MODELTOOL 1.0 – A MODEL TOOLBOX FOR MATLAB/SIMULINK

M. Bakošová, J. Baleja, Ľ. Čirka

Slovak University of Technology in Bratislava, Faculty of Chemical and Food Technology, Institute of Information Engineering, Automation and Mathematics

Abstract

MODELTOOL 1.0 - a model toolbox for MATLAB/Simulink has been developed at the Department of Information Engineering and Process Control IIEAM FCFT STU in Bratislava as a library of mathematical models of some processes from chemical technology: liquid holding tanks, heat exchangers, plate distillation columns and chemical reactors. The library has been developed in the MATLAB simulation environment and has the form of a MATLAB toolbox, which contains Simulink blocks of listed processes. These blocks allow simulation of dynamic behaviour of various types of processes using non-linear or linear mathematical models.

1 Introduction

Two of the main research and teaching areas at the Department of Information Engineering and Process Control of the IIEAM FCFT STU in Bratislava are process modelling/simulation and process control [1]. During the years, there have been created many mathematical models of various types of chemical processes at the department and various simulation environments were used for simulation of their dynamic properties. Many of these models were also used for testing of various control algorithms developed at the department. Nowadays, the MATLAB/Simulink is used as a simulation environment. From the variety of created models arose the necessity to develop a library of basic types of mathematical models of chemical processes. One of the basic demands on this library has been simple using for simulation of dynamic behaviour and also for testing of control algorithms. The result is the MODELTOOL 1.0 - a model toolbox for Matlab/Simulink [2], [3].

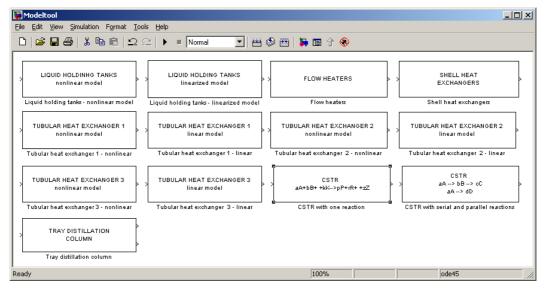


Figure 1: MODELTOOL 1.0 – a toolbox of mathematical models of some processes from chemical technology

2 MODELTOOL 1.0

MODELTOOL 1.0 - a model toolbox for Matlab/Simulink includes blocks of mathematical models of some processes from chemical technology: liquid holding tanks, heat exchangers, tray distillation columns and chemical reactors. All of these models are state-space models, linear or nonlinear. They are derived using mass and energy balances of modelled processes [4], [5], [6]. The basic window of the MODELTOOL is shown in Fig.1. The models in the library are constructed so,

that they can be used for simulation of dynamical behaviour as well as for verifying of various control algorithms for educational and research purposes. According to parameter setting, one block for various situations can represent various types of systems: single-input single-output system or multi-input multi-output system with specified number of inputs and outputs.

3 Liquid holding tanks

Two models of liquid holding tanks are included into the MODELTOOL 1.0 – nonlinear and linearized models. Both models provide the possibility to follow the level heights in liquid tanks connected serially with or without interactions. The input variables are flow rates of inlet streams. Other optional parameters are number of tanks, valves constants, cross section areas of tanks, interactions between tanks. The masks for both models are in Fig. 2. The Liquid Holding Tank – Linearized Model calculates matrices of linear state-space description of tanks and simulates dynamic behaviour of tanks using the linear state-space model.

Block Parameters: Liquid holding tanks - nonlinear model	Block Parameters: Liquid holding tanks - linearized model 🛛 🛛
LIQUID HOLDING TANKS (mask)	LIQUID HOLDING TANKS (mask)
LIQUID HOLDING TANKS - nonlinear model	LIQUID HOLDING TANKS - linearized model
Parameters	Parameters
Number of tanks	Number od tanks
	n
Vector of input variables 0 -no 1 -yes [qvs1 qvsn]	Vector of control variables 0 - no 1 - yes [qvs1 qvsn]
	[1 0 0]
	Input flow rates [qvs1 qvs2 qvsn]
Input flow rates [qvs1 qvs2 qvsn]	[qvs1 qvs2 qvsn]
[qvs1 qvs2 qvsn]	Vector of interactions [101100]
Vector of interactions [1 0 0 1 0 0]	[1 0 10 0]
[1 0 10 0]	Valves constants [k11 k22knn]
Valves constants [k11 k22 knn]	[k11 k22 knn]
[k11 k22 knn]	Cross section surfaces of tanks [F1 F2 Fn]
Cross section surfaces of tanks [F1 F2 Fn]	
[F1 F2 Fn]	[F1 F2 Fn]
· · ·	Vector of level heights [1 3 n - čísla zásobníkov]
Vector of level heights [1 3 n - the number of the tank]	[h1 h2 hi hn]
[h1 h2 hi hn]	Show matrices A,B,C,D
OK Cancel <u>H</u> elp <u>Apply</u>	OK Cancel <u>H</u> elp <u>Apply</u>

