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CHEMICAL KINETICS AND CATASTROPHE THEORY

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Abstract

In this paper a continuous stirred tank reactor (CSTR) model of a first-order, exothermic reaction is examined and the existence of a cusp catastrophe is shown. Analytical solutions are developed for the ignition and quenching boundaries. The significance of the results and further extensions are discussed.

I. Introduction

This paper applies a recently developed mathematical theory--called "catastrophe theory"--to a classic engineering problem, analyzing the stability of a chemical reactor. In particular it treats in detail the case of a continuous flow, perfectly stirred tank reactor (CSTR) with a first-order, irreversible, exothermic chemical reaction. Building on the approach developed in Mehra and Blum [6], we

- demonstrate the application of catastrophe theory to an example typical of a large class of important problems;
- show that catastrophe theory can yield insight even in problems well studied by traditional techniques; and
- lay a foundation for treating more complex problems of interest in fire protection, energy policy, and industrial operation.

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In [6], basic results from catastrophe theory yielded a new criterion for determining the ignition point of flammable paper exposed to thermal radiation, one that improved the agreement of experimental results with previous data. More important conceptually, catastrophe theory showed that

(1) Ignition can be analyzed and explained in terms of equilibrium properties, even though it is usually regarded only as a transient or dynamic phenomenon, and

(2) In analyzing stability behavior such as ignition, primary attention should be paid to the control variables, although one customarily focusses on the state variables (such as composition or temperature) that manifest the instability.

This paper extends this investigation to physical situations described by two or more control variables. A well studied example has been chosen as a base case to simplify the conventional aspects of the analysis and illuminate key points in the method and to provide a basis for comparison and calibration against well tested analyses and computations.

At least since 1953, it has been well known that exothermic chemical reactions, influenced by heat transfer, mass transfer, or both, can exhibit multiple equilibria and bifurcation points (see [1,2,3,4,8]). Indeed, these phenomena have been the subject of so many theoretical and experimental studies that we could not even begin to review the published literature here. What is important to note is that, despite the volume of work, much involving quite sophisticated mathematical techniques, an aspect important for policy--the effects on global stability of simultaneously varying two or more control parameters--appears to remain essentially untouched. And it is to this subject, the stability impacts of multiple control variables, that catastrophe theory is inherently addressed.

An introduction to catastrophe theory is developed in [6]. Suffice it to note here that, based upon the topological properties of flow manifolds, the theory provides a complete classification of all possible "catastrophes" (jump discontinuities between multiple values) for up to five control parameters and a less complete but potentially useful classification in yet higher dimensions.[1] Moreover, it provides this classification, and further insight into system behavior without having to integrate the describing differential equations or to contend with (possibly) large numbers of state variables. Only the equilibrium equations are needed, and the number of control variables is the dimensionality that plays a major role.

The example considered is one of the simplest, realistic chemical reactor models that displays interesting instability. It affords an analytical expression for the catastrophe surface, which exhibits a cusp catastrophe in the control space of residence time versus feed (or coolant) temperature.

II. Chemical Reactor Model

The basic model analyzed represents a continuous flow, perfectly stirred tank reactor (CSTR) in which occurs a first-order, irreversible, exothermic chemical reaction $A \rightarrow B$. Figure 1 depicts the physical situation and explains the nomenclature.

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[1] For six or more control variables, the number of elementary catastrophes is infinite. A finite classification for more than six variables may be obtained under topological, rather than diffeomorphic, equivalence.

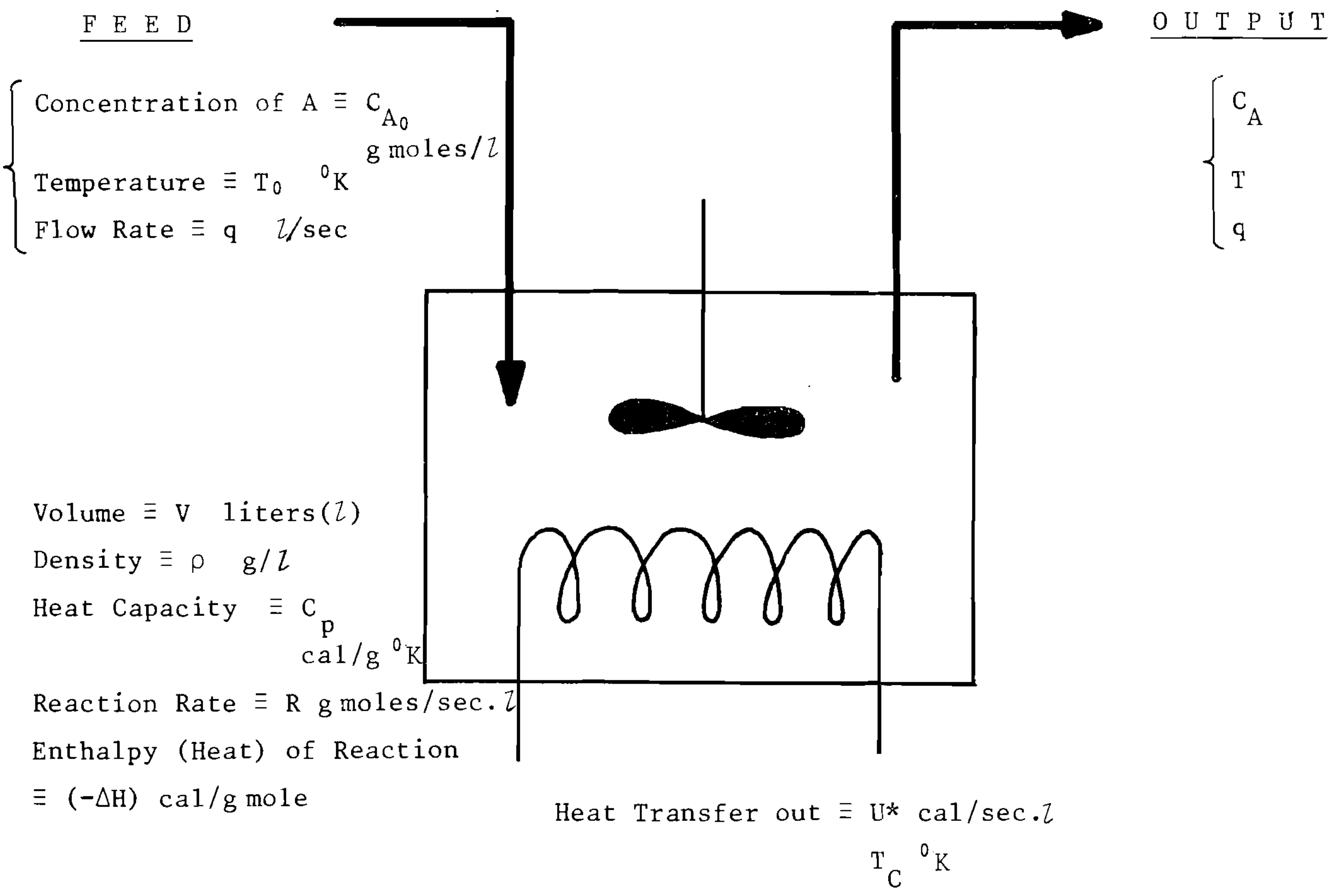

Figure 1. CSTR with heat transfer.

