A study about Exothermic Chemical Reactor by ASM Approach Strategy

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Abstract

In this paper, our aims are accuracy, capabilities and power at solving set of the complex non-linear differential at the reaction chemical . As all experts know most of engineering actual systems behavior in practical are nonlinear process and analytical scrutiny these nonlinear problems are difficult or sometimes impossible.

Our purpose is to enhance the ability of solving the mentioned nonlinear differential equations at chemical engineering and similar issues with a simple and innovative approach which entitled ‘’**Akbari-Sara's Method’’** or ‘’ASM’’.

Introduction and theatrical formulation

Consider a well-mixed continuous stirred tank reactor with the reaction and set of nonlinear differential equations. parameters F(the flow rate), c_{A0} (the initial molar concentration) , T_{A0} (the initial temperature),Q (the rate of heat input to the reactor), V(the volume of the reactor), E, ΔH, k_0 (the pre-exponential constant reaction), c_p and ρ denote the heat capacity and density of the fluid in the reactor.

$$A \to B \quad , \quad r_A = ko \exp\left(-\frac{E}{R\,T} \right) c_A \quad ; \qquad IC:\ c(0) = co \quad , \quad T(0) = To$$

Set of nonlinear differential equations as follows:

$$V \frac{\mathrm{d}}{\mathrm{d}t} C_A(t) = F\left[C_{A0} - C_A(t) \right] - ko\, Exp\left(-\frac{E}{R\,T(t)} \right) V C_A(t)$$

$$V \frac{\mathrm{d}}{\mathrm{d}t} T_A(t) = F\left[T_{A0} - T_A(t) \right] + ko \left(\frac{-\Delta H}{\rho\, cp} \right) Exp\left(-\frac{E}{R\,T(t)} \right) V C_A(t) + \frac{Q}{\rho\, cp}$$

The solution of the mentioned problem by ASM will be obtained as follows:

$$c(t) := \frac{\Gamma}{\psi} - \frac{To^2\,\Delta^2}{\psi} Exp\left(\frac{-\psi\, t}{\Delta\ To^2} \right) \quad ; \quad T(t) := \frac{\Gamma 1}{\psi 1} - \frac{\Delta 1^2\ To^2}{\psi 1} Exp\left(-\frac{\psi 1\, t}{\Delta 1\ To^2} \right)$$

The following new variables are introduced as:

$$\psi = To^2\, co\, \eta\, ko\, e^{-\frac{2\varepsilon}{To}} - co^2 \eta^2 \varepsilon\, e^{-\frac{2\varepsilon}{To}} + 2\, To^2 \beta\, co\, \eta\, e^{-\frac{\varepsilon}{To}} + To\, \beta\, co\, \eta\, \varepsilon\, e^{-\frac{\varepsilon}{To}}$$

$$- To^2\, \alpha 1\, \eta\, e^{-\frac{\varepsilon}{To}} - \alpha 2\, co\, \eta\, \varepsilon\, e^{-\frac{\varepsilon}{To}} - To^3 \beta^2 + To^2\, \alpha 2\, \beta$$

$$\Gamma = To \left(\psi - 2 To^2 \beta\, co\, \eta\, e^{-\frac{\varepsilon}{To}} + To^3 \beta^2 + To\, co^2 \eta^2 e^{-\frac{2\varepsilon}{To}} + 2 To\, \alpha 2\, co\, \eta\, e^{-\frac{\varepsilon}{To}} + To\, \alpha 2^2 \right) ;$$