Figure 2: Block parameters - nonlinear and linear models of liquid holding tanks

4 Heat exchangers

Nowadays, the MODELTOOL contains 8 blocks for heat exchangers. They represent models of serially connected flow heaters, serially connected shell heat exchangers, 3 nonlinear models of tubular heat exchangers derived under various simplifying assumptions (1 – the most simple model, 3-the most complicated model) and 3 linear models of tubular heat exchangers derived also under various simplifying assumptions (1 – the most simple model, 3-the most complicated model). Optional parameters for two of these models can be seen in Fig. 3.

5 Chemical reactors

MODELTOOL includes two models of continuous-time stirred tank reactors (CSTRs). The first one is the model for *m* parallel chemical reactions with *n* reactants. The maximum number of *m* is 3 and the maximum number of *n* is 5. The second one is the model of the reactor with two serial reactions and one parallel reaction according to the scheme $aA \xrightarrow{k_1} bB \xrightarrow{k_2} cC$, $aA \xrightarrow{k_3} dD$. Optional parameters of these models are shown in Fig. 4.

6 Plate distillation column

The block Plate distillation column allows simulation of dynamic behaviour of the plate distillation column for separation of a binary mixture. The mixture can be chosen arbitrarily as well as the number of plates and the feed plate number. Optional parameters are presented in Fig. 5.

Block Parameters: Flow heaters 🛛 🔟	Block Parameters: Tubular heat exchanger 3
FLOW HEATERS (mask)	THREE-CAPACITY CO-CURRENT HEAT EXCHANGER (mask)
FLOW HEATERS - serially connected flow heatres with electrical heating	model
Parameters	Parameters Input - control variables 1-yes 0-no [m1 m3 T1 T3]
Number of flow heaters	[0010]
	Disturbances 1-yes 0-no [m1 m3 T1 T3]
Vector of control valables 0-no 1-yes [Q1., Qn qv1., qvn Tv1., Tvn]	[0 0 0 0]
[010001]	Input temperatures into [inner outer] tube [T1 T3]
Vector of disturbances: 0-no 1-yes [Q1: Qn qv1., qvn Tv1.,Tvn]	[T1 T3]
[000000]	Input mass flow rates in [inner outer] tube [m1 m3]
Input flow rates of heated medium [qv1 qv2 qvn]	[m1 m3]
[qvs1 qvs2 qvsn]	Parameters of medium in inner tube [density cp alpha]
Input temperatures of heated medium [Tv1 Tv2 Tvn]	[ro1 cp1 alfa12] Parameters of medium in outer tube [density_cp_alpha]
[Tv1 Tv2 Tvn]	[ro3 cp3 alfa23]
Input power of heaters in flow heatres	Parameters of tube [density_cp]
[Q1 QiQn]	[ro2 cp2]
Volumes od flow heaters	Diameters of tubes [inner outer wall-thickness]
[V1 ViVn]	[d1 d3 h]
Parameters od heated medium [cp_density]	Length of heat exchanger
	Number of segments for discretization
Vector of output variables yes-1 no-0 [T1TiTn]	n
[101]	Vector of output variables [T(1,i) T(2,i) T(3,i)]
	[1 0 0, 0 0 0, 0 0 0, 0 0 0, 1 0 0]
OK Cancel Help Apply	OK Cancel Help Apply

