

GEOMETRIC CONTROL THEORY AND CLASSICAL PROBLEMS IN CHEMICAL REACTOR DESIGN

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Abstract: A classical problem in chemical reactor design can be stated roughly in the following way: Given a network of chemical reactions and a specified feed, how should one design a chemical reactor to enhance the production of certain desired species while suppressing the production of undesired ones? The purpose of this article is to describe recent work in which geometric control theory provides sometimes surprising answers to classical reactor design questions. As an example it is shown that, associated with a given reaction network (with kinetics) and a given feed composition, there are certain exceptional numbers – something like eigenvalues – having special significance for reactor design: A classical steady-state CFSTR design can have an optimal conversion relative to all other steady-state designs only if the CFSTR residence time assumes one of those exceptional values. *Copyright © 2002 IFAC*

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1. INTRODUCTION

This article is intended to describe ways in which geometric control theory underlies some surprising recent results in the theory of chemical reactor design. It should be kept in mind that this article is written by a reactor theorist, not a control theorist, so there might be some naïvety here. Still, results that geometric control theory give for reactor design seem so striking that it might be interesting for control theorists to see how their work has had impact in another area. The connection to geometric control theory is discussed at greater length in (Feinberg, 2000a,b). These constitute the last two articles of a three part reactor design series that began with (Feinberg and Hildebrandt, 1997).

Expository articles by Kravaris and Kantor (1990a,b) and by Kravaris and Arkun (1991) have already been extremely helpful in bringing geometric control theory to chemical engineering. Moreover, important prior work by Palanki, Kravaris and Wang (1993, 1994) on optimal policies in batch reactor operation

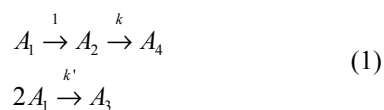
is close in spirit to (Feinberg, 2000b) but somewhat different in context and method. Whereas work by Palanki et al. is based largely on the Pontryagin maximum principle, the results in (Feinberg, 2000a,b) derive directly from a geometric control theory paper by Hermes (1974).

To describe, in a simple way, just how control theory naturally informs reactor design, it will be useful to focus on a very narrow and very old issue in reaction engineering: the suitability of the steady-state CFSTR as a reactor choice for producing an optimal yield. This will pave the way for remarks of a more general nature. For the sake of simplicity, attention is limited to incompressible mixtures and isothermal designs, but it will be clear how control-theoretic ideas enter the scene in a more general setting.

To set the stage, consider a chemistry of N species, A_1, A_2, \dots, A_N , among which might occur many coupled reactions. Suppose that the species formation rate function is $\mathbf{r}(\cdot): \mathbb{R}^N \rightarrow \mathbb{R}^N$. That is, $r_i(\mathbf{c})$ is the

local production rate per unit volume of A_1 , due to the occurrence of all chemical reactions, when the local vector of molar concentrations is $\mathbf{c} = [c_1, c_2, \dots, c_N]$.

Example: The well-studied van de Vusse reaction network taken with the mass-action rate constants



indicated, gives rise to the species formation rate function

$$\mathbf{r}(\mathbf{c}) := [-c_1 - 2k'c_1^2, c_1 - kc_2, k'c_1^2, kc_2]. \quad (2)$$

Now, in the general situation, suppose that a feed stream of composition $\mathbf{c}^{\text{in}} \in \mathbb{R}^N$ is available, and suppose that, as indicated broadly Fig. 1, the stream is passed to some reactor arrangement of unspecified (steady-state) design. The design-dependent effluent composition is denoted \mathbf{c}^{out} . The aim is to choose the reactor arrangement so that \mathbf{c}^{out} is optimal, in a sense to be discussed shortly. The candidate reactor arrangements are broad in scope and might, for example, consist of combinations of classical reactor types – plug flow reactors (PFRs), continuous flow stirred tank reactors (CFSTRs), or differential sidestream reactors (DSRs).

