

IDENTIFICATION OF FUZZY MODELS APPLIED TO A THREE-PHASE CATALYTIC HYDROGENATION REACTOR

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Keywords: Model Identification, Fuzzy modeling, Takagi-Sugeno Model, hydrogenation reactor.

Abstract. This paper proposes the identification of Fuzzy models applied to a three-phase catalytic reactor in which is carried out the o-cresol hydrogenation for obtainment of 2-methyl-cyclohexanol. Through the deterministic model that represents the three-phase catalytic reactor are obtained the data to build the Fuzzy models. The identification of models is an important step for the control design since the Fuzzy model can be presented as an alternative to the model of the Model Predictive Controllers. Two possible control configurations for this reactor is to maintain the exit concentration of o-cresol in the liquid phase at the set point manipulating the reactor feed temperature and to maintain the reaction medium temperature at the exit of the reactor at the set point manipulating the reactor feed temperature. Considering the different order of magnitude of the variables of the first control configuration, in order to procedure with the identification of the model, the codification of such variables is proposed as a first step. The results show a very good approximation of the Fuzzy model and the deterministic model confirming that this Fuzzy model can be used in substitution to the rigorous model of the reactor in control applications. In future works, the Fuzzy model can be used, for instance, as an alternative to the convolution model of the Dynamic Matrix Control, configuring in a Fuzzy-DMC Hybrid Controller.

1 INTRODUCTION

The identification of models is an important step for the control design. Through the identification of models, a controller can be designed by means of various control methods to achieve the required specification. The system identification can be applied as part of control law for instance to design the indirect adaptive control (Alfi and Fateh, 2011).

The serious nonlinearity and uncertainty issues present on the most real systems characterize difficult to develop and to design a suitable model to deal with this problem. In the last four decades, various schemes have been developed, one of the most important of which is fuzzy logic theory (Chen, 2011).

One advantage of the use of Fuzzy models is the fact that they can be constructed using the available information and their complexity can be gradually increased as more information is gathered (Khairy et al., 2010).

There are in literature many works that employ the identification of Fuzzy models. Fuzzy logic is widely used in Model-based predictive control (MPC) (Khairy et al., 2010).

Lima et al. (2010a) presented Takagi–Sugeno Fuzzy models as an alternative modeling tool for the molecular distillation process of heavy liquid petroleum residues and showed that the Fuzzy models obtained were compared with the results generated from the phenomenological model, showing a good agreement.

Lima et al. (2010b) developed a predictive control system based on type Takagi-Sugeno Fuzzy models for a polymerization process. The performance of the projected control system and Dynamic Matrix Control for regulatory and servo problems were compared and the obtained results showed that the control system design is robust, of simple implementation and provides a better response than conventional predictive control.

Causa et al. (2008) proposed a Hybrid Fuzzy Predictive Control strategy (HFPC) in order to regulate the temperature of a batch reactor, minimizing both the trajectory error and the control energy. The authors presented the HFPC based on a Genetic Algorithm as an algorithm that allowed solving NP-hard problems with the HFPC strategy.

Karer et al. (2007) proposed a comparison between MPC employing a hybrid linear model and a hybrid Fuzzy model. It was established that the latter approach clearly outperforms the approach where a linear model is used.

Çetinkaya et al. (2006) implemented a standard Fuzzy-relational matrix version of the classical DMC algorithm in a batch jacketed polymerization reactor showing that the application of a Fuzzy-DMC controller is promising for temperature control of batch polymerization reactors in industrial applications.

The development of reliable mathematical models is important to the control of the three phase catalytic hydrogenation reactors, since it is necessary at the same time to operate with high productivity and within products specifications without causing environmental impact. Hydrogenation reactors have been performed hydrogenation reactors in order to obtain ethanol (Subramani and Gangwal, 2008; Chen et al., 2011; Surisetty et al., 2011).

The deterministic mathematical model of the three phase catalytic reactor, considered in this paper, was developed by Vasco de Toledo (2004), and can be found in Appendix A.

