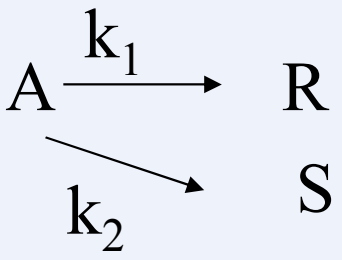
SISTEM
REAKSI KOMPLEKS

Oleh :

Reaksi kompleks :

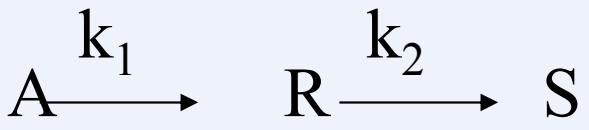
- **Reaksi Paralel** :



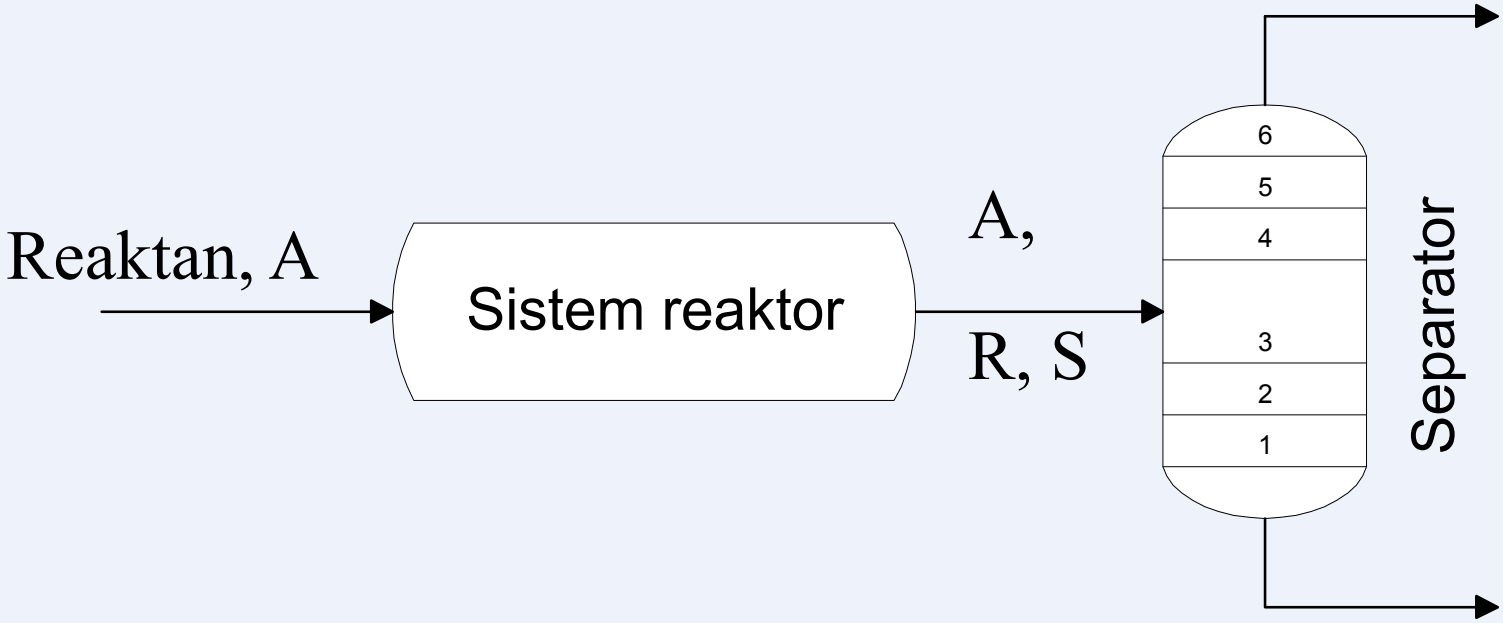
Contoh : $2\ C_4H_9OH \rightarrow 2\ C_4H_8 + 2\ H_2O$

