

The essential role of process control in process intensification

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It is argued that actuation is an overlooked but important aspect of the interaction between process design and control. Actuation is investigated and this leads to an insightful relationship with fluxes. This insight is used and exploited from a (open-loop optimal) control point of view in examples taken from crystallization, reaction and distillation. It is explained that exploitation of actuation means improved interaction with process design or even better with process intensification since the latter offers new possibilities and challenges for actuation and control.

Keywords

Interaction design and control, actuation, optimal control, dynamic optimization, process intensification.

The interaction between process design and control has received considerable attention in the literature. For example Schijndel and Pistikopoulos [1] give over 500 references related to this subject. Lewin [2] recognizes three approaches for the integration of design and control:

- Sequential; the overall design is done in three sequential stages, see Douglas [3]. In the first stage the operation mode (batch or continuous) is chosen, during the second stage the process design is done and finally the control system is designed. Basically this approach means no interaction.
- Anticipating; during the design stage interaction with control is taken into account by using controllability indices. Examples of such indices are the relative gain array (Bristol [4]), the minimum singular value and the closed-loop disturbance gain (Skogestad and Postlethwaite [5]).
- Simultaneous; the process and control stage are fully integrated. This approach typically results in a mixed integer nonlinear dynamic optimization problem. For more information the reader is referred to Bansal [6].

It should be noted that all these approaches have limitations or as Meeuse [7] states it: "One of the main limitations is that all available methods can only analyse the controllability of

given process alternatives. No clues are given on how to generate alternatives with improved controllability."

As a first step in a new direction see figure 1, it shows feedback and feedforward control. Regardless of the type of control it is clear that the process and the controller interact by means of the signal u ; the input or actuation. The very presence of actuation is actually an essential condition to apply control. Surprisingly actuation has not received much attention in the literature indicated above. A possible explanation is that control engineers consider actuation to be the result of process design while process engineers believe that it is fixed for a unit operation. For example a heat exchanger has typically one possibility for actuation; the flow on the utility side. Whatever the reason, actuation is an overlooked aspect of the

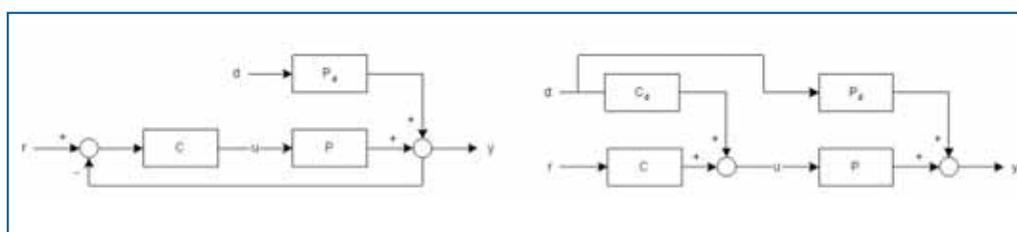


Figure 1 - A process under feedback (left) and feedforward control (right)

interaction between design and control and this seems related to the statement of Meeuse. As a matter of fact the main contribution of this paper is to show the importance of actuation and its potential to improve the interaction between design and control.

The rest of this paper is organized as follows. In the next section, actuation is discussed and this provides an insightful link with fluxes. The section *Control and actuation* illustrates by three examples how actuation can be exploited (read how the interaction between design and control can be improved). The section *Intensification, control and actuation* explains the

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consequences of this exploitation for process design and especially intensification. The last section summarizes the conclusions and does suggestions for further work.

Actuation

What is actuation? In simple terms: Actuation is the possibility to manipulate process behavior continuously over time. In this paper a process is defined as a system which purpose is to convert material and/or energy. Furthermore energy conversion should be associated with material conversion and material conversion should not involve transmutation. In process systems four phenomena play an important role: 1) Chemical reaction, 2) transfer of mass, 3) transfer of heat and 4) transfer of momentum. All these phenomena involve fluxes. So actuation is the possibility to manipulate fluxes continuously over time. As a matter of fact flux equations indicate how a process system can be actuated.