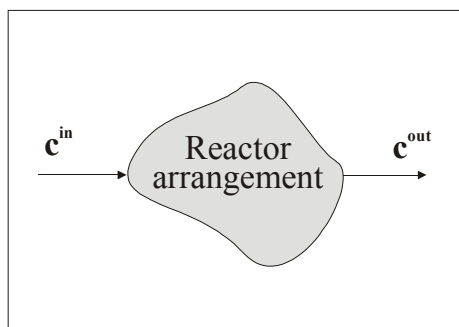


Fig. 1. Schematic of a general reactor configuration

Whatever the design, the relationship between \mathbf{c}^{out} and \mathbf{c}^{in} is constrained by stoichiometry. In fact, if S denotes the smallest linear subspace in \mathbb{R}^N that contains the range of $\mathbf{r}(\cdot)$, then \mathbf{c}^{out} must lie in the set

$$\mathbf{c}^{\text{in}} + S := \{ \mathbf{c}^{\text{in}} + \boldsymbol{\sigma} \in \mathbb{R}^N : \boldsymbol{\sigma} \in S \} \quad (3)$$

(In most instances, S will be the span of the reaction vectors for the underlying network of chemical reactions (Feinberg, 1987).)

A typical objective might be maximization of the effluent concentration of some valued species, say A_N . More generally, one might want to maximize the value of a linear objective function, say

$$\varphi(\mathbf{c}^{\text{out}}) := p_1 c_1^{\text{out}} + p_2 c_2^{\text{out}} + \dots + p_N c_N^{\text{out}}. \quad (4)$$

(Maximization of the effluent concentration of A_N corresponds to the special case $p_1 = p_2 = \dots = p_{N-1} = 0$,

$p_N = 1$.) Still more generally, one might want to maximize the value of some convex function of \mathbf{c}^{out} . In each of these cases, it is not difficult to see that, if the maximum is strict, then the maximizing \mathbf{c}^{out} cannot lie in an open set¹ in $\mathbf{c}^{\text{in}} + S$ consisting of compositions attainable from \mathbf{c}^{in} by steady-state reactor configurations, for then there would be an attainable composition nearby that does as least as well. That is, the maximizing \mathbf{c}^{out} must lie on the boundary of the set of compositions attainable from \mathbf{c}^{in} by steady-state designs.

The narrow question to be considered is this: What can be said, in concrete terms, about circumstances under which a *single classical CFSTR*, operating at steady state and with some judicious choice of residence time, might produce the optimal effluent relative to *all other* steady-state reactor arrangements? More precisely, *we ask about circumstances under which the effluent composition from a single steady-state CFSTR might lie on the boundary of the set of compositions in $\mathbf{c}^{\text{in}} + S$ attainable from \mathbf{c}^{in} by means of all conceivable steady-state reactor configurations.* (This is a *necessary* condition for the CFSTR-only design to provide a maximizing effluent relative to any of the objective functions described earlier.)

It will be argued here, from a control-theoretic viewpoint, that there are only certain exceptional, discrete residence times for which this necessary condition might be satisfied and that these exceptional residence times (if there are any at all) are computable from $\mathbf{r}(\cdot)$ and \mathbf{c}^{in} . (To make a rough analogy, the special residence times are something like eigenvalues.)

2. CRITICAL CFSTRs

Suppose that a perfectly mixed CFSTR with feed composition \mathbf{c}^{in} and residence time $\theta^* > 0$ gives rise to an effluent composition \mathbf{c}^* that lies on the boundary of the set of compositions attainable from \mathbf{c}^{in} by means of *all* steady-state designs (not necessarily CFSTR designs). The simple design under consid-

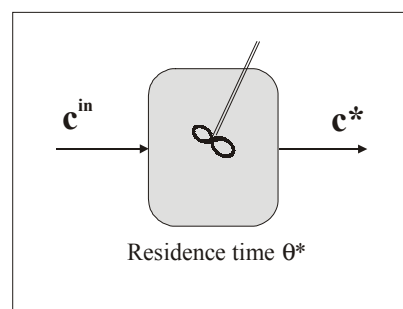


Fig. 2. A critical CFSTR

eration is depicted in Fig. 2. Note that \mathbf{c}^* and θ^* must together satisfy the steady-state CFSTR mole balance

¹ References to open sets, boundary, and interior are to be understood in the sense of the relative topology that $\mathbf{c}^{\text{in}} + S$ inherits from \mathbb{R}^N .

$$\mathbf{r}(\mathbf{c}^*) + \frac{1}{\theta^*} (\mathbf{c}^{\text{in}} - \mathbf{c}^*) = \mathbf{0}. \quad (5)$$

Now consider the arrangement shown in Fig. 3. There, the CFSTR depicted in Fig. 2 is followed by a steady-state differential sidestream reactor (DSR) in which the sidestream composition is \mathbf{c}^{in} . The local sidestream addition rate (volume of sidestream added per unit reactor volume) is denoted $\alpha(\tau)$, where τ denotes the local value of the DSR residence time. (This is the time that a particle entering the mouth of the reactor takes to reach the local axial position. See (Feinberg and Hildebrandt, 1997).)