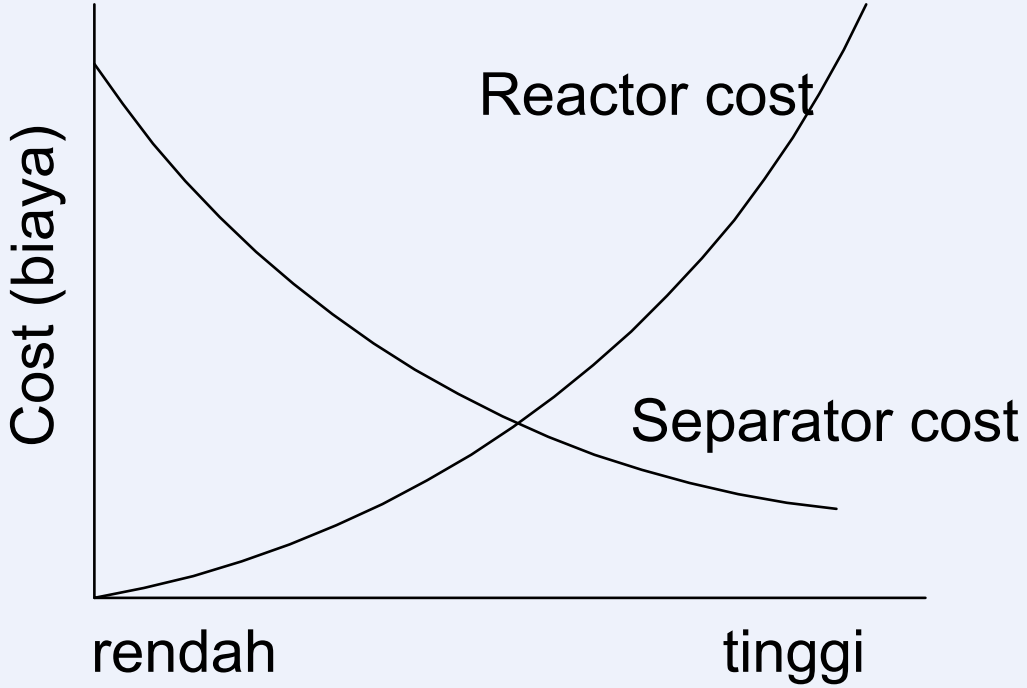
$C_4H_9\text{-}O\text{-}C_4H_9 + H_2O$

- **Reaksi Seri** :



Contoh : $(CH_2)_2O + NH_3 \rightarrow HOC_2H_4NH_2 \rightarrow (HOC_2H_4)_2NH$


Reaktan, A
Sistem reaktor
A,
R, S
6
5
4
3
2
1
Separator


Reactor cost
Separator cost
Cost (biaya)
rendah
tinggi

REAKSI PARALEL

- Reaksi : $A + B \xrightarrow{k_1} R + T$ $\qquad r_R = k_1 C_A^{a1} C_B^{b1}$

  $A + B \xrightarrow{k_2} S + U$ $\qquad r_S = k_2 C_A^{a2} C_B^{b2}$

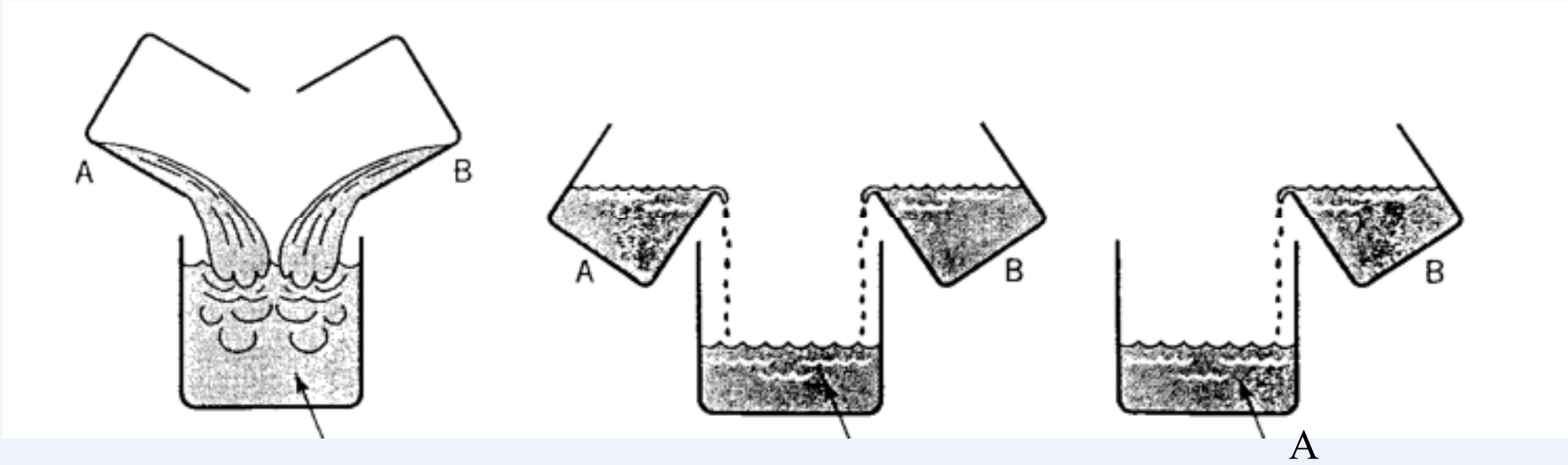
  Bila kedua reaksi paralel berorde sama, maka : $\dfrac{r_R}{r_S} = \dfrac{k_1}{k_2}$