Consider for example the simple heat transfer setup shown in figure 2. A hot flow F transfers heat via a coil to the liquid in the vessel. The heat transfer is given by:

$$F_q = kA\Delta T \tag{1}$$

Here F_q is the heat flow, k the transfer coefficient, A the submerged coil area and ΔT the temperature difference between the hot flow and the liquid in the vessel. Flux equation (1) shows that this process can be actuated via k (stirrer speed), via A (coil submersion) and via ΔT (hot flow). In industrial practice the last option is dominant, however the first two options are occasionally used as well (mixing jets in fluidized beds and flooded condensers). It is worth noticing that in order to go from a flux to a flux equation at least the mechanism should be know. In the case of the simple heat transfer example equation (1) is relevant since the transfer mechanism is conduction.

As a subject flux equations are a part of chemical reaction kinetics, transport phenomena and irreversible thermodynamics. Of course chemical reaction kinetics limits itself to chemical reaction while transport phenomena only deals with the transfer of mass, heat and momentum. Irreversible thermodynamics on the other hand covers all four phenomena. Furthermore irreversible thermodynamics states that the summated product of the so-called conjugate fluxes J_i and the driving force X_i equals the entropy production rate σ :

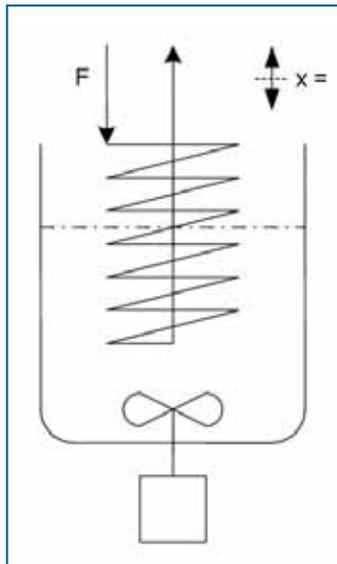


Figure 2 - Actuation of heat transfer

$$\sigma = \sum_i J_i X_i \geq 0 \tag{2}$$

Effectively equation (2) is a reformulation of the second law of thermodynamics. It shows that actuation is a spontaneous process. This is not a trivial matter. From an instrumentation point of view actuation is the opposite of sensing. Sensing is the conversion of the value of a process variable (pressure, temperature etc.) into the value of typically an electric signal (voltage, current etc.). So actuation is the conversion of the value of an electric signal into the value of a process variable. But why would such a conversion be possible? A electric signal represents virtually no material and/or energy while a process variable does. As stated before this conversion is possible because it is associated by an increase of entropy.

This section will be concluded by shortly stating the reasons why actuation is of vital importance for process control. Actuation allows for: 1) Stabilization of the conversion in the face of unknown initial conditions, model uncertainty and disturbances 2) changing the conversion according market demand and 3) optimization of the conversion in a process or economic sense. These reasons correspond directly with the general objectives of process control. It is explained by Huesman et alii [8] that the various objectives can be combined in an optimal control formulation. This rest of this paper will only consider optimal control formulations in an open-loop setting.

Control and actuation

This section will discuss the importance of actuation for control by means of three examples; crystallization, reaction and distillation. In these examples actuation will be increasingly exploited using the relationship with fluxes.

Crystallization

The discussion in this subsection is based on Kalbasenka et alii [9] but the focus is now more on fluxes. Figure 3 shows a typical batch crystallizer with three actuators or Degrees Of Freedom (DOF); seeding, stirrer speed and heat input.

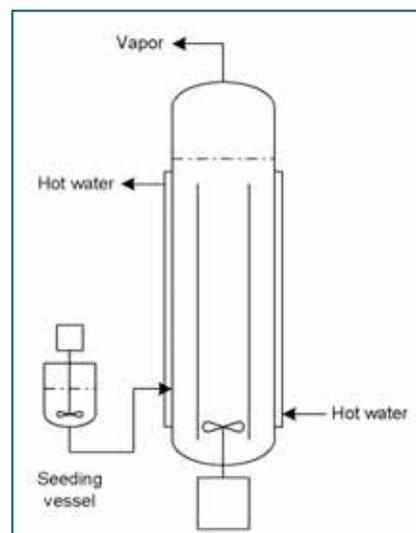


Figure 3 - A batch crystallizer

Obviously the relevant driving force is supersaturation while the relevant flux is from the liquid to the solid phase. Let's analyze the various DOF with respect to this flux. Seeding provides the initial condition for the partial differential equation that describes the Crystal Size Distribution (CSD) development. As such it can be con-

sidered a discrete DOF. Although seeding is very important it has no relationship with the flux and therefore seeding can not help to suppress disturbances like secondary nucleation that happen during the batch. The main function of the stirrer is to avoid settling of the crystals. Also this DOF has no influence on the flux and unfortunately it even causes secondary nucleation. The heat input has a clear influence on the flux and this makes it an effective DOF. However it is not possible to direct the flux to a certain part of the CSD. In other words the total crystal mass can be controlled but not the complete CSD.

