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APPLICATION OF MODELS WITH DIFFERENT COMPLEXITY FOR A STIRRED TANK REACTOR

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Engineering problem solving such as process design, process optimization, safety analysis, etc.; relies widely on mathematical models of the process. To solve various engineering problems various models with different complexity are needed. A stirred tank reactor with a highly exothermic reaction is studied in this work, because in the modern chemical technologies mixing is one of the most important operations, and stirred reactors are widely used in industrial applications. The stirring system of a mixed tank is always an important aspect of the design, because the involved processes (such as reactions, heat and component transport) usually require proper contact and homogeneity of the existing phases. For the suitable homogeneity the design and the size of the moving parts are also important problems. In certain situations attachment of static parts to a stirred tank (such as baffles) may have an important effect too. The primary goal of this study is to create models with different level of complexity and determine which model is the best suited for solving different engineering tasks such as process design, scale-up, or optimisation. etc. To determine which model fits best for a problem, mathematical models were created and compared to find out, how the information can be extracted from these models and be applied to solve engineering problems. Three types of models have been developed: perfectly mixed reactor model, compartment model, and Computational Fluid Dynamics (CFD) models with different dimensions. The reaction of hydrogen peroxide with sodium thiosulphate in a continuously stirred tank reactor is analysed as a case study. The perfectly mixed vessel models and compartment models were solved in MATLAB/SIMULINK program package. The CFD models were implemented in COMSOL Multiphysics.

Keywords: computational fluid dynamics, stirred tank, hydrogen peroxide, model complexity

Introduction

In modern technologies mixing is one of the most important operations. The stirring system of a mixed tank is always an important aspect of the design, because the involved processes (such as reactions, heat or component transport process) require proper contact and homogeneity of the existing phases [1].

Nowadays there are an increasing number of applications of model based methods in the industry too. With a correctly built model there is a possibility to examine the dynamic behaviour of the system as well as the mass, heat and momentum transport processes.

In this study a kinetic model of the reactions of hydrogen-peroxide and sodium thiosulphate from an earlier case-study is analysed [2]. For developing suitable reactor models we followed a sort of hierarchical modelling concept [3]. Three types of models with different complexities have been developed: perfectly mixed reactor model, compartment model, and Computational Fluid Dynamics (CFD) models. Since the examined reaction is highly exothermic the thermal runaway problem must have been investigated thoroughly. For achieving different goals different models might be required. To solve the simplest problems such as preliminary design and control, engineers can use simple models to describe a dynamical system, such as perfectly mixed vessel model, or ideal plug flow reactor model. In the case of a perfectly mixed model the whole vessel is homogenous, and models with concentrated parameters can be used. On the other hand the plug flow reactor models can be applied to calculate the inhomogeneity in a tube reactor in axial direction; in this case the distributed model parameters need to be defined [4].

If a simple model is not detailed enough to solve a problem more complex model have to be created, such as operation fermentation reactor with multiple impellers. The second level of models which is discussed in this paper is the compartment models. These models generally contain two or more well defined compartments, built from perfectly mixed reactor or ideal plug flow reactor models. The most important thing at this level of modelling is to find the proper parameters describing the connections between these models [5]. For example to create a compartment model for a stirred vessel in the basic cases the vessel has to be separated at least two different compartments. The impeller and the region near the impeller can be described by using a perfectly mixed reactor model, and at least one other region must be defined, called circulation loops, or circulation region [6]. To model the connections between these models the

following parameters need to be determined: the exact volume of the compartments, and circulation rates, or other pre-defined parameters [7]. The more difficult the problem is, the more complex model must be created. In the last few years researchers have been trying to create even hybrid CFD-compartment models that are capable of handling more than 100 compartments [8].

