

# Divergence as a Goal Function for Control and On-Line Optimization

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The control and optimization of batch reactors is an active field of research due to the complexity and number of processes that are carried out in these reactors, the strong nonlinearities present in the process, the fact that only few measurements -mainly temperatures- are available in real time, and the safety issues, that is, loss of temperature control leading to a runaway. A considerable amount of techniques have been presented in literature for control and on-line optimization. For a recent review on batch control the reader is referred to Friederich and Perne (1995) and references therein, whereas for on line -optimization see Muske et al. (2004) and Eloy Sequeira et al., (2004).

In a series of recent works (Zaldívar et al., 2003; Bosch et al., 2004a) a new criterion to delimit runaway boundaries was developed, applying techniques from nonlinear dynamical systems theory to characterize the sensitivity of chemical reactors. The runaway detection criterion was defined as when the divergence of the reactor becomes positive on a segment of the reaction path, that is,  $div > 0$ . Furthermore, it was shown that the divergence could be calculated on-line by measuring reactor and jacket temperatures for isoperibolic batch experiments carried out in a 240 L pilot plant reactor (Bosch et al., 2004b).

In this work, we propose the use of the divergence of the system for developing a goal function for control and on-line optimization of chemical reactors. We define as optimum conditions for the operation of batch reactors as those that give

$div = 0$  at any given instant. Therefore, the control system instead of considering the difference between the set point and reactor temperatures,  $(T^{sp} - T_r)$  when working on isothermal mode or set point and jacket temperature  $(T^{sp} - T_j)$ , when working on isoperibolic mode, it considers the divergence  $(0 - div)$  as goal function.

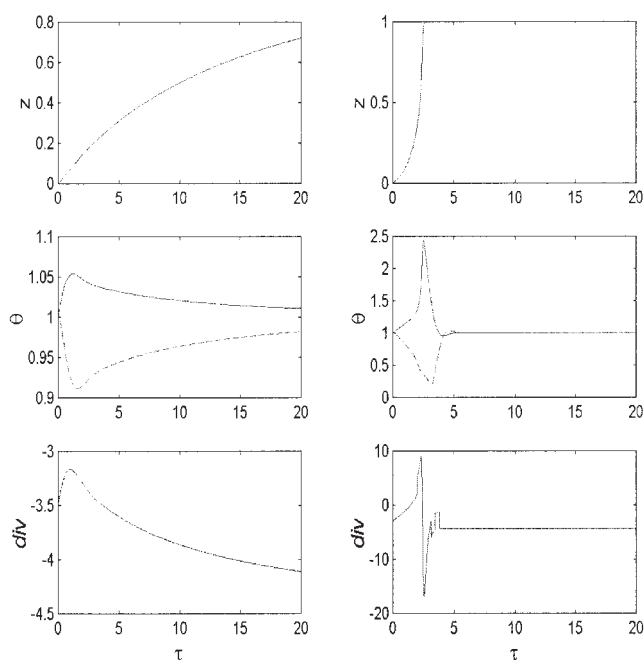
The results for batch simulated experiments show that this control strategy is able to maintain safe conditions in case where traditional control systems will lead to a runaway, and increase the reaction rate for operating conditions where the batch production time would be too long due to the selection of conservative operating conditions.

Furthermore, this approach can be easily extended to SBRs, CSTRs, and to more complex kinetic schemes, for example, parallel, consecutive, polymerizations, and so on, since the divergence has proved to be a reliable criterion of runaway conditions in all these cases (Zaldívar et al., 2003). However, further studies are necessary to compare the results with more conventional techniques aiming at maximize selectivity. Finally, the same approach for SBRs and CSTRs may be applied for controlling the dosing speed instead or in parallel to temperature control.

