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COMPARISON OF MATHEMATICAL MODELS FOR TRAY DISTILLATION COLUMN

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Presented paper deals with mathematical models of a pilot-plant bubble-cup tray distillation column. Two universal models have been derived by the mathematical-physical analysis. Two versions of models have been considered in the simple transfer function form. Step responses and responses to more complex input signals have been measured. Values of models unknown parameters have been estimated from experimental data by the numerical optimisation. The models are verified for more complex input signal and in the closed loop.

Introduction

Distillation column dynamic behaviour description is important for the closed loop control analysis and synthesis. Column trays are usually considered as lumped parameters systems by the mathematical-physical analysis. The whole column dynamic behaviour description is reached by connecting these blocks with mutual bonds (Betlem [1]), (Čermák *et al.* [2]), (Fuentes, Luyben [3]), (Závorka [6]). If theoretical trays count, feed flow rate, feed composition, feed state, feed location and reflux flow rate are known, a system of equations must be solved by an iterative numerical method. Compositions and flow rates of the distillate and bottom product are calculated. Another possibility of obtaining dynamic column model is approximating the plant behaviour with a simple transfer functions (Haber, Unbehauen [4]), (Skogestad, Morari [5]).

Mathematical Models

Mathematical Models M

The models M are created on the mathematical-physical basis. The most complicated model M1 (see Figs 1 – 3) contains equations of total mass balance, mass balance of the light component, equilibrium equations, tray efficiency equations and energy balance equations. Model M1 includes $3 + N * 2$ differential equations, where N is number of column trays. There are considered $N + 1$ algebraic equations for the equilibrium concentration of the light component in the vapour phase and N algebraic equations for the Murphree tray efficiency for this model.

Reboiler

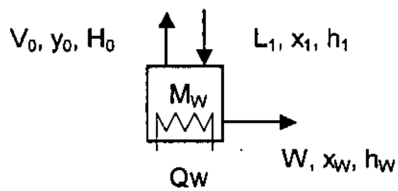

Fig. 1 Reboiler

$$L_1 = V_0 + W + \frac{dM_W}{dt} \quad (1)$$

$$L_1 x_1 = V_0 y_0 + W x_W + \frac{dM_W x_W}{dt} \quad (2)$$

$$\eta_W Q_W + L_1 h_1 = V_0 H_0 + W h_W + \frac{dM_W h_W}{dt} \tag{3}$$

Tray

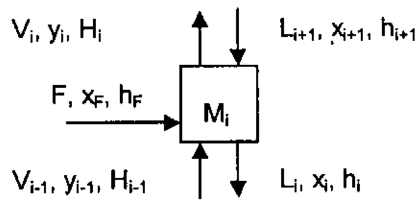

Fig. 2 Tray

$$F + L_{i+1} + V_{i-1} = L_i + V_i + \frac{dM_i}{dt} \tag{4}$$

$$F x_F + L_{i+1} x_{i+1} + V_{i-1} y_{i-1} = L_i x_i + V_i y_i + \frac{dM_i x_i}{dt} \tag{5}$$

$$F h_F + L_{i+1} h_{i+1} + V_{i-1} H_{i-1} = L_i h_i + V_i H_i + \frac{dM_i h_i}{dt} \tag{6}$$

Murphree efficiency

$$\eta_i = \frac{V_i y_i - V_{i-1} y_{i-1}}{V_i y_i^* - V_{i-1} y_{i-1}} \tag{7}$$

Condenser

$$V_N = D + R + \frac{dM_D}{dt} \tag{8}$$

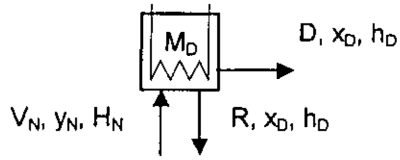

Fig. 3 Condenser

$$V_N y_N = (D+R)x_D + \frac{dM_D x_D}{dt} \tag{9}$$

The simplified model M2 (see Figs 4 – 6) is obtained, if additional assumptions are considered. The liquid and vapour molar flows beside the column are constant and the model does not contain the energy balance equations. Model M2 comprises $2+N$ differential equations. The number of algebraic equations for the liquid-vapour equilibrium and for the Murphree tray efficiency is identical as in model M1. Model M2 contains one additional algebraic equation for the calculation of the vapour phase flow dependence on the reboiler electric heating input (Eq. (12)).

