Real-Time Optimization in Nonlinear Chemical Processes: Need For Global Optimizer

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Large chemical processes are complex systems that can operate under a range of conditions described by variables such as flow rates, temperatures, pressures, and so on. The economic profit derived from a process is a function of these operating condition variables, and the profit depends parametrically on the prices of the products, raw materials, and utilities. The profit can be a nonlinear function of the operating conditions variables, and there may be many local maxima, minima, and saddle points of the profit in the operating condition variable space. The profit function in the operating condition variable space can be called a "profit landscape" to emphasize the possibility of many local maxima, minima, and saddle points. The optimum operation of the process occurs at the conditions corresponding to the global maximum of the profit landscape. The profit landscape changes with time, due to changes in the prices of raw materials, products, and utilities, and real-time optimization can be used to periodically adjust the operating conditions to follow the profit maximum (for example, Biegler et al., 1997).

This article shows that real-time optimization can in certain cases lead to inferior performance even if the process is perfectly modeled. Real-time optimization is normally based on local (rather than global) optimization, due to the computational intensity of global optimization procedures and the need to carry out the real-time optimization quickly. As shown below, using local optimization in real-time optimization can sometimes lead to inferior process performance (compared to the case with no real-time optimization) when a parameter fluctuates.

As a simple example, we consider a biodesulfurization process to increase the value of a crude oil stream, with economic parameters used previously for studying pooling processes (Haverly, 1979; Adhya et al., 1999). A reactor is used to remove sulfur from a crude oil stream with initial sulfur concentration y_o and a flow rate V. The aqueous phase containing the biological cells is initially free of sulfur, and is used at the flow rate L. The sulfur concentration in the oil phase, (y) and in the aqueous phase (x) exiting the reactor is modeled by an effective Henry's law

$$y = mx \tag{1}$$

where m is an effective Henry's law parameter that is obtained from measurements on the process (since Henry's law may not accurately describe the system, the parameter m may depend on the process conditions). Combining the effective Henry's law with a mass balance, the sulfur concentration in the crude oil exiting the reactor as a function of the aqueous phase flow rate is given as

$$y(L/V;m,y_0) = \frac{y_0}{1+\frac{(L/V)}{m}} \tag{2}$$

The cost of operating the reactor is taken to be the cost of purchasing (or recovering) the sulfur-free aqueous phase containing the biological cells; this cost is denoted as α per unit volume. The profit, on a per unit basis of the crude oil stream, is then given by

$$\text{Profit}[L/V;m,\alpha,y_o] = \text{Value}[y(L/V;m,y_o)] - \text{Value}[y_o] - \alpha(L/V) \tag{3}$$

where the crude oil value as a function of sulfur concentration, Value [y] is shown in Figure 1; a cubic spline interpolation is used to extend the set of Haverly economic parameters at several concentrations (Haverly, 1979; Adhya et al., 1999) to intermediate concentrations.

We investigate first the operation of the process with the cost of the aqueous phase $\alpha = 3$, the effective Henry's law parameter $m = 2$, and the sulfur concentration of the initial crude oil stream $y_o = 0.03$. The profit as a function of L/V is shown in Figure 2. There are two profit maxima: a high-L/V profit maximum at L/V = 2 and a low-L/V profit maximum at L/V = 0.4. The high-L/V profit maximum is the global

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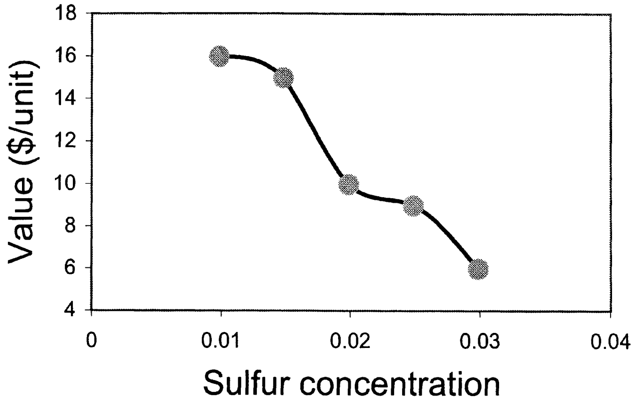

Figure 1. Value of crude oil stream as a function of sulfur concentration.

