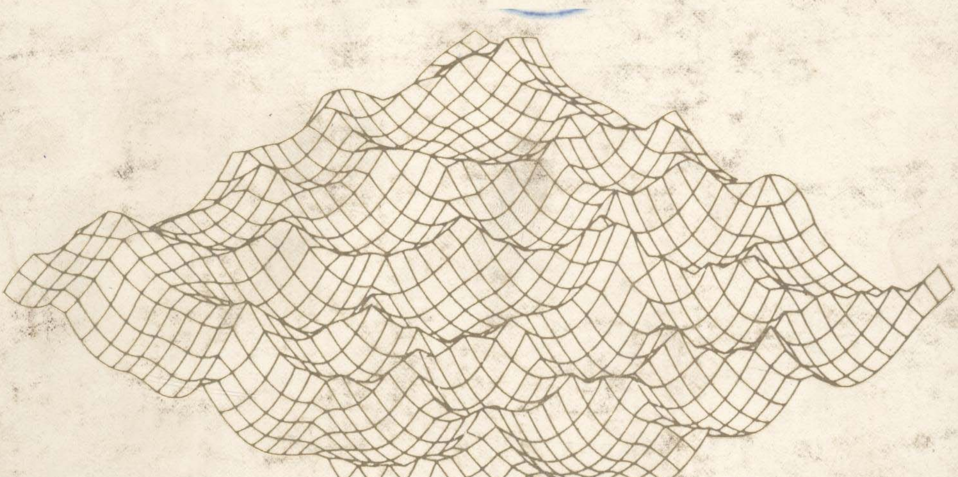
Reacting Flows:

Combustion and Chemical Reactors

Part 2



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Part 2

G.S.S. Ludford, Editor

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Reacting Flows:

Combustion and Chemical Reactors

Part 2

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CHEMICAL REACTORS

Lectures in Applied Mathematics
Volume 24, 1986

STABILITY AND HOPF BIFURCATION IN ISOTHERMAL CATALYSTS*

José M. Vega and Ignacio E. Parra

ABSTRACT. It is considered a well-known model for the evolution of a distributed concentration and a uniform temperature in an isothermal catalyst, which occupies a bounded domain $\Omega \subset \mathbb{R}^p$ ($p=1,2,3$) with smooth boundary. It is assumed that the Sherwood number is large.

For a not too large Thiele modulus, the boundary condition for the concentration is of the Dirichlet type in first approximation. An analysis of the linearized stability of the steady state in the slab geometry ($p=1$), shows that oscillatory instabilities may appear for appropriate values of the parameters. Bifurcation diagrams are reminiscent of those for the C.S.T.R.

For a sufficiently large Thiele modulus and arbitrary shapes of the domain Ω, an approximate one-dimensional model is considered, which accounts for the fact that the concentration vanishes, to leading order, outside a thin reaction layer. A linearized stability analysis shows that oscillatory instabilities may appear again.

A local Hopf bifurcation analysis is carried out, in order to know whether such bifurcation is sub-critical or super-critical.

1. INTRODUCTION. A well-known model, see Aris [1], for the evolution of the concentration u and temperature v, in an isothermal catalyst, is considered

$$\frac{\partial u}{\partial t} = \Delta u - \phi^2 u \exp\left(\gamma \frac{v-1}{v}\right) \text{ in } \Omega, \tag{1}$$

* This research was partially supported by the Comisión Asesora de Investigación Científica y Técnica under Contract N/r 2291-83.

$$\frac{\partial u}{\partial n} = \sigma(1-u) \text{ at } \partial\Omega, \quad (2)$$

$$\frac{dv}{dt} = \lambda\mu(1-v) + \lambda\phi^2 \exp(\gamma\frac{v-1}{v}) \int_\Omega u\, dx. \quad (3)$$

Here, n is the outward unit normal to the smooth boundary of the bounded domain $\Omega \subset \mathbb{R}^p$ (p=1,2,3). The Damköhler number ϕ^2, the activation energy γ, and the parameters λ and μ are positive. The Serwood number, σ, will be assumed to be large.

Such model is a first approximation, as $\gamma\beta \to 0$ and $\nu \to 0$, of the fully non-isothermal model, in which the temperature is spatially distributed, and given by

$$\frac{1}{L}\frac{\partial v}{\partial t} = \Delta v + \beta\phi^2 u \exp(\gamma\frac{v-1}{v}) \text{ in } \Omega \ ; \ \frac{\partial v}{\partial n} = \nu(1-v) \text{ at } \partial\Omega. \quad (4)$$

In this limit, the parameters λ and μ of (3) are

$$\lambda = \beta L/V_\Omega, \ \mu = \nu\, S_\Omega/\beta,$$

in terms of the Prater, Lewis and Nusselt numbers, β, L and ν, and of the volume, V_Ω, and external area, S_Ω, of the domain Ω. For p=1, if $\Omega =]-1,1[\subset \mathbb{R}$, then $S_\Omega = V_\Omega = 2$.

