Simulation of a batch reactor and its monofluid heating-cooling system

M. G. Balaton, L. Nagy, F. Szeifert
Department of Process Engineering, University of Pannonia – Veszprem, Egyetem str. 10,
Veszprem, Hungary H-8200, e-mail: balatonm@fmt.uni-pannon.hu, tel.: +36-88-62-4295

Batch technologies in chemical industry

A large number of industrial processes, such as the production of fine chemicals, pharmaceuticals, bioproducts, as well as other products for which continuous production is not feasible, are operated batchwise. In many cases this mode of operation is used to manufacture a variety of products that need significantly different characteristics such as conversion time, heat of reaction ...etc. Good control in such reactors is quite often difficult to achieve due to their flexible and multipurpose character and is essentially a problem of temperature control.[3]

Moreover, the control performances are mainly dependent on the heating-cooling system associated with the reactor. Two main types of heating-cooling systems are commonly used in industry: the alternate system or multifluid system and the monofluid system. The well-known alternate system makes utility fluids flow alternatively in the jacket. The monofluid system uses a single-fluid, the temperature of which can be modified to achieve the desired reactor temperature by an intermediate thermal loop which may include heat exchangers, power heaters, etc. An example for this kind of system can be seen on Figure 1. [2], [4]
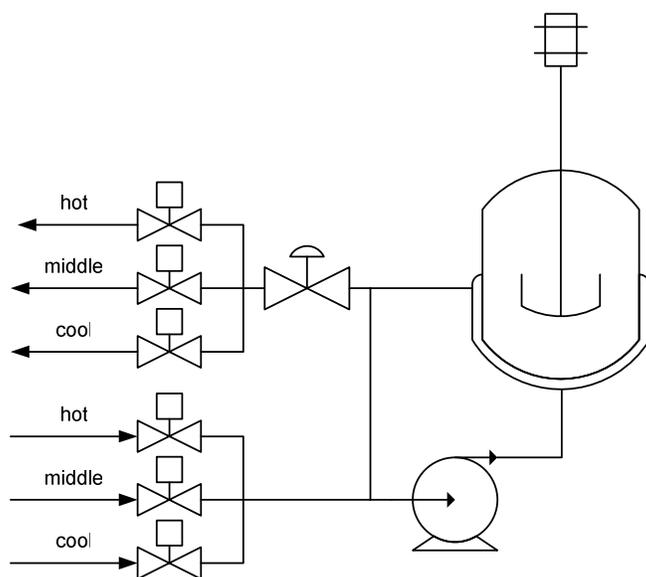

Figure 1: Batch reactor with monofluid heating-cooling

The monofluid heating-cooling system

In our laboratory a 50 litre stirred batch reactor with a monofluid jacket heating-cooling including three temperatures can be found. Besides the main economic advantage of the system with three temperatures (not only two temperatures on the boundary of the temperature range, a cheap, water controlled middle temperature can be set), it can provide the necessary (for batch reactors) homogeneous temperature distribution in the jacket, however the ball valves and control valve must be operated in accordance. With this system more economic benefit can be achieved if the recurring fluid from the jacket returns to the tank with the closest temperature. Unnecessary heating and cooling and disturbances can be avoided.
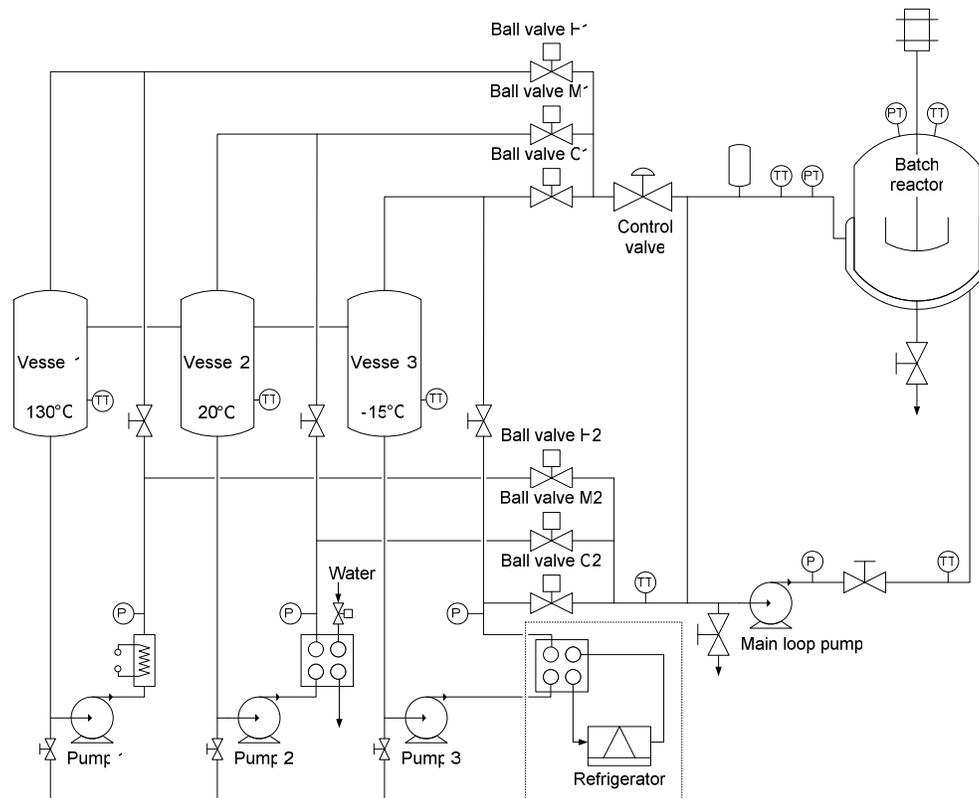