Circles: Haverly parameters (Haverly, 1979; Adhya et al., 1999). Line: Cubic spline interpolation based on Haverly parameters.

maximum for which the sulfur concentration in the product is $y = 0.015$ and a profit of $3/unit is obtained. The low-L/V profit maximum is a local profit maximum, for which the sulfur concentration in the product is $y = 0.025$ and a profit of $1.80/unit is obtained.

Changes in the economic parameters (α in the present process), model parameters (m in the present process), and process inputs (y_o in the present process) alter the profit landscape. Figure 2 shows the changes in the profit landscape due to changes in the cost of the aqueous phase α. The increase in the cost of the aqueous phase distorts the profit landscape such that: (1) the profit maxima shift to lower values of L/V as α increases; (2) the high-L/V profit maximum, which is the global maximum at $\alpha = 3$, is no longer the global maximum for $\alpha > 3.76$; (3) the high-L/V profit maximum disappears completely for $\alpha > 5.85$.

These changes in the profit landscape can be used to address process performance as α increases from its initial value of $\alpha = 3$ (with m constant; the more general case is discussed below), using real-time optimization based on a local optimizer. The process initially operates at the high-L/V profit maximum in Figure 2, which is the global maximum. Since the high-L/V profit maximum shifts to lower L/V as α increases, real-time optimization will decrease L/V to track the changing position of the profit maximum. Figure 3 shows the decrease in L/V specified by real-time optimization, along with the resulting product concentration and the profit. As α exceeds 3.76, process operation is maintained at the high-L/V profit maximum even though it is no longer the global maximum, because the real-time optimization is based oa local optimization procedure. As α exceeds 5.85, the high-L/V profit maximum disappears, and a steepest ascent path suddenly becomes available that leads the real-time optimizer to the low-L/V profit maximum; as shown in Figure 3, the sudden appearance of a steepest ascent path causes the real-time

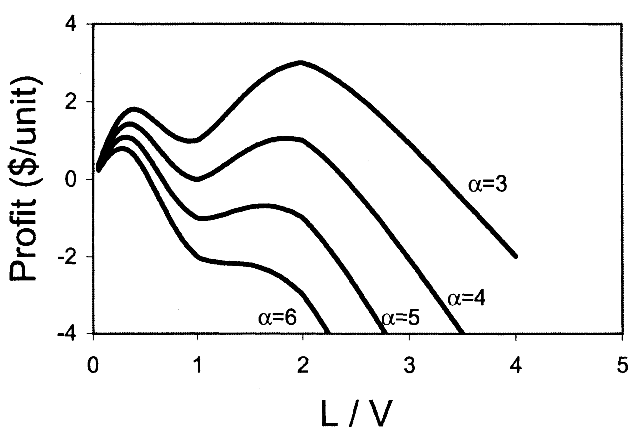

Figure 2. Profit landscapes for various values of the cost of the aqueous phase containing the biological cells (α).

