially taken into account in this work.

Integrated Computer Aided System (ICAS) is a computer-aided tool for modelling developed by Computer Aided Process Engineering Center (CAPEC) at Technical University of Denmark. ModDev and MoT are modelling tools integrated with ICAS; both have established work-flow defined by the computer-aided modelling frameworks. But, *why do we need to use ModDev and MoT together?* Because through their interaction, model equations for a specific equipment, process or operation would be developed by ModDev; and then translated, analyzed and solved through MoT with almost zero programming effort, and thereby, producing customized simulators for a particular process.

2.1. ModDev

ModDev [6] is a knowledge-based modelling system that is able to generate process models. It employs a graphical user-interface to convert the modeller's perception of the process in terms of phenomena, accumulation, and constraints, and aggregates them to form models of the unit operation defined in terms of boundaries, connections, and states. In ModDev, fundamental modelling objects are used to create generic building blocks. The fundamental modelling objects and the generic building blocks are then aggregated to form the desired process model. The equation set representing the process model is then analyzed and translated for integration with a solver. The translated model may be used as an equation set in equation-oriented simulators (MoT).

2.2. ICAS-MoT

Model Test-bed (MoT) [7] is a tool within ICAS and is an equation based modelling/simulation tool and allows the user to perform simulations of a process without having to write any source code. The translated model can be solved, after satisfying mathematical consistency requirements. After the model equations have been successfully solved, the user has the option to generate a COM-object of the model to transfer and use it in external software. COM-object of other models, in this way, can also be used for different terms of a model, for example, different sets of compound properties, reaction kinetics and

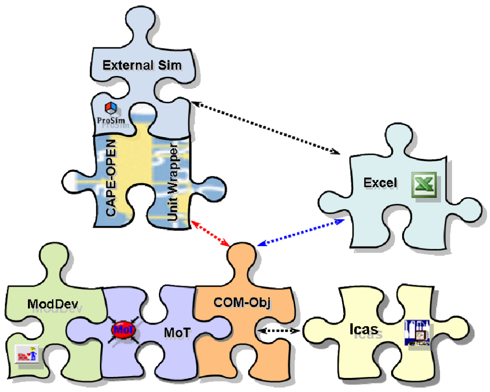

Fig. 1. Computer-Aided Modelling Framework behaviour

equipment sizing data. On the other hand, the connection of these COM-Objects with external software or commercial simulator (such as ProSim) can be done through a CAPE-OPEN link. Also, MoT-COM is able to interact with the ICAS simulation environment generating a new unit operation that can be used with other already available unit operation models and used with other ICAS features. Furthermore, some of the external simulators can operate with EXCEL at the same time it is working with MoT-COM without additional work and providing a high-quality interaction between them (see figure 1).

2.3. Case Study

In order to illustrate the connection between the different parts according to the computer-aided modelling framework, a multiscale model for a fuel cell is chosen from the open literature [8]. Multiscale issue can be seen between scale-phenomena connection carried out in the different parts of the fuel cell; for instance, between the charge balance and mass balance. The equations representing the direct methanol fuel-cell are listed in table 1.
In this case study, use of ModDev to generate the model equations is not necessary as a published model [8] is used. However, ModDev can also be used to verify the model.
Once the model equation for the unit has been derived/generated, MoT is used to make the translation, analysis and solution. As far as model analysis is concerned, the degrees of freedom, determination of the structure of the equation system, index analysis, partitioning and ordering of the model equations and numerical analysis can be carried out in this part. The next step is to solve the model equation analyzed in the previous step.

Table 1. The DAE model for DMFC in various components [8].

