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Model Structure Identification Algorithm for Stirred Systems

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Abstract: **Solving engineering problems, such as design or optimization relies widely on the mathematical models of the process. To solve more complex problems, the more sophisticated model must be developed. To predict the dynamic behaviour of mixed reactors, the perfectly mixed reactor model with concentrated parameters is applied most widely because of its simplicity. The hydrodynamic behaviour of the real mixed reactor can be taken into account by using compartment models. With the proper compartment structure the changes in the state-variables of the system can be described more precisely. The main modelling tasks using compartment models is to define the structure of the compartment model, and the connection parameters between the compartments. Hence, a qualitative trend analysis based approach was developed to support the identification process.**

The most critical aspect of compartment modelling is to describe the system with the possible least number of compartments. For this purpose an algorithm is proposed, that capable of generating and evaluating compartment structures from one to few dozen compartments. The proposed algorithm can be applied to identify the proper structures based on the comparison of measured and simulated data. The mathematical model and the identification algorithm were implemented in MATLAB/Simulink.

Keywords: stirred reactor, structure identification, qualitative method, compartment model

I. INTRODUCTION

In modern technologies mixing is one of the most crucial process 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 processes) 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. With the help of 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.

To solve the simplest problems engineers can use simple models to describe a stirred system, such as perfectly mixed reactor, or ideal plug flow reactor model. In the case of a perfectly mixed reactor model the whole vessel is assumed to be homogenous, and models with concentrated parameters can be applied to calculate the trajectories of the state-variables. On the other hand the plug flow reactor models can be applied to calculate the inhomogeneity in a tube reactor; in this case distributed model parameters need to be defined [2].

Solving more complex practical problems Computation Fluid Dynamics (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 [3]. CFD models can also serve as excellent design tools.

The compartment models can make a connection between the perfectly mixed reactor models, and the more complex CFD models. By more detailed modelling of macro mixing effects, a more complex model can be obtained, and it can describe the real system more accurately.

Compartment models can be used for:

- modelling biological systems [4];
- modelling aired systems [5];
- optimization tasks [6];
- on – line control;
- to define the residence time.

Before starting the model building the detailed examination of the whole system must be performed. The first step of building a compartment model is to define the number and the type of compartments. There are several basic points to be investigated at this level of model development:

- type of the impeller (mechanical, pneumatic etc.);
- recirculation loops;
- the investigated system contains injection or not;
- baffles and the flow near the walls;
- phases (gas, liquid, solid – such as. fluidized bed, etc.) [7].

Based on the velocity field, and hydrodynamics, there are four basic types of compartments:

- Perfectly Mixed Reactor: has an exact volume and chemical reaction takes place within; can be modelled with algebraic, and/or differential equations, homogeneous hydrodynamic conditions. It has one input and one output stream.
- Ideal Plug Flow Reactor: similar to the perfectly mixed reactor model, but the hydrodynamic conditions are plug flow. Ideal Plug Flow Reactor can be modelled as a series of perfectly mixed reactors.
- Mixer: does not have volume; the specifications of the outlet stream can be determined using algebraic equations. It has one output and at least two input stream.
- Distributor: does not have a volume; the specifications of the outlet stream can be determined using algebraic equations. It has one input and at least two output streams.

There are a lot of on-going research projects in the field of multi impeller systems by using compartment models, because the reactions in these systems are difficult to model, and modelling with CFD is difficult especially in more complex systems [8].

In the field of compartment modelling the model can be described with the number and the type of the compartments and connections - such as circulation, transport, and diffusion - between them. The connections between the compartments can be represented with the incidence matrix. Incidence matrix is a matrix that shows the connection between compartments in one structure. If a stream does not connect to a compartment the corresponding element is zero. If the stream leaves the compartment the value is -1, and if the stream enters the compartment the value is 1.

The most difficult task in the field of compartment modelling is to identify the adequate model structure. For solving this problem a qualitative approach can be useful. Qualitative data intensive methods are widely applied because of their statistical nature, however they always require prior knowledge to analyse the results. Usually prior knowledge is available in the form of qualitative or tendency models of the process. Hence, qualitative analysis of complex systems is an important task at the design of control and process monitoring algorithms. Qualitative models require the interpretable description not only of the historical process data but also the operating regimes of the process [9].

The qualitative method in this case refers to the method by which the data are processed. The method uses first and second derivatives to determine primitive episodes and finally to define a structure based on measurement data [10]. Based on recent studies and the proposed algorithm experimental data can be processed and the proper structure can be identified for a further dynamic evaluation. For qualitative analysis seven primitive episodes were used, based on the first and second derivatives of the measured data.