The process variables in this model are the linear velocity of gas (ug), the linear velocity of liquid (ul), the linear velocity of coolant (ur), the hydrogen concentration in the gas phase in the reactor feed (Agf), the hydrogen concentration in the liquid phase in the reactor feed (Alf), the o-cresol concentration in the liquid phase in the reactor feed (Blf), the feed reactor temperature (Tf) and the feed coolant temperature (Trf). The output variables are exit concentrations of hydrogen both in the gas phase (Ag) and in the liquid phase (Al), exit

concentration of o-cresol in the liquid phase (Bl), reaction medium temperature at the exit of the reactor (T) and temperature of the coolant fluid at the exit of the reactor (Tr). Rezende et al. (2008) showed a dynamic behavior of the reactor in terms of two important output variables (Bl and T). The authors appointed the influence of the T_f on Bl and the influence of the T_f on T . This suggests a suitable SISO control configuration in which T_f is the manipulated variable and Bl and T are the controlled variables. Aiming the future reactor control, the present work proposes the identification of Fuzzy models. Using the deterministic model of the reactor as data generator, the Fuzzy models are built. In a future work, the Fuzzy model will be employed as internal model of a DMC control algorithm leading to a new predictive control, a Fuzzy model-based predictive control.

In the present work, the type of functional Fuzzy models employed is the Takagi-Sugeno Fuzzy models. Since in a first control configuration, the order of magnitude of the controlled and manipulated variables is different, the codification of such variables is proposed. The results obtained show a good approximation between the Fuzzy model and the deterministic model.

2 IDENTIFICATION OF FUNCTIONAL FUZZY MODELS

According to Lima et al. (2010a), the first point to be considered in the procedure of Fuzzy modeling is the definition of the Fuzzy model structure that make up the system rule base. The Takagi-Sugeno (T-S) Fuzzy model is a special case among functional Fuzzy models. Its structure was proposed by Takagi and Sugeno (Takagi and Sugeno, 1985).

The T-S type fuzzy models combine linguistic rule descriptions with the traditional functional description of the system operations (Chen, 2011).

T-S fuzzy models are suitable for modeling a large class of nonlinear systems. They consist of fuzzy IF-THEN rules which represent local linear input-output relations of a nonlinear system (Khairy et al., 2010).

The Takagi-Sugeno model for generation of Fuzzy rules from a given input-output data set, which has two-inputs x_1 and x_2 , and output y , can be written in the following way:

$$\text{IF } x_1 \text{ is } X_1 \text{ and } x_2 \text{ is } X_2 \text{ THEN } y \text{ is } y = f(x_1; x_2) \quad (1)$$

where X_1 and X_2 are Fuzzy sets (membership functions) of x_1 and x_2 , respectively, and $y = f(x_1, x_2)$ is a crisp consequent function.

The generalization of Eq. 1, for a linear structure with an entrance number n , leads to the Takagi-Sugeno model, as following by Eq. 2:

$$\text{IF } (x_i \text{ is } X_{i;1}) \text{ and } (x_2 \text{ is } X_{i;2}) \text{ and } \dots \text{ and } (x_j \text{ is } X_{i;j}) \text{ and } \dots \text{ and } (x_n \text{ is } X_{i;n}) \text{ THEN } y_i = a_{i1} \cdot x_1 + a_{i2} \cdot x_2 + \dots + a_{ij} \cdot x_j + \dots + a_{in} \cdot x_n \quad (2)$$

where $i = 1, \dots, R$, being R the number of rules of the Fuzzy model; $j = 1, \dots, n$ and a_{ij} are parameters of the consequent function of the Fuzzy model.

For a given input, the output of the Fuzzy model is inferred by the weighted average of referring output i to each rule, calculated by: Eq. 3:

$$y = \frac{\sum_{i=1}^R f_i \cdot \mu_i(x)}{\sum_{i=1}^R \mu_i(x)} \quad (3)$$

where $\mu_i(x)$ are membership functions and f_i is a consequent function to each rule i (Lima et al., 2010b).

In this paper, the type of functional Fuzzy models employed is the Takagi-Sugeno Fuzzy

models. The Subtractive Clustering method is the chosen method to be used to determine the rule number and parameters of the membership functions. Consequent function parameters are obtained through an optimization problem solved by a least square based algorithm. This work employs Gaussian membership functions given by Eq. 4:

$$\mu_i = \exp\left[-\frac{1}{2}\left(\frac{x_i - c_i}{\sigma_i}\right)^2\right] \quad (4)$$

where c_i is the i^{th} center of the membership function and σ_i is a constant related to spread of the i^{th} membership function.