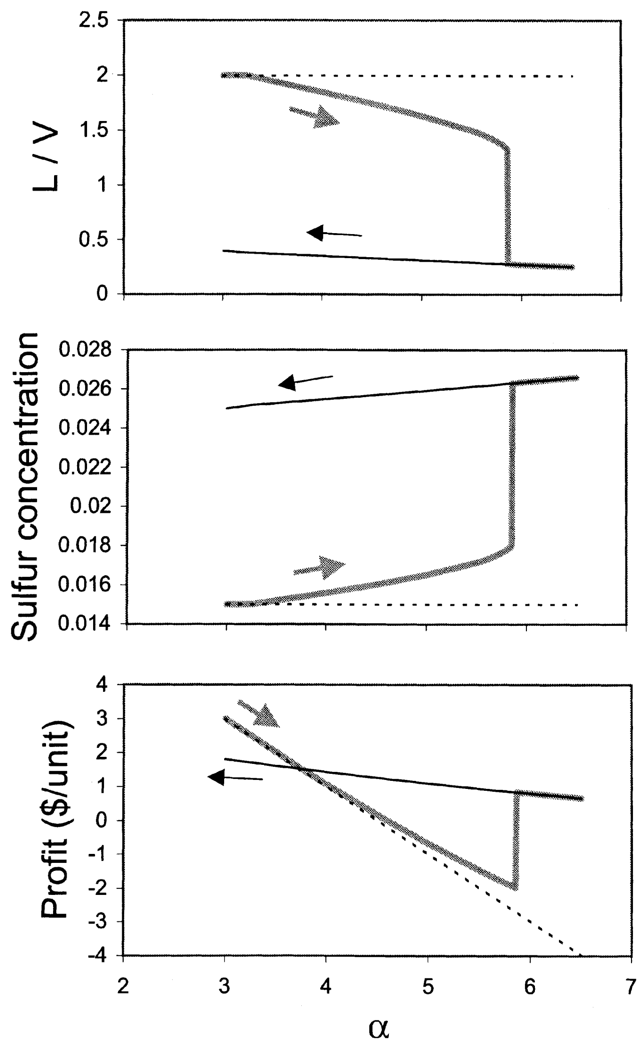

Figure 3. Process performance as the cost of the aqueous phase containing the biological cells (α) changes.

Dashed line: no real-time optimization (either increasing or decreasing α). Thick solid line: real-time optimization (based on local optimizer), increasing α. Thin solid line: real-time optimization (based on local optimizer), decreasing α.

optimizer to decrease L/V discontinuously, with a resulting discontinuous increase in profit.

The profit landscapes shown in Figure 2 can also be used to address process performance as α decreases back from large $\alpha(\alpha > 5.85)$ to the initial value of $\alpha = 3$. As discussed in the previous paragraph, real-time optimization will cause the process to operate at the low-L/V profit maximum when $\alpha > 5.85$. If α then decreases back to $\alpha = 3$, process operation is maintained at the low-L/V profit maximum even though it is no longer the global maximum, because the real-time optimization is based on a local optimization procedure. Thus, as shown in Figure 3, the cycle of changes in α in combination with real-time optimization causes the process to operate at a lower profit at the initial value of α.

If real-time optimization is not used, the process always operates at the initial operating conditions (L/V = 2), even as α changes. The profit as a function of α in this case is also shown in Figure 3. In contrast to the case with real-time optimization, the process operates at the globally optimum conditions after the cycle of changes in α (since the operating conditions do not change when real-time optimization is not used, the process does not get stuck at a different profit optimum). Thus, the process performance after this cycle of changes in α is better when real-time optimization is not used.

Real-time optimization also utilizes periodic measurements on the actual process to update parameters for the model used to obtain the profit function. In the present process, the effective Henry's law constant m is a parameter that would be periodically updated by such measurements. Changes in m lead to the same distortions of the profit landscape as shown above for changes in α. In particular, the cost of operating the process increases as m increases because more aqueous phase is required to remove a specified amount of sulfur, and the large-L/V profit maximum disappears for $m > 3.9$. Thus, the consequences of real-time optimization discussed above in terms of changes in α will also occur due to changes in m. (The actual dynamics may be more complex when m changes. Since the model used in real-time optimization is not a perfect representation of the actual process, the value of m can change with changing L/V; thus, while changes in m lead the real-time optimizer to change L/V, those changes in L/V can lead to further changes in m, and so on. However, the more complex dynamics will not change the fundamental picture described above, which is due to the disappearance of a profit maximum).