Figure 2: The 50 litre batch reactor and its monofluid thermoblock

On figure 2 the batch reactor and its heating-cooling system can be seen. It has four closed loops. Three loops represent the monofluid thermoblock, where the three different temperatures can be produced. The fourth recirculation loop is for the reactor's jacket providing homogeneous temperature distribution.

The highest temperature can be adjusted with an electric heater, the middle with a heat exchanger cooled with tap water and the coolest with a refrigerator.

The fluid with the required temperature can be chosen with on-off ball valves and the fluid rate can be controlled with a control valve.

The UniSim™ Design simulation software

The simulator is made with Honeywell's UniSim™ Design Suite, which is based on HYSYS® software. It offers steady-state and dynamic simulation, design, performance monitoring, optimization and business planning for the oil and gas production, gas processing, petroleum refining and chemical industries.

Chemical plants are never truly at steady state. Feed and environmental disturbances, heat exchanger fouling, and catalytic degradation continuously upset the conditions of a smooth running process. The transient behaviour of the process system is best studied using a dynamic simulation tool like UniSim™ Design.

A variety of control strategies can be designed and tested before choosing one that is suitable for implementation. The dynamic response to system disturbances can be examined and the tuning of controllers can be optimized. Dynamic analysis provides feedback and improves the steady state model by identifying specific areas in a plant that have difficulty achieving the steady state objectives.

Numerical integration is used to determine the process behaviour at distinct time steps. The smaller the time step, the more closely the calculated solution matches the analytic solution. However, this gain in rigour is offset by the additional calculation time required to simulate the same amount of elapsed real time. A reasonable compromise is achieved by using the largest possible step size, while maintaining an acceptable degree of accuracy without becoming unstable.

UniSim™ Design uses lumped models for all of the unit operations, because the distributed models need more calculating capacity and time. The operations with volume are divided into several sub-volumes which are considered to be lumped. The reaction rate, temperature and compositions are constant through each sub-volume, varying only with time. With this method the whole volume is calculated likewise a distributed model.

In dynamic mode UniSim™ Design uses a pressure flow solver that contains two basic equations which define most of the pressure flow network and these equations only contain pressure and flow as variables. Resistance equations, which define flow between pressure hold-ups and volume balance equations, which define the material balance at pressure hold-ups.

"One Model, Many Uses". The single model concept allows the user to build one model of the process and migrate it through the various stages of the Lifecycle. During the design stage, a model can be used for conceptual design, real process design, detailed engineering design, and finally, for operability design. Once the asset has been built, this same model can be used for operations improvement, operator training, safety studies, and asset optimization. In addition to delivering simulation capabilities that support the Lifecycle, UniSim™ Design also serves as the platform for modelling across the entire range of the chemical and hydrocarbon processing industries. [5]

The simulator

Long since in chemical industry creating the simulation of existing technologies for the reasons mentioned above has been a good practice. This is the reason why we managed to create the simulator of the batch reactor and its monofluid jacket heating-cooling system and. With this dynamic simulator new control structures can be tested without reference to the real system. Besides it can be used for training laboratory instructors and for education, for example in laboratory practices more students can work at the same time than using the real system.