## Batch Reactors Case Study

In order to discuss this new approach to control and on-line optimization of process plants lets use the simulated temperature data obtained for an isothermal batch reactor in which a  $n$ th-order reaction takes place. The differential equations that describe the dynamic behavior of a controlled batch reactor

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**Figure 1. Conversion, dimensionless reactor and jacket temperatures and divergence during a nonrunaway ( $B = 1.8$ ) and a runaway ( $B = 2.9$ ) simulation.**

Parameters:  $Da = 0.05$ ;  $St = 1$ ;  $\gamma = 0.1$ ;  $\delta = 0.33$ ;  $Kp_1 = 2$ ;  $Kp_2 = 3$ ;  $Q_{Rmax} = 0.8$ ;  $Q_{Rmin} = -0.8$ .

with an exothermic  $n$ th-order reaction  $A \xrightarrow{r_1} B$ , can be written, in dimensionless form, as (Zaldívar et al., 2003)

$$\frac{dz}{d\tau} = Da \cdot R_1 \quad (1)$$

$$\frac{d\theta}{d\tau} = B \cdot Da \cdot R_1 - St \cdot (\theta - \theta_w) \quad (2)$$

$$\frac{d\theta_w}{d\tau} = \delta \cdot St \cdot (\theta - \theta_w) + Q_R \quad (3)$$

where  $Da$ ,  $B$ ,  $St$  and  $\delta$  are the Damköhler number, the dimensionless heat of reaction parameter, the Stanton number and the cooling dimensionless time of the heat-transfer fluid system, respectively. The dimensionless reaction rate is given by the following expression

$$R_1 = \exp\left(\frac{\gamma \cdot \theta}{\gamma + \theta}\right) \cdot (1 - z)^n \quad (4)$$

where  $\gamma$  is the dimensionless activation energy. As can be seen the reaction rate equation is the main source of nonlinearities in these systems due its exponential temperature dependence.

The control configuration may be summarized as follows, when the process is carried out under isothermal conditions, the

reactor temperature is maintained at its desired value, set point, by adjusting the temperature set point for the heat-transfer fluid circulating through the reactor jacket. This is accomplished by the master controller. The temperature of the heat-transfer fluid, which circulates through the reactor jacket, is controlled using a slave controller. Hence, the controller of the outer loop corrects deviations of the reactor temperature,  $\theta$ , from the set value,  $\theta^{sp}$ , following a proportional criterion

$$\theta_w^{sp} = \theta^{sp} + Kp_1(\theta^{sp} - \theta) \quad (5)$$

providing the set value for the heat-transfer fluid temperature  $\theta_w^{sp}$ , which is adjusted by the inner loop controller by means of another proportional controller. This configuration is typical of reaction calorimeters (Zaldívar et al., 1996), and it has been used in pilot-plant reactors (Zaldívar et al., 1993). Expressing this in terms of heat balance, it is possible to write

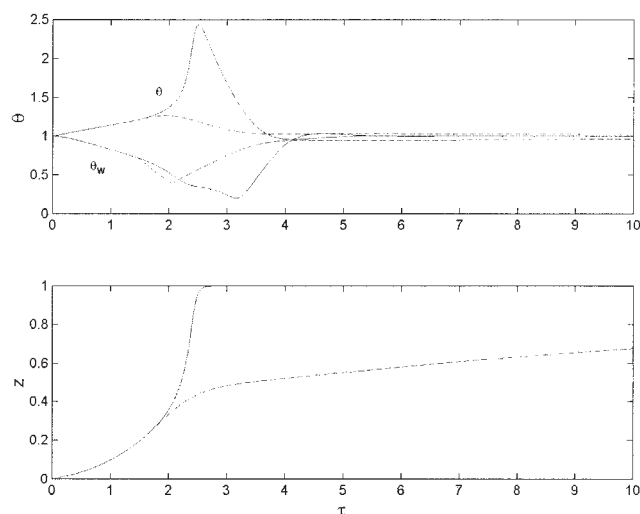
$$Q_R = Kp_2(\theta_w^{sp} - \theta_w) \quad (6)$$

In order to consider control saturation during transients, the manipulated variable  $Q_R$  is constrained as follows: if the required  $Q_R$  is higher than the maximum heating capacity of the system  $Q_{Rmax}$ , this parameter takes this maximum value, and if  $Q_R$  is lower than the maximum cooling capacity then the parameter is equal to  $Q_{Rmin}$ .

The typical behavior of this control system can be shown in Figure 1, where a nonrunaway and runaway simulation are shown.