Type		Equations	
Electrode kinetics		$r_1 = k_1 \exp\left(\frac{\alpha_1 F}{RT}\eta_a\right)\left\{\theta_{Pt}^3 c_{CH_3OH}^{CL} - \frac{1}{K_1}\exp\left(-\frac{F}{RT}\eta_a\right)\theta_{Pt-COH}\right\}$	*Eq. (1)*
		$r_5 = k_5 \exp\left(\frac{\alpha_5 F}{RT}\eta_c\right)\left\{1-\exp\left(-\frac{F}{RT}\eta_c\right)\left(\frac{p_{O_2}}{p^0}\right)^{3/2}\right\}$	*Eq. (2)*
Mass Balance	Anode	$\frac{dc_{CH_3OH}}{dt} = \frac{1}{\tau}\left(c_{CH_3OH}^F - c_{CH_3OH}\right) - \frac{k^{LS}A^S}{V_a}\left(c_{CH_3OH} - c_{CH_3OH}^{CL}\right)$	*Eq. (3)*
		$\frac{dc_{CO_2}}{dt} = \frac{1}{\tau}\left(c_{CO_2}^F - c_{CO_2}\right) - \frac{k^{LS}A^S}{V_a}\left(c_{CO_2} - c_{CO_2}^{CL}\right)$	*Eq. (4)*
	Cathode	$\frac{dc_{CH_3OH}^{CL}}{dt} = \frac{k^{LS}A^S}{V_a^{CL}}\left(c_{CH_3OH} - c_{CH_3OH}^{CL}\right) - \frac{A^S}{V_a^{CL}}n_{CH_3OH}^M - \frac{A^S}{V_a^{CL}}r_1$	*Eq. (5)*
		$\frac{dc_{CO_2}^{CL}}{dt} = \frac{k^{LS}A^S}{V_a^{CL}}\left(c_{CO_2} - c_{CO_2}^{CL}\right) + \frac{A^S}{V_a^{CL}}r_1$	*Eq. (6)*
Charge Balance	Anode	$\frac{d\eta_a}{dt} = \frac{1}{C_a}\left(-i_{cell} - 6Fr_1\right)$	*Eq. (7)*
	Cathode	$\frac{d\eta_c}{dt} = \frac{1}{C_c}\left(-i_{cell} - 6F\left(r_5 + n_{CH_3OH}^M\right)\right)$	*Eq. (8)*

Solution of the model for a direct methanol fuel cell (table 1) is presented below. The results are in agreement with the experimental data, which are indicated by the points (see figure 2).

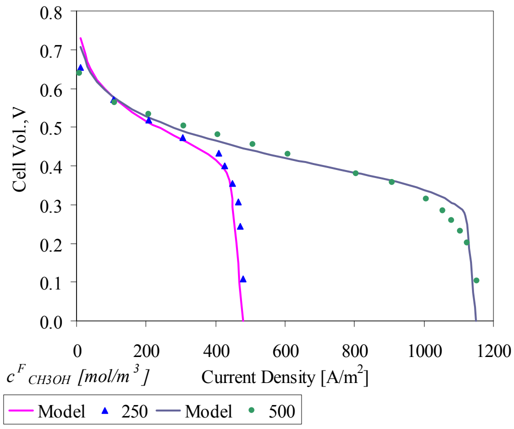

Fig. 2. Simulation for two methanol feed concentration in the fuel cell.

The second example highlights the solution of model equations for a short-path evaporator [9] where a model object is generated through MoT for use in EXCEL which is used as a visual interface and for simulation of different operational scenarios. Figure 3 is highlighting the results obtained and the easy way to handle the results (producing the necessary graphics, reports and so on) obtained from the simulation carried out previously in MoT-EXCEL interaction through COM-objects.

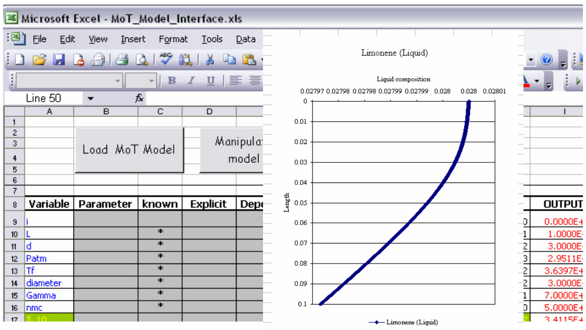

Fig. 3. Example for MoT-Excel Interaction

3. Conclusions and future work

The development of a Computer-Aided modelling framework for multiscale modelling is a very important tool for the development of chemical process models. It has been shown that the combination and interaction between different computer-aided tools and external software provide the additional modelling/simulation features needed for design/analysis of specific processes and also simultaneously obtaining customized process simulators, while performing the modelling tasks more easily and efficiently.

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