In regard to the robustness of the conclusions, we note that the details of the process are not crucial—any reasonable cost function that increases with the amount of sulfur removed would lead to similar results. The crucial aspect is the nonlinear dependence of the stream value on composition; this nonlinear dependence is also the crucial aspect that makes pooling processes possible (that is, mixing two or more streams to yield a product stream of higher value).

The process optimization phenomenon described here is analogous to phenomena involving glassy materials under stress, as illustrated with the landscape paradigm. For example, experiments show that a cycle of compression and decompression changes the favorable open-framework structure of silica glass to a denser, but less favorable, structure (Grimsditch, 1984). These experimental results have been explained in terms of energy landscapes (that is, energy as a function of atomic configuration), which are analogous to profit landscapes, but inverted; energy minima are favored, in contrast to profit maxima. As the glass is compressed, the energy landscape deforms and the atoms move so as to remain near an energy minimum; this adjustment of atomic positions is a local optimization. These landscape distortions eventually cause the energy minimum that the system is in to disappear (as in Figure 2, but inverted), after which the system is forced to an alternate energy minimum corresponding to a denser structure (Lacks, 1998, 2000). As the glass is decompressed, the system remains trapped in the denser structure, which is less favorable at low pressure.

The landscape paradigm also leads to analogies between process optimization and biological evolution. The analogies become evident when biological evolution is described in terms of a fitness landscape, which represents the fitness for survival as a function of genotype (Wright, 1932). We have shown that regressive evolution (that is, evolution to a less fit state) can result from fluctuations in the environment, in the same way that real-time optimization can cause a process to operate at lower profit conditions after process parameters fluctuate (Lacks, 2001).

In summary, the present results show that running a process with real-time optimization based on a local optimizer can cause the process to operate at a lower profit. This lower-profit performance occurs if price fluctuations cause the profit maximum at which the process operates to disappear at some point in the fluctuation. Note that this effect is not just that the real-time optimizer fails to find other higher profit maxima as prices change, but rather that the real-time optimizer guides the process to lower-profit performance. This effect is also not due to inadequate modeling of the real process, and it occurs even if the real process is modeled perfectly.

The lower-profit performance caused by real-time optimization arises from the use of a local optimizer—this problem can be averted by using a global optimizer in the real-time optimization procedure. Although global optimization is much more computationally intensive than local optimization, advances in global optimization methods (for example, Floudas, 2000) and computer hardware may allow the use of global optimizers in real-time optimization to become feasible.

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Literature Cited

Adhya, N., M. Tawarmalani, and N. V. Sahinidis, "A Lagrangian Approach to the Pooling Problem," *Ind. Eng. Chem. Res*, **38** 1956 (1999).

Biegler, L. T., I. E. Grossmann, and A. W. Westerberg, *Systematic Methods of Chemical Process Design*, Prentice-Hall, NJ (1997).

Floudas, C. A., *Deterministic Global Optimization: Theory, Algorithms and Applications*, Kluwer Academic Publishers, Dordrecht, The Netherlands (2002).

Grimsditch, M., "Polymorphism in Amorphous SiO_2," *Phys. Rev. Lett.*, **52**, 2379 (1984).

Haverly, C. A., "Studies of the Behavior of Recursion for the Pooling Problem," *ACM SIGMAP Bull.*, **25**, 29 (1979).

Lacks, D. J., "Localized Mechanical Instabilities and Structural Transformations in Silica Glass under High Pressure," *Phys. Rev. Lett.*, **80** 5385 (1998).
Lacks, D. J., "First-Order Amorphous-Amorphous Transformation in Silica," *Phys. Rev. Lett.*, **84**, 4629 (2000).
Lacks, D. J., "Regressive Biological Evolution due to Environmental Change," *J. Theoretical Biology*, **209**, 487 (2001).
Wright, S., "The Roles of Mutation, Inbreeding, Crosslinking, and Selection in Evolution," *Proc. 6th Int. Cong. On Genetics*, **1**, 356 (1932). (Reprinted in: Wright, S., Evolution: Selected Papers, University of Chicago Press, Chicago (1986).)

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