5.4) Consider Example 3.7 for a CSTR with a cooling jacket operating in a steady state in which the exothermic reaction $A + B \xrightarrow{k} C$ takes place. The mass and energy balances that represent this reactor are rewritten as follows:

$$\text{Mass balance for A (mol/min):}\quad Q(C_{A\text{in}} - C_A) - kC_AC_BV = 0 \tag{3.12}$$

$$\text{Mass balance for B (mol/min):}\quad Q(C_{B\text{in}} - C_B) - kC_AC_BV = 0 \tag{3.13}$$

$$\text{Mass balance for C (mol/min):}\quad Q(C_{C\text{in}} - C_C) + kC_AC_BV = 0 \tag{3.14}$$

$$\text{Energy balance for the reactor (J/min):}\quad Q\rho c_p(T_{\text{in}} - T) + UA(Tj - T) + kC_AC_BV(-\Delta H)_R = 0 \tag{3.15}$$

$$\text{Energy for the cooling fluid (J/min):}\quad Q_j\rho_j c_{p_j}(Tj_{\text{in}} - Tj) + UA(T - Tj) = 0 \tag{3.16}$$

Using the numerical values in Tables 3.1 and 3.2, solve the nonlinear algebraic equations system using the NR approach (Sect. 5.2) and obtain the concentrations of A, B, and C, and the temperatures of the reactor and the cooling jacket in a steady state. Try to solve this problem using the *Solver* tool (Sect. 5.3) and observe that this approach is not robust (due to a highly nonlinear characteristic of this system).

References

Lona, L.M.F., A step by step Approach to the Modeling of Chemical Engineering Process: Using Excel for Simulation, Ed. Springer, 2018

Chapra S.C. e Canale R.P., Métodos Numéricos para Engenheiros, Mac Graw Hill.

Jenson, V.G. e Jeffreys, G.V., Mathematical methods in chemical engineering, 2.ed., London : Academic Press, 1977.

Luyben, W.L., Process modeling, simulation, and control for chemical engineers, 2.ed., London: McGraw-Hill, 1990.

Davis, M.E., Numerical methods and modeling for chemical engineers, N.Y.: J. Wiley.

Conte S.P. e Carl de Boor, ElementaryNumericalAnalysis.

Ingham J.; Dunn I.J.,Heinzle, E; Pfenosil, J.E., Chemical Engineering Dynamics: An Introduction to Modelling and Computer Simulation, Wiley-VCH