The seven primitive episodes cover all the combinations of the first and second derivatives. By the shape there are convex, concave, and linear shapes with positive or negative gradient and constant value. Figure 1 shows the applied primitive episodes.

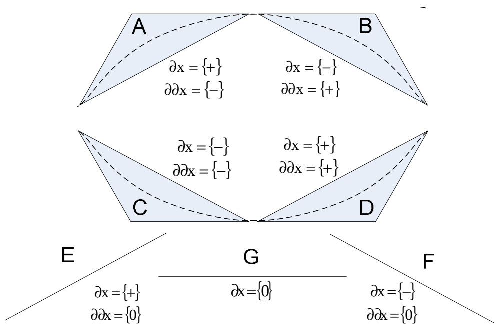

Figure 1 The applied primitive episodes

The primary goal of this study is to develop an algorithm that is capable of describing a stirred system as a compartment structure. Qualitative methods were used for the identification of the compartment structure, and MATLAB/Simulink was applied for the implementation of the algorithm. The first half of the paper presents the methods and algorithm, and the second half of this paper shows the results of the research.

II. ALGORITHM DEVELOPMENT

Figure 1 shows the flowsheet of the developed algorithm. The first step of the algorithm is the generation of all compartment combinations, which was solved by a suitable algorithm. When all the combinations have been computed a filtering step has to be done. There are well defined restrictions are applied to avoid repetition, and some false structures. The restrictions were:

- every structure must contain at least one reactor compartments (perfectly mixed reactor or plug flow reactor);
- the number of mixers and distributors has to be equal;
- if two plug flow compartments follow each other, these compartments are changed for one plug flow reactor compartment;
- those structures where mixer and distributor compartments are connected directly, has to be eliminated.

The most important objective is, to describe a system with the possible least compartment. After the filtering step a dynamic simulation must take place. Before the simulations can be started the connection between the compartments has to be defined.

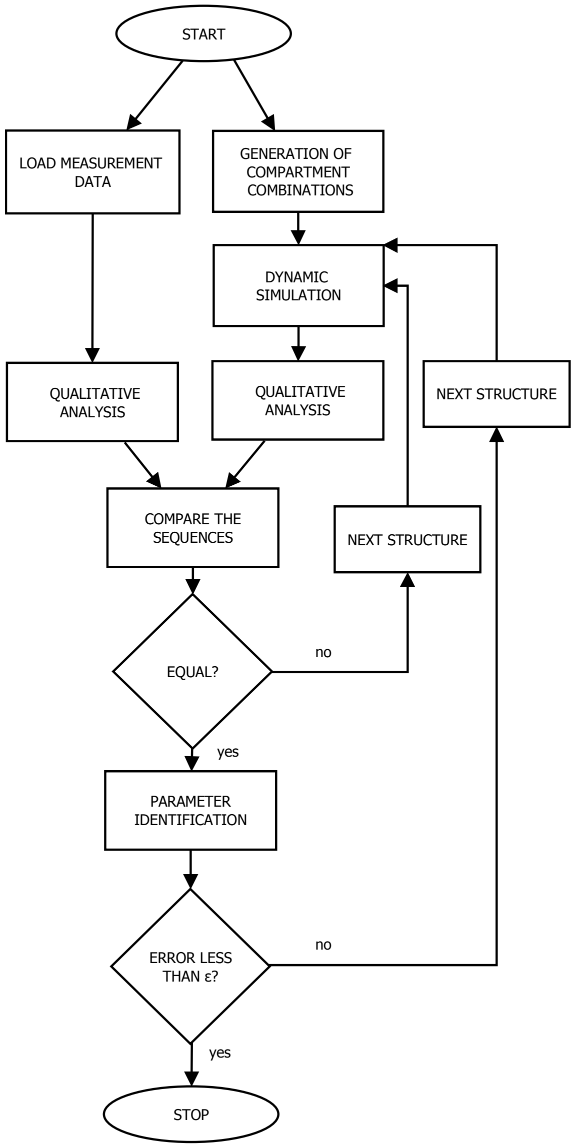

Figure 2 The flowsheet of the proposed algorithm

In the simulation we describe plug flow reactor compartment as a series of perfectly mixed reactors. To describe the connections an incidence matrix was defined. The simulation goes from simpler to more complex compartment structures. The measured and the simulated data have to be compared in order to determine which structure fits between an acceptable margin of error.

To determine the adequate structure a qualitative method was applied for the measured and simulated data too, using the earlier introduced primitive episodes.

Using the qualitative approach an individual sequence can be identified for each individual structure. If the sequence of the simulated data is identical to the measured data, a parameter identification step must be done to identify the model parameters. Two types of parameters were identified, the circulation numbers (α), and the volume ratios (V=V1/V2) between reactor compartments. In this step it is important to determine the influence of the model parameters.