The CFD models are the most complex models examined in this work. The CFD models can be applied to determine the entire hydrodynamics of the system, to define flow patterns, or concentration distributions, or thermal hotspots. With validated CFD models the system can be examined at a completely new level, and engineers can model anomalies such as thermal runaway, and prevent hazardous situations [9]. CFD models can also serve as excellent design tools [10]. In this paper we have created models with different complexities in order to determine how these models can be used to solve various engineering problems in the field of design and control of chemical processes. The perfectly mixed vessel models and compartment models were solved in MATLAB/SIMULINK program package. The CFD models were implemented in COMSOL Multiphysics.

Modelling approach

At every level of modelling the same exothermic reaction with a well-known kinetics is used [2]. This is the reaction of hydrogen-peroxide with sodium thiosulphate.

$$2Na_2S_2O_3 + 4H_2O_2 \rightarrow Na_2S_4O_6 + 2Na_2SO_4 + 4H_2O \quad (1)$$

The analysed highly exothermic reaction is the oxidation of sodium thiosulphate with hydrogen peroxide. The kinetic parameters of the analysed reaction were determined in an earlier case-study [2]. *Table 1* contains the model parameters.

Table 1: Model parameters

Revolution speed	20	[1/min]
Density	1000	[kg/m^3]
Volume	0.375	[m^3]
Feed	2e-4	[m^3/s]
Viscosity	0.001	[Pas]
Component diffusion C_A - sodium thiosulfate, C_B - hydrogen-peroxide, C_C - sodium - trithionate	10^{-5}	[m^2/s]

The examined stirred vessel is a continuous tank reactor. All the implemented models have the same model parameters for describing reactor geometry (apart from the parameters of the impeller, since the impeller was implemented only in the CFD simulations).

Because of the exothermic reaction the temperature dependence of the reaction is high, thus it is necessary to define heat balance equations too. In every model component and heat balances was implemented.

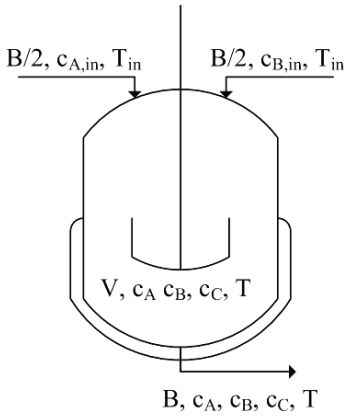

Figure 1: Scheme of the reactor

Component balances

$$\frac{dc_i}{dt} = \frac{B}{V} \cdot (c_{i,be} - c_i) + \upsilon_i \cdot r \qquad (2)$$
$$i = \{Na_2S_2O_3, H_2O_2, Na_2S_4O_6, Na_2SO_4, H_2O\}$$

Heat balance

$$\frac{dT}{dt} = \frac{1}{\rho c_p} \cdot r \cdot (-\Delta H) + \frac{B}{V} \cdot (T_{IN} - T) \qquad (3)$$

In CFD models a momentum balance was also added besides component and heat balances.

Momentum balance

$$\rho \frac{\partial u}{\partial t} + \rho(u \cdot \nabla) \cdot u = \nabla[-pI + \tau] + F \qquad (4)$$

Results and discussion

Perfectly mixed reactor model

In the perfectly mixed reactor model a mathematical formulation based on the modified Dahmköhler-equations is applied to describe material and heat balances. The model was implemented and solved in MATLAB. *Fig. 2* shows the results of the dynamic simulation of the perfectly mixed reactor model with the previously mentioned reaction implemented. The perfectly mixed reactor model can be used to:

- calculate the maximum productivity and conversion;
- support optimization and design of the reactor;
- study control functions;
- examine runaway situations in the system level;
- etc.

The figure shows, that the product concentration reaches a stationary value within a short time, but, the temperature rises 45 K, therefore it is important to control the reaction temperature to avoid hazardous situations.