The validation of the Fuzzy models is quantified by the average quadratic error between the predicted output from the Fuzzy models and the real output (phenomenological model) through the Eq. (5):

$$Error = \sqrt{\frac{\sum_{k=1}^m (\bar{y}_k - y_k)^2}{m}} \quad (5)$$

where k is the time point, m is the number of considered discrete instants, \bar{y}_k is the predicted output from the Fuzzy model in instant k and y_k is the real output in instant k (Lima et al., 2010a).

The identification of Fuzzy models is important step to proceed with process control. The Fuzzy model can be presented as an alternative to the convolution model of the Dynamic Matrix Control in a future work generating a Fuzzy-Predictive Hybrid Control. A control configuration possible for this reactor is to maintain the exit concentration of o-cresol in the liquid phase at the set point manipulating the reactor feed temperature and to maintain the exit concentration of o-cresol in the liquid phase at the set point manipulating the reactor feed temperature. The results obtained by this configuration are presented in the next heading.

3 RESULTS AND DISCUSSIONS

In order to deal with the identification of the model, the data generation must to be performed through the deterministic model. Considering a range of 0 to 15%, disturbances of +/-1% was applied to the manipulated variable and the respective effect on the controlled variable is verified in order to generate data for training (generation) of the Fuzzy model, as following by Tables 1-2 and Tables 2-3. In this work, the studied control configuration considers Tf (feed reactor temperature) as manipulated variable and Bl (exit concentration of o-cresol in the liquid phase) and T (reaction medium temperature at the exit of the reactor) as controlled variables.

Disturbance (%)	Tf (K)	Bl (Kmol/m ³)
0	540.0	0.01299
+1	545.4	0.01239
-1	534.6	0.01360
+3	556.2	0.01120
-3	523.8	0.01482
+5	567.0	0.01007
-5	513.0	0.01601
+7	577.8	0.00900

-7	502.2	0.01715
+9	588.6	0.00801
-9	491.4	0.01821
+11	599.4	0.00710
-11	480.6	0.01918
+13	610.2	0.00627
-13	469.8	0.02003
+15	621.0	0.00552
-15	459.0	0.02077

Table 1: Data for training (generation) of the Fuzzy model of the exit concentration of o-cresol in the liquid phase (BI).

Disturbance (%)	Tf (K)	T (K)
0	540.0	539.11
+1	545.4	543.48
-1	534.6	534.74
+3	556.2	552.19
-3	523.8	526.00
+5	567.0	560.85
-5	513.0	517.27
+7	577.8	569.44
-7	502.2	508.61
+9	588.6	577.95
-9	491.4	500.02
+11	599.4	586.37
-11	480.6	491.53
+13	610.2	594.72
-13	469.8	483.16
+15	621.0	602.98
-15	459.0	474.90

Table 2: Data for training (generation) of the Fuzzy model of the reaction medium temperature at the exit of the reactor (T).

Thereafter, considering a range of 0 to 14%, disturbances of +/-2% was applied to the manipulated variable and the respective effect on the controlled variables is verified in order to generate data for testing (validation) of the Fuzzy model, as following by Tables 3-4:

Disturbance (%)	Tf (K)	BI (Kmol/m ³)
0	540.0	0.01299
+2	550.8	0.01179
-2	529.2	0.01421
+4	561.6	0.01063
-4	518.4	0.01542
+6	572.4	0.00952
-6	507.6	0.01659

+8	583.2	0.00849
-8	496.8	0.01769
+10	594.0	0.00754
-10	486.0	0.01871
+12	604.8	0.00667
-12	475.2	0.01962
+14	615.6	0.00588
-14	464.4	0.02042

Table 3: Data for testing (validation) of the Fuzzy model of the exit concentration of o-cresol in the liquid phase (Bl).

Disturbance (%)	Tf (K)	T (K)
0	540.0	539.11
+2	550.8	547.84
-2	529.2	530.36
+4	561.6	556.53
-4	518.4	521.63
+6	572.4	565.15
-6	507.6	512.93
+8	583.2	573.70
-8	496.8	504.30
+10	594.0	582.17
-10	486.0	495.76
+12	604.8	590.56
-12	475.2	487.33
+14	615.6	598.86
-14	464.4	479.02

Table 4: Data for testing (validation) of the Fuzzy model of the reaction medium temperature at the exit of the reactor (T).

