React. Kinet. Catal. Lett., Vol. 15, No. 2, 215–220 (1980)

STABILITY OF HYPERBOLIC REACTORS

P. Réti

Central Research and Planning Institute of the Silicate Industry,
Budapest, P.O.B 112, 1300

Received June 17, 1980
Accepted July 15, 1980

For the one-phase tubular reactor, a new mathematical model is suggested, viz. a hyperbolic system of first order partial differential equations instead of the usual second order parabolic ones. This physically better model is investigated from the point of view of stability via the second Lyapunov method.

Была предложена новая математическая модель для однофазного трубчатого реактора с использованием гиперболической системы парциальных дифференциальных уравнений первого порядка вместо обычных параболических систем второго порядка. Эта физически более обоснованная модель была исследована с точки зрения стабильности с помощью второго метода Ляпунова.

INTRODUCTION

Recently many publications emphasized the more than a century old idea of replacing those constitutive equations which result in parabolic systems of partial differential equations. These equations are the so-called reaction-diffusion type, having the unpleasant consequence of the unphysical infinite speed of the propagation of disturbances. This fact was first pinpointed by Maxwell /1/, for detailed references, see Gyarmati /2/.

The aim of this paper is to elaborate some questions of the qualitative behavior of such models for isothermal tubular chemical reactors, i.e. in the simplest case. The necessary theory of stability for distributed parameter systems is given in Zubov's book /3/.

HYPERBOLIC REACTORS

To model an isothermal reactor with a hyperbolic system of equations, one has to complete the usual Fick or Fourier type constitutive relations with a term which accounts for relaxation effects. Thus one obtains the following equation:

$$J = -DC_x - T(J_t + vJ_x) \qquad (1)$$

where J is the flux of the chemical component, c is its concentration, D and T are the diffusion and relaxation constants, respectively, v is the rate of convection.

With the conservation equation

$$C_t + vC_x + J_x - q = 0 \qquad (2)$$

(here q is the reaction rate, generally a non-linear function of polynomial type), a system of first order partial diffential equations of hyperbolic type (for the notion of hyperbolicity, see Ref. /4/) is obtained.

Introducing the following notations:

$$\hat{C} = \begin{pmatrix} C \\ J \end{pmatrix}, \quad A = \begin{bmatrix} v & 1 \\ \frac{D}{T} & v \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{T} \end{bmatrix}, \quad f = \begin{bmatrix} -q \\ 0 \end{bmatrix}, \qquad (3)$$

one obtains the following equation:

$$\hat{C}_t + A\hat{C}_x + B\hat{C} + f = 0$$

From eq. (3) the so-called canonical form is easily obtained. For this purpose the eigenvalues of A should be computed ($k_{1,2} = v \pm\sqrt{D/T}$), then the corresponding eigenvalues are $x_{1,2} = \begin{bmatrix} 1 \\ \pm\sqrt{D/T} \end{bmatrix}$ and with $Z = [x_1 \; x_2]$ A can be transformed into a diagonal matrix $Z^{-1}\ AZ = K = \begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix}$. Intoducing new variables $Z^{-1}\ \hat{C} = w$, we obtain the canonical form

$$w_t + Kw_x + Ew + u = 0 \tag{4}$$

(Here $E=Z^{-1}\ BZ$, $u=Z^{-1}\ f$).

Equation (4) with the necessary initial and boundary conditions is the mathematical model of the one-phase hyperbolic reactor. As concerns these conditions, they are treated thoroughly in another paper /5/, their general form is

$$\sum_{i=1}^{2} \alpha_i w_i \text{ (either 0 or 1)} = 0$$

and their number is determined by signs of elements of K.

STABILITY OF THE STEADY STATE

Our goal is to examine the stability of the steady-state solution of eq. (4). It turns out that as in the case of parabolic equations the simplest step is the examination of the linearized equation. In the isothermal reactor, this is the case if the reaction is of the first order.

If eq. (4) is linearized, the following equation is obtained (w^x denotes its solution):

$$w^x_t + Kw^x_x + Ew^x + u^x = 0 \tag{5}$$

Here u^x is already a linear function.