It can be concluded that the actuation of batch crystallizers is limited. There are several ways to deal with this. The first possibility is to simply accept the limitation; from a control point of view this implies designing a controller that controls the growth rate rather than the CSD. As a matter of fact this approach has been rather successful, see Mesbah [10]. Another possibility is to extend the actuation such that the flux can be directed to a specific part of the CSD. In a sense this is done in practice by classification (for example fine extraction in an annular zone) followed by dissolution (a negative flux!). The last possibility is to create new actuation by redesign, for steps in that direction see Lakerveld et alii [11]. The following subsections will focus more on the extension or intensification of actuation.

Reaction

In a batch reactor component A is converted in the components B and C; $A \rightarrow B$ and $2A \rightarrow C$. The first reaction is desired while the second one is not. The reaction rates or fluxes J_B and J_C are given by:

$$J_B = k_B A = 10^6 e^{-\frac{45000}{RT}} A \text{ and } J_C = k_C A^2 = 5.10^{11} e^{-\frac{90000}{RT}} A^2 = 0.5 k_B^2 A^2 \quad (3)$$

Here k_B and k_C denote the specific rates, A the concentration of A, R the universal gas constant and T the absolute temperature. Suppose that in the normal case the batch reactor is actuated by a transformed temperature k_B (see figure 4, left). From the fluxes the flows can be derived:

$$F_B = k_B A_R V_R \text{ and } F_C = 0.5 k_B^2 A_R^2 V_R \quad (4)$$

So it should be possible not only to actuate the system by k_B

but also by the concentration of A in the reactor A_R and the volume in the reactor V_R . Both variables are influenced by an inlet flow of A to the reactor; F_1 (see figure 4, right). Note that an outlet flow from the reactor would only influence V_R . Therefore the actuation is extended or intensified by adding F_1 as a DOF.

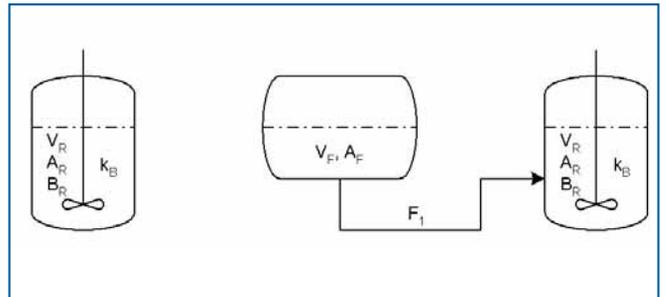


Figure 4 - A reactor system with normal (left) and intensified actuation (right)