To connect the simulator with process control software through OPC (OLE for process control) interface Honeywell's UniSim™ Operations Suite is needed instead of UniSim™ Design.

These engineering softwares like UniSim™ Design have limits in case of batch technologies, because they are designed and mostly used for continuous technologies. In UniSim™ Design no jacketed batch reactor models are provided, so approximation have to be made. We tested a couple of differently detailed models for the approximation. In this paper the differences and the deficiencies of the models and dynamic simulation results compared to measured values from the real system are presented. The rest of the simulator (monofluid system) was made of the models of UniSim™ Design.
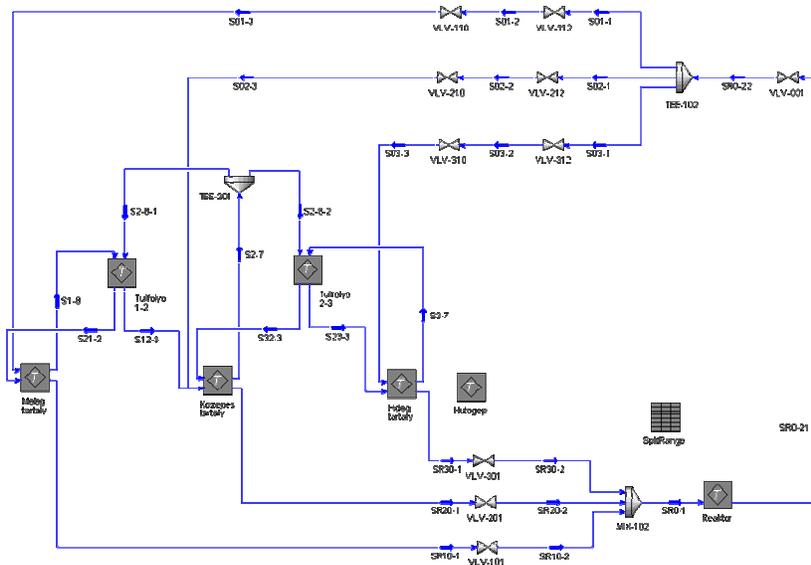
Figure 3: The flowsheet of the batch reactor and its monofluid thermoblock in UniSim™ Design

According to our basic concept the jacketed batch reactor was built up from a CSTR and a 1-1 shell-tube heat exchanger. The two models were connected through heat flow. The duty of the CSTR is set equal to the heat exchanger's (which represents the jacket) duty. The heat exchanger's tube side inlet stream has the same composition and temperature as the reaction mixture, and its flow rate can be adjusted according to the stirrer's speed. The PFD in UniSim™ Design of this concept can be seen on Figure 4. [1]

The connection was achieved with UniSim™ Desgin's flexible module called "Spreadsheet". It allows accessing all the variables in the simulator, but only the user defined variables can be modified with it. It's very similar to Microsoft Excel, it has 10×4 cells as default, and the calculations can be done through cell links.
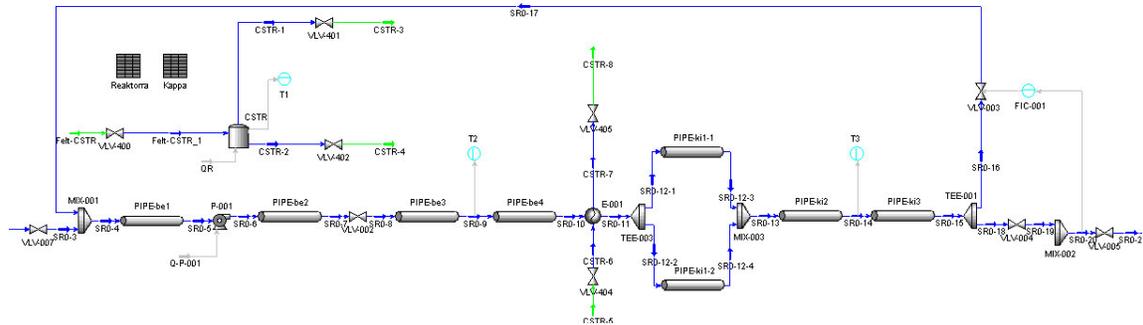