In this case the divergence ( $div$ ) of the system may be easily calculated as

$$div(t) = \frac{\partial(dz/d\tau)}{\partial z} + \frac{\partial(d\theta/d\tau)}{\partial \theta} + \frac{\partial(d\theta_w/d\tau)}{\partial \theta_w} \quad (7)$$



**Figure 2. (a) Reactor and jacket temperatures in a batch experiment without (continuous line) Eq. 6, and with the  $div$  in the control, Eq. 8 actuation, and (b) conversion.**

Parameters: the same as Figure 1b and  $K_{div} = 2$ .

### Divergence as an on/off controller

Let us first study the case in which the divergence is used as an active system when a runaway initiation is detected. Figure 2 shows the reactor and jacket temperatures for the control system given by Eq. 6. As can be seen in this case a runaway would occur inside the reactor (Figure 1) under this operating conditions and control parameters. However, if we apply the following equation to the controller when  $div > 0$

$$Q_R = K_{p2}(\theta_w^{sp} - \theta_w) + K_{div} \cdot (0 - div) \quad (8)$$

it is possible to see (Figure 2) that the controller would have had time to act and to control the reactor, avoiding a dangerous situation. Because of high parametric sensitivity conditions, a small change would suffice to change the dynamics of the system.

### Divergence as a goal function for optimization and control

When operating chemical reactors, the main objective is to maximize production and in parallel to increase the safety. In this sense, the criterion to distinguish between nonrunaway and runaway conditions (Strozzi et al., 1997) says that we are in a dangerous situation when  $div > 0$ . On the contrary, we are in a safe situation when  $div < 0$ . Therefore, it seems natural to conclude that if we want to maximize production (reducing time between batches) and work on safety conditions, we should impose  $div=0$  as our controller set point.

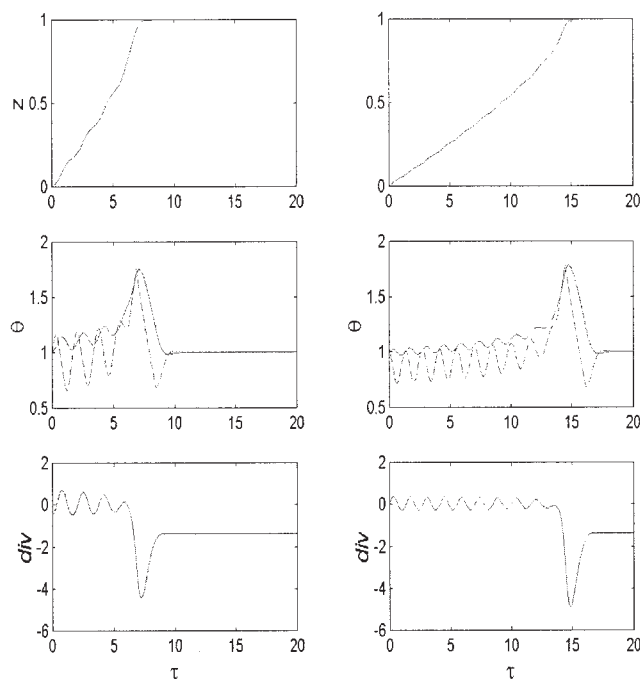
Figure 3 shows the result of the divergence controller applied to the two processes previously described in Figure 1. In this case a proportional control, based on the divergence of the system has been used, that is

$$Q_R = K_{pdiv} \cdot (0 - div) \quad (9)$$

As can be seen, by using this control function we are able to conduct nonrunaway and runaway reactions in an optimal way, reducing the time necessary to obtain a complete conversion, but maintaining safe conditions. For the nonrunaway case, it can be seen in Figure 3 (at  $\tau \approx 7$ ,  $z \approx 1$ ) the reduction in time obtained when comparing with Figure 1 (at  $\tau = 20$ ,  $z \approx 0.7$ ). For the runaway case, the controller is able to maintain the reactor in safe conditions, as can be seen by the low increase in reactor temperature. In conclusion, using  $div$  as a goal function, when conditions are safe the system tries to increase the conversion by increasing jacket temperature, whereas when we are in runaway situation the controller tries to reduce the rate of heat production inside the reactor.

When the reaction is almost completed  $div$  is always negative (chemical reactors are dissipative systems). In this case, to avoid excessive heating, the standard control can act and put the reactor in some desired set point. This effect can be observed in Figure 3 by a sharp change in jacket temperature.