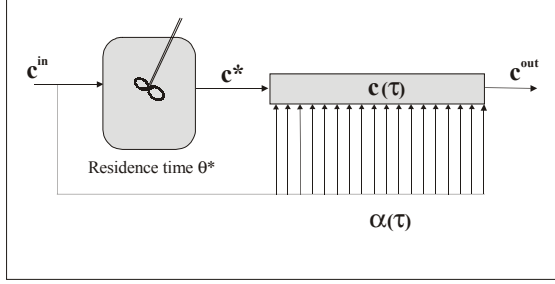


Fig. 3 . A CFSTR-DSR series

The differential equation governing the mixture composition in the DSR is

$$\dot{\mathbf{c}}(\tau) = \mathbf{r}(\mathbf{c}(\tau)) + \alpha(\tau)(\mathbf{c}^{\text{in}} - \mathbf{c}(\tau)) \quad (6)$$

subject to the initial condition

$$\mathbf{c}(0) = \mathbf{c}^*. \quad (7)$$

Here the overdot indicates differentiation with respect to τ . The sidestream addition rate policy is chosen by the designer.

Note that if $\alpha(\cdot)$ is chosen such that $\alpha(\tau) = 1/\theta^*$ for all $\tau \geq 0$, then eq. (5) implies that $\mathbf{c}(\tau) \equiv \mathbf{c}^*$ is a solution of eqs. (6)-(7). This is to say that the composition will remain unchanged along the DSR, and, in particular, that $\mathbf{c}^{\text{out}} = \mathbf{c}^*$.

Now consider small variations of the choice $\alpha(\tau) \equiv 1/\theta^*$, in particular those of the form

$$\alpha(\tau) \equiv \frac{1}{\theta^*} + \varepsilon(\tau), \quad (8)$$

where $\varepsilon(\cdot)$ takes small values. (At the very least, we require that $|\varepsilon(\cdot)| < 1/\theta^*$ so that $\alpha(\cdot)$ takes positive values in eq. (8).) If, by suitable manipulations of $\varepsilon(\cdot)$, it is possible to attain, at the DSR outlet, all compositions in a small open ball around \mathbf{c}^* , then \mathbf{c}^* could not lie on the boundary of all compositions attainable from \mathbf{c}^{in} (contrary to what had been supposed).

Thus, for \mathbf{c}^* (and θ^*) to be critical in the sense supposed, it is necessary that, with respect to the differential equation

$$\dot{\mathbf{c}} = \mathbf{r}(\mathbf{c}) + \frac{1}{\theta^*} (\mathbf{c}^{\text{in}} - \mathbf{c}) + \varepsilon(\tau) (\mathbf{c}^{\text{in}} - \mathbf{c}), \quad (9)$$

there are, in every (small) open ball around \mathbf{c}^* , compositions that cannot be accessed any choice of (small) $\varepsilon(\cdot)$. In control-theoretical terms, this is to say that eq. (9) should not be locally controllable from \mathbf{c}^* . For the given $\mathbf{r}(\cdot)$ and \mathbf{c}^{in} , the *denial* of local controllability will turn out to constrain \mathbf{c}^* (and θ^*) severely.

3. RESULTS DERIVED FROM A PAPER BY HERMES

(Hermes, 1974) contains deep controllability results that play a crucial role in both (Feinberg, 2000a) and (Feinberg, 2000b). These results subsume, but are not limited to, questions about controllability from a rest point of the uncontrolled differential equation. More broadly, the Hermes results address issues of controllability along a nontrivial trajectory of the uncontrolled equation. Although earlier results (from other authors) about controllability from a rest point would have sufficed to discuss critical CFSTRs, we cite the Hermes paper in particular because its wider scope has implications for broader questions about optimal reactor design. These are discussed briefly in Section 4 and, more generally, in (Feinberg, 2000a.)