Figure 4: The PFD of the reactor, the jacket and the jacket's recirculation loop

The user interface can be seen on Figure 5, it shows the window on the spreadsheet module in the top left, the configuration window of the CSTR in the bottom left corner, the model palette on the right side and the part of the PFD in the background.
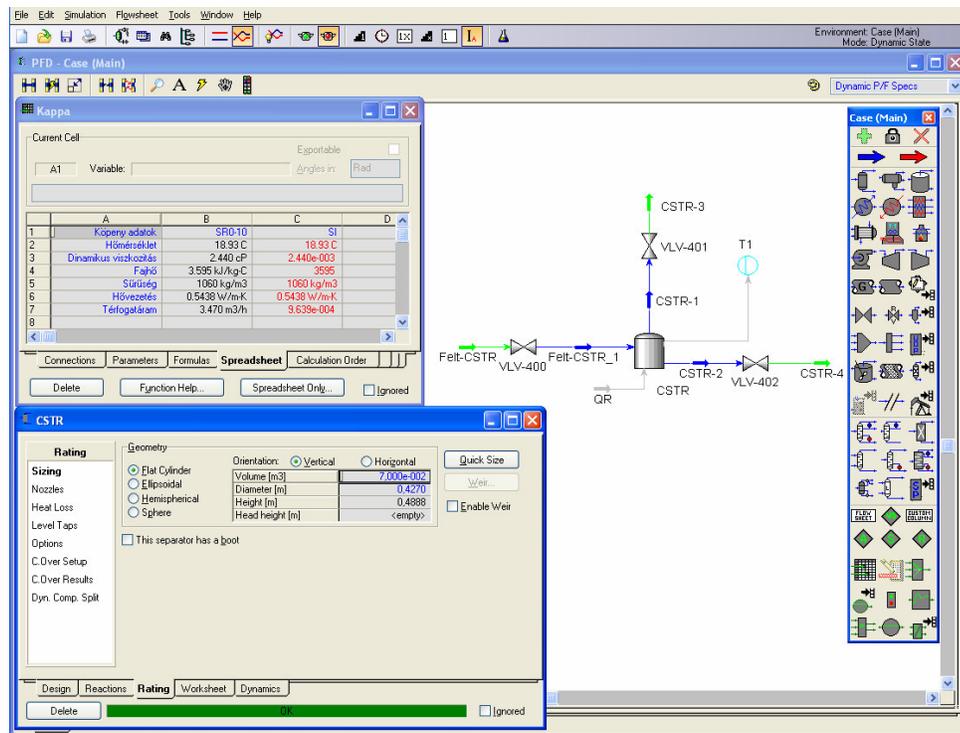

Figure 5: UniSim™ Design user interface

According to our first consideration we used a simple equation for heat transfer calculation (Equation 1-4.) the same as the built in for heat exchanger in UniSim™ Design.

The simulation results of the simple model compared with the measured data is presented on Figure 6. We only used two different temperatures (hot and middle) of the three available. The simulated temperatures show good approximation compared to the measured data, except the reactors temperature on the cooling part, where increasing differences occur.

This model doesn't contain any information about the viscosity of the fluid that is highly temperature dependent and affects the heat transfer coefficient significantly. This is the reason why the cooling part doesn't fit to the measured data (system parameters were fitted to the heating part).

Used equations:

Transferred heat flow:

$$Q = \kappa A \Delta T_{LM} F_t \tag{1}$$

Dynamic correction factors:

$$F_T = \frac{2 f_1 f_2}{f_1 + f_2} \tag{2}$$

$$f_1 = \left(\frac{M_{cs}}{M_{cs,ref}} \right)^{0,8} \tag{3}$$

$$f_2 = \left(\frac{M_k}{M_{k,ref}} \right)^{0,8} \tag{4}$$
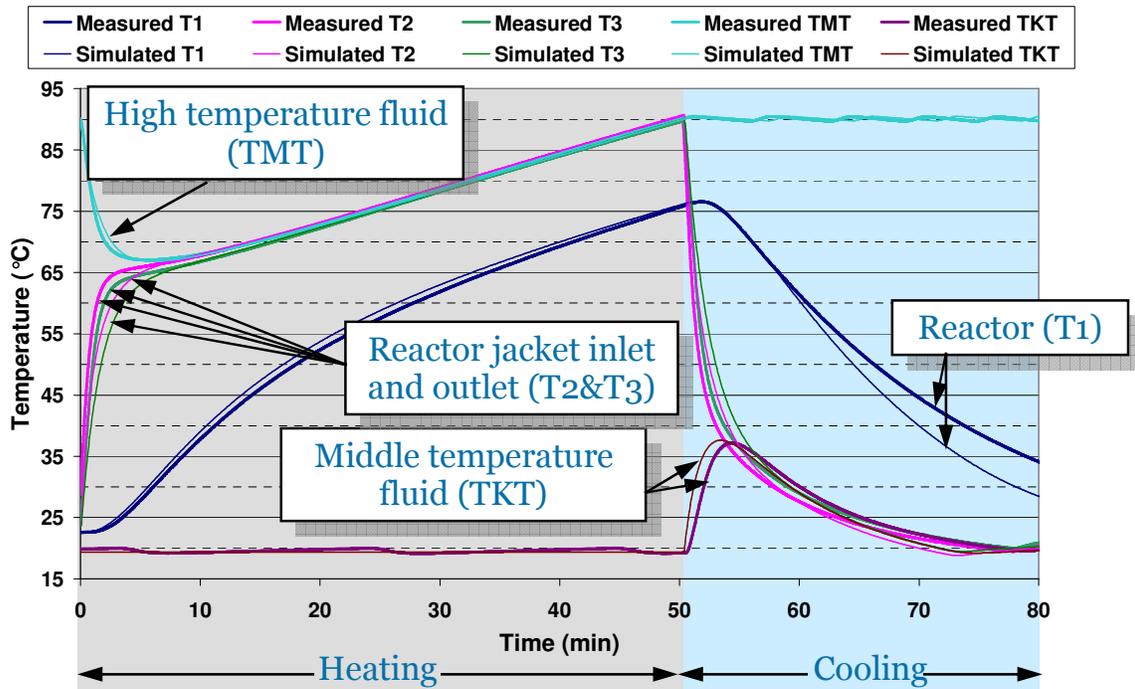

Figure 6: The results of the simple model

To eliminate the deficiencies of the simple model, we built a detailed model containing temperature dependent viscosity. It calculates the heat transfer coefficient in every time step from the constant physical dimensions and dynamic fluid properties of the system (Equation 5-10). We this change the constant overall heat transfer coefficient became dynamic.

The results of the detailed model are shown on Figure 7, where the approximation of the reactor temperature is better (<1 °C) in both heating and cooling parts due to the detailed model.

<u>Used equations:</u>

Overall heat transfer coefficient:

$$\kappa = \cfrac{1}{\cfrac{1}{\alpha_{reactor}} + \cfrac{1}{\alpha_{jacket}} + \cfrac{\delta_{wall}}{\lambda_{wall}} + \cfrac{\delta_{glass}}{\lambda_{glass}}} \qquad (5)$$

Reactor side heat transfer coefficient:

$$\alpha_{reactor} = Nu \cdot \frac{\lambda}{D_{inside}} \qquad (6)$$

Nusselt number on reactor side (Chilton correlation):

$$Nu = C \cdot \mathrm{Re}^{2/3} \cdot \mathrm{Pr}^{1/3} \cdot \left(\frac{\mu}{\mu_{wall}}\right)^{0,14} \qquad (7)$$

Jacket side heat transfer coefficient:

$$\alpha_{jacket} = Nu \frac{\lambda}{d_h} \qquad (8)$$

Equivalent diameter in the jacket:

$$d_h = \frac{4 \cdot f}{U} \qquad (9)$$

Nusselt number on jacket side (Sieder-Tate correlation):