- Distribusi produk bergantung pada k_1/k_2
  (ukuran reaktor tak berpengaruh)
- Pengendalian dapat dilakukan dengan dua cara :
  1. Ubah temperatur , bila nilai energi aktivasi kedua reaksi berbeda
  2. Gunakan katalis yang selektif (cara ini lebih efektif).

Bila orde reaksi berbeda : $\frac{r_R}{r_S} = \frac{k_1}{k_2} C_A^{a1-a2} C_B^{b1-b2}$

- **Reaktor partaian** (tidak bersinambung) :

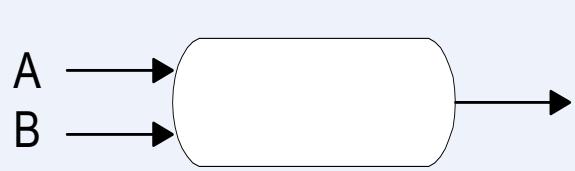
C_A ,C_B tinggi	C_A, C_B rendah	$C_A$tinggi, C_B rendah

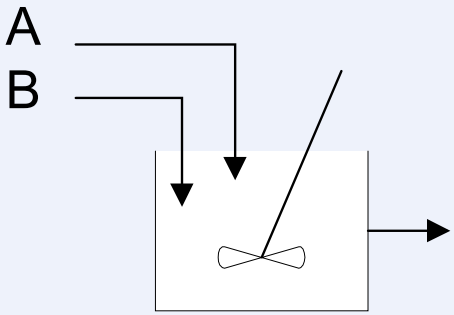


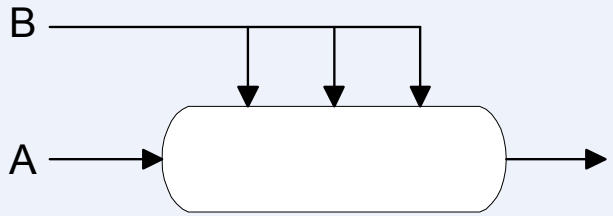
A,B cepat A,B lambat A ditambah B lambat

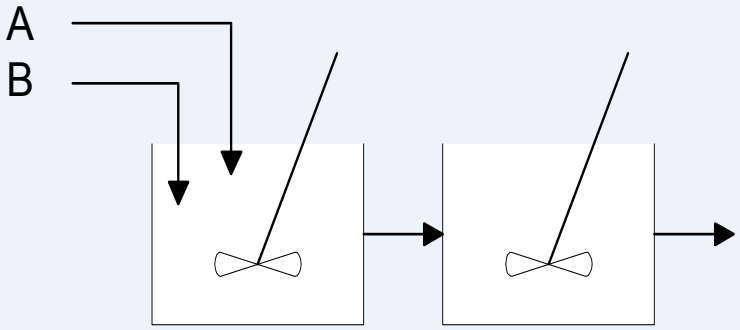
- **Reaktor sinambung (kontinyu) :**

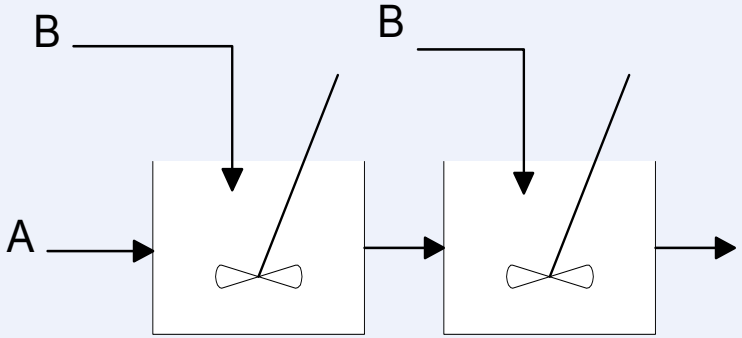
C_A ,C_B tinggi	C_A, C_B rendah	$C_A$tinggi, C_B rendah