To cast the critical CFSTR question into a standard control-theoretical form, let

$$\mathbf{f}(\mathbf{c}) := \mathbf{r}(\mathbf{c}) + \frac{1}{\theta^*} (\mathbf{c}^{\text{in}} - \mathbf{c}) \quad (10)$$

and

$$\mathbf{g}(\mathbf{c}) := \mathbf{c}^{\text{in}} - \mathbf{c}. \quad (11)$$

Then eq. (9) becomes

$$\dot{\mathbf{c}} = \mathbf{f}(\mathbf{c}) + \varepsilon(\tau) \mathbf{g}(\mathbf{c}). \quad (12)$$

Note that \mathbf{c}^* is a rest point of the uncontrolled equation $\dot{\mathbf{c}} = \mathbf{f}(\mathbf{c})$.

In this case we say that we say that eq. (12) is *locally controllable from \mathbf{c}^** if there is an open ball (in $\mathbf{c}^{\text{in}} + S$) with center at \mathbf{c}^* such that each point in that ball is, by means of a suitable choice of $\varepsilon(\cdot)$, reachable from \mathbf{c}^* along a solution of eq. (12).

Adapted to the situation at hand, the results in (Hermes, 1974) indicate that for eq. (12) *not* to be locally controllable from \mathbf{c}^* , it is necessary that the following condition be satisfied (Feinberg, 2000b):

$$\det[\mathbf{c}^* - \mathbf{c}^{\text{in}}, \mathbf{d}\mathbf{r}(\mathbf{c}^*)(\mathbf{c}^* - \mathbf{c}^{\text{in}}), (\mathbf{d}\mathbf{r}(\mathbf{c}^*))^2(\mathbf{c}^* - \mathbf{c}^{\text{in}}), \dots, (\mathbf{d}\mathbf{r}(\mathbf{c}^*))^{s-1}(\mathbf{c}^* - \mathbf{c}^{\text{in}}), \mathbf{m}_1, \mathbf{m}_2, \dots, \mathbf{m}_{N-s}] = 0 \quad (13)$$

Here $\mathbf{d}\mathbf{r}(\mathbf{c}^*)$ denotes the derivative of $\mathbf{r}(\cdot)$ at \mathbf{c}^* , $(\mathbf{d}\mathbf{r}(\mathbf{c}^*))^k$ is the k^{th} power of $\mathbf{d}\mathbf{r}(\mathbf{c}^*)$, s is the dimension of S , and $\{\mathbf{m}_1, \mathbf{m}_2, \dots, \mathbf{m}_{N-s}\}$ is any fixed linearly independent set of vectors orthogonal to S . (The particular choice of the \mathbf{m}_i is of no consequence. If

eq. (13) is satisfied for one such choice, it will be satisfied for all others.)

For reasons explained at the close of Section 2, eq. (13) becomes a necessary condition that \mathbf{c}^* must satisfy if it is to lie on the boundary of all compositions attainable from \mathbf{c}^{in} by means of steady-state designs.

Now let

$$\Delta(\mathbf{c}) := \det[\mathbf{c} - \mathbf{c}^{\text{in}}, \mathbf{d}\mathbf{r}(\mathbf{c})(\mathbf{c} - \mathbf{c}^{\text{in}}), (\mathbf{d}\mathbf{r}(\mathbf{c}))^2(\mathbf{c} - \mathbf{c}^{\text{in}}), \dots, (\mathbf{d}\mathbf{r}(\mathbf{c}))^{s-1}(\mathbf{c} - \mathbf{c}^{\text{in}}), \mathbf{m}_1, \mathbf{m}_2, \dots, \mathbf{m}_{N-s}]. \quad (14)$$

Loosely speaking, the scalar equation $\Delta(\mathbf{c}) = 0$ defines an $N - 1$ dimensional surface in \mathbb{R}^N_+ consisting of all compositions that might satisfy the non-controllability condition.

On the other hand, the vector equation

$$\mathbf{r}(\mathbf{c}) + \frac{1}{\theta}(\mathbf{c}^{\text{in}} - \mathbf{c}) = \mathbf{0} \quad (15)$$

describes the locus in \mathbb{R}^N_+ of compositions that might emerge from a CFSTR having feed composition \mathbf{c}^{in} . It is useful, though not always accurate, to think of that locus as a curve in \mathbb{R}^N_+ parameterized by θ .