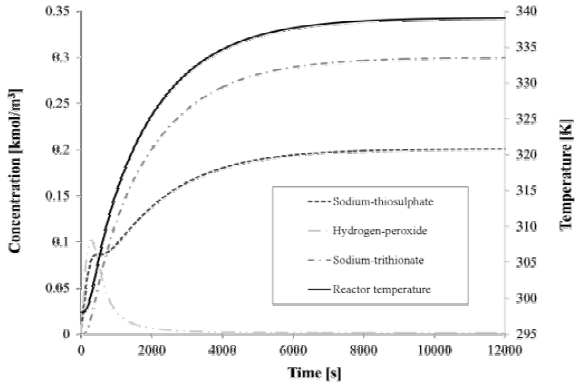

Figure 2: Results of the perfectly mixed reactor model

Compartment model

At this stage of the work four types of compartment are applied to model macro mixing conditions. The following compartments are applied:

- perfectly mixed reactor;
- mixer;
- distributor;
- dead zone.

The first cell is identical to the previously discussed perfectly stirred reactor model. The mixer and the distributor have zero volume, and these compartments are capable of modelling circulation loops. The distributor distribute the flow directly, and the mixer use mixing equation to calculate the outlet variables. The output variables were computed from the input variables using algebraic equations. The dead zone cell represents a cell with real volume; however there is no flow in it. The circulation numbers – describe the ratio of distribution – have constant values at this time and describe the rate of circulation between impeller zone and circulation zones. *Fig. 3* represents the compartment approach and *Fig. 4* shows the structure of the compartment model. Eight compartments have been used: one dead zone, three perfectly mixed reactor models for impeller top and bottom circulation zones, two mixers and two distributors. The volume of the dead zone is 15 % of the total volume, and each reactor cell has the same volume.

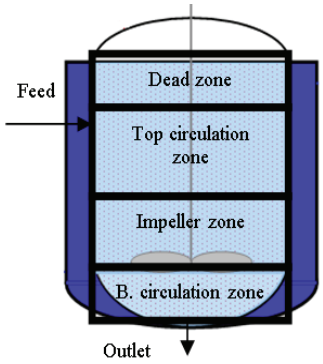

Figure 3: Compartment model for a stirred tank reactor

The compartment model can be used to:

- support advanced control and design;
- examine macro mixing and model complex reaction systems;
- examine heat transfer at a more complex level;
- etc.

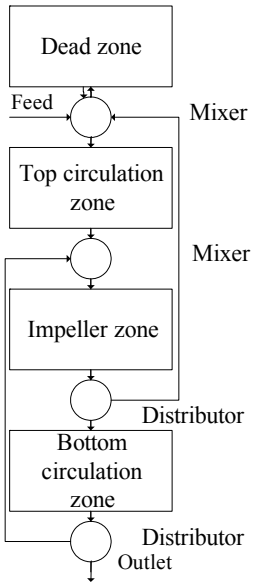

Figure 4: Compartment model structure

Two- and three-dimension CFD models

To simulate the behaviour of the system in a CFD environment COMSOL Multiphysics program package was applied. The investigated impeller is a standard six bladed Ruston turbine in the 3D simulations and a simple blade in the 2D analysis. The revolution of the impeller is 20 RPM in the first investigation. The revolution of the impeller is low, because a laminar model was used in this case, and laminar models can only work at low impeller revolution. In the future a turbulent model will be implemented to examine higher revolution speed. In case of the 2D analysis the same continuous system cannot be simulated, since the investigated geometry is a slice of the 3D geometry, i.e. the slice in the centre of impeller zone. In the 3D simulations the same continuous reactor is investigated as in the two dimensional simulations. The results of the CFD simulation are shown in *Fig. 5* and *Fig. 6*. The velocity field are calculated in 2 and 3D.

The CFD models can be used for:

- examining of runaway reactions in three dimension;
- studying different impeller geometries;
- testing of new vessel constructions;
- applying multi-level optimisation;
- etc.