$$Nu = 0{,}023 \cdot \mathrm{Re}^{4/5} \cdot \mathrm{Pr}^{1/3} \cdot \left(\frac{\mu}{\mu_{wall}}\right)^{0,14} \qquad (10)$$
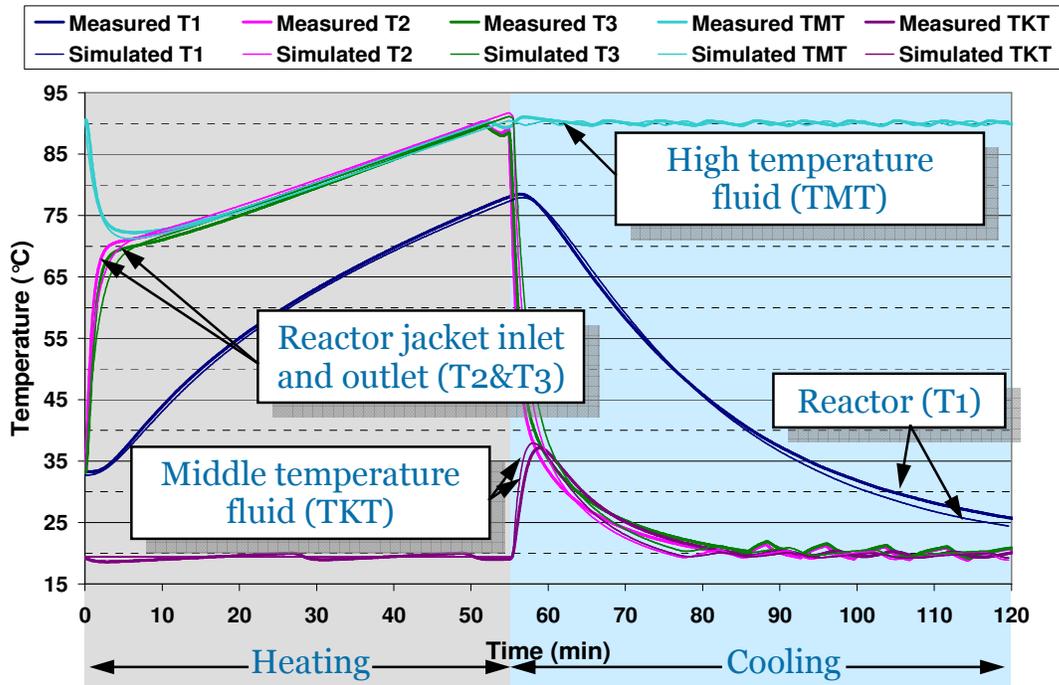
Figure 7: The results of the detailed model

Conclusion

In result we made a simulator responding likewise the real system; with this corrected model more accurate controllers can be designed. To connect the simulator with process control software through OPC (OLE for process control) interface Honeywell's UniSim™ Operations Suite is needed instead of UniSim™ Design. The connected dynamic simulator can be a useful tool for controller design and testing and for student laboratory practices.

Acknowledgement

Nomenclature

α	Heat transfer coefficient
δ	Wall thickness
κ	Average heat transfer coefficient
λ	Conductive heat transfer coefficient
μ	Dynamic viscosity of reaction mixture
μ_{wall}	Dynamic viscosity of reaction mixture at the temperature of the wall
A	Heat transfer area
C	Constant
$CSTR$	Completely stirred reactor
D_{inside}	Inner diameter of the reactor
d_h	Equivalent diameter
f	Cross-section of flow
F_t	LMTD correction factor
M_{cs}	Tube side flow rate (reactor side)
$M_{cs,ref}$	Tube side reference flow rate (reactor side)
M_k	Shell side flow rate
$M_{k,ref}$	Shell side reference flow rate
Nu	Nusselt-number
PFD	Process flow diagram
Pr	Prandtl-number
Q	Heat
Re	Reynolds-number
$T1$	Reactor temperature
$T2$	Reactor jacket circulating loop jacket inlet temperature
$T3$	Reactor jacket circulating loop jacket outlet temperature
TKT	Middle temperature vessel's temperature
ΔT_{LM}	Log mean temperature difference
TMT	High temperature vessel's temperature
U	Wetted perimeter

References

[1] *M. G. Balaton., L. Nagy:* Simulation of a batch unit, MKN '09, Veszprém, 2009 (in Hungarian language)

[2] *J. E. Edwards:* Dynamic modelling of batch reactors & batch distillation, Batch Reactor Systems Technology Symposium, Teesside, 2001

[3] *Z. Louleh, M. Cabassud, M.V. Le Lann, A. Chamayou, G. Casamatta:* A new heating-cooling system to improve controllability of batch reactors, Chemical Engineering Science, Vol. 51, 1996

[4] *Z. Louleh, M. Cabassud, M.V. Le Lann:* A new strategy for temperature control of batch reactors: experimental application, Chemical Engineering Journal 75, 1999

[5] UniSim™ Design Dynamic Modelling Guide