ODE Model System: Dynamics of a jacketed CSTR in the presence of a first-order exothermic reaction

Reference paper : Uppal, A., Ray, W.H., and Poore, A. (1974). On the dynamic behavior of continuous stirred tank reactors, *Chem. Eng. Sci. 29*, 967-985.

Balance Equations in dimensionless form :

$$
\begin{aligned}
\frac{dx}{dt} &= -x + Da\,(1-x)\,\mathrm{e}^{f(y)} \\
\frac{dy}{dt} &= -(1+\beta)\,y + B\,Da\,(1-x)\,\mathrm{e}^{f(y)}
\end{aligned}
\qquad (1)
$$

where $f(y) = y/(1+y/\gamma)$, x and y are the dimensionless reactant concentration and temperature, respectively and B, β, γ and the Damkölher number Da the model parameters.

This model system can exhibit steady-state multiplicity and limit cycles, depending on the values of model parameters. For a thorough presentation of the bifurcation structure please refer to the original paper by Uppal, Ray and Poore (1974).

We focus on the following two cases:

(1) $B = 10$, $\beta = 1.8$, $\gamma = 35$, $Da = 0.1$.
The system exhibits
(i) a unique stable equilibrium point $\mathbf{z}_{eq} = (x_{eq}, y_{eq}) \simeq (0.141, 0.504)$ characterized by a pair of complex conjugate eigenvalues (with negative real part)
(ii) a saddle point-at-infinity $\mathbf{u}_{eq}^{\infty} = (u_1, u_2) = (0, 1)$ of the corresponding Poincaré projected system
(iii) an invariant slow manifold represented by the heteroclinic connection between the stable equilibrium point $\mathbf{z}_{eq}$ and the saddle point at infinity (Figure 1)

(2) $B = 10$, $\beta = 1.8$, $\gamma = 35$, $Da = 0.2$.
The system exhibits
(i) a unique unstable equilibrium point $\mathbf{z}_{eq} = (x_{eq}, y_{eq})$ characterized by a pair of complex conjugate eigenvalues (with positive real part)

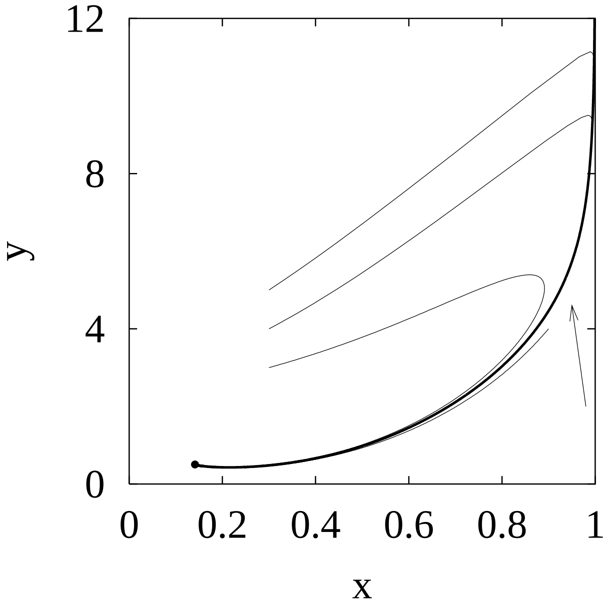

Fig. 1. Phase plot of the orbit structure in the UPR model at $\beta = 1.8$ $\gamma = 35$ and $Da = 0.1$. Dot (•) indicates the stable equilibrium point. Thicker line is the slow manifold.

(ii) a stable limit cycle surrounding the unstable equilibrium point
(iii) a saddle point-at-infinity $\mathbf{u}_{eq}^{\infty} = (u_1, u_2) = (0, 1)$ of the corresponding Poincaré projected system
(iv) orbits collapsing towards an invariant one-dimensional template (the slow manifold) connecting the the saddle point at infinity with the limit cycles and rolling up infinitely times around the limit cycle itself (Figure 2)

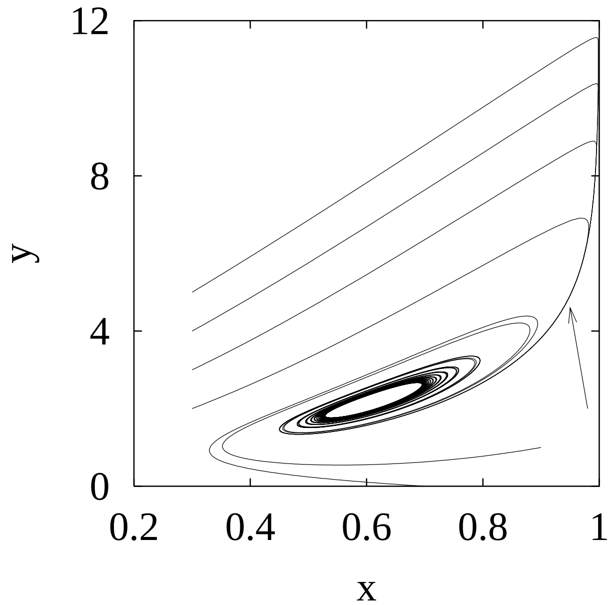

Fig. 2. Phase plot of the orbit structure in the UPR model at $\beta = 1.8$ $\gamma = 35$ and $Da = 0.2$. Thicker line is the slow manifold.