CE 329, Fall 2015

Assignment 19

Problem Statement

Recall the problem statement for Assignment 18: Reagent A undergoes an essentially irreversible isomerization reaction that obeys first-order kinetics (A → B). Both A and B are liquids at room temperature and both have extremely high boiling points. The rate constant at 163 ˚C is 0.2 h^{-1} and the activation energy associated with the rate constant is 28,960 cal mol^{-1}. The heat of reaction is constant and is equal to –20,750 cal mol^{-1}. The heat capacities of species A and B may be assumed to be identical and equal to 125 cal mol^{-1} $˚C^{-1}$. The initial charge to a perfectly mixed batch reactor contains no B, and it contains A at a concentration of 3.6 millimoles cm^{-3} and at 163 ˚C. You need to determine how long it will take to reach 97% conversion and what the final temperature will equal if the reactor operates adiabatically.

One might reasonably ask how the initial charge was heated to 163 ºC without any reaction taking place. In a slightly more realistic scenario the initial charge (3.6 mmol A cm^{-3} and no B) to the 100 cm^3 reactor would be at 300 K. In the first stage of processing, a heating jacket (heat transfer area of 11.2 cm^2, heat transfer coefficient of 12.1 cal cm^{-2} h^{-1} K^{-1}) surrounding the reactor contains a well-mixed fluid at 200 ºC. Once the reactor contents reaches 160 ºC, the reactor is instantaneously (and magically?) switched to adiabatic operation which then continues until 97% conversion is attained. What will the total processing time be?

Notes: 1. The ODEs in this problem may be stiff. 2. With the use of an “IF” statement, it is possible to solve the ODEs for both stages using a single call to the numerical ODE solver.