R6.1 The Attainable Region

A technique developed by Professors Glasser and Hildebrandt[1] allows one to find the optimum reaction system for certain types of rate laws. The WWW[1] uses modified van de Vusse kinetics, that is,

$$A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B \xrightarrow{k_3} C$$

A: CSTR
B: PFR
C: CSTR & PFR

$$2A \xrightarrow{k_4} D$$

to illustrate what combination of reactors PFR/CSTR should be used to obtain the maximum amount of B. The combined mole balance and rate laws for these liquid-phase reactions can be written in terms of space time as

van de Vusse kinetics

$$\frac{dC_A}{d\tau} = -k_1C_A + k_2C_B - k_4C$$

$$\frac{dC_B}{d\tau} = k_1C_A - k_2C_B - k_3C_B$$

PFR

$$\frac{dC_C}{d\tau} = k_3C_B$$

$$\frac{dC_D}{d\tau} = \frac{k_4}{2}C_A^2$$

One can solve this set of ODEs to obtain the plot of C_B as a function of C_A shown in Figure R6-1.1.

In a similar fashion one can solve the combined CSTR mole balances and rate laws, that is,

CSTR

$$C_{A0} - C_A = \tau[k_1C_A - k_2C_B + k_4C_A^2]$$
$$C_B = \tau[k_1C_A - k_2C_B - k_3C_B]$$

These equations can be solved to give C_A and C_B as a function of space time and also C_B as a function of C_A. The latter is shown as the dashed line in Figure R6-1.1.

The values of the specific reaction rates or $k_1 = 0.01\ s^{-1}$, $k_2 = 5\ s^{-1}$, $k_3 = 10\ s^{-1}$, $k_4 = 100\ \frac{m^3}{kmol \cdot s}$.

The WWW[1] shows how to use these plots along with the attainable region technique to maximize the amount of B produced.

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[1] Department of Chemical Engineering, Witswatersrand University, Johannesburg, South Africa. See also D. Glasser, D. Hildebrandt, and C. Crowe, *IEC Res.*, *26*, 1803 (1987). *www.engin.umich.edu/~cre/Chapters/ARpages/Intro/intro.htm* and *www.wits.ac.za/fac/engineering/procmat/ARHomepage/frame.htm*

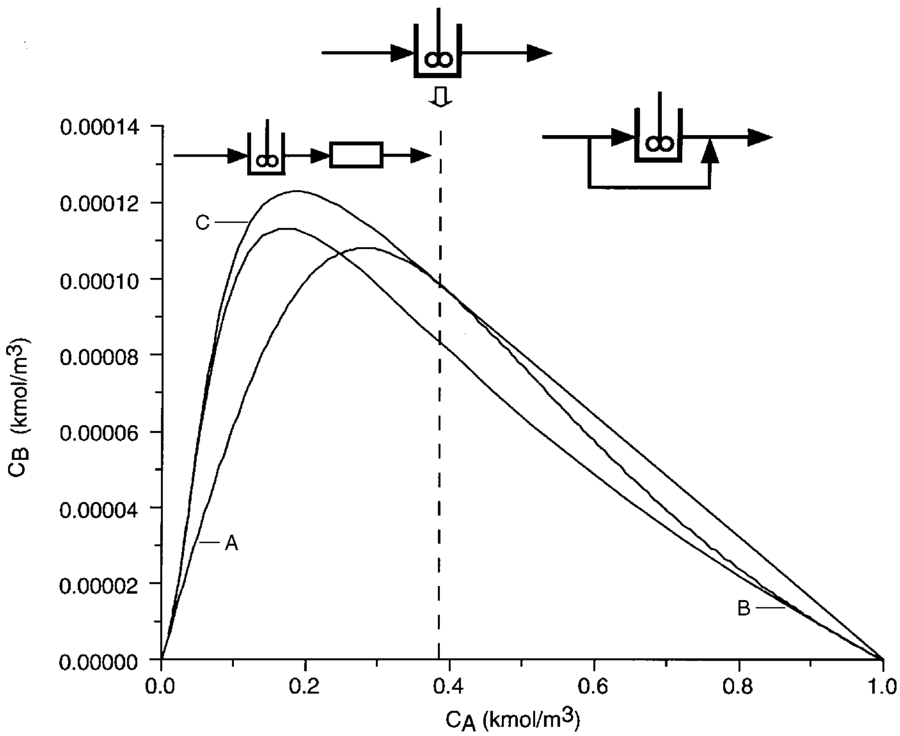

Figure R6-1.1 Phase plane plots of C_B as a function of C_A.

From Figure R6-1.1, we see that if the space time is such that the effluent concentration of A is between 0.38 and 1.0 kmol/m^3, a CSTR with by-pass will give us the maximum concentration of B. If the effluent concentration A is exactly 0.38, then a single CSTR is the best choice. Finally, if the total space time ($\tau = \tau_{PFR} + \tau_{CSTR}$) is such that the effluent concentration is below 0.38 kmol/m^3, then a CSTR followed by a PFR will give the maximum amount of B.