Reboiler

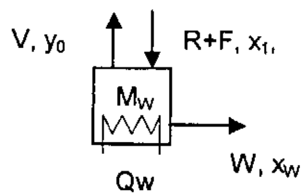

Fig. 4 Reboiler

$$R+F = V+W \tag{10}$$

$$(R+F)x_1 = Vy_0 + Wx_W + M_W\frac{dx_W}{dt} \tag{11}$$

$$V = kQ_W + q \tag{12}$$

Tray

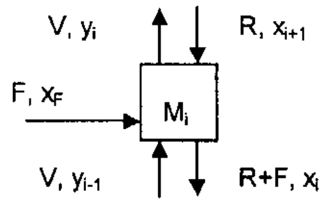

Fig. 5 Tray

$$Fx_F + Rx_{i+1} + Vy_{i-1} = (R + F)x_i + Vy_i + M_i\frac{dx_i}{dt} \tag{13}$$

Murphree efficiency

$$\eta_i = \frac{y_i - y_{i-1}}{y_i^* - y_{i-1}} \tag{14}$$

Condenser

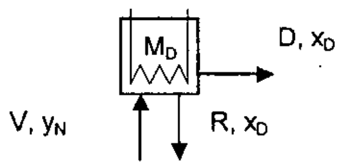

Fig. 6 Condenser

$$V = D + R \tag{15}$$

$$Vy_N = (D + R)x_D + M_D\frac{dx_D}{dt} \tag{16}$$

Mathematical Models P

The dynamic behaviour of the distillation column can well be approximated in the neighbourhood of the working point by the low order transfer functions - models P. Simple model P1 (see Fig. 7) is a linear two-dimensional transfer function matrix $\boldsymbol{F}$. Transfer functions F_{ij} in terms of Laplace transform are given

$$F_{ij} = \frac{Z_{ij}}{\tau_{ij}s + 1} \qquad i, j \in \{1, 2\} \tag{17}$$

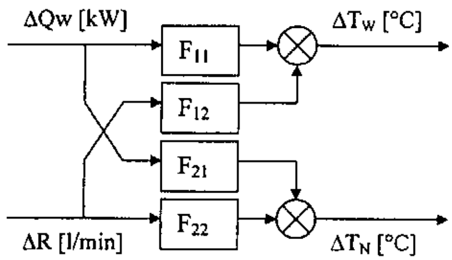

Fig. 7 Two-dimensional system

Model P2 contains linear dependences of the steady state gains on the model inputs

$$Z_{ij} = a_{ij} + b_{ij}\Delta Q_W + c_{ij}\Delta R \tag{18}$$

This function causes non-linear behaviour of the model P2.

Estimation of the Unknown Parameters

Models M need prior information about the plant. The equilibrium data for the methanol-water mixture are searched. The dependence of mixture density on the composition and temperature is used for the conversion between volume rate of flow and molar flow. Model M1 contains equations for the enthalpy of liquid and vapour phase calculation. Models P do not involve additional information except the working point.

The models are converted into the Simulink block schemes. Step responses and two responses to more complex input signals are measured on the pilot-plant column. These data serve for the estimation of the model unknown parameters. The reflux flow rate and the reboiler heating input are changed during the experiments. The temperatures in the reboiler and on the column trays are chosen for the plant outputs. The temperature of the boiling mixture corresponds for the given pressure with the liquid phase composition.

The model parameters are estimated by means of the numerical optimisation. Matlab function FMINS is used for the minimization of the function of several variables. SIM command starts the simulation and the objective function is evaluated after the simulation ends. Criterion for the optimisation is the measure of coincidence between temperatures computed from the model and measured temperatures in the heater and on the column trays. The sum of squared differences divided by data count is used.