The operation range of the Fuzzy model is determined by the definition of the minimal and maximal values of the variables, as following by Table 5:

Minimal values	Variables	Maximal values
459.0	Tf (K)	621.0
0.01360	Bl (Kmol/m ³)	0.02077

Table 5: Minimal and maximal values of the variables Tf and Bl.

The operation range of the Fuzzy model is determined by the definition of the minimal and maximal values of the variables, as following by Table 6:

Minimal values	Variables	Maximal values
459.0	Tf (K)	621.0
474.90	T (K)	602.98

Table 6: Minimal and maximal values of the variables Tf and T.

Using the Matlab software (Matlab 7.0), the data were trained and the model parameters were evaluated.

The configuration of parameters that provided a good approximation of the Fuzzy model of the exit concentration of o-cresol in the liquid phase was:

- 1) Range of influence = 0.5
- 2) Squash factor = 1.25
- 3) Accept ratio = 0.5
- 4) Reject ratio = 0.15

For the case of the Fuzzy model of the reaction medium temperature at the exit of the reactor, the configuration of parameters that provided a good approximation was:

- 1) Range of influence = 0.5
- 2) Squash factor = 0.625
- 3) Accept ratio = 0.5
- 4) Reject ratio = 0.15

Finally, the model is validated through the test data.

In the control configuration that considers T_f (feed reactor temperature) as manipulated variable and Bl (exit concentration of o-cresol in the liquid phase) as controlled variable, as such variables have different order of magnitude, it was verified that is essential to codify such variables, as following by Eqs 6 and 7:

$$Tf_{cod} = \frac{Tf - Tf_{min}}{Tf_{max} - Tf_{min}} \quad (6)$$

$$Bl_{cod} = \frac{Bl - Bl_{min}}{Bl_{max} - Bl_{min}} \quad (7)$$

where,

Tf is the value that will be codified.

Tf_{min} is the Tf minimal value in the range of the values of Tf (Tables 5 and 6).

Tf_{max} is the Tf maximal value in the range of the values of Tf (Tables 5 and 6).

Bl is the value that will be codified.

Bl_{min} is the Bl minimal value in the range of the values of Bl (Tables 5 and 6).

Bl_{max} is the Bl maximal value in the range of the values of Bl (Tables 5 and 6).

The generated Fuzzy model for the exit concentration of o-cresol in the liquid phase (Bl) is represented by three rules and the Fuzzy model for the reaction medium temperature at the exit of the reactor (T) is represented by five rules.

Table 7 and 8 show the parameters for the Fuzzy cognitive models (input) and the parameters for the Fuzzy cognitive models (output) for the exit concentration of o-cresol in the liquid phase (Bl) and for the reaction medium temperature at the exit of the reactor (T), respectively.

Rule	Input		Output	
	c_i	σ_i	b_i	a_i

1	0.51329250	0.19521458	0.93563407	-0.86876139
2	0.85595731	0.19473479	0.66189259	-0.66725742
3	0.13587435	0.17953994	1.0023190	-0.78018940

Table 7: Parameters for the Fuzzy cognitive models – input and output for the exit concentration of o-cresol in the liquid phase (Bl).

Rule	Input		Output	
	c_i	σ_i	b_i	a_i
1	28.637824	540	-21.513812	1.037861
2	28.637824	577.8	-15.706127	1.011522
3	28.637824	502.2	-4.9096879	1.024277
4	28.637824	610.2	74.472645	0.845209
5	28.637824	469.8	92.515496	0.841145

Table 8: Parameters for the Fuzzy cognitive models – input and output for the reaction medium temperature at the exit of the reactor (T).