$$\Delta := \eta\, co\, e^{-\frac{\varepsilon}{To}} - \beta\, To + \alpha 2$$

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$$\psi 1 = -To^2\, co\, ko^2 e^{-\frac{2\varepsilon}{To}} + co^2\,\eta\, ko\,\varepsilon\, e^{-\frac{2\varepsilon}{To}} - 2\,To^2\,\beta\, co\, ko\, e^{-\frac{\varepsilon}{To}} - To\,\beta\, co\, ko\,\varepsilon\, e^{-\frac{\varepsilon}{To}}$$
$$+ To^2\,\alpha 1\, ko\, e^{-\frac{\varepsilon}{To}} + \alpha 2\, co\, ko\,\varepsilon\, e^{-\frac{\varepsilon}{To}} - To^2\,\beta^2\, co + To^2\,\alpha 1\,\beta$$
$$\Gamma 1 = co^3\,\eta\, ko\,\varepsilon\, e^{-\frac{2\varepsilon}{To}} - To\,\beta\, co^2\, ko\,\varepsilon\, e^{-\frac{\varepsilon}{To}} - To^2\,\alpha 1\, co\, ko\, e^{-\frac{\varepsilon}{To}} + \alpha 2\, co^2\, ko\,\varepsilon\, e^{-\frac{\varepsilon}{To}}$$
$$- To^2\,\alpha 1\,\beta\, co + To^2\,\alpha 1^2 \;;\quad \Delta 1 = ko\, co\, e^{-\frac{\varepsilon}{To}} + \beta\, co - \alpha 1$$
$$\alpha 1 := \frac{F}{V} co\,;\ \alpha 2 := \frac{F}{V} To + \frac{Q}{\rho\, cp\, V}\,;\ \beta := \frac{F}{V}\,;\ \eta := ko\left(-\frac{\Delta H}{\rho\, cp}\right);\ \varepsilon := -\frac{E}{R}$$

By selecting the physical values at below:

$$V := 20\ (L); R := 8.314\ \frac{J}{mol.K}; co := 0.6\frac{mol}{L}; To := 310\ K; \Delta H := -4.78\cdot 10^4 \frac{J}{mol}; ko := 7.20$$
$$\cdot 10^{-2}\,\mathrm{min}^{-1}; E := 83.1\frac{J}{mol}; cp := 0.539\ \frac{J}{g.K}; \rho := 1000\frac{g}{L}; F := 2\frac{L}{\mathrm{min}}; Q := 100\frac{L}{\mathrm{min}}$$

The solution is rewritten as follows:

$$c(t) := 332.7146555 - 22.71465617\, e^{-0.1745968863\ t}$$
$$T(t) := 0.3447209382 + 0.2552790620\, e^{-0.1747717806\ t}$$

Comparing the achieved solutions by Numerical Method and ASM (Akbari Sara's Method)

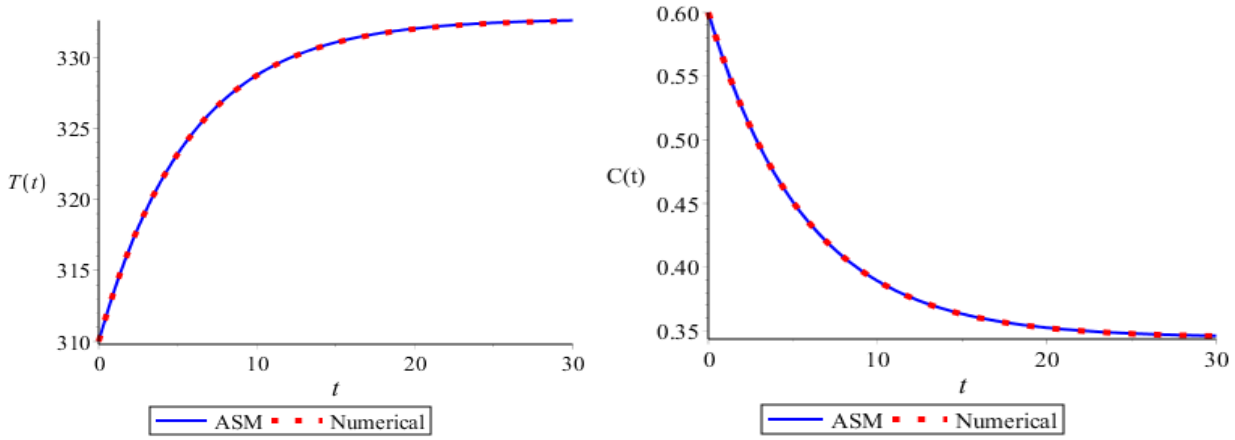


Fig. A comparison between ASM and Numerical solution for concentration and temperature.

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