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Compartment model structure identification of stirred reactors based on qualitative method

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ABSTRACT

Engineering problem solving such as process design, process optimization, safety analysis, etc.; relies widely on mathematical models of the process. To solve complex problems related to mixing detailed models are required such as compartment or computational fluid dynamic models. The compartment modelling based on at least three different types of basic compartments: the mixer, the distributor and the perfectly mixed reactor. Obviously, the compartment set can be expanded with the ideal plug flow reactor. The main modelling tasks using compartment models is to define of the structure of the compartment model, and the parameters of connections between the compartments. Hence, a qualitative approach has been developed to support the identification process. Qualitative methods are widely applied to analyse experimental data and to compress the information content of a time series. The primary goal of this study is to present an algorithm based on qualitative analysis that can be used to identify a compartment model structure based on the results of physical experiments performed in a stirred reactor.
(Keywords: stirred reactor, structure identification, qualitative method, compartment model)

ÖSSZEFOGLALÁS

Kevert tankreaktor cellás modelljének struktúra identifikációja kvalitatív módszerek alkalmazásával

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A mérnöki problémák megoldása – például tervezés, folyamatoptimalizálás, biztonság-technikai analízis stb. – nagymértékben függ a folyamat leírására használt matematikai modelltől. A keveréshez kapcsolódó bonyolultabb problémák megoldása esetén összetettebb modellek használata lehet szükséges, ezek legtöbbször a cellás modellek, vagy a numerikus áramlástani modellek. A cellás modellek általában legalább három, vagy több elemi cellatípust tartalmaznak: keverőt, elosztót és tökéletesen kevert üstöt. Emellett az elemi készlet kiegészíthető például ideális csőreaktorral. A fő modellezési feladat cellás modellek esetén a megfelelő cellás struktúra definiálása, valamint a cellák közötti kapcsolatok paramétereinek meghatározása. A kvalitatív megközelítés segítheti a struktúra identifikációt. A kvalitatív módszerek alkalmasak időfüggő mérési adatok feldolgozásával a kevert rendszerek leírására. A dolgozat elsődleges célja, hogy bemutasson egy algoritmust, amely képes kvalitatív módszerek alkalmazásával egy adott valós rendszerre alkalmazható cellás modell struktúrájának meghatározására, kevert üstön végzett fizikai kísérleteket alapul véve.
(Kulcsszavak: kevert reaktor, struktúra identifikáció, kvalitatív módszer, cellás modell)

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 (*Paul et al*., 2004).

Nowadays there are an increasing number of applications of model based methods in the industry. 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.

To solve the simplest problems engineers can use simple models to describe a stirred system, such as perfectly mixed, or ideal plug flow reactor model. In the case of a perfectly mixed 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 the distributed model parameters need to be defined (*Perry et al*., 1997).

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 (*Milewska et al*., 2007). CFD models can also serve as excellent design tools (*COMSOL News*, 2010).

The compartment models can make a connection between the perfectly mixed reactor models, and the more complex CFD models. With better 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 (multi impeller fermentors) (*Alves et al*., 1997);
- modelling aired systems (multiphase) (*Znad et al*., 2004);
- optimization tasks (cost, or product) (*Penry et al*., 1986);
- on-line control;
- defining residence time.

Before starting the model buildings 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 the 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, packed reactor, etc.) (*Claudel et al*., 2003).

There are different compartments based on the velocity field and hydrodynamics. There are four basic types of compartments:

- Perfectly Mixed Reactor: has an exact volume, 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 of 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 researches in the field of multi impeller systems by using compartment models, because modelling reactions in these systems with CFD is difficult especially in larger systems (*Alexopoulos et al*., 2002). These models might be more complex, because at least two impeller regions and the connections between each region need to be described. For multi impeller system models more compartments might be needed from two to a few dozen compartments.

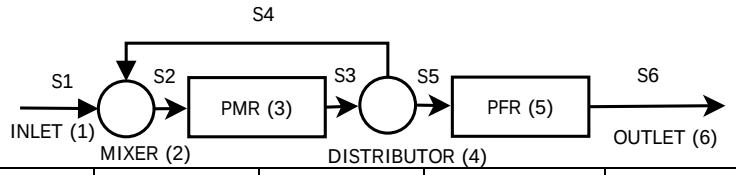
The fermentors are multi impeller systems; and in the design of these systems the most important aspect is the development of optimal oxygen distribution along the system (*Alves et al*., 1997). There are other important variables to deal with, such as gas and fluid hold-up.