Parameters Estimation from Step Responses

For the models M1 and M2 only parameters influencing the static properties are estimated at first. Volume holdups of reboiler, trays and condenser are guessed from the plant geometric dimensions. Temperature in the reboiler and temperatures on all trays in 10 steady states are used for calculating the criterion $K_{US\,1-8}$. Temperature step response 2 for model M1 is shown in the Fig. 8 (the heating input is kept constant and the reflux flow rate is changed). Calculated temperatures are plotted with the bold line in all following figures. The highest curve corresponds to the reboiler temperature. The temperature responses on the first, second, ..., last tray follow downwards.

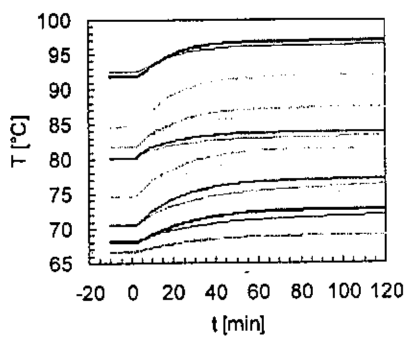

Fig. 8 Step response 2 – model M1

Model M1 describes the real plant behaviour better than the model M2.

The second set of unknown parameters for models M1 and M2 is estimated. The criterion is calculated only from reboiler temperature and temperature on the last tray (the same criterion as for the models P). All model parameters are estimated (including the volume holdups). The reboiler holdup is identified significantly smaller than the corresponding plant dimension. On the other hand, the tray holdup is twofold than the quessed value. The model well approximates the reality for the temperature in the reboiler and on the last tray. Agreement between the model and the real plant for all other temperatures is worse than the if the criterion for all temperatures is considered.

Unknown parameters of the models P (models in the simple transfer function form) are estimated. The working point for the models is chosen in the middle of the model M1 working area. All parameters of models P (gains and time constants) are estimated. The model output variables are temperature in the reboiler and on the last column tray. Criterion $K_{PCH\,1,8}$ is calculated from these two temperatures only. Due to the non-linear behaviour, the value of the criterion for model P2 is reduced three times compared to the model P1.

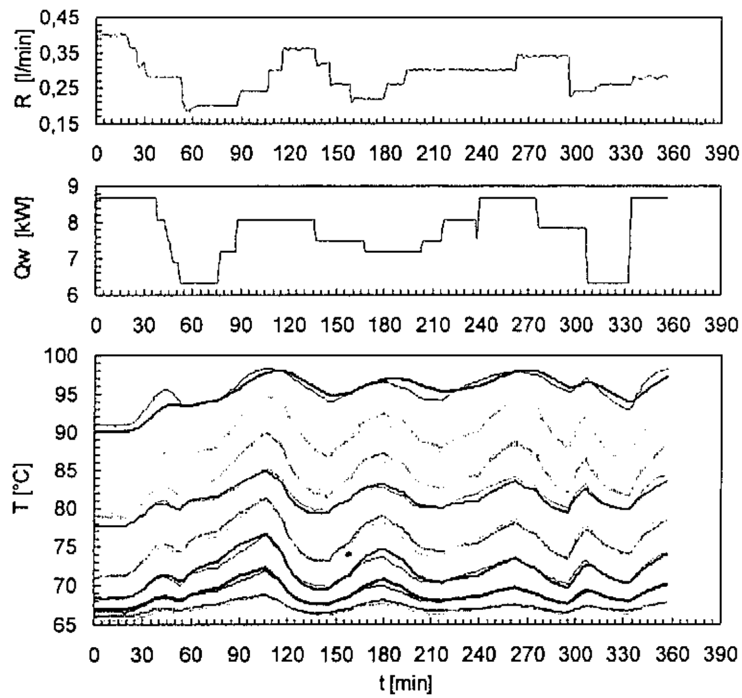

Fig. 9 More complex signal I – model M1

Parameters Estimation from More Complex Signal

All parameters of the models M and P are estimated from a more complex input signal. The plant inputs (R and Q_W) and temperature responses are shown in Fig. 9.

For the models M the criterion $K_{SS\,1-8}$ is calculated from all the temperatures. For the $K_{SS\,1,8}$ criterion calculation only temperatures in the reboiler and on the last tray are used.

