PDE Model System: Non-isothermal model simulating the self-ignition dynamics of a coal stockpile

Reference papers :
(1) G. Continillo, V. Faraoni, P.L. Maffettone and S. Crescitelli, Non-linear dynamics of a self-ignited reaction-diffusion system, Chem. Engng. Sci. 56 (2000) S1071-S1076.
(2) A. Adrover, M. Giona, Modal reduction of PDE models by means of Snapshot Archetypes, Physica D 182 (2003) 2345.

Balance Equations in dimensionless form :

$$\begin{aligned} \frac{\partial c}{\partial t} &= Le \frac{\partial^2 c}{\partial x^2} - \phi^2 c \exp(-\gamma/T) \, , \\ \frac{\partial T}{\partial t} &= \frac{\partial^2 T}{\partial x^2} + \beta \phi^2 c \exp(-\gamma/T) \, , \qquad x \in (0,1) \, , \end{aligned} \tag{1}$$

equipped with the boundary conditions

$$T(0,t) = T(1,t) = 1 \, , \qquad \left. \frac{\partial c}{\partial x} \right|_{x=0} = 0 \, , \qquad c(1,t) = 1 \, , \qquad \text{for } t > 0 \, , \tag{2}$$

where c and T are respectively dimensionless reactant concentration and temperature, Le is the Lewis number (ratio of mass and heat diffusivities), ϕ the Thiele modulus, β the dimensionless heat of reaction, and γ the dimensionless activation energy.

The dynamical behavior of the model system has been numerically obtained by means of collocation methods, (sinc collocation by Adrover and Giona with $N = 39$ internal collocation points and classical orthogonal collocation with Lagrange interpolating polynomials in Continillo et al. with $N = 12$ collocation points) that are very simple and efficient in the presence of non polynomial nonlinearities, such as the Arrhenius dependence of the kinetic rates on temperature.

The coal stockpile model displays a rich dynamical structure. By letting the activation energy γ vary in the interval $[11, 14]$, (for fixed values of the other parameter: $Le = 0.2333$, $\phi^2 = 70000$ and $\beta = 4.287$), the system exhibits the complex bifurcation diagram. Starting from lower values of γ, corresponding to a stable equilibrium solution, a stable periodic branch emerges from a first Hopf bifurcation $\gamma = \text{HB}_1$. As the bifurcation parameter is further increased, a period doubling cascade, leading to chaos is observed. The bifurcations diagrams obtained by Adrover and Giona and by Continillo et al. are slightly different because of different collocation approaches and different collocation points have been used. For example, two Hopf-bifurcations are detected for $\gamma = \text{HB}_1 = 12.2043$ and $\gamma = \text{HB}_2 = 13.5557$ by Adrover and Giona. The same Hopf bifurcations are observed by Continillo et al. at $\gamma = \text{HB}_1 = 12.033$ and $\gamma = \text{HB}_2 = 13.3783$.

The table below reviews some of the values of the bifurcation parameter γ at which it is possible to observe sone characteristic dynamical behaviors of the system, equilibrium solutions, periodic oscillations and chaos.

asymptotic behavior	Continillo et al.	Adrover and Giona
equilibrium solution	$\gamma = 11.5$	$\gamma = 11.5$
period 1 limit cycle	$\gamma = 12.2$	$\gamma = 12.55$
period 2 limit cycle	$\gamma = 12.395$	$\gamma = 12.59$
chaos	$\gamma = 12.6$	$\gamma = 12.61$