In some of the cases the compartment model may be less complex than CFD model, but both models need validation. To validate these models Doppler anemometry, particle velocimetry or mixing time measurements needs to be performed (*Vrabel et al*., 1999).

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. The incidence matrix is a matrix that shows the connection between two compartments, and contains column equal to the number of compartments, and rows equal to the number of stream between them. The incidence matrix describes the structure of a network, all of the connections between compartments in one structure. If a stream does not connect to a compartment the value is zero. If the stream leaves the compartment the value is -1, and if the stream enters the compartment the value is 1. *Figure 1* shows a possible compartment structure with the incidence matrix, which describes the structure of the compartment model; S refers to streams.

Figure 1

A compartment structure and its incidence matrix



	MIXER	PMR	DISTRIBUTOR	PFR
S1	1	0	0	0
S2	-1	1	0	0
S3	0	-1	1	0
S4	1	0	-1	0
S5	0	0	-1	1
S6	0	0	0	-1

1. ábra: Egy cellás struktúra és az azt leíró kapcsolati mátrix

Betáplálás(1), Keverő(2), Tökéletesen kevert üst(3), Elosztó(4), Ideális cső(5), Elvétel(6)

In some cases the compartment model of a stirred system does not have to contain more than two compartments, the impeller zone and the circulation zone. The impeller and the zone near the impeller can be described by using a perfectly mixed reactor model, and at least one other region called circulation loop must be defined. Applying empirical equations the circulation numbers can be determined (*Alexopoulos et al*., 2002). The circulation numbers describe the rate of circulation between the impeller zone and circulation zones.

Compartment models can also be used in granulation systems, or in pharmaceutical applications (*Portillo et al*., 2006). Nowadays there are research efforts towards fuzzy solution or possibility theory, and these efforts can support the compartment model approach (*Claudel et al*., 2003).

Besides, the compartment models can be used not only in process industries, but in meteorology, or biomass processing (*Iliuta et al*., 2010). In these fields the application of compartment model is necessary, because the parts in ecological systems are often more complex than in the process industries. But some devices in industrial applications also demand more complex compartment models such as slurry reactors, or bubble columns (*Iliuta et al*., 2008).

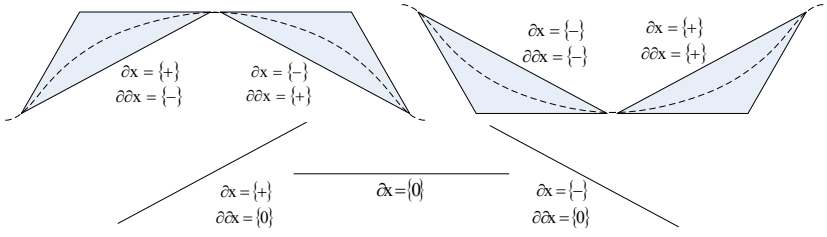
The most difficult task in the field of compartment modelling is to identify the adequate model structure. For solving this problem a qualitative approach can be useful. Qualitative data-intensive methods are widely applied because of their statistical nature, but they always require prior knowledge 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 (*Varga et al*., 2008).

The qualitative method in this case refers to the method by which the data have been processed in this study. The method uses first and second derivatives to determine primitive episodes and finally to define a structure based on measurement data (*Cheung et al., 1990).* By using the 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.

After the derivatives of the experimental data have been computed, the primitive episodes can be used to characterize the changes of the state variables during the experiments according to the shape of the diagram. 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 or constant value. *Figure 2* shows the primitive episodes used in this study.