Models P approximate real plant behaviour better than models M if the criterion $K_{SS\,1-8}$ is considered. If the $K_{SS\,1,8}$ criterion is used for the models M, the value of criterion for the models M1, M2 and P1 will be approximately identical. The value of this criterion for the model P2 is twice smaller.

Parameters Estimation Results

Models with parameters estimated from more complex signal give half value of the criterion than those from the step responses. The parameters for the models M and P are shown in Tables I – IV (US = parameters from step responses, SS = parameters from more complex signal). Two parameters sets are considered for the models M according to the estimation criterion used.

Table I Parameters – model M1

	M_W, l	M_i, l	M_D, l	η_W	η_1	η_2	dp, Pa	Criterion
US	4.00	0.50	0.50	0.876	0.767	0.805	232	$K_{US\,1-8}$ = 0.90
	2.83	0.94	0.97	0.872	0.598	1.000	246	$K_{PCH\,1,8}$ = 0.31
SS	11.89	0.67	0.17	0.869	0.893	0.785	192	$K_{SS\,1-8}$ = 0.34
	2.23	1.25	0.55	0.849	0.674	0.970	397	$K_{SS\,1,8}$ = 0.17

Table II Parameters – model M2

	M_W, l	M_i, l	M_D, l	k	q	η_1	η_2	dp, Pa	Criterion
US	4.00	0.50	0.50	2.72×10^{-5}	-2.41×10^{-2}	0.673	0.682	419	$K_{US\,1-8}$ = 1.09
	0.61	1.25	0.43	2.73×10^{-5}	-2.48×10^{-2}	0.504	0.967	347	$K_{PCH\,1,8}$ = 0.36
SS	8.48	0.59	0.39	2.43×10^{-5}	-6.93×10^{-3}	0.810	0.742	359	$K_{SS\,1-8}$ = 0.61
	1.39	0.85	0.26	2.76×10^{-5}	-3.54×10^{-2}	0.555	0.998	231	$K_{SS\,1,8}$ = 0.21

Table III Parameters – model P1

	τ_{11}, s	τ_{12}, s	τ_{21}, s	τ_{22}, s	Z_{11}	Z_{12}	Z_{21}	Z_{22}	Criterion
US	626.9	655.2	88.0	727.1	4.81×10^{-3}	-76.51	1.92×10^{-3}	-33.84	$K_{PCH\,1,8}$ = 0.59
SS	1632.5	1892.3	73.1	377.8	5.90×10^{-3}	-90.25	4.11×10^{-4}	-12.71	$K_{SS\,1,8}$ = 0.18

Table IV Parameters – model P2

	a_{11}	a_{12}	a_{21}	a_{22}	b_{11}	b_{12}	b_{21}	b_{22}
US	5.38×10^{-3}	-78.3	1.91×10^{-3}	-34.6	-7.34×10^{-7}	-8.79×10^{-3}	1.30×10^{-6}	-3.18×10^{-3}
SS	6.81×10^{-3}	-110.8	5.00×10^{-4}	-11.5	-5.23×10^{-8}	1.92×10^{-2}	2.70×10^{-7}	1.55×10^{-2}

c_{11}	c_{12}	c_{21}	c_{22}	τ_{11}, s	τ_{12}, s	τ_{21}, s	τ_{22}, s	Criterion
2.04×10^{-2}	36.7	-2.05×10^{-2}	143.8	462.7	659.0	2053.5	1725.4	$K_{PCH\,1,8}$ = 0.21
1.58×10^{-2}	-335.5	-4.09×10^{-2}	195.5	1876.6	2221.9	1432.0	1087.3	$K_{SS\,1,8}$ = 0.13

Models Validation

Validation for More Complex Signal

The mathematical models obtained are verified for the second more complex input signal. The plant inputs (R and Q_W) and temperature responsres are shown in Fig. 10. Models approximation quality criterion of the real plant dynamic behaviour is computed. Values of criterion are shown in Table V for all the models (models with parameters estimated from step responses and from more complex input signal). Two parameters sets are used for the models M according to the estimation criterion used. Essentially smaller criterion values are reached if unknown parameters are estimated from a more complex signal than from the step responses.

