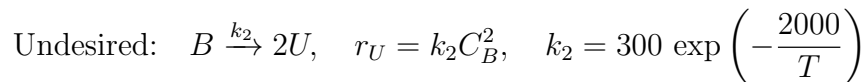
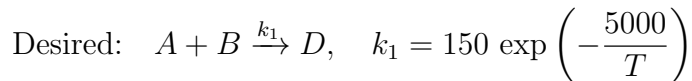


# Solution

## (a) Instantaneous Selectivity $S_{D/U}$

Reactions:



For the desired product  $D$ :

$$r_D = k_1 C_A C_B$$

For the undesired product  $U$ :

$$r_U = k_2 C_B^2$$

The instantaneous selectivity is:

$$S_{D/U} \equiv \frac{r_D}{r_U} = \frac{k_1 C_A C_B}{k_2 C_B^2} = \frac{k_1}{k_2} \cdot \frac{C_A}{C_B}$$

Substituting the Arrhenius forms:

$$\frac{k_1}{k_2} = \frac{150 e^{-5000/T}}{300 e^{-2000/T}} = \frac{1}{2} e^{-3000/T}$$

Thus:

$$S_{D/U} = \frac{1}{2} e^{-3000/T} \cdot \frac{C_A}{C_B}$$

**Interpretation:** Higher  $T$  increases  $S_{D/U}$  since the desired step has higher activation energy. Large  $C_A$  and low  $C_B$  also improve selectivity.

## (b) Reactor Systems and Operating Conditions

### 1. Semibatch Reactor (Charge A, Feed B Slowly)

- **Schematic:** Agitated tank with temperature control; charge with excess  $A$  at  $t = 0$ , feed  $B$  continuously.
- **Rationale:**  $r_U \propto C_B^2$ , so keeping  $C_B$  low suppresses the undesired second-order pathway while  $r_D \propto C_A C_B$  still proceeds efficiently due to high  $C_A$ .
- **Operating conditions:**
  - Maintain high  $T$  (within safety limits) to favor the desired path.
  - Large initial  $C_A$ , slow  $B$  feed to keep  $C_B$  small.
  - Stop the run as soon as  $A$  is mostly consumed to avoid further decomposition of  $B$ .

## 2. Plug Flow Reactor (PFR) with Distributed $B$ Injection

- **Schematic:** Start the reactor with  $A$  only; inject small quantities of  $B$  at several points along the reactor.
- **Rationale:** Keeps  $C_B$  low at all points in the reactor, ensuring the desired reaction dominates.
- **Operating conditions:**
  - High, uniform temperature profile.
  - Split  $B$  into multiple side feeds; control feed spacing and rate to cap  $C_B$  at a low value.
  - Large excess of  $A$  at inlet.

### General tips for both systems:

- Use dilution or solvent flow to further lower  $C_B$ .
- Minimize residence time to avoid excessive  $B \rightarrow 2U$  conversion.
- Preheat  $B$  only immediately before mixing with  $A$  to reduce decomposition risk.