When the flow rate and volume are constant, the system equations become [1]:

<u>Mass Balance</u>:

$$V\frac{dC_A}{dt} = q(C_{A_0} - C_A) - VR \quad . \tag{1}$$

<u>Energy Balance</u>:

$$\rho C_p V\frac{dT}{dt} = \rho C_p q(T_0 - T) - VU^* + (-\Delta H)RV \quad . \tag{2}$$

Note that if all the reactant A_0 in the feed were to react adiabatically, the total heat released (H_M) would be

$$H_M = (-\Delta H)C_{A_0} \quad . \tag{3}$$

Thus, the maximum temperature rise attainable is

$$\Delta T_M = \frac{(-\Delta H)C_{A_0}}{\rho C_p} \quad , \tag{4}$$

and the fraction of the maximum temperature rise actually attained

$$\frac{\Delta T}{\Delta T_M} \equiv \frac{T - T_0}{T_M - T_O} = \frac{\rho C_p}{(-\Delta H)C_{A_0}}(T - T_0) \equiv \eta - \eta_0 \quad , \tag{5}$$

where η and η_0 are dimensionless temperatures. With this definition, the maximum dimensionless temperature attainable is simply

$$\eta_M = \eta_0 + 1 \quad . \tag{6}$$

Now multiply equation (2) through by $\rho C_p/[(-\Delta H)C_{A_0}q]$ and divide equation (1) through by (qC_{A_0}). Define the additional dimensionless variables

$$\xi \equiv C_A/C_{A_0} \qquad U \equiv VU^*/[(-\Delta H)qC_{A_0}) = U^*/[H_M/\theta]$$

$$\theta \equiv V/q \qquad P \equiv VR/qC_{A_0} = \theta R/C_{A_0}$$

$$\tau \equiv t/\theta \quad .$$

Then the system equations become, respectively,

$$\frac{d\xi}{d\tau} = (1-\xi) - P(\xi,\eta) \quad , \tag{7}$$

and

$$\frac{d\eta}{d\tau} = (\eta_0 - \eta) - U(\eta) + P(\xi,\eta) \quad . \tag{8}$$

If the reaction is first-order and irreversible, then

$$P(\xi,\eta) = (\theta/C_{A_0}) \cdot [A \exp(-E/rT)]C_A \text{ [2]}$$

$$\equiv (A\theta)\xi \exp(-\alpha/\eta) \quad , \tag{9}$$

where

$$\alpha \equiv \frac{E}{r(\Delta T_M)} \quad . \tag{10}$$

The simplest realistic heat transfer (cooling) function is $U(\eta) = U_S(\eta - \eta_C)$, simple convective cooling with water, say, at a constant flow rate and temperature η_C. If one wanted to impose control, to operate the system at a naturally unstable point, one could add proportional flow control with bounded magnitude, e.g.,

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[2] In this Arrhenius expression for the reaction rate, E, is the activation energy and r (usually R) is the gas constant, $r = 1.9872$ cal/g mole^{0}K.

$$U(\eta) = \begin{cases} U_M(\eta - \eta_C) & \eta > \eta^+ \\ [U_S + K(\eta - \eta_S)](\eta - \eta_C) & \eta^+ \geq \eta \geq \eta_- \\ 0 & \eta < \eta_- \end{cases} \quad . \tag{11}$$

Here η_S is an equilibrium temperature (achieved with $K = 0$) about which the system is to be controlled and

$$\eta^+ \equiv \eta_S + (U_M - U_S)/K$$

$$\eta_- \equiv \eta_S - U_S/K \quad .$$

In this model, there are two state variables--η and ξ--and four nominal control parameters: η_C, η_0, K, and θ. Physically, the first three control parameters have the same kind of effect, i.e., to vary the net influx of thermal energy; indeed the effects of η_C and η_0 are essentially identical, as we shall see below. The residence time θ, controlled by varying the flow rate q, has a different physical effect--to give the reaction time to take place. The next section examines the effects of varying energy flux--residence time pairs on the stability properties of equations (7) and (8).

III. Application of Catastrophe Theory

In catastrophe theory (see [7,9,10,11,12]) it is assumed that the control parameters vary slowly compared to the motion of the state variables, so that one may consider the system as moving from one equilibrium point to another. At an equilibrium point (ξ^*, η^*)

$$\frac{d\xi^*}{d\tau} = 0 \quad \text{and} \quad \frac{d\eta^*}{d\tau} = 0 \quad . \tag{12}$$

With (9), equation (7) then yields

$$\xi^* = \frac{1}{1 + A\theta e^{-\alpha/\eta^*}} \quad , \tag{13}$$

which when substituted into (8) gives the equation for the equilibrium surface

$$f(\eta^*,\eta_0,\eta_C,\theta,K) = (\eta^* - \eta_0) + U_S(\eta^* - \eta_C) + K(\eta^* - \eta_C)(\eta^* - \eta_S) - \frac{A\theta e^{-\alpha/\eta^*}}{1 + A\theta e^{-\alpha/\eta^*}} = 0 \quad , \tag{14}$$

with appropriate modifications in the control portion for $\eta > \eta^+$ and $\eta < \eta^-$.

Equation (14) is of fundamental importance in studying the equilibrium manifold in the (η^*,η_0,θ) space or (η^*,η_C,θ) space. In particular, we are interested in the locus of points in (η_0,θ) space at which there are catastrophic changes in η^*. The main theorem of catastrophe theory [7] tells us that, in general, this locus is a cusp, the interior of which corresponds to unstable equilibria. At catastrophe points, the differential equation $\frac{d\eta}{d\tau} = f(\eta,\eta_0,\theta)$ changes from a locally stable equation to a locally unstable equation. Thus $\frac{\partial f}{\partial \eta^*}$ changes sign and passes through zero value at the catastrophe points. The equations of the catastrophe locus are thus $f = 0$ and $\frac{\partial f}{\partial \eta^*} = 0$, i.e., equation (14) and equation (15) below

$$\frac{\partial f}{\partial \eta^*} = (1 + U_S) + K(2\eta^* - \eta_C - \eta_S) - \frac{\alpha(A\theta e^{-\alpha/\eta^*})}{(\eta^*)^2\left(1 + A\theta e^{-\alpha/\eta^*}\right)^2} = 0 \quad , \tag{15}$$

for $\eta^+ > \eta^* > \eta_-$. ($U(\eta)$ has a step function in the derivative at $\eta^* = \eta_-$ and $\eta^* = \eta^+$.)

