Intermittency in Nonisothermal CSTR

G. T. Caneba, Barbara Densch

Department of Chemistry and Chemical Engineering Michigan Technological University Houghton, MI 49931

Intermittency has been a well-known phenomenon in fluid turbulence (Berge et al., 1980; Siggia, 1981; Chen and Lumley, 1984) and in other dynamic systems (Bak et al., 1985; Lister, 1983; Heffernan, 1985). At present, there has been no reported occurrence of this dynamic behavior in nonisothermal chemical reactors. In this work, we present simulation results of a periodically perturbed nonisothermal continuous stirred-tank reactor (CSTR), with $A \rightarrow B$ kinetics, that exhibits intermittency. The mathematical model of the unperturbed reactor follows that of Uppal et al. (1974). The phase plot for this portion of the reactor system corresponds to two concentric limit cycles in which one is stable and the other unstable. The possibility of obtaining intermittency from this kind of geometric structure has been shown in a system with two competing frequencies, in which the transition is caused by interaction and overlap of mode-locked resonances (Bak et al., 1985). In the geometric sense, this could imply the overlap of two limit cycles by periodic forcing of system parameters. Indeed, intermittency is observed in this case.

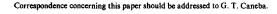
In the reactor, periodic perturbations are applied to the volumetric feed rate F, and the cooling fluid temperature T_C :

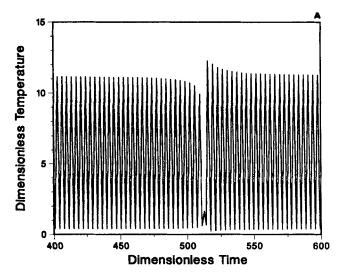
$$F = F_o[1 + \zeta \sin(\omega_F t)]$$

$$T_C = T_{Co}[1 + \xi \sin(\omega_T t)]$$
(1)

Resulting dimensionless quantities for the unperturbed portion of the system are the same as those in Uppal et al. (1974) except that F_o is substituted for F and T_{Co} for T_C . Perturbation parameters are $\eta = \beta \gamma \xi$, ξ , ω_T , and ω_F . Simulation of the set of nonlinear ordinary differentials is done through the IMSL package, DGEAR, with a relative tolerance of 10^{-8} .

The phase plot of the unperturbed system, corresponding to the structure of two concentric limit cycles, is shown in Figure 20 of Uppal et al. (1974). Parameter values are: Da = 0.12823, $\beta = 3$, B = 16.2, and $\gamma \rightarrow \infty$. When periodic perturbations ($\eta = 0.9862$, $\zeta = 0.2$, $\omega_F = \omega_T = 1.7718$) are applied to the volumetric





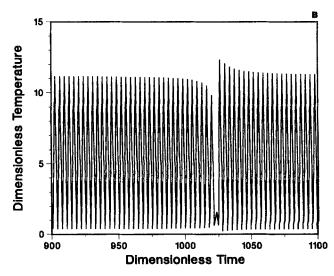
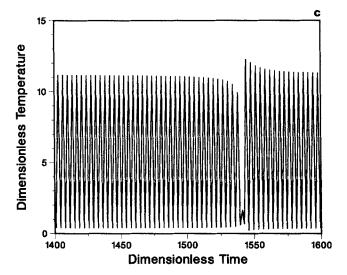


Figure 1. Integral plots of dimensionless temperature vs. dimensionless time.

Apparent limit cycle behavior is interrupted by short bursts; the period between bursts seems to be constant at a dimensionless time of 510



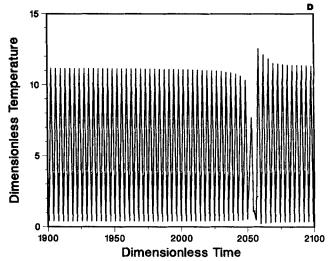


Figure 1. (Continued)

feed rate and cooling fluid temperature, the system seems to exhibit limit cycle behavior. However, when one extends the simulation run to a dimensionless time of 600, a dramatic deviation from this behavior is observed at dimensionless times of around 510–520, Figure 1a. Then the system returns to its limit cycle behavior. A continuation of the simulation run results in the periodic occurrence of this behavior, Figures 1b–1d, with a period of about 510.

To verify that this behavior is indeed that of intermittency, a plot of the Poincare return map for the dimensionless temperature y, Figure 2, shows that there is a series of points that seem to run parallel to the diagonal line. Points in this region are dense, indicating that the system seems to converge into a limit cycle. However, the system eventually escapes, and again

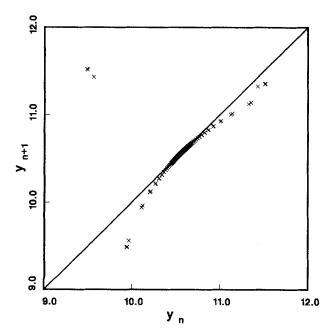


Figure 2. Poincare return map of dimensionless temperature y.

In center region points seem to run parallel and very close to the diagonal line

returns to the dense region after a relatively short period of time. Thus, we have the bursting behavior occurring in a system that seems to behave like a limit cycle.

Notation

B = heat of reaction

Da = Damkohler number, rate of reaction

F = volumetric feed rate

T = absolute temperature

y =dimensionless temperature

Greek letters

 β = rate of cooling

 γ = activation energy

 η = defined as $\beta \gamma \xi$

 ζ = amplitude of feed rate perturbation

 ξ = amplitude of cooling fluid perturbation

 ω = frequency

Subscripts

C = cooling fluid

F = feed

T =cooling fluid temperature

n, n + 1 = nth, (n + 1)th intersection of phase trajectory with an arbitrary surface

0 = average quantity

Literature Cited

Bak, P., T. Bor, and M. H. Jensen, "Mode-Locking and the Transition to Chaos in Dissipative Systems," *Physica Scripta*, **79**, 50 (1985).

Berge, P., M. Dubois, P. Manneville, and Y. Pomeau, "Intermittency in Rayleigh-Benard Convection," J. Physique—Lettres, 41, L-341 (1980).

Chen, J.-Y., and J. L. Lumley, "Second-Order Modeling of the Effect of Intermittency on Scalar Mixing," 20th Int. Symp. Combustion, Combustion Inst., 359 (1984).

Hefernan, D. M., "Multistability, Intermittency and Remerging Feigenbaum Trees in an Externally Pumped Ring Cavity Laser System," Physics Lett., 108A(8), 413 (1985).

Lister, C. R. B., "On the Intermittency and Crystallization Mechanisms of Sub-Seafloor Magma Chambers," *Geophys. J. R. Astr. Soc.*, 73, 351 (1983)

Siggia, E. D., "Numerical Study of Small-scale Intermittency in Three-Dimensional Turbulence," J. Fluid Mech., 107, 375 (1981).

Uppal, A., W. H. Ray, and A. B. Poore, "On the Dynamic Behavior of Continuous Stirred-Tank Reactors," *Chem. Eng. Sci.*, 29, 967 (1974).

Manuscript received July 9, 1987 and last revision on Aug. 5, 1987.