Figure 2

The applied primitive episodes



2. ábra: A használt primitív epizódok

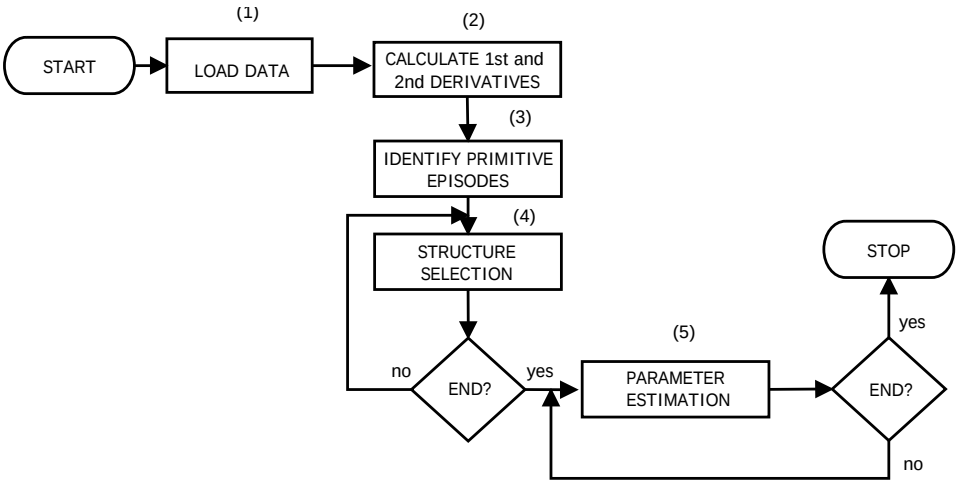
The primary goal of this study is to develop an algorithm that is capable of describing a stirred system as a compartment structure. Qualitative methods were used for the identification of the compartment structure; and MATLAB/Simulink was applied for the implementation of the algorithm. The first half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

MATERIAL AND METHOD

The developed algorithm is based on a qualitative method. *Figure 3* shows the flowsheet of the proposed algorithm.

Figure 3

Flowsheet of the proposed algorithm



3. ábra: A kidolgozott algoritmus folyamatábrája

Adatok betöltése(1), Első és második derivált számítása(2), Primitív epizódok azonosítása(3), Struktúra kiválasztása(4), Paraméterek becslése(5)

The first step of the algorithm is the processing of experimental data by filtering, and the second step is the analysis of the filtered data by qualitative methods.

To examine the hydrodynamic behaviour of the investigated system test signals must be used. In most of the cases impulse or step functions can be applied as test signals. However there are other signals can be used for studying hydrodynamic behaviour such as PRBS or trigonometric functions. The processed data in this case represents residence time distribution or residence time distribution density, obtained from experimental measurements. The residence time distribution of a chemical reactor is a probability distribution function that describes the amount of time that a fluid element could spend inside the reactor. Chemical engineers use the residence time distribution function to characterize the mixing and flow within reactors and to compare the behaviour of real reactors to ideal models. The residence time distribution function is

useful, not only for troubleshooting existing reactors, but also in estimating the yield of a given reaction and designing future reactors.

The qualitative approach is applied in the next step of the algorithm. The first and second derivatives have to be computed. Based on the derivatives the primitive episodes are assigned to the appropriate time domains. For the identification step the previously mentioned seven primitive episodes have been used. The series of these episodes gives a sequence, that is specific for the structure of the investigated process unit.

The experimental data must be filtered, to avoid the short episodes and to compensate the noise. The filtering coefficient is the minimal length of one episode and must be carefully chosen and has to be lower than the sampling time of the experimental data. After the generation of the sequence based on the measurement data, the next step in the algorithm is to create a database of compartment models that contains all combinations of the applied compartments. These compartments at this stage of the development are:

- perfectly mixed reactor (PMR);
- ideal plug flow reactor (PFR);
- distributor;
- mixer.

Reaction takes place only in the reactor compartments. There are some heuristic rules which can be applied to model the net of the compartments:

- the model must contain at least one reactor compartment;
- the model has to contain equal number of distributors and mixers;
- the ideal plug flow reactor modelled by a series of ten perfectly mixed reactors in the compartment structure.

For identification purposes a database has been developed with all possible compartment structures, containing series of PFR-s and PMR-s and parallel reactor structures alike. At this stage of the development the goal is to create the model with the least number of compartments with an acceptable tolerance of error.

The essence of the next step is to define the incidence matrix for the generated structures.