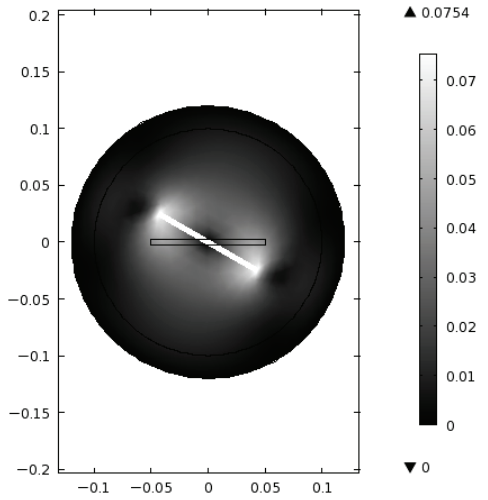

Figure 5: Results of the 2D CFD model

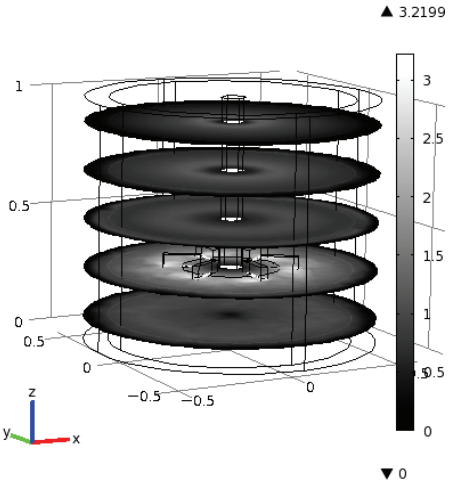

Figure 6: Results of the 3D CFD model

Comparison of the models

In the final step of our investigation the simulation results of the developed three models are compared. The results are shown in *Fig. 7*. The concentration refers to the concentration of the product. The results of the CFD model are much more different than the other two, because in this model the real geometry of the reactor has been implemented, and this makes the system more inhomogeneous. Because the lack of the validation the question which model is the best is hard to answer. To obtain validated models hydrodynamic measurements will be taken in a glass reactor at our department.

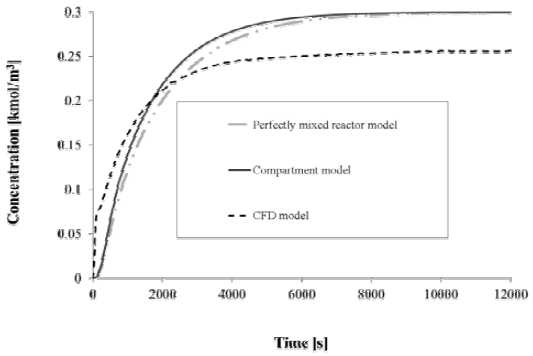

Figure 7: Comparison of the models

Conclusion

The predefined goal – to create models with different complexity – has been achieved. The developed models can be applied in a wide range of industrial purposes, from the design of a reactor to control or solving optimisation problems. At every level of modelling some of the possible applications have been discussed.

This approach is expected to be used to determine which level of hierarchical modelling have to be applied to solve a given engineering problem, and to implement the simplest model suitable to work at this level. It is important that all the simulation results need to be validated based on experimental data from real systems. The physical experiments will be the next step in our work.

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APPENDIX

Appendix 1: The construction parameters of the reactor

Impeller length	0.6	[m]
Impeller width	0.1	[m]
Impeller height	0.01	[m]
Inner diameter	1	[m]
Outer diameter	1.2	[m]
Vessel height	1	[m]
Feed diameter	0.02	[m]

NOTATION

Name	Description	Unit
c_A	hydrogen-peroxide concentration	[kmol/m^3]
c_B	sodium - thiosulfate concentration	[kmol/m^3]
c_C	sodium - trithionate concentration	[kmol/m^3]
c_{in}	inlet concentration	[kmol/m^3]
V	reactor volume	m^3
B	Feed	[m^3/h]
k	Reaction rate	1/s
ρ	Density	[kg/m^3]
cp	Heat capacity	[J/mol/K]
T_{IN}	Feed temperature	[K]
T	Reactor temperature	[K]
u	velocity vector	[m/s]
t	time	[s]
τ	shear force tensor	
g	grav. acceleration	[m/s^2]
∇	differentialoperator	
F	Force vector	N

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