Figure 3: Block parameters – flow heaters and tubular heat exchanger

Block Parameters: CSTR	Block Parameters: C5TR with serial reactions
CONTINUOUS-TIME STIRRED TANK REACTOR (mask)	CONTINUOUS-TIME STIRRED TANK REACTOR - nonlinear model (mask)
CONTINUOUS-TIME STIRRED TANK REACTOR - nelinear model Maximum number of reactions: 3, maximum number of reactants: 5, only serial reactions are considered.	CONTINUOUS-TIME STIRRED TANK REACTOR - nonlinear model for reactions according to the scheme: $aA \rightarrow bB \rightarrow cC$ $aA \rightarrow dD$
Parameters Number of [reactions reactants products]	(e.g. cyklopenthadiol preduction).
[n r p]	Input-control variables yes-1 no-0 [q Tv Qc cv]
Input - congtrol variables yes-1 no-0 [q qc Tv Tvc cv]	[0001]
[0 1 0 0 0]	Disturbances yes-1 no-0 [q Tv Qc cv]
Disturbances yes-1 no-0 [q qc Tv Tvc cv]	[0000]
[0 0 0 0 0]	Matrix of stechiometric coefficients
Matrix of stechiometric coeficients	[a1 b 0 0;0 b c 0;a2 0 0 d]
[a1 b1 ;a2 b2; a3 b3]	Vector of input concentrations
Vector of input concentrations	[cA cB cC cD]
[cA cn]	Parameters [g Tv mc Tvc]
Input floe rates [reaction-mixture coolant]	[q Tv mc Tvc]
[q qc]	Vector of reaction rate constants [kr1 kr2 kr3]
Input temperatures [reaction-mixture coolant]	[kr1 kr2 kr3]
[T Tc]	Vector of reaction energies [E1 E2 E3]
Vector of reaction rate coeficents	[E1 E2 E3]
[kr1 kri krn]	Vector of reaction enthalpies
Vector of reaction energies	[h1 h2 h3]
[E1 Ei En]	Heat flow trasfered into the coolant Oc
Vector of reaction enthalpies	
[h1 hi hn]	
Constants [reaction-mixture-density coolant-density	Parameters [reaction-mixture-density reaction-mixture-cp cp-coolant
[ro roc cp cpc]	[ro cp cpc]
Constants [reaction-mixture-V coolant-V A-heat-transfer-surface	Parameters [V-reaction-mixture A-heat-transfer-area k-coefficient fo
[V Vc A k]	[V A k]
Vector of output variables yes-1 no-0 [ci cn T Tc]	Vector of output variables yes-1 no-0 [cA cD T Tc]
[1 0 1 0 1]	[00001 1]
OK Cancel Help Apply	OK Cancel Help Apply

Figure 4: Block parameters – CSTRs

Block Parameters: Plate distillation column	×
PLATE DISTILLATIN COLUMN (mask)	
Etážová rektifikačná kolona - nelineárny model	
Parameters	
Input - control variables yes-1 no-0 [nF xF nL nD nV nW]	
[001000]	
Disturbances yes-1 no-0 [nF xF nD nL nV nW]	
[0 0 0 0 0]	
Number of plates	
n	
Feed plate	
F	
coeficients of equilibrium dependence y=(ax^2+bx+c)/(dx^2+ex+1)	
[abcde]	
Efficiencies [plates reboiler] in %	
[ni nv]	
Mole feed flow rate and mole fraction of feed [nF xF]	
[nF xF]	
Mole feed flow rate of destillate and bottom product [nD nW]	
[nD nW]	
Mole feed flow rate of reflux and mole vapour flow rate [nL nV]	
[nL nV]	
Hold-up [plates reboiler]	
[Hi Hiv]	
Vector of output variables xi-yi 1 - yes 0 - no [., xi-yi.,]	
[1010000]	
OK Cancel <u>H</u> elp <u>Apply</u>	

Figure 5: Block parameters – plate distillation column

7 Conclusions

The toolbox MODELTOOL is an opened system and mathematical models of other processes from chemical technology will be gradually added to it. The using of individual blocks is simple and it does not demand special knowledge on modeling. The toolbox can be used especially for educational but also for research purposes.

Acknowledgements

The authors are pleased to acknowledge the financial support of the Scientific Grant Agency of the Slovak Republic under grants No. 1/1046/04 and No. 1/3081/06 and of the Cultural and Educational Grant Agency of the Slovak Republic under the grant No. 3/3121/05.

References

- [1] Mikleš, J., Fikar, M. Process modelling, identification and control II. STU Press, Bratislava, 2004.
- [2] Baleja, J. Development of a library of mathematical models of processes from chemical technology. Diploma thesis (in Slovak). DIEPC FCFT STU, Bratislava, 2005.
- [3] Bakošová, M., Baleja, J., Ondrovičová, M. *MODELTOOL 1.0 toolbox matematických modelov chemickotechnologických procesov* (in Slovak). AT&P Journal 12, 12, 59-60, 2005.
- [4] Ingham, J., Dunn, I. J., Heinzle, E., Přenosil, J. E. *Chemical engineering dynamics*. VCH Verlagsgesellschaft, Weinheim, 1994.
- [5] Ogunnaike, B. A., Ray, W. H. *Process dynamics, modeling and control.* Oxford University Press, New York, 1994.
- [6] Mészáros, A., Rusnák, A., Fikar, M. *Adaptive neural PID control. Case Study: Tubular chemical reactor.* Comp. and Chem. Engng. Sup., 1999, S847-S850.

Monika Bakošová

Slovak University of Technology in Bratislava, Faculty of Chemical and Food Technology, Institute of Information Engineering, Automation and Mathematics, Radlinského 9, 812 37Bratislava, Slovakia, e-mail: <u>monika.bakosova@stuba.sk</u>

Ján Baleja e-mail: jan.baleja@post.sk

Ľuboš Čirka e-mail: <u>lubos.cirka@stuba.sk</u>