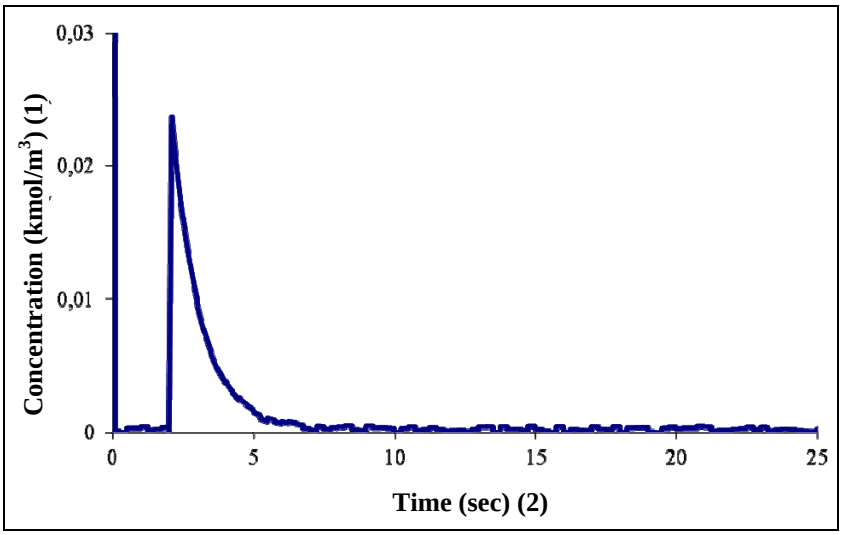
After the construction of the structure database the next step is to determine which model fits the best for the processed experimental data. A dynamic simulation has to be run for every structure in the database, and a qualitative analysis has to be done. After the qualitative step the measured and the simulated sequences have to be compared to find the proper structure. Having the proper structure the model parameters - such as volume of the reactor compartments and circulation ratios - the only information remains to be determined. Hence, in the parameter estimation step two parameters have to be identified: the circulation ratio (α), and the volume ratio of the reactor compartments (β). To find the correct parameters an optimizer algorithm is applied based on the minimization of the difference between experimental and simulated data.

RESULTS AND DISCUSSION

In the case study a perfectly mixed reactor and a consecutive ideal plug flow reactor have been used with one feed-forward stream. *Figure 4* shows the residence time distribution density of the investigated system that was used as measured data. To make the defined data set more realistic some noise was superposed on the data.

Figure 4

The measurement data



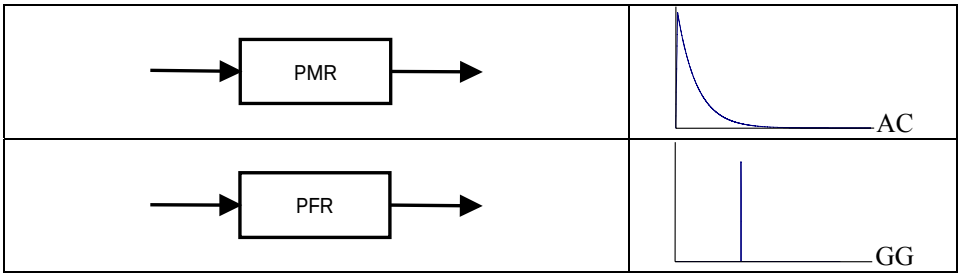
4. ábra: A mérési adatok

Koncentráció (kmol/m^3)(1), Idő (sec)(2)

In this particular case the system have been identified with a combination of 'GGAC'. The letter G may refer three different things. If G is only the last episode of the sequence that means the function has reached the stationary state. If G is the only episode that means there is not any reactor compartment in the system. And if there are more than one G in the sequence that means at least one plug flow reactor compartment has to be built into the structure. The other letters refer, that there are other reactor cells in the system. *Figure 5* shows the length of the identified primitive episodes in the order of 'G' 'G' 'A' and 'C'.

