King Fahd University of Petroleum & Minerals
Chemical Engineering Department
CHE 560 –Numerical Methods in Chemical Engineering
2010 - 2011 (102)

HW#3

Due: Sun. 27-March-2011

This problem is about Hydrodealkylation of Mesitylene in a PBR. The production of m-Xylene (*X*) by the hydrodealkylation of mesitylene (*M*) over a Houdry Detrol catalyst involves the following reactions:

$$\text{Reaction 1:} \quad M + H_2 \rightarrow X + CH_4$$

m-xylene (*X*) can also undergo hydrodealkylation to form toluene (*T*):

$$\text{Reaction 2:} \quad X + H_2 \rightarrow T + CH_4$$

The second reaction is undesirable, because m-Xylene sells for a higher price than toluene. Thus we see that there is a significant incentive to maximize the production of m-xylene. The hydrodealkylation of mesitylene is to be carried out isothermally at 1500^oR and 35 atm in a packed-bed reactor (PBR) in which the feed is 66.7% mol hydrogen and 33.3 % mol mesitylene. The volumetric feed rate is 476 ft^3/h and the reactor volume is 238 ft^3.

The rate laws for reaction 1 and 2 are, respectively, $-r_{1M} = k_1 C_M C_H^{0.5}$ and $-r_{2T} = k_2 C_X C_H^{0.5}$

where the subscripts are: *M* = Mesitylene, *X* = m-Xylene, *T* = Toluene, *Me* = Methane, and *H* = Hydrogen (H_2).

At 1500^oR the specific reaction rate constants are: k_1 = 55.20 $(ft^3/lbmol)^{0.5}\ h^{-1}$, k_2 = 30.20 $(ft^3/lbmol)^{0.5}\ h^{-1}$. The bulk density of the catalyst has been included in the specific reaction rate (i.e., $k_1 = \rho_s k_1^{'}$).

Solution Methodology:

Reaction 1: $M + H \rightarrow X + Me$
Reaction 2: $X + H \rightarrow T + Me$

Mole balances:

Hydrogen: $\frac{dF_H}{dV} = r_{1H} + r_{2H}$, Mesitylene: $\frac{dF_M}{dV} = r_{1M}$, Xylene: $\frac{dF_X}{dV} = r_{1X} + r_{2X}$,
Toluene: $\frac{dF_r}{dV} = r_{2T}$, Methane: $\frac{dF_{Me}}{dV} = r_{1Me} + r_{2Me}$

Rate laws: Reaction 1: $-r_{1H} = k_1 C_H^{0.5} C_M$; Reaction 2: $-r_{2T} = k_2 C_H^{0.5} C_X$;

***Stoichiometry*:** ($v = v_o$). $-r_{1H} = -r_{1M} - r_{1X} = r_{1Me}$, $-r_{2H} = -r_{2X} - r_{2T} = r_{2Me}$

Flow rates: $F_H = v_0 C_H$, $F_M = v_0 C_M$, $F_X = v_0 C_X$,

$F_{Me} = v_0 C_{Me} = F_{H0} - F_H = v_0 (C_{H0} - C_H)$, $F_T = F_{M0} - F_M - F_X = v_0 (C_{M0} - C_M - C_X)$

If we know C_M, C_H, and C_X, then C_{ME} and C_T can be calculated from the reaction stoichiometry. Consequently, we need only to solve three equations. Combining and substituting in terms of the space time: $\tau = V / v_0$

$$\frac{dC_H}{d\tau} = -k_1 C_M C_H^{0.5} - k_2 C_X C_H^{0.5} \qquad (1)$$

$$\frac{dC_M}{d\tau} = -k_1 C_M C_H^{0.5} \qquad (2)$$

$$\frac{dC_X}{d\tau} = k_1 C_M C_H^{0.5} - k_2 C_X C_H^{0.5} \qquad (3)$$

Parameter evaluation:

$C_{H0} = y_{H0} P_0 / RT = (0.667)(35)/(0.73)(1500) = 0.021 \ \ Ibmole/ft^3$,

$C_{M0} = 0.5\, C_{H0} = 0.0105\, lbmole/ft^3$, $C_{X0} = 0$, $\tau = V/v_0 = 238\, ft^3 / 476\, ft^3/h = 0.5h$

Assignment:

(a) (5 Points) Non-dimensionalize the above IVP's (1, 2 and 3) and their initial conditions. Use C_{H0} and $1/C_{H0}^{0.5} k_1$ to non-dimensionalize the concentrations and space time, respectively. Also, define any resulting dimensionless groups.

(b) (30 Points) Using the following methods:

  1) 2nd-order explicit Adams-Bashford formula.
  2) Predictor-Corrector method by combining 2nd-order Adams-Bashford and 2nd-order Adams-Moulten formulae.
  3) 2nd-order implicit Adams-Moulten formula.

  Set up the equations that allow the numerical solution of the IVP's showing all required details (algorithm, recursive formulas, residual equations, Jacobian matrix ... etc.)

(c) (20 Points) Solve the equations derived in part (b) using the sample program provided for you in class. COMMON statements should be used appropriately in the main program and subroutines. Upload this program to WebCT (call it yourname-hw4.f).

(d) (5 Points) Using the 2nd-order explicit Adams-Bashford formula, tabulate the values of dimensionless concentrations at τ = 0.5 h for different values of time steps to demonstrate convergence.

(e) (5 Points) For the most reasonable value of the time step in part (d), plot C_M, C_H, C_X, C_{ME} and C_T as functions of dimensionless space time.