REAKSI SERI (orde – 1)

Contoh 1 :

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$$r_1 = k_1 C_A$$

$$r_2 = k_2 C_B$$

Reaktor batch/ RAS :

$$\frac{dC_A}{d\tau} = -r_1 = -k_1 C_A$$

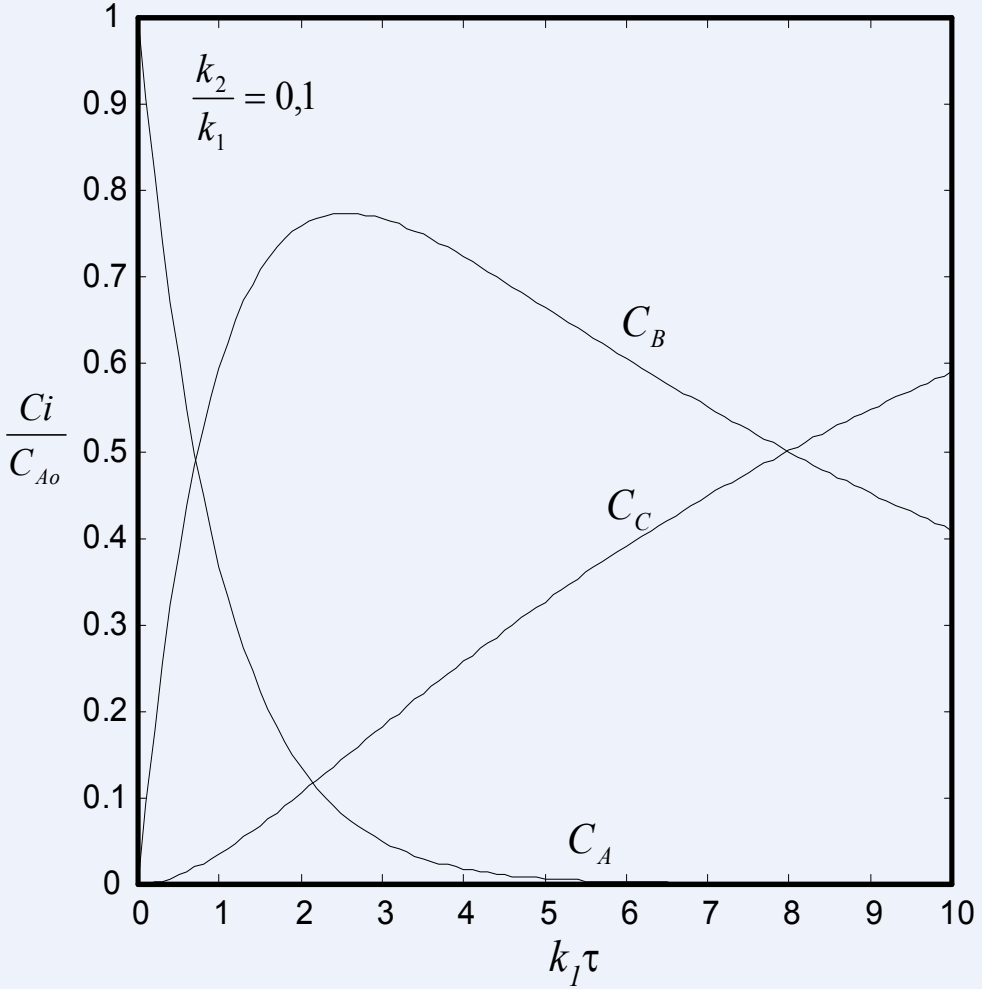
$$\frac{dC_B}{d\tau} = r_1 - r_2 = k_1 C_A - k_2 C_B$$