We can now vary η^* as a parameter in equations (14) and (15) and solve (15) for θ and (14) for η_0 or η_C, keeping all other quantities constant. This procedure yields explicit equations for the catastrophe locus--which, in this case, we know a priori must be a cusp. Alternatively, we can eliminate θ by merging (14) and (15), obtain an analytical solution for the values of η^* at which catastrophes (jumps) occur, and use this solution to obtain an analytical expression for the cusp. To illustrate the procedure most clearly, let us focus for now on the case $K = 0$, i.e., the reactor with simple cooling.

IV. Analytical Solution

For $K = 0$, equations (14) and (15) become

$$(\eta^* - \eta_0) + U_S(\eta^* - \eta_C) = \frac{Y}{1 + Y} \quad , \tag{14a}$$

$$(1 + U_S) = \frac{\alpha}{(\eta^*)^2} \frac{Y}{(1 + Y)^2} \quad , \tag{15a}$$

where for convenience we have defined

$$Y \equiv (Ae^{-\alpha/\eta^*})\theta \quad . \tag{16a}$$

Let us also define a combined thermal control variable

$$\eta_1 \equiv \eta_0 + U_S\eta_C \quad ; \tag{16b}$$

η_1 and θ form the two dimensions of our control space. We can solve equations (14a) and (15a) analytically, thus obtaining

- an explicit analytical form for the boundaries in control space of the region within which multiple equilibria occur, and
- analytical criteria for ignition and quenching (extinction), important phenomena as yet incompletely understood.

Dividing (14a) by (15a) yields

$$Y = \frac{\alpha}{\eta^*} - \frac{\eta_1\alpha}{(1 + U_S)(\eta^*)^2} - 1 \quad , \tag{17a}$$

or

$$\Theta = \left[\frac{\alpha}{\eta^*} - \frac{\eta_1}{(1 + U_S)\alpha}\left(\frac{\alpha}{\eta^*}\right)^2 - 1\right] A^{-1} \exp\left(\frac{\alpha}{\eta^*}\right) \quad . \tag{17b}$$

Let us now solve for η^*. Since $1/(1 + Y) = 1 - Y/(1 + Y)$, we have from (14a)

$$\frac{Y}{(1 + Y)^2} = \left[\eta^*(1 + U_S) - \eta_1\right]\left[1 + \eta_1 - \eta^*(1 + U_S)\right] = \left(\frac{1 + U_S}{\alpha}\right)(\eta^*)^2 \quad , \tag{18}$$

which yields the quadratic equation

$$[1 + \alpha(1 + U_S)](\eta^*)^2 - \alpha(1 + 2\eta_1)\eta^* + \alpha\eta_1(1 + \eta_1)/(1 + U_S) = 0 \quad . \tag{18a}$$

The solution yields the two equilibrium temperatures along the catastrophe locus:

Ignition Temperature = η^*_-
Quenching Temperature = η^*_+,

where the subscripts indicate the sign before the square root in

$$\eta^*_{\pm} = \frac{\alpha}{2[1 + \alpha(1 + U_S)]}\left[(1 + 2\eta_1) \pm \left(1 - \frac{4\eta_1(1 + \eta_1)}{\alpha(1 + U_S)}\right)^{\frac{1}{2}}\right] \quad . \tag{19}$$

A necessary condition for multiple equilibria is thus

$$\alpha(1 + U_S) \geq 4\eta_1(1 + \eta_1) \quad . \tag{20}$$

Since $Y/(1+Y)^2 \leq 1/4$, we also have from (15a)

$$\eta^* \leq \tfrac{1}{2}\sqrt{\alpha/(1+U_S)} \tag{21}$$

for equilibrium temperatures along the catastrophe locus. Together, (20) and (21) characterize the surface near the tip of the cusp's tail.

Having solved for η^*, we can readily obtain through (17b) the projection $\theta(\eta_1)$ of the catastrophe locus on the θ,η_1 control plane.

From (18a), the product of the roots

$$\eta^*_- \eta^*_+ = \alpha\eta_1(1+\eta_1)/[(1+U_S)(1+\alpha(1+U_S))] \quad , \tag{22}$$

so that

$$\frac{\alpha}{\eta^*_-} = \frac{\alpha(1+U_S)}{2\eta_1(1+\eta_1)}\left[1 + 2\eta_1 + \left(1 - \frac{4\eta_1(1+\eta_1)}{\alpha(1+U_S)}\right)^{\frac{1}{2}}\right] \quad ; \tag{23}$$

α/η^*_+ is the same except with a minus sign before the square root.

The form of (23) invites the approximation

$$(1 - X)^{\frac{1}{2}} \approx 1 - \tfrac{1}{2}CX \quad , \tag{24}$$

where $C \approx 1$ if X is small compared to 1 and $C \approx 1.069 + 0.287X$ (derived from a four-term Chebyshev polynomial fit to the usual power series expansion of the square root) approximates the function well for $X < 0.8$.[3] Using this approximation (23)

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[3] Alternatively, one can use the exact C for the middle of the range of interest. At X = 0.64, for example, C = 1.25; with this value (24) holds to within 3.2% at X = 0.40 and 6.2% at X = 0.75.

simplifies to

$$\frac{\alpha}{\eta^*_-} \cong \frac{\alpha(1 + U_S)}{\eta_1} - C \tag{25a}$$

$$\frac{\alpha}{\eta^*_+} \cong \frac{\alpha(1 + U_S)}{1 + \eta_1} + C \quad , \tag{25b}$$

which yield the approximations

$$\eta^*_- \cong \frac{\alpha\eta_1}{\alpha(1 + U_S) - C\eta_1} \cong \frac{\eta_1}{(1 + U_S)}\left[1 + \frac{C\eta_1}{\alpha(1 + U_S)}\right] \tag{26a}$$

$$\eta^*_+ \cong \frac{\alpha(1 + \eta_1)}{\alpha(1 + U_S) + C(\eta_1 + 1)} \cong \frac{(\eta_1 + 1)}{(1 + U_S)}\left[1 - \frac{C(\eta_1 + 1)}{\alpha(1 + U_S)}\right] . \tag{26b}$$

More clearly than (19), these approximate forms reveal how the ignition and quenching temperatures vary with the major parameters on regions of the equilibrium surface.