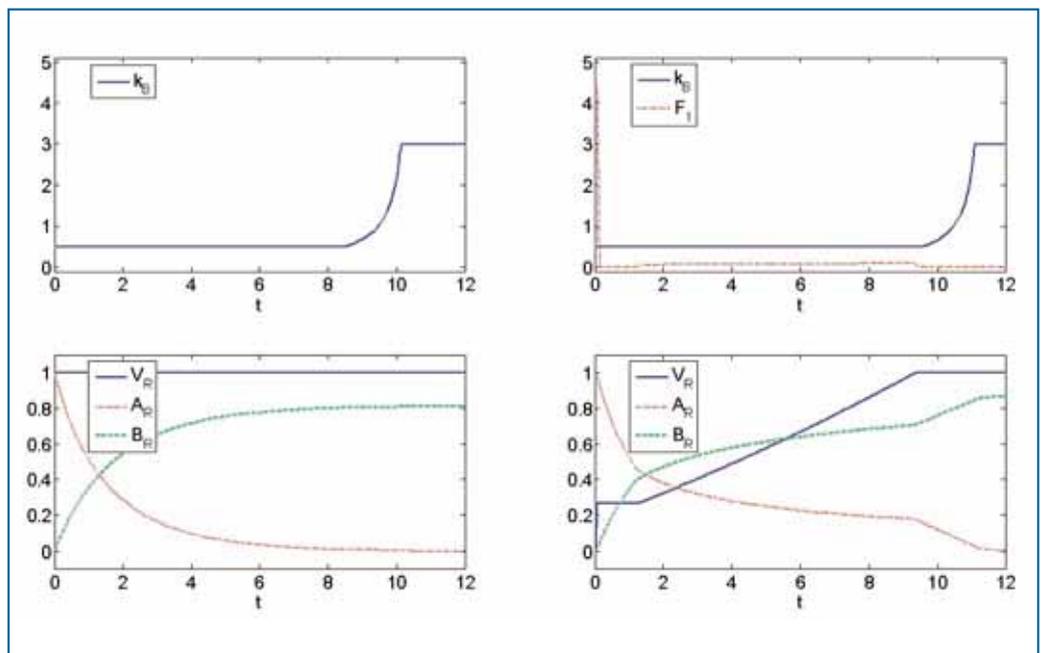


Figure 5 - The reactor system results for normal (left) and intensified actuation (right)

Both systems were used to solve an optimal control problem. The objective was to maximize $V_R(t_f)B_R(t_f)$ with t_f being the time horizon subject to system behavior (mass and component balances) and operational constraints (state and input limitations). The objective reflects the total production of component B. Great care was taken to ensure a fair comparison between the normal and intensified case. The optimal control problem was solved using dynamic optimization; the simultaneous approach based on an implicit Euler transcription. The implementation was done in the algebraic language Gams with the solver Conopt. The results are shown in figure 5. In the case of normal actuation the objective value was 0.8317 while in the case of intensified actuation it increased to 0.8710; an improvement of 7%.

The results can be explained from a process point of view. In the normal case the reaction starts at high values for V_R and A_R . In other words initially there is a large flow to component C compared to B. In the case of intensified actuation first the value of A_R is lowered after which V_R is slowly increased.

Distillation

In a continuous distillation column a mixture of the components A and B is separated and B is stored in a product tank. In the normal case the distillation column is actuated by the feed F , the boilup V and the reflux L_{10} (see figure 6, left). The fluxes between the liquid and vapor phase depend on the

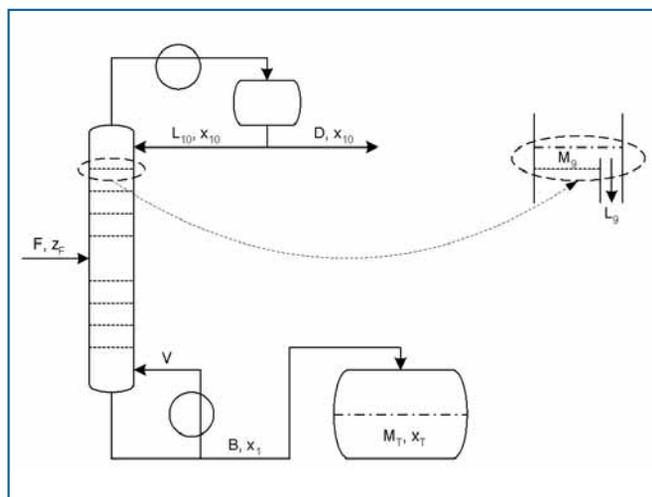


Figure 6 - A distillation system with normal (left) and intensified actuation (right)