According to Eqs. 3 and 4 and the values shown in Table 7, the Fuzzy model for the exit concentration of o-cresol in the liquid phase (Bl) can be written as following by Eq.8:

$$\begin{aligned}
 Bl_{cod} = & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf_{cod} - 0.5132}{0.1952}\right)^2\right) \right) \times (0.9356 - 0.867 \times Tf_{cod}) + \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf_{cod} - 0.8559}{0.1947}\right)^2\right) \right) \times (0.6618 - 0.6672 \times Tf_{cod}) + \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf_{cod} - 0.1358}{0.1795}\right)^2\right) \right) \times (1.0023 - 0.7801 \times Tf_{cod}) / \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf_{cod} - 0.5132}{0.1952}\right)^2\right) \right) + \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf_{cod} - 0.8559}{0.1947}\right)^2\right) \right) + \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf_{cod} - 0.1358}{0.1795}\right)^2\right) \right)
 \end{aligned} \tag{8}$$

Equation 8 considers the code values of the manipulated and controlled. Equation 9 decodes the values obtained by Eq.8:

$$Bl = 0.00588 + Bl_{cod} \times (0.02042 - 0.00588) \tag{9}$$

According to Eqs. 3 and 4 and the values shown in Table 8, the Fuzzy model for the reaction medium temperature at the exit of the reactor (T) can be written as following by Eq.10:

$$\begin{aligned}
 T = & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf - 540}{28.63}\right)^2\right) \right) \times (-21.51 + 1.037 \times Tf) + \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf - 577.8}{28.63}\right)^2\right) \right) \times (-15.70 + 1.011 \times Tf) + \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf - 502.2}{28.63}\right)^2\right) \right) \times (-4.90 + 1.024 \times Tf) + \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf - 610.2}{28.63}\right)^2\right) \right) \times (74.47 + 0.845 \times Tf) + \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf - 469.8}{28.63}\right)^2\right) \right) \times (92.51 + 0.841 \times Tf) / \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf - 540}{28.63}\right)^2\right) \right) + \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf - 577.8}{28.63}\right)^2\right) \right) + \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf - 502.2}{28.63}\right)^2\right) \right) + \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf - 610.2}{28.63}\right)^2\right) \right) + \\
 & \left(\exp\left(-\frac{1}{2} \times \left(\frac{Tf - 469.8}{28.63}\right)^2\right) \right)
 \end{aligned}
 \tag{10}$$

Figures 1 and 2 illustrate the identification data for the output variables (Bl) and (T), respectively.

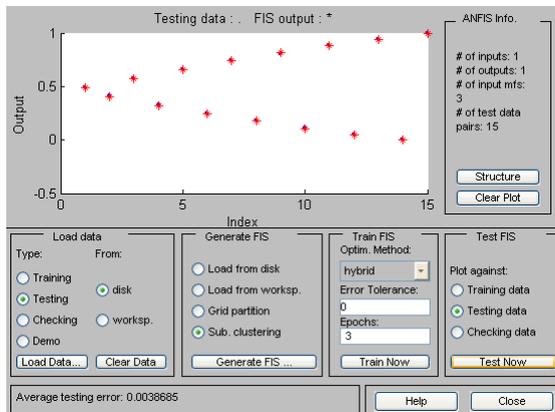


Figure 1: Data identification of the Fuzzy model for the exit concentration of o-cresol in the liquid phase (Bl).

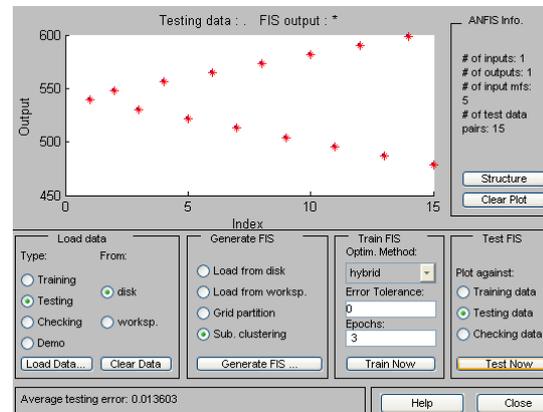


Figure 2: Data identification of the Fuzzy model for the reaction medium temperature at the exit of the reactor (T).

The medium error associated to the model for Bl variable is equal to 0.0038685 Km³/m³ and the medium error associated to the model for T is 0.013603 K.

The validation of the Fuzzy model for the concentration of o-cresol in the liquid phase (Bl) is shown in Figure 3.