Finally, substituting (23) into (17b) gives, after rearranging and collecting terms,

$$\theta_{\pm} = \left(\frac{\eta_1}{1 + \eta_1}\right)\left[\frac{\alpha(1 + U_S)}{2\eta_1(1 + \eta_1)}\left(1 \pm \sqrt{1 - \frac{4\eta_1(1 + \eta_1)}{\alpha(1 + U_S)}}\right) - 1\right]A^{-1}\exp\left(\frac{\alpha}{\eta^*_{\pm}}\right) , \tag{27}$$

where $\theta_+(\eta_1)$--the quenching locus -- takes the plus sign before the square root and η^*_+, and $\theta_-(\eta_1)$--the ignition locus--takes the minus sign and η^*_-. The exponential's argument is equation (23), with the appropriate sign before the square root. If we define the function

$$Q(\eta_1) \equiv \frac{\alpha(1 + U_S)}{4\eta_1(1 + \eta_1)} \quad , \tag{28}$$

then the cusp equations can be written more compactly as

Ignition Boundary:

$$\theta_-(\eta_1) = \left(\frac{\eta_1}{1 + \eta_1}\right)[2Q(1 - \sqrt{1 - 1/Q}) - 1]A^{-1} \exp [2Q(1 + 2\eta_1 + \sqrt{1 - 1/Q})] \; . \tag{27a}$$

Quenching Boundary:

$$\theta_+(\eta_1) = \left(\frac{\eta_1}{1 + \eta_1}\right)[2Q(1 + \sqrt{1 - 1/Q}) - 1]A^{-1} \exp [2Q(1 + 2\eta_1 - \sqrt{1 - 1/Q})] \; . \tag{27b}$$

IV. Numerical Results

Figure 2 displays the catastrophe surface--$f(\eta_1, \theta, \eta^*) = 0$ --computed from equation (14) with $K = 0$, $A = \exp(25)$, $U_s = 1$ and $\alpha = 50$. Catastophe theory shows that all potentially unstable systems having two principal control dimensions and one free state dimension must manifest a surface of this general type. Moreover, it shows that the catastrophe locus for systems of this kind must be a cusp.[4]

Figure 2 emphasizes the structure of the catastrophe surface for small θ (flow residence times). Specifically, the coordinates of the surface's "corners," written as they

[4] Though for some systems, where no control variable imposes a limit on behavior (as low θ, which does not permit enough reaction to occur to generate instability, does here), the cusp may degenerate into a simple fold catastrophe locus, of the type considered in [6].

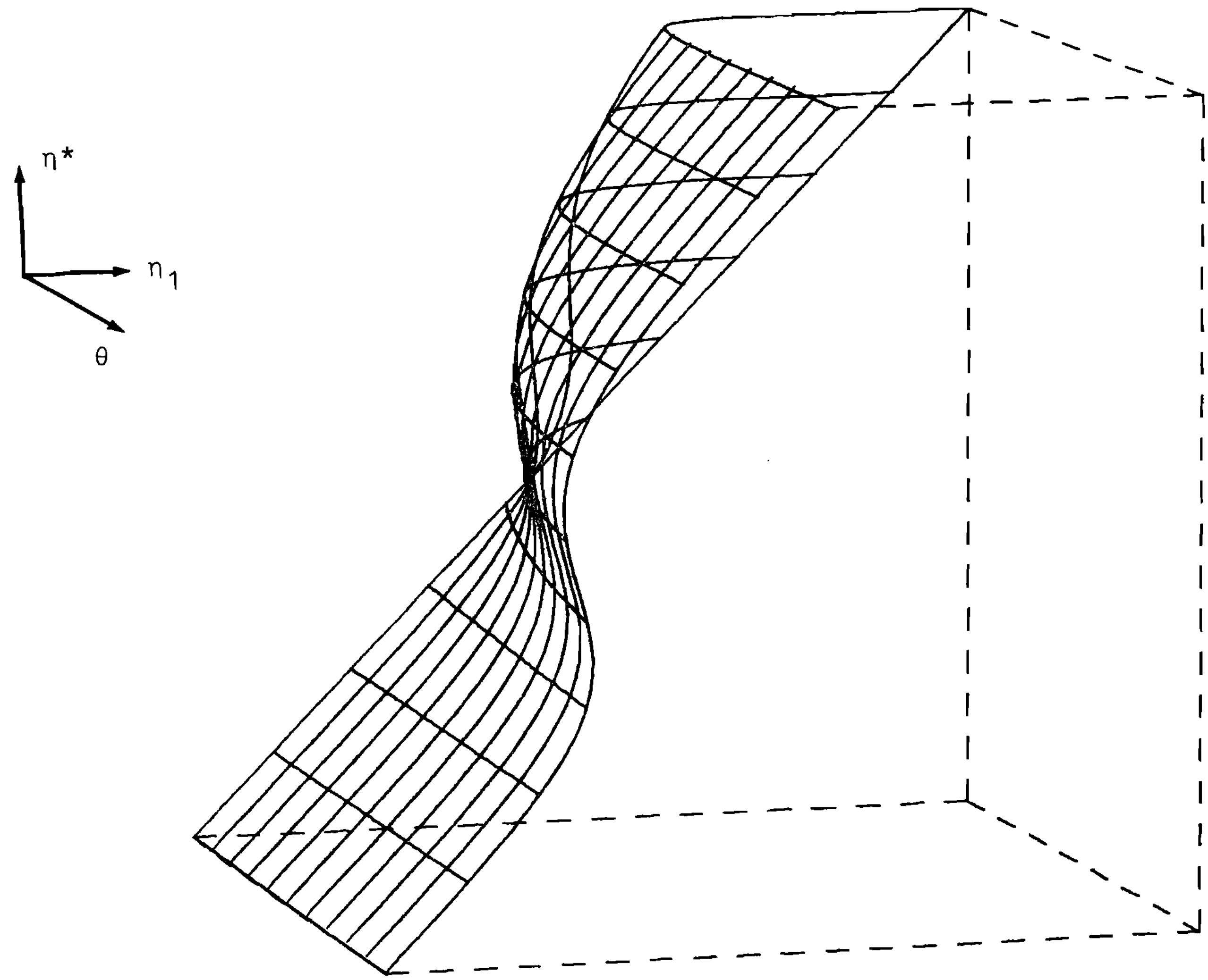

Figure 2. Catastrophe surface for perfectly stirred, continuous flow tank reactor with first-order, irreversible exothermic chemical reaction.

appear in Figure 2, are

$\theta = 0$
$\eta_1 = 5.6$
$\eta^* = 2.8$

$\theta = 0.1$
$\eta_1 = 4.6078$
$\eta^* = 2.8$

$\theta = 0$
$\eta_1 = 3.4$
$\eta^* = 1.7$

$\theta = 0$
$\eta_1 = 3.3988$
$\eta^* = 1.7$

Here the surface is depicted using a perspective transformation, with viewing elevation 8° and rotation 75°.