Figure 5

Structures, residence time distribution functions and identified sequences



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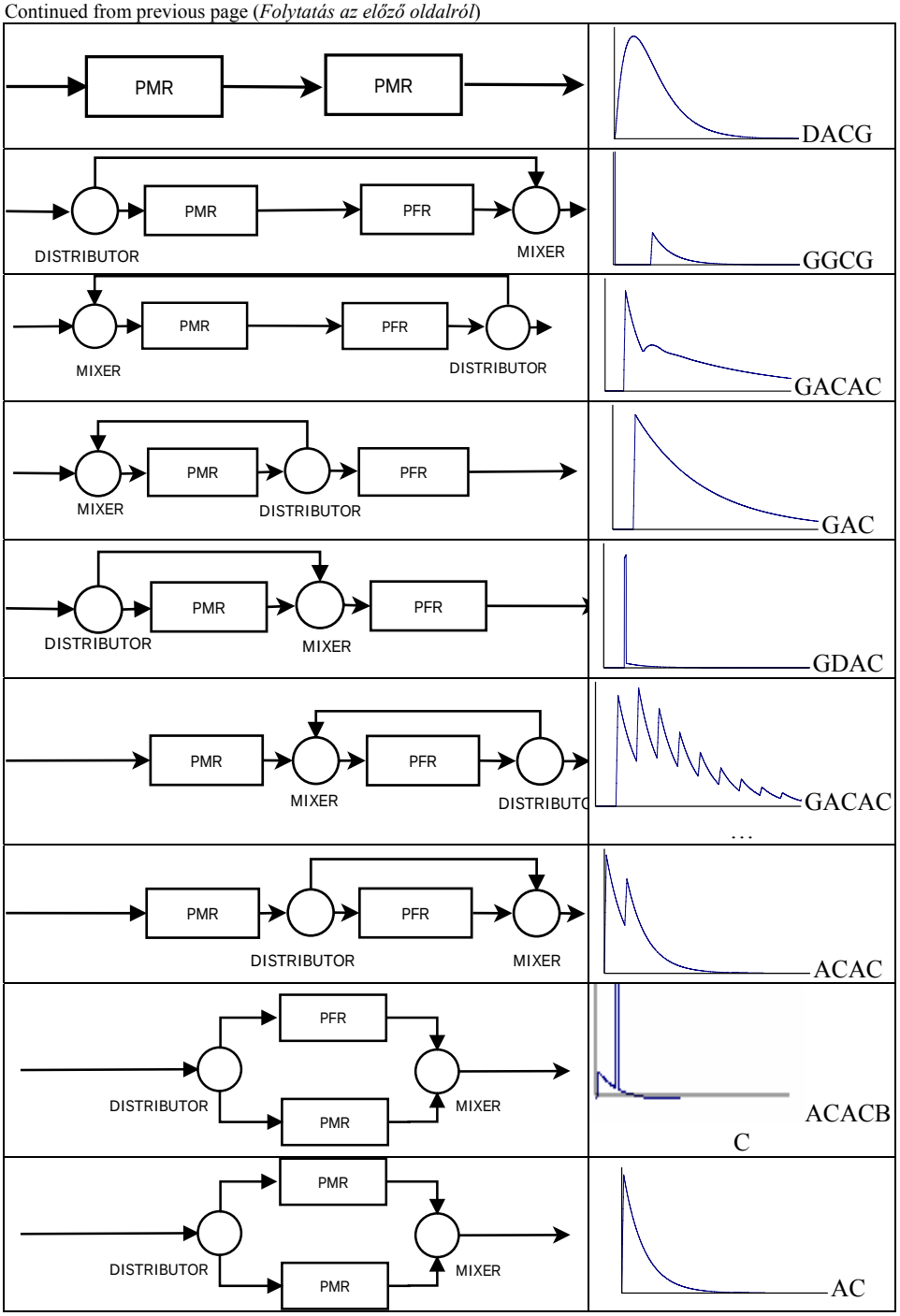


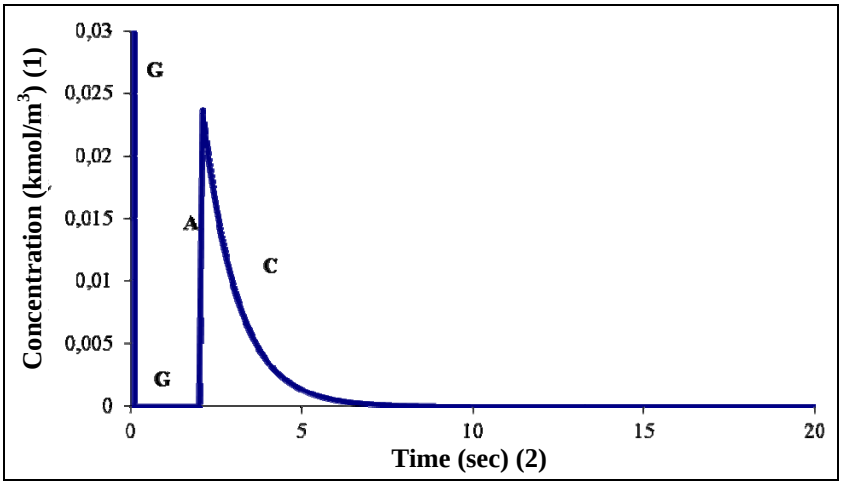
5 ábra: Struktúrák, Dirac deltára adott válaszuk és az azonosított szekvenciák