Thus, the intersection of compositions that solve eq. (15) with those that solve $\Delta(\mathbf{c}) = 0$ is the set of all possible CFSTR effluent compositions that might be critical. That is, these are the **only** CFSTR effluent compositions that might lie on the boundary of the set of compositions attainable from \mathbf{c}^{in} by means of all possible steady state designs (not necessarily CFSTR designs).

The situation is depicted schematically in Fig. 4. The figure suggests just why, for given $\mathbf{r}(\cdot)$ and \mathbf{c}^{in} , there are (at most) certain exceptional residence times for which a CFSTR might produce an effluent composition that is optimal relative to the class of objective functions discussed earlier.

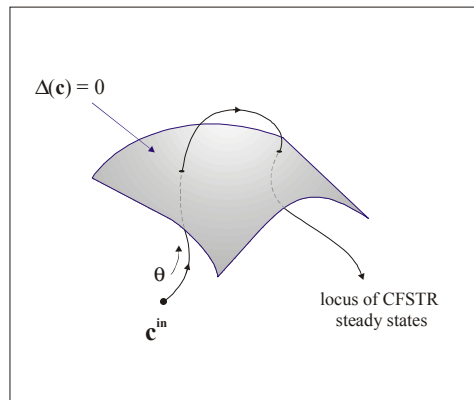


Fig. 4. The intersection of solutions of $\Delta(\mathbf{c}) = 0$ with the locus of CFSTR steady states.

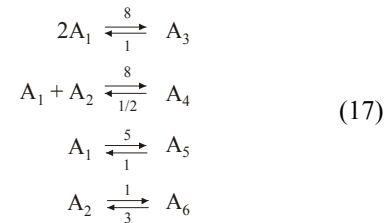
4. EXAMPLES

Detailed calculations for two examples – one analytic and one numerical – are given in (Feinberg, 2000b). Here we present only the results.

4.1. The van de Vusse Example. For the van de Vusse system (1) and for a feed composition $\mathbf{c}^{\text{in}} = [1, 0, 0, 0]$, it is necessary that a CFSTR residence time satisfy eq. (16) if it is to give rise to an effluent composition that respects eq. (13). That is, the CFSTR residence time must satisfy eq. (16) if its effluent composition is to lie on the boundary of all compositions attainable from \mathbf{c}^{in} by steady-state designs. Note that there is precisely one such (positive) residence time when $k < 2k'$ and no such (positive) residence time when $k > 2k'$. In the latter case, no single CFSTR operating at steady-state can produce an optimal effluent (relative to all other steady-state designs), so long as the objective function is in the class described earlier.

$$\theta^* = \frac{1 - \sqrt{\frac{k}{2k'}}}{k + \sqrt{\frac{k}{2k'}}}. \quad (16)$$

4.2. A more complex example. Consider the reaction network depicted in (17). The kinetics is mass-action



with rate constants as indicated. For a feed

$$\mathbf{c}^0 = [1/2, 1/2, 0, 0, 0, 0]$$

it turns out that there are precisely two positive CFSTR residence times for which eq. (13) is satisfied:

$$\theta^* = 0.1216 \quad \text{and} \quad \theta^* = 0.8252.$$

These are the “exceptional” residence times for which a single steady-state CFSTR design might produce an optimal effluent (relative to all other steady-state reactor designs) for the class of objective functions described earlier.

4. CRITICAL SIDESTREAM REACTORS

So far, attention has been restricted to conditions under which a single steady-state CFSTR might provide an effluent that is, with respect to certain objectives, optimal relative to all other steady-state reactor designs. The aim has been to show how control-theoretic ideas enter naturally in a simple situation. The picture becomes substantially more complex when similar questions are asked about differential

sidestream reactors (DSRs). In this case, geometric control theory enters in a stronger, more sophisticated way. For this reason, it will only be possible here to discuss critical DSRs briefly and to indicate the kind of results that geometric control theory gives. More extended discussions are available in Feinberg, 1999, 2000a)