Figure 3A displays the same surface, showing below it the projection of the multiple equilibrium region, computed directly from the surface by numerical differentiation. The same surface and cusp are shown from a different viewing angle (elevation 30°, rotation 290°) in Figure 3B.

Figure 4A displays the cusp $\theta\ (\eta_1)$, computed from equations (27a) and (27b), for $\alpha(1+U_S) = 100$, $A = \exp(25)$. Figure 4B plots the same curve in terms of $\log\theta$ versus η_1, which reduces the curvature and lets us examine the tip of the cusp's tail.

Analytically, the equations show that the cusp terminates at an end-point $(\eta_1^E, \theta_E, \eta_E^*)$ given by

$$\eta_1^E = \tfrac{1}{2}(\sqrt{1 + \alpha(1 + U_S)} - 1)$$

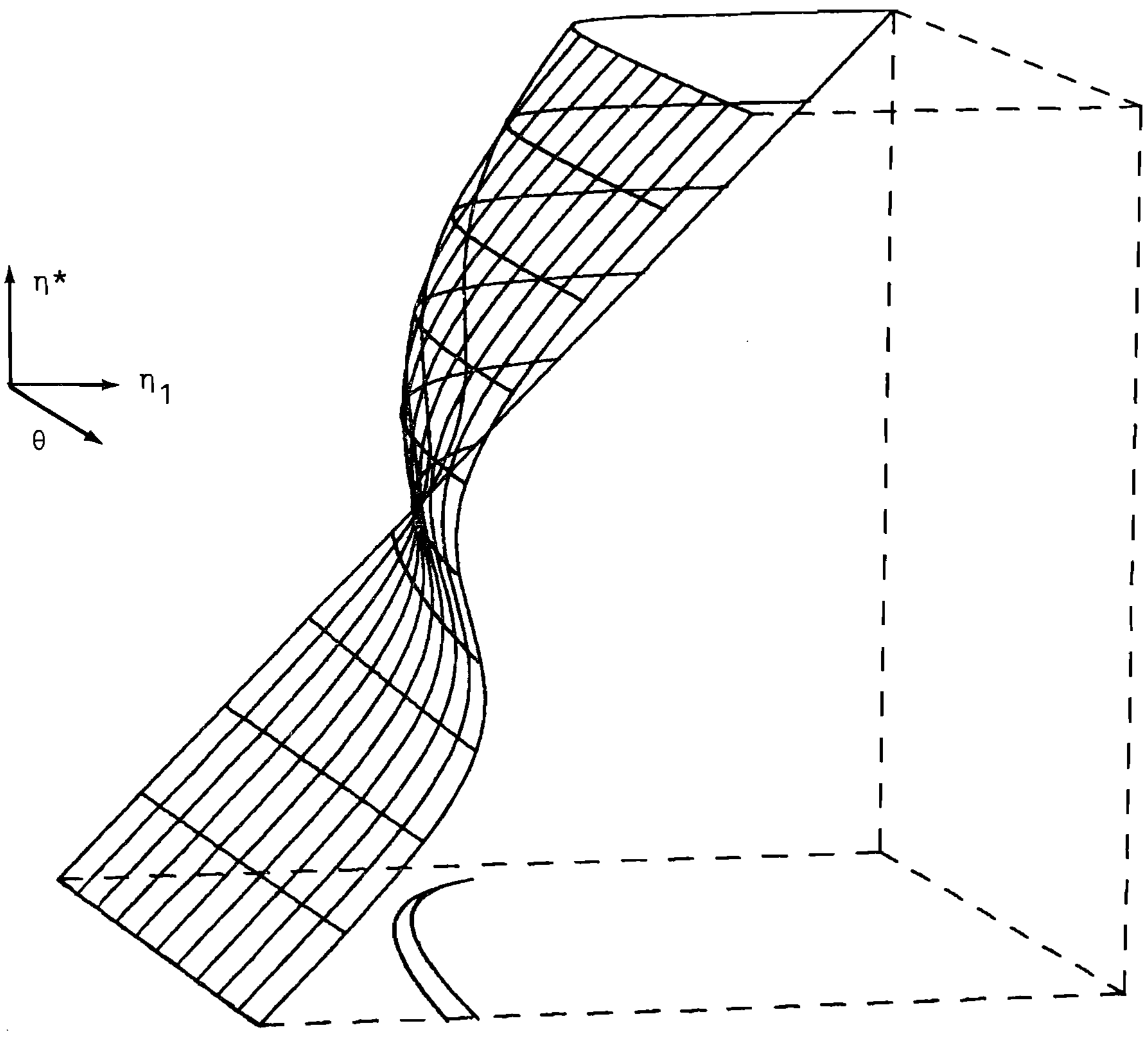

Figure 3A. Catastrophe surface with projection of multiple equilibrium region: view in the direction of decreasing residence time.