Let $\{u_s(x), v_s\}$ be a steady state of (1-3). If

$$\phi_s^2 = \phi^2 \exp[\gamma(v_s-1)/v_s] << \sigma^2, \quad (5)$$

the boundary condition (2) may be replaced by

$$u = 1 \text{ in } \partial\Omega, \quad (6)$$

in first approximation (as $\sigma \to \infty$), when analyzing the nonlinear stability of the steady state under small perturbations. Model (1,3,6) will be referred to as Model 1 in the sequel. It was considered by Amundson and Raymond, [2], for the slab geometry (p=1). In that work, it was apparently proved that the possible instabilities of the steady state are of the non-oscillatory type, and that they appear only at the bending points of the response curve v_s-ϕ. A slippery gap in their use of Rouche's theorem prevent their conclusion from being true. In fact, as we shall see in Section 2, oscillatory instabilities do take place in a region of the response curve, if $\lambda\mu > 8.889...$ and γ is such that $\gamma_{c1}(\lambda,\mu) < \gamma < \gamma_{c2}(\lambda,\mu)$, for some critical parameters, γ_{c1} and γ_{c2}.

If condition (5) is not satisfied, i.e., in the limit $\phi_s \to \infty$, the boundary condition (6) may not be used. But, in this limit, it is easily shown, see Murray [3], that the steady state concentration, $u_s(x)$, vanishes to leading order outside a thin boundary layer, of thickness ϕ_s^{-1}, which is close to the boundary of the domain. A Singular Perturbation analysis, which is a straightforward extension of that of [3], shows that the transient concentration profile has the same structure as that of the steady state one, if the initial values of u and v are close to the steady state ones. In the distinguished limit $\phi_s \sim \lambda \sim \mu \sim \sigma$, the above-mentioned analysis leads to the following model

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial \xi^2} - \Phi^2 u \exp\left(\gamma \frac{v-1}{v}\right) \text{ in } -\infty < \xi < 0, \tag{7}$$

$$u = 0 \text{ at } \xi = -\infty, \quad u_\xi = 1-u \text{ at } \xi = 0, \tag{8}$$

$$\frac{dv}{d\tau} = lm(1-v) + l\Phi^2 \exp\left(\gamma \frac{v-1}{v}\right) \int_{-\infty}^{0} u\,d\xi \tag{9}$$

where

$$\Phi = \phi/\sigma, \ l = \lambda\, S_\Omega/\sigma, \ m = \mu/\sigma\, S_\Omega, \ \tau = t\sigma^2, \ \xi = \eta\sigma,$$

and η is a co-ordinate along the outward unit normal to $\partial\Omega$. Again, if $\Omega =]-1,1[\subset\mathbb{R}$, then $S_\Omega = 2$. Model (7-9) will be referred to as Model 2 in the sequel. It could be obtained also, as a first approximation, from the non-isothermal model (1,2,4). Observe that Model 2 is independent of the shape of the domain Ω; it depends on the overall properties of Ω, S_Ω and V_Ω, only through the parameters l and m.

In Sections 2-4, we shall analyze linear stability and local Hopf bifurcation for Model 2. For the sake of brevity, many details of the analysis will be omitted; they may be found in

[4]. In order to obtain close-form solutions of the equations, only the slab geometry will be considered for Model 1. Some global stability results for problem (1-3) and for: (a) arbitrary shapes of the domain Ω, (b) more general type of kinetic laws, and (c) arbitrary positive values of the Sherwood number σ (not necessarily large), will be presented in [5].

2. LINEAR STABILITY FOR MODEL 1. Let us consider Model 1 in $\Omega =]-1,1[\subset \mathbb{R}$. It may be easily seen that no properties concerning nonlinear stability are lost if one considers the symmetric case, i.e.,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - \phi^2 u \exp\left(\gamma \frac{v-1}{v}\right) \text{ in } 0 < x < 1, \tag{10}$$

$$\partial u/\partial x = 0 \text{ at } x = 0, \quad u = 1 \text{ at } x = 1, \tag{11}$$

$$\frac{dv}{dt} = \lambda\mu(1-v) + 2\lambda\phi^2 \exp\left(\gamma\frac{v-1}{v}\right) \int_0^1 u \, dx. \tag{12}$$

The steady state solutions of (10-12) are given by

$$u_s = \frac{\cosh \phi_s x}{\cosh \phi_s}, \quad v_s = 1+2\frac{\phi_s}{\mu} \tanh\phi_s, \tag{13}$$

in terms of the parameter

$$\phi_s^2 = \phi^2 \exp[\gamma(v_s-1)/v_s].$$

The linearized problem around the steady state has non-trivial solutions, of the form $u-u_s = U(x)\exp(\omega t)$, $v-v_s = V\exp(\omega t)$, if and only if ω satisfies

$$\omega(\omega+\lambda\mu) = \frac{2\lambda\mu^2\gamma\phi_s^2}{(\mu+2\phi_s\tanh\phi_s)^2}\left[\frac{\phi_s^2 \tanh\sqrt{\omega+\phi_s^2}}{\sqrt{\omega+\phi_s^2}} + \frac{(\omega-\phi_s^2)\tanh\phi_s}{\phi_s}\right] \tag{14}$$

for $\omega \neq 0$, or

$$\gamma = \frac{(\mu\cosh\phi_s + 2\phi_s\sinh\phi_s)^2}{\mu\phi_s(\phi_s+\sinh\phi_s\cosh\phi_s)} \tag{15}$$