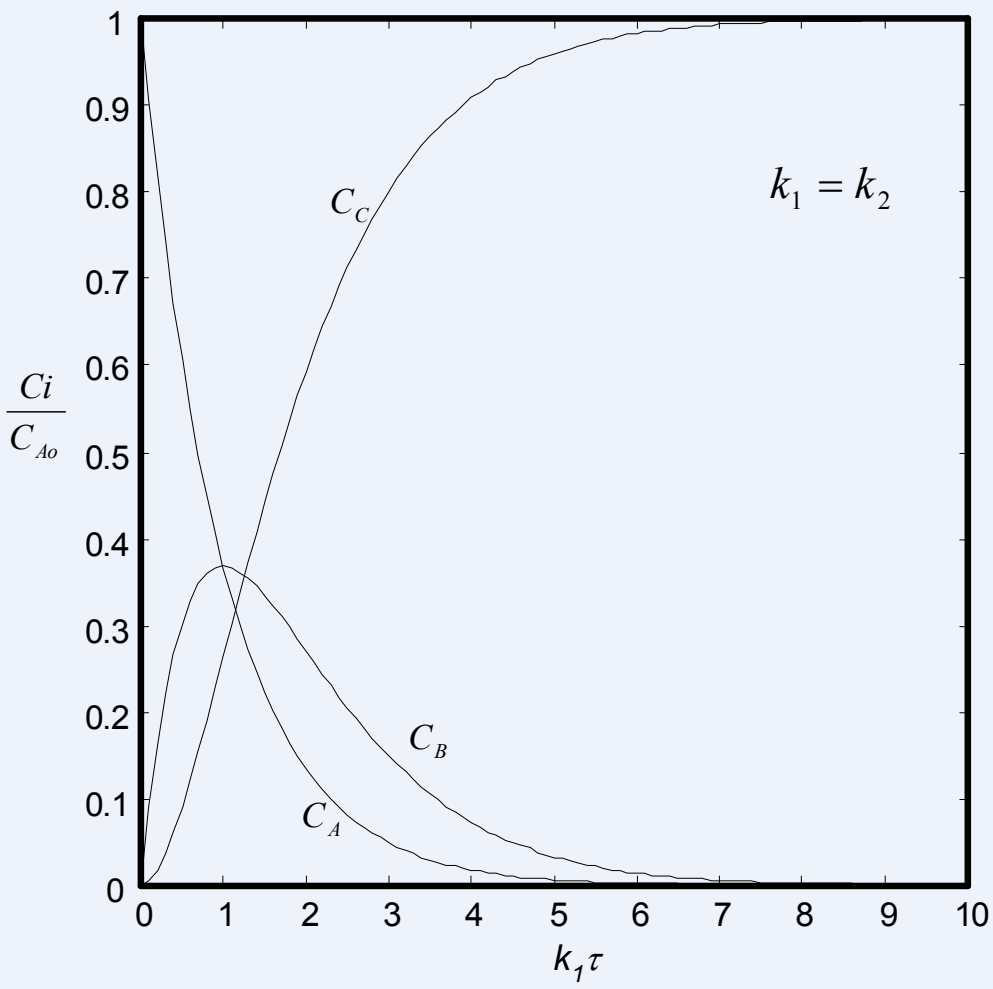
$$\frac{dC_C}{d\tau} = r_2 = k_2 C_B$$

$$C_A = C_{Ao} e^{-k_1 \tau}$$

$$C_B = C_{Ao} \frac{k_1}{k_2 - k_1} \left(e^{-k_1 \tau} - e^{-k_2 \tau} \right)$$

$$C_C = C_{Ao} \left(1 - \frac{k_2}{k_2 - k_1} e^{-k_1 \tau} + \frac{k_1}{k_2 - k_1} e^{-k_2 \tau} \right)$$