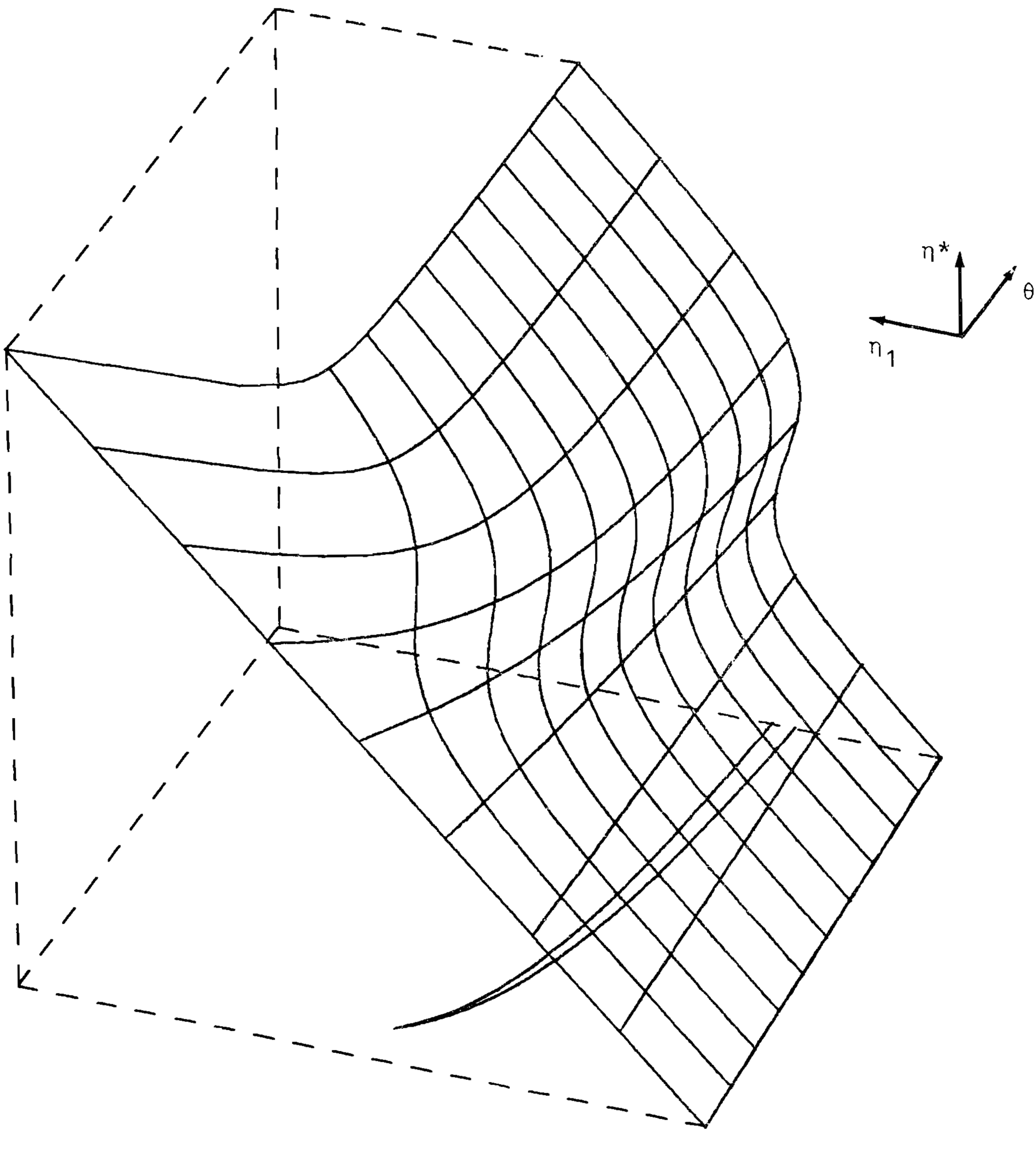

Figure 3B. Catastrophe surface with projection of multiple equilibrium region: view in the direction of increasing residence time.

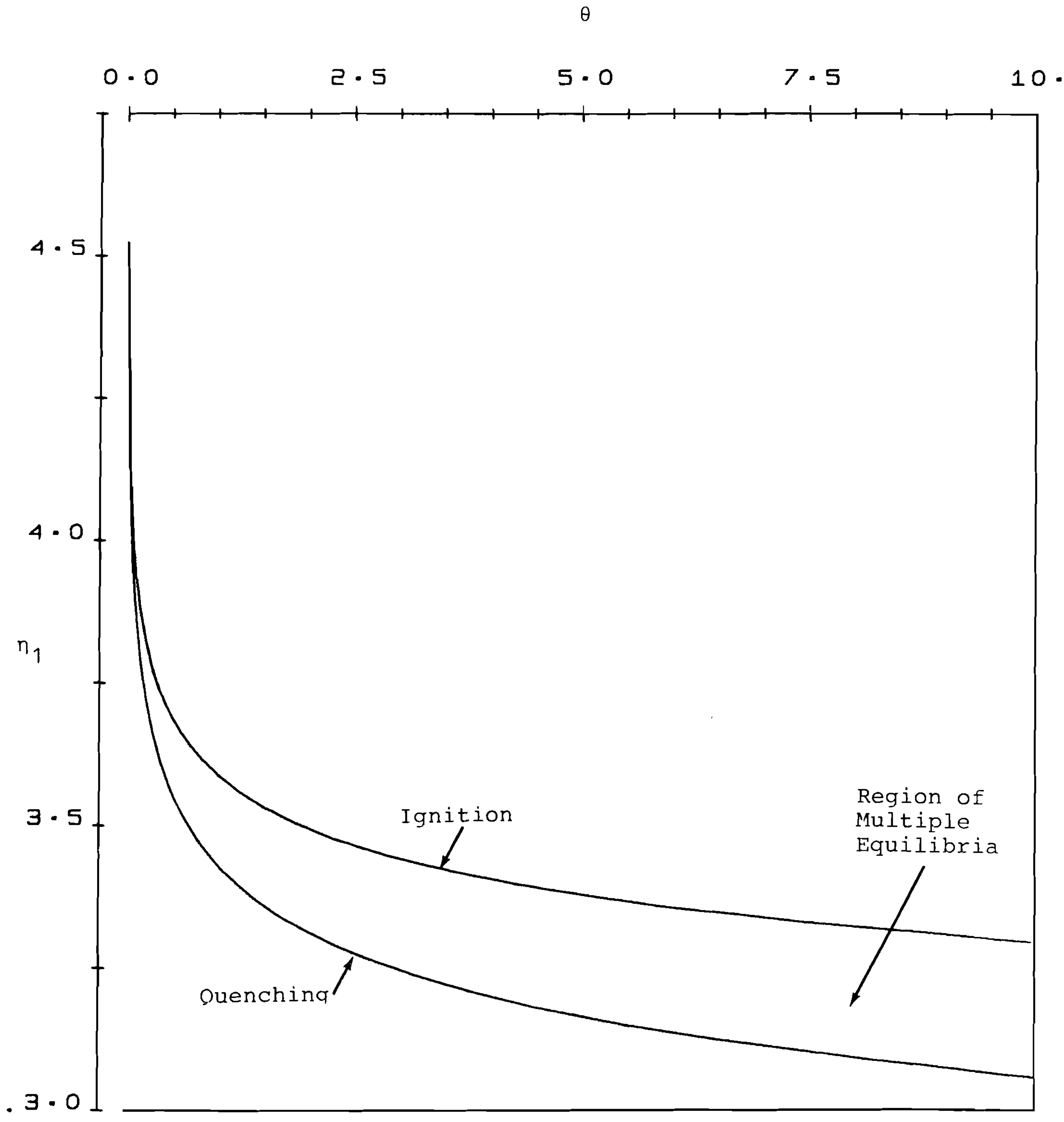

Figure 4A. Cusp catastrophe locus.