In this sense, better control could be obtained using the typical PID equation, but with  $div$  as a goal function instead of the error between reactor or jacket and set point temperature



**Figure 3. Conversion, dimensionless reactor and jacket temperatures and divergence during the non-runaway ( $B=1.8$ ), and a runaway ( $B=2.9$ ) simulations in Figure 1, using  $div = 0$  as a goal function for control and on-line optimization.**

Parameters: the same as Figure 1 and  $K_{div} = 2$ .

$$Q_R = K_{pdiv} \cdot (0 - div)$$

$$+ K_{idiv} \int_0^t (0 - div) \cdot d\tau + K_{ddiv} \frac{d[0 - div]}{dt} \quad (10)$$

### State space reconstruction of the divergence using experimental data

In order to calculate on-line the divergence without the need to know the differential equations of the system, we have used the theory of embedding. The theory of embedding is a way to move from a temporal time series of measurements  $s(t) = h[x(t)]$ , which is related to the state variables  $x(t)$ , by a unknown function  $h$ , to a state space similar—in a topological sense—to that of the underlying dynamical system we are interested in analyzing. Techniques of state space reconstruction were introduced by Packard et al. (1980) and Takens (1981), who showed it is possible to address this problem using time delay embedding vectors of the original measurements, that is  $\{s(t), s(t - \Delta t), s(t - 2\Delta t), \dots, s(t - (d_E - 1)\Delta t)\}$ .

The extension of this theory for the case of batch and semi-batch chemical reactors is complicated by the dynamic nature (nonstationarity) of the system that implies that embedding parameters, that is, time delay,  $\Delta t$  (the lag between data when reconstructing the state space), and embedding dimension  $d_E$  (the dimension of the space required to unfold the dynamics) are changing during the process. However, as it was discussed in Zbilut et al. (2002) and Bosch et al. (2004a), an

appropriate value for these parameters can be chosen to allow state space reconstruction. Furthermore, several methods of reconstruction of state space: time delay embedding vectors; derivative coordinates and integral coordinates may be used (Bosch et al., 2004a). However, the more robust to noise is the one based on delayed vectors, that is,  $\{T(t), T(t - \Delta t)\}$  (Bosch et al., 2004b), and for the cases studied an embedding dimension of two is sufficient to reconstruct the divergence.

Once the state space has been reconstructed, using measurements of a variable of the system, it is possible to calculate the divergence,  $div$ . The divergence gives the rate of expansion or contraction of the phase space ( $PS$ ), and as it was shown in Strozzi et al. (1999) it may be calculated as

$$div = \frac{\dot{V}_{PS}(t)}{V_{PS}(t)} \quad (11)$$

Phase space volume (area) at time  $t$  may be calculated using the determinant between close points in state space as

$$V(t) = \left| \det \begin{bmatrix} T(t) - T(t - \Delta t) & 0 \\ 0 & T(t - \Delta t) - T(t - 2\Delta t) \end{bmatrix} \right| \quad (12)$$

The robustness to noise and numerical errors depend on the selection of the appropriate state space and the reconstruction parameters, that is, time delay and embedding dimension. Experimental analysis using bench-scale, pilot plant and industrial reactor data show that it is possible to reconstruct the divergence for runaway experiments (Bosch et al., 2004b) being more affected by noise “safe” experiments that have low values of  $V_{PS}$ , and small variation of  $\Delta V_{PS}$ . Furthermore, from industrial data, it has been observed that time delayed vectors are more robust to noise than earlier reconstruction schemes proposed using the derivatives (Bosch et al., 2004a).

## Conclusions

An on-line optimization and control system for batch chemical reactors easily applicable to other type of process has been developed. The system is based on the use of the divergence of the process as a goal function. The divergence can be calculated on-line using state space reconstruction techniques (Bosch et al., 2004a,b; Zaldívar et al., 2004) applied to reactor

and jacket temperatures. This means that the batch process may be optimized on-line automatically using this control strategy. Furthermore, there is no need to have a model of the system for applying this control strategy. This methodology, when completely developed, would reduce considerably the time needed to find optimum operating conditions in terms of production and safety.

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