Consider the (steady-state) design shown in Fig. 5. In the figure, $\bar{\alpha}(\cdot)$ indicates sidestream addition rate “law” – that is, a function of composition that tunes the volumetric sidestream addition rate (per unit reactor volume) to the local reactor composition. (The value of $\bar{\alpha}(\mathbf{c})$ is the local addition rate when the local reactor composition is \mathbf{c} .) The DSR is governed by the differential equation

$$\dot{\mathbf{c}} = \mathbf{r}(\mathbf{c}) + \bar{\alpha}(\mathbf{c})(\mathbf{c}^{\text{in}} - \mathbf{c}) \quad (18)$$

subject to the initial condition

$$\mathbf{c}(0) = \mathbf{c}^{\text{in}} \quad (19)$$

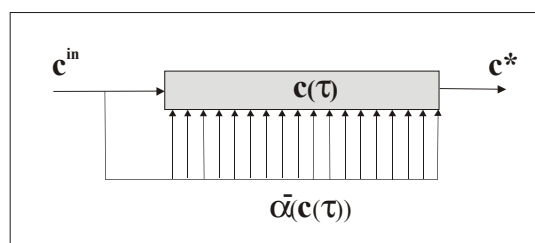


Fig. 5. A critical DSR

Now suppose that $\bar{\alpha}(\cdot) > 0$ is piecewise smooth and that it has been chosen to produce an effluent composition \mathbf{c}^* that lies on the boundary of all compositions attainable from \mathbf{c}^{in} by means of steady state reactor designs. Moreover, consider perturbed DSR sidestream addition rates governed by

$$\alpha(\tau) \equiv \bar{\alpha}(\mathbf{c}(\tau)) + \varepsilon(\tau), \quad (20)$$

where $\mathbf{c}(\tau)$ is the local composition (in the perturbed DSR) at residence time τ and where $\varepsilon(\cdot)$ takes small values. That is, addition rate distributions given by

$$\bar{\alpha}(\mathbf{c}) = \frac{2c_1^4 c_3^2 - 2c_1^3 c_2 c_3^2 - 4c_1^3 c_3^3 - 2c_1^3 c_3^2 c_4 + 2c_1^2 c_2 c_3^3 + 4c_1^2 c_2 c_3^2 c_4 + 2c_1^2 c_3^4 + 2c_1^2 c_3^3 c_4 - 4c_1^2 c_3^2 c_4^2 - 4c_1^3 c_3^2 + 10c_1^2 c_2 c_3^2 + 8c_1^2 c_3^3 - 6c_1^2 c_3^2 c_4 - 4c_1 c_2 c_3^3 - 8c_1 c_2 c_3^2 c_4 - 4c_1 c_3^4 - 4c_1 c_3^3 c_4 + 8c_1 c_3^2 c_4^2 + 2c_1^3 c_3 - c_1^3 c_4 + 2c_1^2 c_2 c_4 + 13c_1^2 c_3^2 - 11c_1^2 c_3 c_4 + 2c_1^2 c_4^2 - 2c_1 c_2^2 c_3 - c_1 c_2^2 c_4 - 6c_1 c_2 c_3^2 + 8c_1 c_2 c_3 c_4 - 2c_1 c_2 c_4^2 - 16c_1 c_3^3 - 11c_1 c_3^2 c_4 + 12c_1 c_3 c_4^2 - c_1 c_4^3 - c_2^2 c_3^2 - c_2^2 c_3 c_4 + 6c_2 c_3^3 + 10c_2 c_3^2 c_4 - c_3^4 - 5c_3^3 c_4 - 3c_3^2 c_4^2 + c_3 c_4^3 - 6c_1^2 c_3 + 3c_1^2 c_4 - 4c_1 c_2 c_4 - 18c_1 c_3^2 + 26c_1 c_3 c_4 - 4c_1 c_4^2 + 2c_2^2 c_3 + c_2^2 c_4 + 2c_2 c_3^2 - 4c_2 c_3 c_4 + 2c_2 c_4^2 + 8c_3^3 + 11c_3^2 c_4 - 8c_3 c_4^2 + c_4^3 + 8c_1 c_3 - 3c_1 c_4 + 2c_2 c_3 + 2c_2 c_4 + 9c_3^2 - 9c_3 c_4 + 2c_4^2 - 4c_3 + c_4}{4c_3(-c_1^2 c_3 + c_1^2 c_4 - c_1 c_2 c_3 - c_1 c_2 c_4 + c_1 c_3^2 + 2c_1 c_3 c_4 - c_1 c_4^2 + 2c_1 c_3 - 2c_1 c_4 + c_2 c_3 + c_2 c_4 - c_3^2 - 2c_3 c_4 + c_4^2 - c_3 + c_4)}$$