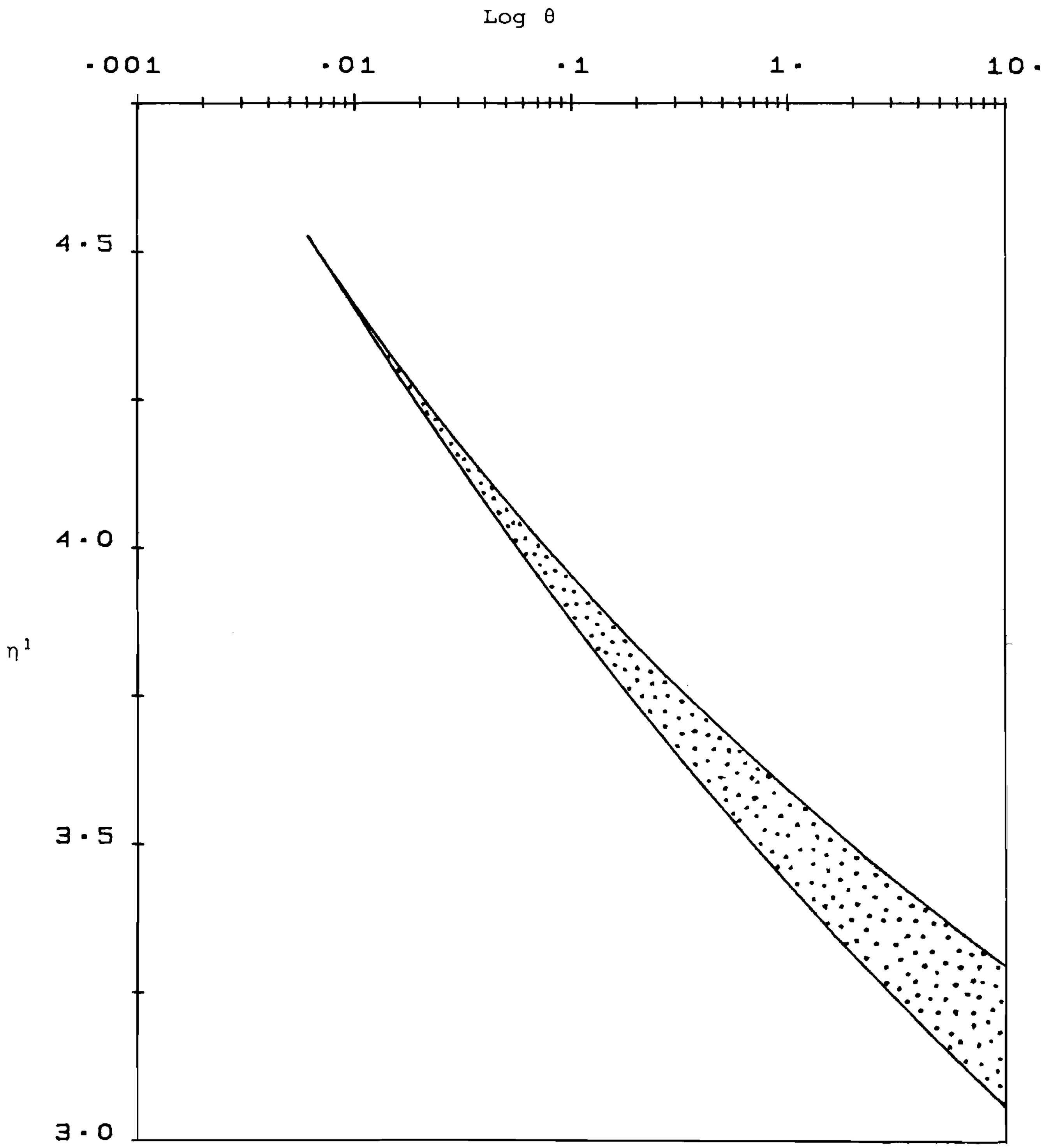

Figure 4B. Cusp catastrophe locus (logarithmic plot).

$$\theta_E = \left(\frac{\sqrt{1 + \alpha(1 + U_S)} - 1}{\sqrt{1 + \alpha(1 + U_S)} + 1} \right) A^{-1} \exp(2\sqrt{1 + \alpha(1 + U_S)})$$

$$\eta_E^* = \frac{\alpha}{2\sqrt{1 + \alpha(1 + U_S)}} \quad .$$

In Figures 2-5, this point is

$$\eta_1^E \cong 4.52494$$

$$\theta_E \cong 6.09725 \times 10^{-3}$$

$$\eta_E^* \cong 2.48759 \quad .$$

In the terminology of catastrophe theory (see [7,9,10,11]), θ is thus a "splitting factor." In physical terms, high flow rates (low θ) "blow out" the reaction, much as one blows out a flame; the reactants are out and away before the reaction can become self-sustaining. That there must exist small values of θ for which there is only one steady-state solution (e.g., one value of η^*) has been proved in general for CSTR's [3, p. 36]. (Gavalas' corresponding result, that the steady state must also become unique for sufficiently large values of θ, does not apply to this model, since an irreversible reaction has no unique stable state except $\xi \to 0$ as $\theta \to \infty$.)

Let us briefly examine Figures 2-4. First, note that the interior of the cusp fully defines the region within which multiple steady states--and hence jumps between them--can occur. For any values of η_1, multiple equilibria can occur if and only if $\theta_+ \leqslant \theta \leqslant \theta_-$. For $\theta < \theta_+$, only low temperature equilibria are possible, and for $\theta > \theta_-$, only high temperature equilibria occur. This behavior is depicted in another fashion in Figure 5, which shows slices through the catastrophe surface at selected values of θ, plotting η^* vs. η_1. The middle part of the fold