If the sequences match and in the parameter identification step the error is reasonable, then the identified compartment structure is adequate. Otherwise the next compartment structure must be simulated according to the flowsheet.

III. RESULTS AND DISCUSSION

All of the compartment combinations were created in order to solve the structure identification task. One of the most important aspects of this level is, to understand the parameter dependence of the sequence. For this analysis a number of simulations were examined with different model parameters but the same compartment structure. Figure 3 shows the examined structure and the parameters.

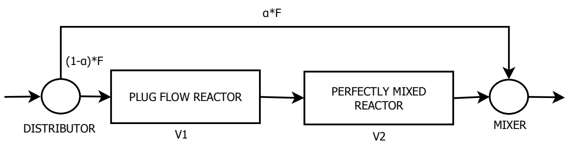

Figure 3 The structure and the model parameters

The input of the system was an impulse function, and the residence time distribution function has been studied. Figure 4 and 5 shows the results, and the identified sequences. In every case a four-compartment structure was used. It consists of a distributor, a plug flow reactor, a perfectly mixed reactor, and a mixer.

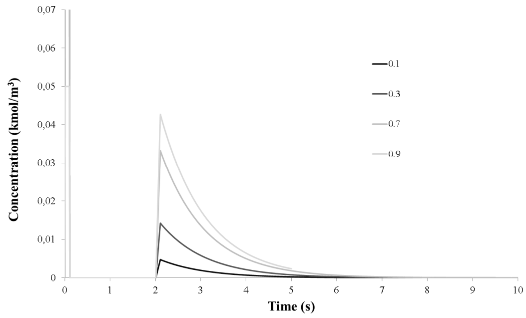

Figure 4 Circulation number dependence of the sequence

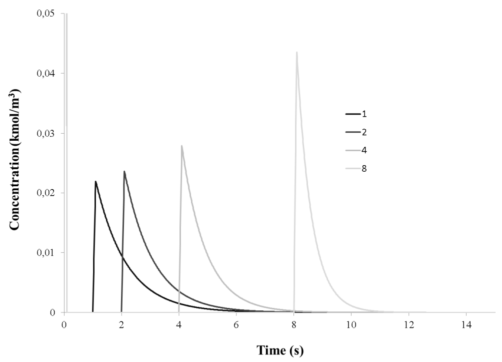

Figure 5 Volume ratio dependence of the sequence

The shape of the response function was clearly the same, but the intensity of the function was different in every case. The identified sequence was 'GGAC' in every parameter combinations, as Table 1 shows, so the sequence is independent from the parameters. In this case, the sequence was independent from the model parameters, the structure and the parameter identification step can be separated. In this stage of the development only the parameter independent structures have been investigated. After the parameter dependence test a dynamic simulation was applied to compare measured, and computed data, based on error minimalization. Figure 6 shows one structure (contain one circulation loop, a plug flow and a perfectly mixed reactor cell) as an illustrative example, and the difference between measured and computed data.

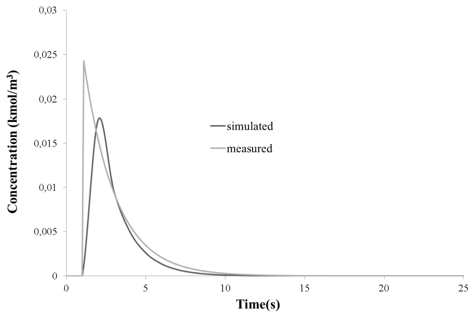

Figure 6 Comparison of measured and computed data

Figure 6 shows a little difference between the shapes of the data, because in the simulation ten perfectly mixed reactors was used to simulate the behaviour of the plug flow compartment.

IV. CONCLUSIONS

The developed algorithm is capable of describing stirred system in a more detailed level, and it can be a useful tool for engineers. The algorithm is capable of processing time domain data, and identifies a proper compartment structure to describe it. Furthermore, based on the compartment structure, dynamic simulation can be applied to identify and validate the unknown model parameters of the compartment model. The most important aspect of this study is that a suitable structure identification algorithm was created, and tested. Based on the developed algorithm engineers can make various compartment models which, can be used for on-line control, engineering design and modelling systems at a more detailed level.

Based on the analysis of the compartment structure, the influence of model parameters was revealed. For further understanding of model parameter infulence, the other cases eill be investigated, where the structure and the parameter identification step can not be separated.

In the future the algorithm will be improved to handle other structures such as structures contain reactor cells in circulation loops, and the basic compartment models will be extended to handle more compartment classes such as dead zone.

V. ACKNOWLEDGEMENT

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