Validation in Closed Loop

Three closed-loop control experiments were carried out on the pilot-plant distillation column. Two PS controllers were used for the temperature control in the reboiler and on the last tray. One set of regulators parameters was applied for all experiments. The set points for the temperature are alternating in the first two experiments (in two different operating point). The third experiment represents a

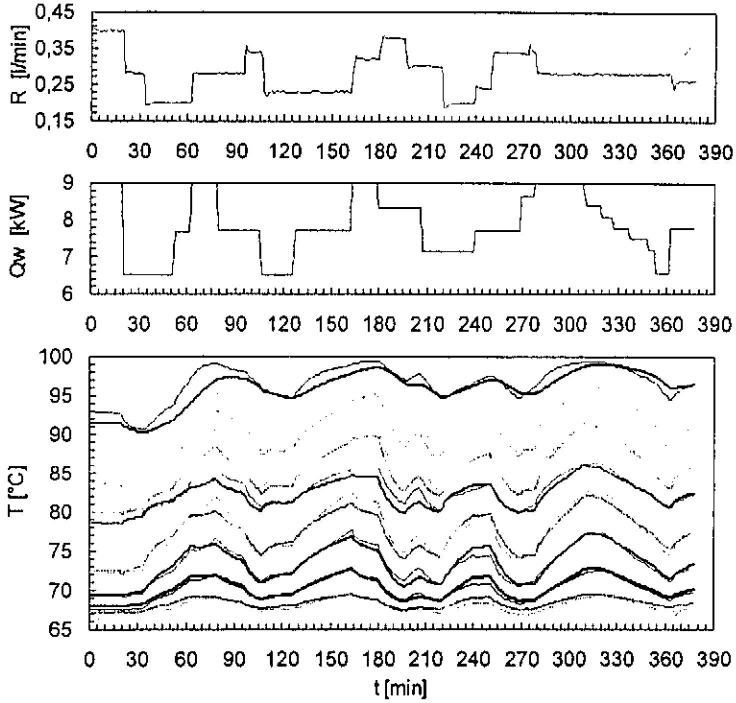

Fig. 10 More complex signal II – model M1

Table V Approximation criterions for more complex signal

Model	Parameters from US		Parameters from SS	
	$K_{SS\ 1-8}$	$K_{SS\ 1,8}$	$K_{SS\ 1-8}$	$K_{SS\ 1,8}$
M1	*2.05*	0.84	0.69	0.8
	7.63	0.79	2.29	0.56
M2	2.98	1.48	0.68	0.93
	18.37	2.73	5.66	0.7
P1	-	2.1	-	0.7
P2	-	2.35	-	0.53

crossing between the two working points with linearly changing set points.

Closed loop control responses are computed for all models (regulator parameters are identical as for the experiments). Models parameters estimated

Table VI Approximation criterions for validity in closed loop

	Control process 1	Control process 2	Control process 3
M1	2.25	7.49	1.50
	1.20	7.62	1.09
M2	1.17	6.52	1.28
	0.42	5.22	0.78
P1	10.17	15.78	8.76
P2	-	15.36	2.00