As it was explained at least two reactor cells are needed to describe the examined system. This will be the lower boundary of the number of the cells. For two cells there are only three combinations if the system has to contain at least one plug flow reactor cell. These combinations are PMR-PFR, or PFR-PMR or a series of two PFR-s. Using four compartments it is possible to describe a system with four consecutive reactor compartments, or to define maximum one circulation loop with two reactor compartments.

The generated structure database contains all of the combinations between the defined boundaries according to the defined limitations. The algorithm at this point examines the combinations, and finds the proper one. *Figure 6* shows the processed data, and *Figure 7* shows the structure of the compartment model.

Figure 6

The filtered data and the identified episodes

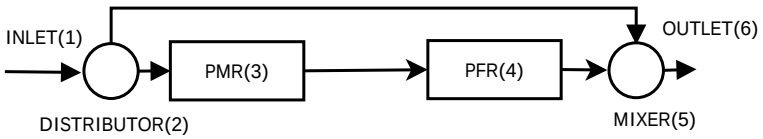


6. ábra: A szűrt adatok és az identifikált primitív epizódok

Koncentráció (kmol/m^3)(1), Idő (sec)(2)

Figure 7

The identified compartment structures



7. ábra: Az identifikált cellás struktúrák

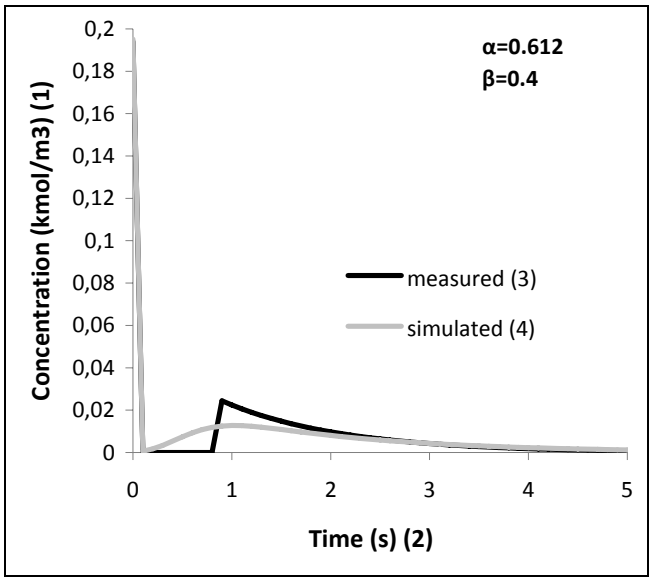
Betáplálás(1), Elosztó(2), Tökéletesen kevert üst (PMR)(3), Ideális cső (PFR)(4), Keverő(5), Elvétel(6)

In this case two structures have been identified. Each structure contains four compartments and in both cases the first compartment is a distributor and the last one is a mixer. The compartments between them have the same response to the impulse function, so swapping them does not conclude any changes in the results.

After the structure selection the parameter estimation step could be done, and the circulation ratio and the volume ratio were identified. *Figure 8* shows the measured data compared to the simulated data and the identified model parameters. There is a difference between the experimental and simulated data, because in the simulation we used ten perfectly mixed reactors for modelling a plug flow compartment instead a time delay.

Figure 8

Comparison of measured and simulated data and the identified parameters



8. ábra: A mért és szimulált adatok összehasonlítása, valamint az identifikált paraméterek (α=cirkulációs arány, β=térfogat arány)

Koncentráció (kmol/m^3)(1), Idő (sec)(2), Mért(3), Szimulált(4)

The algorithm found the adequate structures to describe the measurement data, and could identify the proper parameters. The proposed algorithm can be a useful tool to identify compartment structures for optimisation and solving other engineering problems.

CONCLUSIONS

An algorithm was developed in order to determine an adequate compartment structure for an experimental data set. 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.

In the future the algorithm will be improved to identify more complex structures, and the basic compartment models will be extended to handle more compartment classes such as dead zone.

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