Fig. 6. A critical sidestream addition rate law.

eq. (20) are small perturbations of those one would get by adhering to the $\bar{\alpha}(\cdot)$ “law”. If every composition in a small ball around \mathbf{c}^* could be attained in a DSR from \mathbf{c}^{in} by means of a suitable $\varepsilon(\cdot)$ choice, then the original $\bar{\alpha}(\cdot)$ “law” could not have had the critical properties attributed to it.

This is to say that if $\bar{\alpha}(\cdot)$ is to be critical in the sense described, then it must be governed by controllability considerations. These can be formulated in the following way: Let $\mathbf{f}(\mathbf{c}) := \mathbf{r}(\mathbf{c}) + \bar{\alpha}(\mathbf{c})(\mathbf{c}^{\text{in}} - \mathbf{c})$ and $\mathbf{g}(\mathbf{c}) := \mathbf{c}^{\text{in}} - \mathbf{c}$. Then the differential equation

$$\dot{\mathbf{c}} = \mathbf{f}(\mathbf{c}) + \varepsilon(\tau) \mathbf{g}(\mathbf{c}) \quad (21)$$

should *not* be controllable along the trajectory given by eqs. (18) and (19). (Eq. (18) is just $\dot{\mathbf{c}} = \mathbf{f}(\mathbf{c})$.) Denial of controllability imposes strong constraints on the relationship that $\bar{\alpha}(\cdot)$ can bear to $\mathbf{r}(\cdot)$ and \mathbf{c}^{in} . These relationships are complex and again derive from results in (Hermes, 1974). Here it suffices to say that iterated Lie brackets of $\mathbf{r}(\cdot)$ and $\mathbf{g}(\cdot)$ play a prominent role. (See (Feinberg, 1999, 2000a) for more detail and for connections to earlier intuitive ideas (Glasser and Hildebrandt, 1990) about DSRs in three dimensions. See also (Palanki, et al, 1993,1994) for work in a different context but in a very similar spirit.)

An example from (Feinberg, 2000a) will provide the basis for some concluding remarks.

Example. Consider the reaction network (22) taken with mass-action kinetics. For the purpose of the



example, all rate constants are set to 1. For a DSR of the kind shown in Fig. 5, let $\mathbf{c}^{\text{in}} = [1,0,0,0,0]$. Theory in (Feinberg, 2000a) indicates that, for the effluent to be on the boundary of the set of all compositions attainable from \mathbf{c}^{in} via steady-state reactor designs, then the only possible piecewise smooth sidestream addition rate “law” is the one shown in Fig. 6.

Note that the sidestream addition rate law in the example is already quite complicated despite the relative simplicity of the chemistry. When the chemistry gets more complicated – in particular when the number of linearly independent reactions increases – not only does the complexity of the sidestream addition rate law increase dramatically, so do the control-theoretic equations from which the law derives. This results from the fact that, with increasing dimensions, higher order Lie brackets of $\mathbf{r}(\cdot)$ and $\mathbf{g}(\cdot)$ come into play. The increase in complexity becomes dramatically evident in (Feinberg, 2000a). To make matters worse, computations of higher order Lie brackets invoke increasingly higher order derivatives of $\mathbf{r}(\cdot)$. In view of the uncertainty associated with the kinetics of even moderately complex reaction systems and in view of the complexity of the resulting formulae, it is difficult to know if *practical* results about *exactly* optimal DSR sidestream addition rates can emerge.

5. CONCLUDING REMARK

Geometric control theory gives answers to *seemingly* simple classical problems in reactor design, problems that are not explicitly control-theoretical in character. It is not a fault of the theory that some answers turn out to be far more complex than might have been supposed. The complexity *is intrinsic to the problem at hand*, not to the powerful theory that reveals its solution. If it turns out that *approximately* optimal solutions are all that can be hoped for in a practical sense, then geometric control theory has the virtue of telling us what, in fact, is being approximated.

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