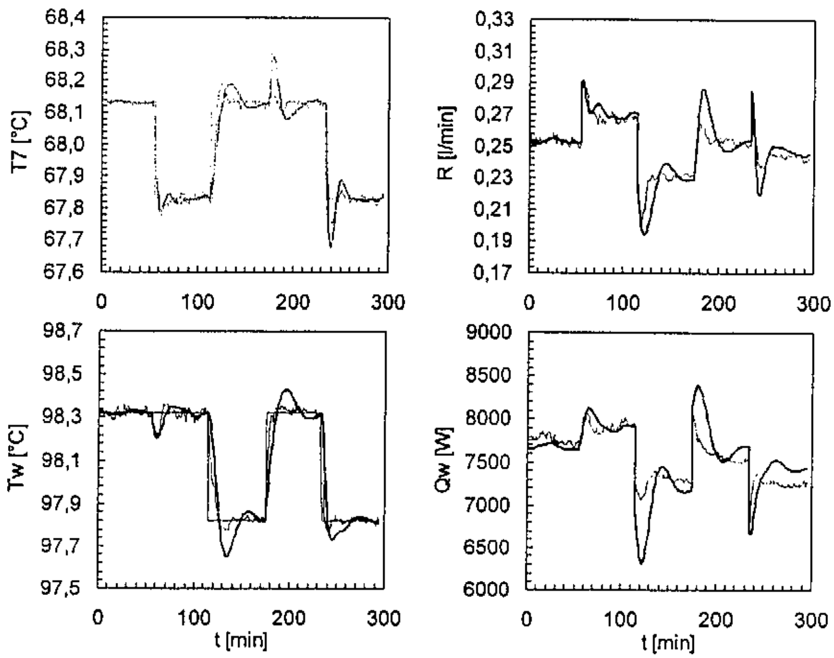

Fig.11 Control process 1 – model M1

from more complex signal are used. For the models M two sets of parameters are used according to the estimation criterion. Only set points temperatures enter the simulation. The manipulated variable Qw and R and the plant responses are calculated from the closed loop model simulation. Approximation criterions are calculated from measured and simulated temperatures in the reboiler and on the last tray (see Table VI).

All the models M display similar approximation criterion values in the closed loop. Model M2 with parameters estimated from two temperatures offers the best agreement between the model and the real plant. Criterion values for the models P are many times higher than those for the models M. Disagreement between the models P and the real plant arises by the closing the two control loops at the same time.

Conclusion

The main results can be summarized in the following points:

1. Two models were derived on the mathematical-physical basis. Two models were considered in the simple transfer function form. The models were specified for the particular column and converted into the Simulink block schemes.
2. The data for unknown parameters estimation and models verification were measured on a pilot-plant. Five step responses and two responses to more complex input signal were obtained. Step responses and more complex signals were chosen to cover whole column working area.
3. The estimation of the models parameters was carried out from experimental data by using the Matlab optimising function. The models were validated for the second more complex signal. For additional models verification closed loop was used.

Model construction using the mathematical-physical analysis is rather complicated but due to the prior information the models give better results than models in general transfer function form. Models in the simple transfer function form are valid only in the near neighbourhood of the working point. The unknown parameters number disproportionately increases by extending of the model order. For the non-linear models, the question of non-linearity type and model form remains open.

Comparable criterion values are achieved for all models by the verification with more complex input signal. Disagreement between the models arises within the verification in the closed loop. Agreement between the models in the simple transfer function form and the real plant is rather insufficient.

The inputs and model parameters can be changed within the simulation. From this point of view the Simulink models are convenient for the simulation of the plant dynamic behaviour (even in real time). Simulink models are suited also for the control loop design. It is possible in short time to debug and try out different approaches to the process control.

Symbols

D distillate (top product) rate
dp pressure drop on the tray
η_1 Murphree efficiency below feed location
η_2 Murphree efficiency above feed location
η_W reboiler efficiency
F feed flow rate
F_{ij} transfer function
h_D distillate enthalpy
h_F feed enthalpy
h_i enthalpy of liquid leaving tray i
H_i enthalpy of vapour leaving tray i
h_W bottom product enthalpy
i tray index ($i = 1, 2, ..., N$)
k coefficient for vapour flow rate dependence on reboiler heating input
L_i liquid flow rate leaving tray i
M_D liquid holdup in condenser
M_i liquid holdup on tray
M_W liquid holdup in reboiler
N total number of trays (for pilot-plant column $N = 7$)
q coefficient for vapour flow rate dependence on reboiler heating input
Q_W heating input into the reboiler
R reflux flow rate
$T_1, ..., T_N$ temperature on the first, ..., last tray
T_W temperature in reboiler
τ_{ij} time constant
V_i vapour flow rate leaving tray i
W bottom product rate
x_D mole fraction of light component in distillate
x_F mole fraction of light component in feed
x_i mole fraction of light component in liquid on tray i
x_W mole fraction of light component in bottom product
y_i mole fraction of light component in vapour on tray i
y_i^* equilibrium mole fraction of light component in vapour on tray i
Z_{ij} steady state gains

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