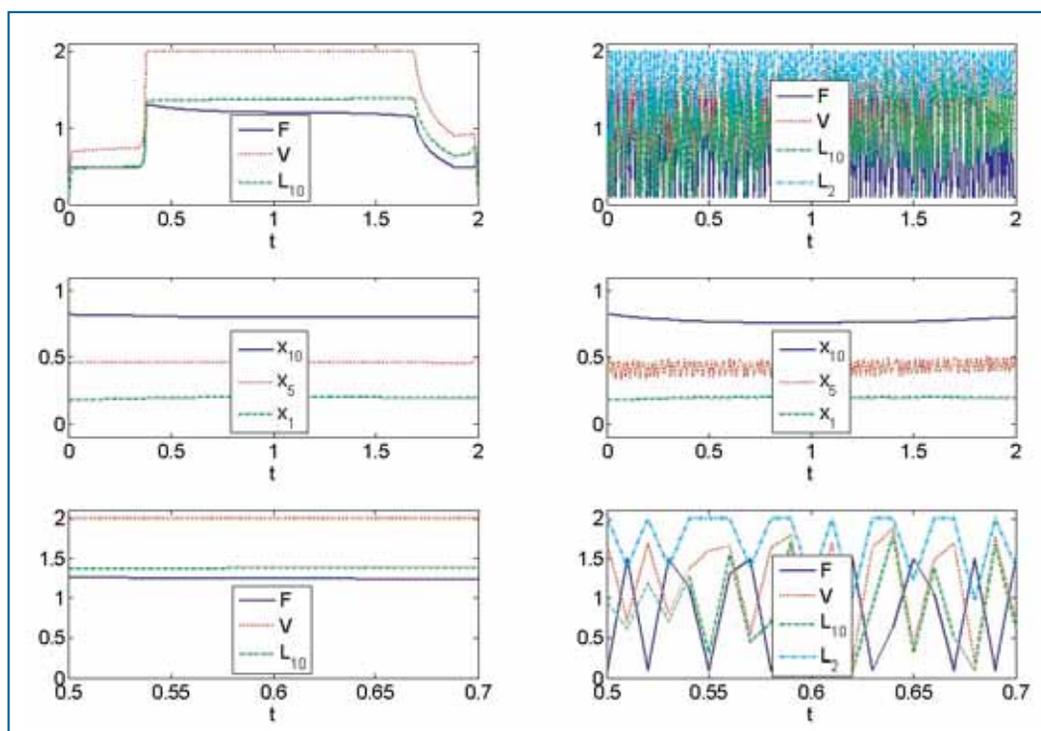


Figure 7 - The distillation system results for normal (left) and intensified actuation (right)

transfer coefficient and the distance from equilibrium. The latter is easy to influence by the liquid flow in the downcomers; for example L_o (see figure 6, right). So the actuation can be intensified by adding $L_2 - L_o$ as DOF. This gives a significant increase in the number of DOF (from 3 to 11); this is a direct result of the distributed nature of distillation columns.

Again both systems were used to solve an optimal control problem. The objective was to minimize the integral $wF(t)+V(t)dt$ from 0 to t_f subject to system behavior, operational constraints and the constraints $M_T(t_f) = 1.1$ and $x_T(t_f) = 0.2$. The objective reflects the operational costs; feed plus energy, with w being the cost of feed over the cost of energy. Again great care was taken to ensure a fair comparison. The optimal control problem was solved in the same way as the batch reactor example. The normal case is described in detail by Huesman et alii [12].

The results are shown in figure 7. In the case of normal actuation the objective value was 7.2327 while in the case of intensified actuation it could at least go as low as 4.6417; an improvement of 35%.

Figure 7 clearly shows that intensified actuation results in, roughly, periodic operation. That this form of operation (also known as controlled cycling) is indeed attractive has been reported before. Douglas [13] gives a nice overview of the relevant literature; the superiority of periodic operation has been proven both analytically as well as experimentally. The reason for the better performance is that a higher time-average driving force for mass transfer is obtained with controlled cycling.

Intensification, control and actuation

It is evident that going from the first to the last example actuation was increasingly exploited. However it should be noted that there are consequences for the process design. In the crystallization case no concrete changes are proposed but in the reaction example an open shut valve must be replaced by a complete flow control loop. And in the distillation case downcomers, trays etc. should be modified such that all downcomer flows can be manipulated.

It is doubtful if these consequences go well with traditional process design (sequential approach, see first section of this article). On the other hand process intensification that aims to improve processes and equipment may consider

these consequences opportunities.

According to Gerven and Stankiewicz [14] process intensification is based on four domains. All domains are discussed below including their relationship with control and actuation:

- Spatial; the drastic reduction of characteristic dimensions to micrometer up to nanometer scale. However even on the traditional process scale improvements are possible. Worth mentioning is the idea developed at the Delft University of Technology of small floating sensors and actuators that communicate via ultra-wideband radio and enable an innovative form of spatial process control.
- Thermodynamic; the application of alternative driving forces such as gravitational, electromagnetic or acoustic fields. Given the relationship between driving forces, fluxes and actuation, this opens complete new possibilities for actuation. For instance, the application of microwaves is a fundamentally different way of heating compared to the conventional heating by conduction.
- Functional; the integration of various functions within a single unit operation. A well-known example is reactive distillation. Although this is attractive since it leads to compact designs it may well reduce the possibilities for actuation.
- Temporal; the dramatic shortening of the characteristic times and the use of deliberate non steady state operation. The last point was clearly illustrated in the distillation example.