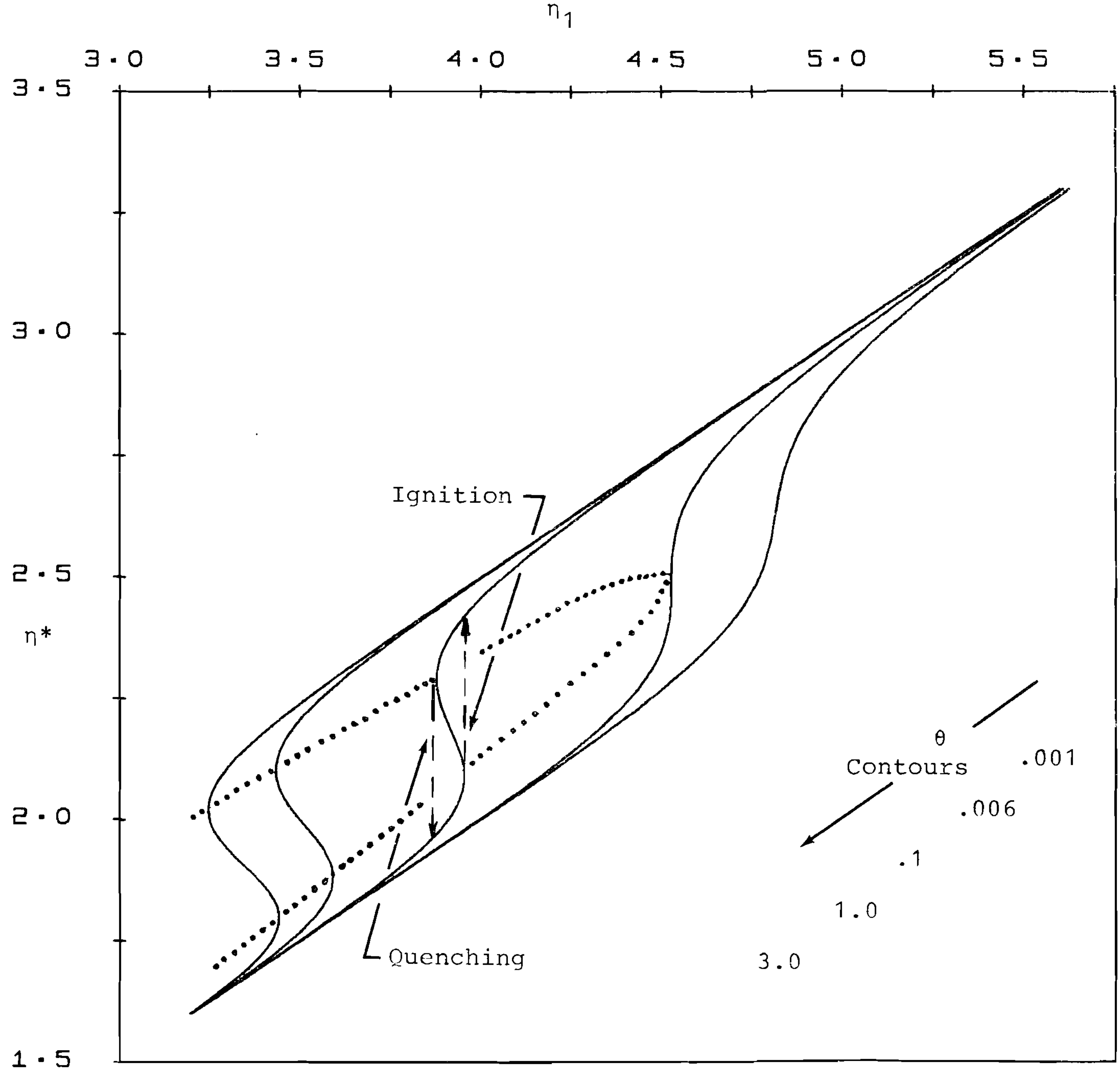

Figure 5. System behavior with multiple equilibria.

curve consists of unstable equilibria. The catastrophic jumps occur at the points where $\frac{\partial f}{\partial \eta^*}$ vanishes; these are also the points $\eta^*(\eta_1)$ given by equation (19), which is superimposed. At the upper extreme, all the curves converge to the line $\eta_1=(1+U_s)\eta^*-1$; the lower asymptote is $\eta_1=(1+U_s)\eta^*$.

Figures 2-5 show how the system behaves as the control parameters are varied. As we know, the right arm of the cusp corresponds to "ignition" or accelerating of the reaction and the left arm corresponds to "quenching" or sudden slowing of the reaction. There is an increase in temperature η^* and a decrease in the reactant concentration variable ξ^* on the ignition boundary. For example, if θ is kept fixed at 1 and η_1 is varied, the reaction will start at η_1 = 3.59 and the temperature will jump from 1.88 to 2.27. Similarly for θ = .5, the temperature suddenly increases from 1.93 to 2.26 at η_1=3.68 and suddenly decreases from 2.15 to 1.8 at η_1=3.55. Notice that for large values of η_1, the cusp is very narrow so that a small change in θ can cause the reaction to accelerate or to quench. Further uses of Figures 2-5 will be discussed in the next section.

V. Discussion of Results and Extensions

In addition to revealing interesting qualitative properties of the reaction mechanism, Figures 2 to 5 also have potential operational value. One may, for example, consider strategies for a chemical reactor in which both θ and η_1 are varied simultaneously. Figures 2-5 (and the equations they depict) may then be used to come up with effective policies. A number of design and control questions may also be studied in terms of cusps similar to Figures 3 and 4.

In considering the control of fires, for example, optimal strategies for quenching may be studied using similar catastrophe analysis--with the more complex catastrophe types met as the number of control variables increases--in the oxygen partial pressure-/cooling rate space. Extending the analysis begun here and in [6] should shed light on ignition phenomena and ways of minimizing unwanted ignitions. And, since catastrophe theory concerns global stability, it may help in examining effects of large disturbances and in counteracting the effect of these disturbances through automatic controls.

Catastrophe theory [7,9,10,11,12] also gives generic or canonical forms for each catastrophe. For example, the canonical form for the cusp catastrophe is

$$\frac{dx}{dt} = x^3 + C_1 x + C_2 \ , \tag{29}$$

where x is the state variable and C_1 and C_2 are control parameters.

The main theorem of Thom [7] states that equation (29) can be obtained from equations (7) - (8) by a diffeomorphism-- i.e., a one-to-one differentiable and inverse differentiable mapping from (η^*, η_1, θ) space to (x, C_1, C_2) space. This indicates that model simplifications are possible, though there is no well-defined way for constructing such diffeomorphisms. This is one of the unsolved problems in the application of Catastrophe theory to practical problems. A solution to this problem might contribute to the identification problem for non-linear systems in the same way that canonical models contribute to linear system identification [5].

Several further extensions of the work reported here are possible. One can consider more realistic situations having more general chemical reactions with more than two control variables and more than three equilibrium points. One would then observe other catastrophes, such as the "butterfly" catastrophe in four control variables. The existence of an infinite number of catastrophes for more than five control variables may have important implications for certain complicated chemical reaction situations. And the construction of the diffeomorphisms discussed above even for simple cases would be of interest.

VI. Conclusions

Chemical kinetics and reactor dynamics are a very fruitful area for the application of catastrophe theory. It has been demonstrated that a cusp catastrophe exists for a simple first-order irreversible reaction in the residence time--thermal input (coolant temperature or feed temperature) space. Analytical formulas have been obtained for the ignition and quenching boundaries, which may provide a basis for understanding more complex ignition and quenching phenomena.

Acknowledgment

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