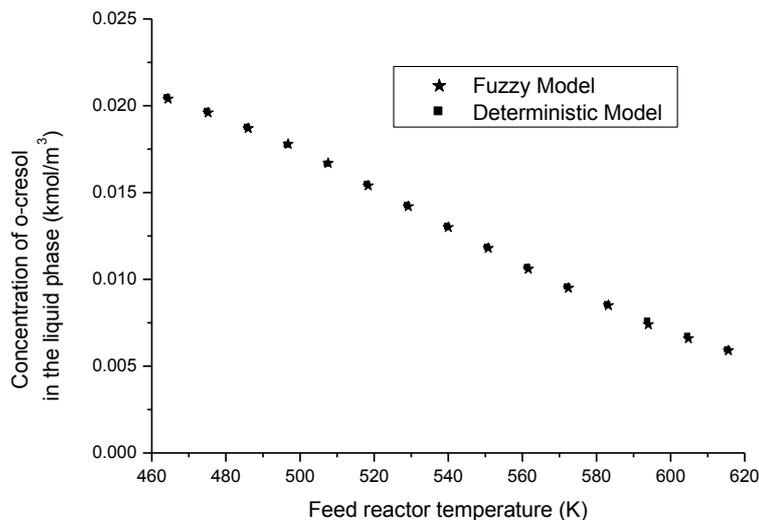


Figure 3: Validation of the Fuzzy model for the exit concentration of o-cresol in the liquid phase (BI).

Figure 3 shows that the Fuzzy model is close to the deterministic model. The values of the output variable (concentration of o-cresol in the liquid phase - BI) in relation to the input variable (feed reactor temperature - Tf) obtained by Fuzzy model presented a very good approximation to the values derivate from deterministic model.

The validation of the Fuzzy model for the reaction medium temperature at the exit of the reactor (T) is shown in Figure 4.

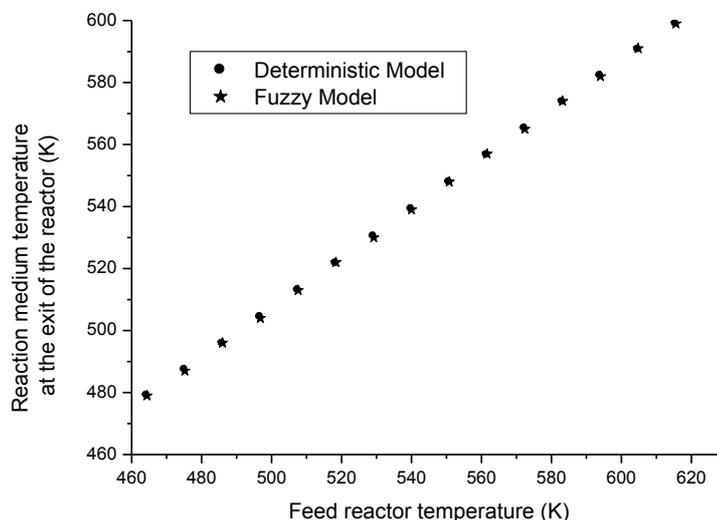


Figure 4: Validation of the Fuzzy model for the reaction medium temperature at the exit of the reactor (T).

Through Figure 4, is possible to see that the values of the output variable (reaction medium temperature at the exit of the reactor - T) in relation to the input variable (feed reactor temperature - Tf) obtained by Fuzzy model presented a very good approximation to the values derivate from deterministic model.

These results confirm that the Fuzzy models can be used to represent the o-cresol hydrogenation reactor considered here and can be employed in substitution to the rigorous

model of the reactor in control applications. In future works, the Fuzzy models can be used as an alternative to the convolution model of the Dynamic Matrix Control, configuring in a Fuzzy-DMC Hybrid Controller.

4 CONCLUSIONS

In this paper, the identification of Fuzzy models applied to a three-phase catalytic reactor in which is carried out the o-cresol hydrogenation for obtainment of 2-methyl-cyclohexanol was performed in order to obtain a suitable model for control applications. The control configurations considered for this reactor was to maintain the exit concentration of o-cresol in the liquid phase at the set point manipulating the reactor feed temperature and to maintain the reaction medium temperature at the exit of the reactor at the set point manipulating the reactor feed temperature. Considering the different order of magnitude of the variables in the first control configuration, the codification of such variables was performed. The obtained results showed that the Fuzzy models are close to the deterministic model proving a very good approximation between these both model types. The results confirm that the Fuzzy models obtained in this work are a potential model to be employed in control applications, for instance, as an alternative to the convolution model of the Dynamic Matrix Control, configuring in a Fuzzy-DMC Hybrid Controller.