Summarizing, there are new and exciting possibilities for process intensification and control to cooperate in which actuation will play a central role.

Finally Freund and Sundmacher [15] point out in a convincing manner that process intensification requires a shift from thinking in unit operations to thinking in underlying fundamental physical and chemical processes and fluxes. This seems to imply that process design in the sense of process intensification and the design of actuation can be performed simultaneously thereby improving the interaction between control and design.

Conclusions and future work

The main conclusions of this paper are:

- An overlooked but important aspect of the interface of process design and control is actuation.
- Actuation boils down to the possibility to manipulate fluxes continuously over time.
- Actuation can be used to improve or intensify process performance.
- Process intensification offers new possibilities and challenges for actuation and control.

Future work will concentrate on:

- The benefits of intensified actuation in the case of closed-loop control.
- Application of intensified actuation to distributed systems and systems with new driving forces.
- The integration of process intensification and actuation by focusing on fluxes.

References

[1] J. van Schijndel, E.N. Pistikopoulos, "Towards the inte-

gration of process design, process control and process operability: current status and future trends", in M.F. Malone, J.A. Trainham, B. Carnaham, editors, *Proc. of the 5th international conference on Foundations of Computer-Aided Process Design*, pp. 99-112, 2000.

[2] D.R. Lewin, "Interaction of design and control", in *Proc. of the search IEEE Mediterranean conference on control and automation*, Haifa, 1999.

[3] J.M. Douglas, *Conceptual Design of Chemical Processes*, McGraw-Hill, New York, pp. 406 and 414, 1988.

[4] E.H. Bristol, On a new measure of interaction for multivariable process control. *IEEE Transactions on Automatic Control*, 11, p. 133, 1966.

[5] S. Skogestad, I. Postlethwaite, *Multivariable feedback control, analysis and design*, Wiley, Chichester, 1996.

[6] V. Bansal, *Analysis, design and control optimisation of process systems under uncertainty*. PhD thesis, Imperial College, London, 2000.

[7] F.M. Meeuse, *On the design of chemical processes with improved controllability characteristics*, PhD thesis, Delft University of Technology, Delft, p. 25, 2002.

[8] A.E.M. Huesman, O.H. Bosgra, P.M.J. Van den Hof, "Integrating MPC and RTO in the process industry by economic dynamic lexicographic optimization; an open-loop exploration", in *Proc. of the 100th AIChE Annual Meeting*, Philadelphia USA, 2008.

[9] A. Kalbasenka, A. Huesman, H. Kramer, O. Bosgra, "Controllability analysis of industrial crystallizers", in M. Jones, J. Ulrich, editors, In *Proc. of the 12th International Workshop on Industrial Crystallization*, pp. 157-164, Halle Germany, 2005.

[10] A. Mesbah, A.N. Kalbasenka, A.E.M. Huesman, H.J.M. Kramer, P.M.J. Van den Hof, "Real-time dynamic optimization of batch crystallization processes", in *Proc. of the 17th Ifac World Congress*, pp. 3246-3251, Seoul Korea, 2008.

[11] R. Lakerveld, H.J.M. Kramer, P. Jansens, J. Grievink, "The application of a task-based concept for the design of innovative industrial crystallizers", *Computers and Chemical Engineering*, (accepted), 2009.

[12] A.E.M. Huesman, O.H. Bosgra, P.M.J. Van den Hof, "Degrees of freedom analysis of economic dynamic optimal plantwide operation", in B. Foss, J. Alvarez, editors, *Prepr. of the 8th Ifac International Symposium on Dynamics and Control of Process Systems*, volume 1, pp. 165-170, Cancun Mexico, 2007.

[13] J.M. Douglas, *Process Dynamics and Control Volume 2 Control System Synthesis*. Prentice-Hall, New Jersey, pp. 383-392, 1972.

[14] T. van Gerven, A. Stankiewicz, "Structure, Energy, Synergy, Time - the Fundamentals of Process Intensification", *Ind. Eng. Chem. Res.*, 48, (accepted), 2009.

[15] H. Freund, K. Sundmacher, "Towards a methodology for the systematic analysis and design of efficient chemical processes Part1. From unit operations to elementary process functions", *Chemical Engineering and Processing: Process Intensification*, 47, pp. 2051-2060, 2008. ■