Let us suppose that the corresponding equa tion for the steady state has only one solution – this means that a local Lipschitz criterion is satisfied (for this statement, see Ref. /6/) – and let us denote this solution by w^{xx}, $u^{xx} = u(w^{xx})$, so

$$Kw_x^{xx} + Ew^{xx} + u^{xx} = 0 \tag{6}$$

The (small) perturbation from the steady state is

$$s = w^x - w^{xx}. \tag{7}$$

Then $w^x = s + w^{xx}$ and with notation $E^x w^{xx} = Ew^{xx} + u^{xx}$ one obtains this equation for $s + w^{xx}$:

$$(s + w^{xx})_t + K (s + w^{xx})_x + E^x (s + w^{xx}) = 0 \tag{8}$$

From eq. (8) a linear equation is obtained for s using eq. (6):

$$s_t + Ks_x + E^x s = 0 \tag{9}$$

The asymptotic stability of w^{xx} is ascertained if a Lyapunov functional could be constructed for s. This could be done in the following way.

It is easy to prove that

$$(s^t s)_t + (s^t Ks)_x + s^t (E^x + E^{xt}) s = 0 \tag{10}$$

where the superscript t denotes a transposed vector or matrix. More than one possibility exist for obtaining a Lyapunov functional. If eq. (10) is integrated then

$$\frac{d}{dt} \int_0^1 (s^t s)\, dx = - \int_0^1 (s^t (E^x + E^{xt}) sdx \tag{12}$$

and

$$v(t) = \int_0^1 s^t sdx \geqslant 0 \tag{11}$$

and

$$\frac{d}{dt} v(t) < 0 \quad \text{if} \quad E + E^{xx} \text{ is positive} \tag{13}$$

If condition (13) is met, functional $v(t)$ will be a Lyapunov functional for eq. (9) and therefore the steady-state solution will be asymptotically stable.

Another possibility (if condition (13) is not met) is to multiply eq. (9) by K^{-1} from the left:

$$K^{-1} s_t + s_x + K^{-1} E^* s = 0 \tag{14}$$

If both of the characteristic velocities are positive (elements in K), similar arguments lead to the statement that asymptotic stability is proved

with

$$v_1 (t) = \int_0^1 s^t K^{-1} sdx \tag{15}$$

if

$$\frac{d}{dt} v_1 (t) < 0 \tag{16}$$

In this case v_1 (t) will be a Lyapunov functional. If one of the characteristic velocities is non-positive, then $v_1(t) \geq 0$ is not true. In this case, a Q matrix with constant elements could be found so that $Q K^{-1}$ be positive, then $v_2(t) = \int_0^1 = s^t Q K^{-1} sdx$ can be a Lyapunov functional with the same conditon and with similar arguments.

CONCLUSIONS

Stability of one-phase hyperbolic chemical reactor models in the isothermal case was examined. Conditions for asymptotic stability were stated for the case of linearized equations. If the chemical reaction occurring in the tubular reactor is of first order, this result can be used immediately because of the linearity of equations. In the non-linear cases, namely when the reactor is not isothermal and/or the order of the chemical reaction is not equal to one, the problem reduces to the usual but very hard question of relation between the qualitative behavior of linearized equations and that of non-linear ones. This question is far from being solved.

Acknowledgement. Many problems in this article were developed during discussions with Dr. J. Holderith, to whom due thanks are hereby expressed.

REFERNCES

1. J.C. Maxwell: Phil. Trans. Roy. Soc., London, 49, 157 (1857).
2. J. Gyarmati: J. Non-Equil. Thermodyn. 2, 233 (1977).
3. V.I. Zubov: Methods of A.M. Lyapunov and their Application. Groningen 1964.
4. R. Courant: Partial Differential Equations. Interscience, New York 1962.
5. J. Holderith, P. Réti: Ann. Univ. Sci. Budap., R. Eötvös, Sec. Chim., 1979.
6. N.I. Vasilyev, Yu.A. Klokov: Foundations of the Theory of Boundary Problems for Ordinary Differential Equations (in Russian). Zinatie, Riga 1978.