ACKNOWLEDGEMENTS

The authors would like to thank FAPESP (Fundação de Amparo à Pesquisa do Estado de São Paulo), for the financial support, process number [2008/01230-1](#).

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APPENDIX A

This Appendix presents the mass and energy balances (Equations A1-A17) that constitutes the mathematical model of the three-phase reactor considered in this work and illustrated in Figure A.1. Details about the model, kinetic, mass transfer, heat and design parameters can be found in Vasco de Toledo et al. (2004).

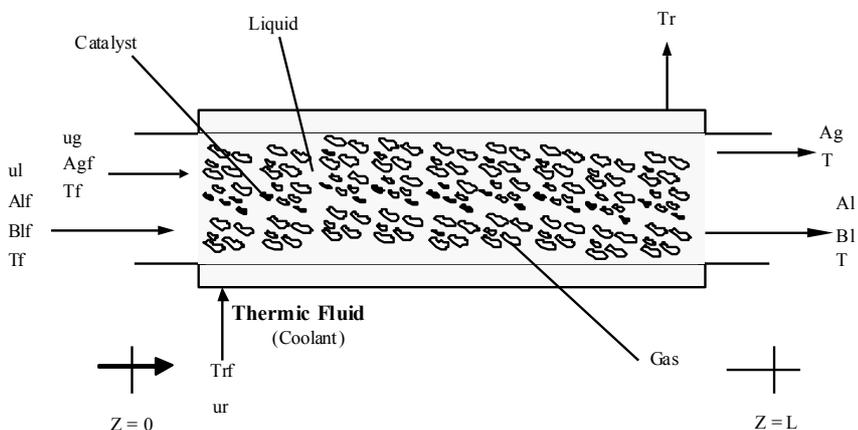


Figure A.1: Schematic drawing of a three-phase slurry reactor.

Mass Balance for reactant A (hydrogen) in gas phase:

$$\epsilon_g \frac{\partial A_g}{\partial t} = \frac{D_{eg}}{L^2} \frac{\partial^2 A_g}{\partial z^2} - \frac{u_g}{L} \frac{\partial A_g}{\partial z} - (K_{gl})_A a_{gl} (A^* - A_l) \quad (\text{A1})$$

$$\text{Boundary Conditions: } \left. \frac{D_{eg}}{L} \frac{\partial A_g}{\partial z} \right|_{z=0} = u_g (A_g - A_{gf}) \quad (\text{A2})$$

$$\left. \frac{\partial A_g}{\partial z} \right|_{z=1} = 0 \quad (A3)$$

Mass Balance for reactant A (hydrogen) in liquid phase:

$$\varepsilon_1 \frac{\partial A_l}{\partial t} = \frac{D_{el}}{L^2} \frac{\partial^2 A_l}{\partial z^2} - \frac{u_l}{L} \frac{\partial A_l}{\partial z} + (K_{gl})_A a_{gl} (A^* - A_l) - (K_{ls})_A a_{ls} (A_l - A_s^s) \quad (A4)$$

$$\text{Boundary Conditions: } \left. \frac{D_{el}}{L} \frac{\partial A_l}{\partial z} \right|_{z=0} = u_l (A_l - A_{lf}) \quad (A5)$$

$$\left. \frac{\partial A_l}{\partial z} \right|_{z=1} = 0 \quad (A6)$$

Mass Balance for reactant B (o-cresol) in liquid phase:

$$\varepsilon_1 \frac{\partial B_l}{\partial t} = \frac{D_{el}}{L^2} \frac{\partial^2 B_l}{\partial z^2} - \frac{u_l}{L} \frac{\partial B_l}{\partial z} - (K_{ls})_B a_{ls} (B_l - B_s^s) \quad (A7)$$

$$\text{Boundary Conditions: } \left. \frac{D_{el}}{L} \frac{\partial B_l}{\partial z} \right|_{z=0} = u_l (B_l - B_{lf}) \quad (A8)$$

$$\left. \frac{\partial B_l}{\partial z} \right|_{z=1} = 0 \quad (A9)$$

Energy Balance in the fluid phase:

$$\begin{aligned} (\varepsilon_g \rho_g C_{pg} + \varepsilon_l \rho_l C_{pl}) \frac{\partial T}{\partial t} = \frac{(\varepsilon_g \lambda_g + \varepsilon_l \lambda_l)}{L^2} \frac{\partial^2 T}{\partial z^2} - \frac{(\varepsilon_g \rho_g C_{pg} u_g + \varepsilon_l \rho_l C_{pl} u_l)}{L} \frac{\partial T}{\partial z} \\ + h_s a_{ls} (T_s^s - T) - \frac{4U}{D_t} (T - T_r) \end{aligned} \quad (A10)$$

$$\text{Boundary Conditions: } \left. \frac{(\varepsilon_g \lambda_g + \varepsilon_l \lambda_l)}{L} \frac{\partial T}{\partial z} \right|_{z=0} = (\varepsilon_g \rho_g C_{pg} u_g + \varepsilon_l \rho_l C_{pl} u_l) (T - T_r) \quad (A11)$$

$$\left. \frac{\partial T}{\partial z} \right|_{z=1} = 0 \quad (A12)$$

Energy Balance for the coolant:

$$\rho_r C_{pr} \frac{\partial T_r}{\partial t} = - \frac{\rho_r C_{pr} u_r}{L} \frac{\partial T_r}{\partial z} + \frac{4U}{D_t} (T - T_r) \quad (A13)$$

$$\text{Boundary Conditions: } T_r = T_{rf}, \quad z = 0 \quad (A14)$$

Mass Balance for reactant A (hydrogen) in solid phase:

$$(1 - \varepsilon) \varepsilon_s \frac{\partial A_s}{\partial t} = (K_{ls})_A a_{ls} (A_l - A_s) - \frac{(1 - \varepsilon) \rho_s}{A_{ref}} R_w (A_s, B_s, T_s) \quad (A15)$$

Mass Balance for reactant B (o-cresol) in solid phase:

$$(1 - \varepsilon) \varepsilon_s \frac{\partial B_s}{\partial t} = (K_{ls})_B a_{ls} (B_l - B_s) - \frac{v(1 - \varepsilon) \rho_s}{B_{ref}} R_w (A_s, B_s, T_s) \quad (A16)$$

Energy Balance in solid phase:

$$(1 - \varepsilon) \rho_s C_{ps} \frac{\partial T_s}{\partial t} = h_s a_{ls} (T_s - T) + \frac{(1 - \varepsilon) \rho_s (-\Delta H_R)}{T_{ref}} R_w (A_s, B_s, T_s) \quad (A17)$$

NOMENCLATURE

- a surface area, m⁻¹
- A hydrogen concentration, kmol/m³

A*	solubility of the component A, kmol/m ³
Ag	exit concentration of hydrogen in the gas phase, kmol/m ³
Al	exit concentration of hydrogen in the liquid phase, kmol/m ³
Agf	feed concentration of hydrogen in the gas phase, kmol/m ³
Alf	feed concentration of hydrogen in the liquid phase, kmol/m ³
B	o-cresol concentration, kmol/m ³
Bl	exit concentration of o-cresol in the liquid phase, kmol/m ³
Blf	feed concentration of o-cresol in the liquid phase, kmol/m ³
Cp	heat capacity, kJ/kg K
De	effective diffusivity, m ² /s
D _t	reactor diameter, m
h	heat transfer coefficient, kJ/m ² s K
k	kinetic constant, kmol/kg-catalysts.s;
K	mass transfer coefficient between the phases, cm/s
L	reactor length, m
R _w	reaction rate, kmol/kg catalysts.s
T	reaction medium temperature at the exit of the reactor, K
T _f	reactor feed temperature, K
T _r	temperature of the coolant fluid at the exit of the reactor
T _{rf}	feed coolant temperature, K
u	linear velocity, m/s
u _g	linear velocity of gas, m/s
u _l	linear velocity of liquid, m/s
u _r	linear velocity of coolant, m/s
U	global heat transfer coefficient, kJ/m ² s K
z	dimensionless reactor axial position

Greek Letters

ΔH _R	heat of reaction, kJ/kmol
ε	porosity
λ	heat conductivity, kJ/m s K
ν	stoichiometric coefficient
ρ	density, kg/m ³

Subscripts:

A	component A (hydrogen)
B	component B (o-cresol)
f	feed
g	gas phase
gl	gas-liquid
l	liquid phase
ls	liquid-solid
p	particle
r	coolant fluid
ref	reference value used to turn the equations dimensionless
s	solid

Superscripts:

s	catalyst surface
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