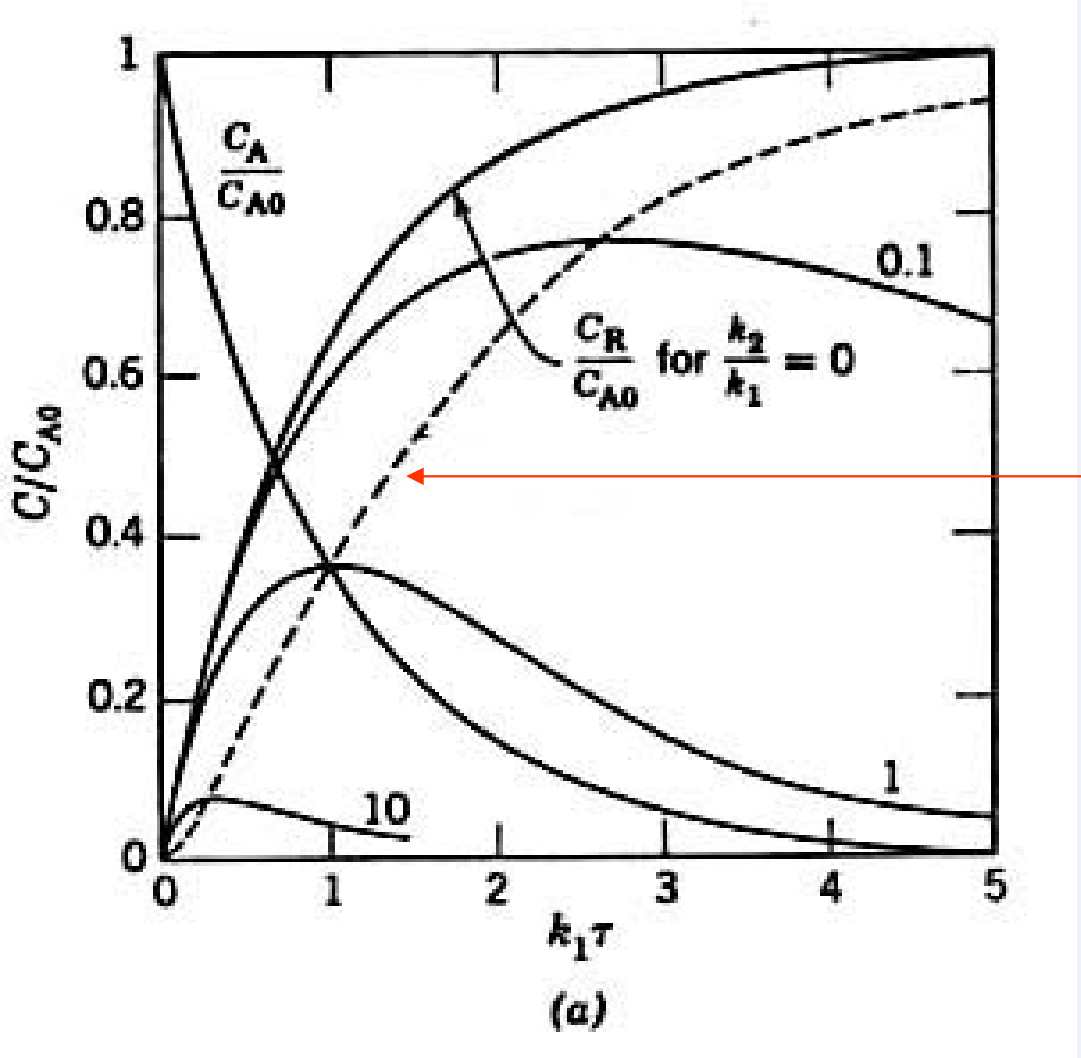

$\frac{k_2}{k_1} = 0{,}1$
C_B
C_C
C_A
$\frac{Ci}{C_{Ao}}$
$k_1\tau$


$k_1 = k_2$
C_C
C_B
C_A
$\frac{Ci}{C_{Ao}}$
$k_1\tau$

$k_2/k_1 = 0{,}1$

$k_2 = k_1$

Reaktor partaian / RAS



$$A \xrightarrow{k_1} R \xrightarrow{k_2} S$$

Orde-1,

Tempat kedudukan $C_R$max

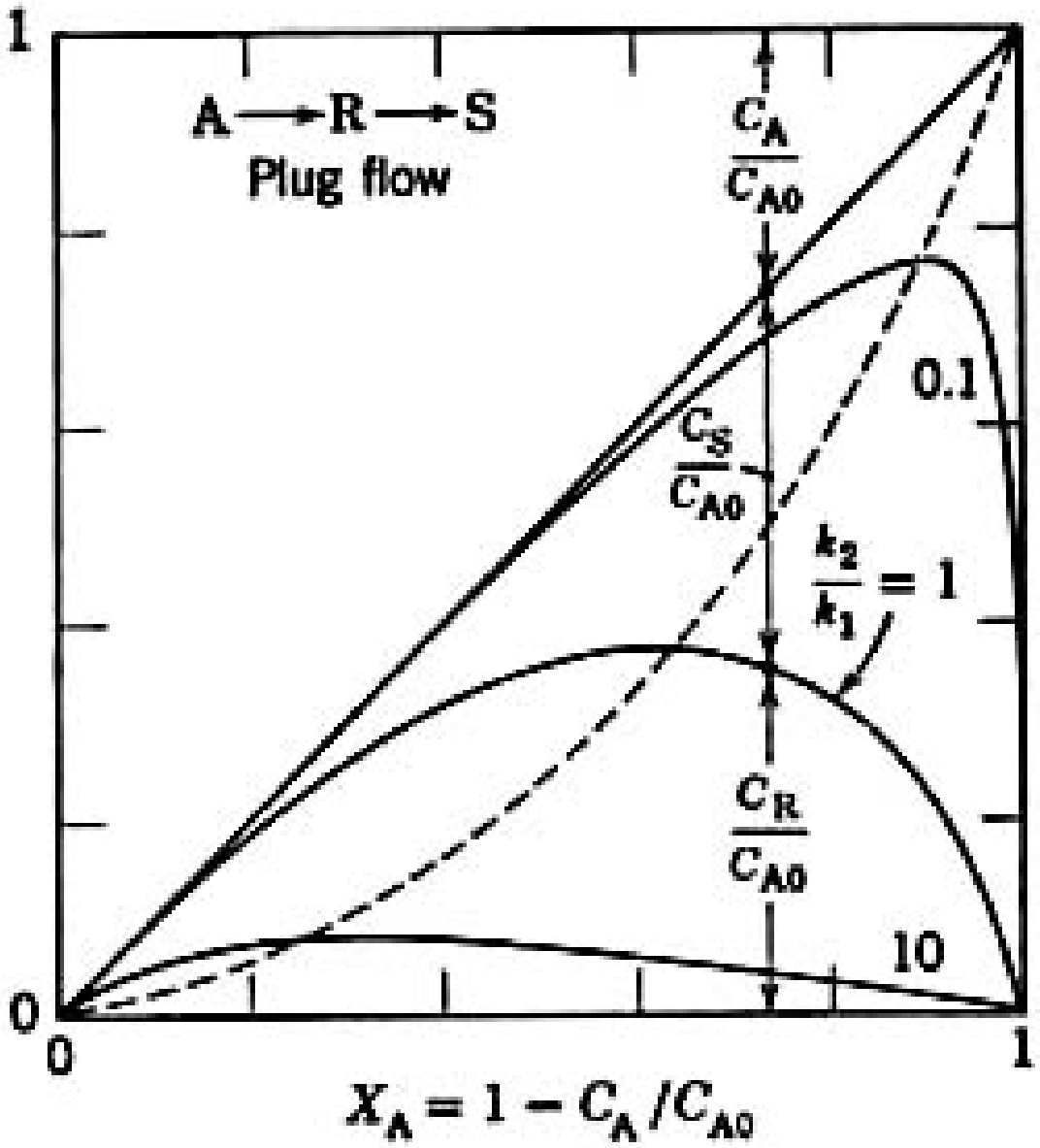
$$\frac{C_A}{C_{A0}} = e^{-k_1\tau}$$

$$\frac{C_R}{C_{A0}} = \frac{k_1}{k_2 - k_1}\left(e^{-k_1\tau} - e^{-k_2\tau}\right)$$

$$\frac{C_S}{C_{A0}} = \left(1 - \frac{k_2}{k_2 - k_1}e^{-k_1\tau} + \frac{k_1}{k_2 - k_1}e^{-k_2\tau}\right)$$

Perbandingan C_A, C_R, dan C_S

Pada RAS



Produk intermediet maksimum :

$$\frac{dC_B}{d\tau} = 0 = \frac{k_1 C_{Ao}}{k_2 - k_1}\left(-k_1 e^{-k_1\tau} + k_2 e^{-k_2\tau}\right)$$

$$\tau_{\max} = \frac{\ln(k_2/k_1)}{k_2 - k_1} \qquad C_{B,\max} = C_{Ao}\left(\frac{k_1}{k_2}\right)^{\frac{k_2}{k_2 - k_1}}$$

Selektivitas :

$$S = \frac{\text{mol zat yang diinginkan (R)}}{\text{total mol zat produk + zat lain yang terbentuk}}$$

Contoh 2 :

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D$$

$$C_A = C_{Ao} e^{-k_1 t}$$

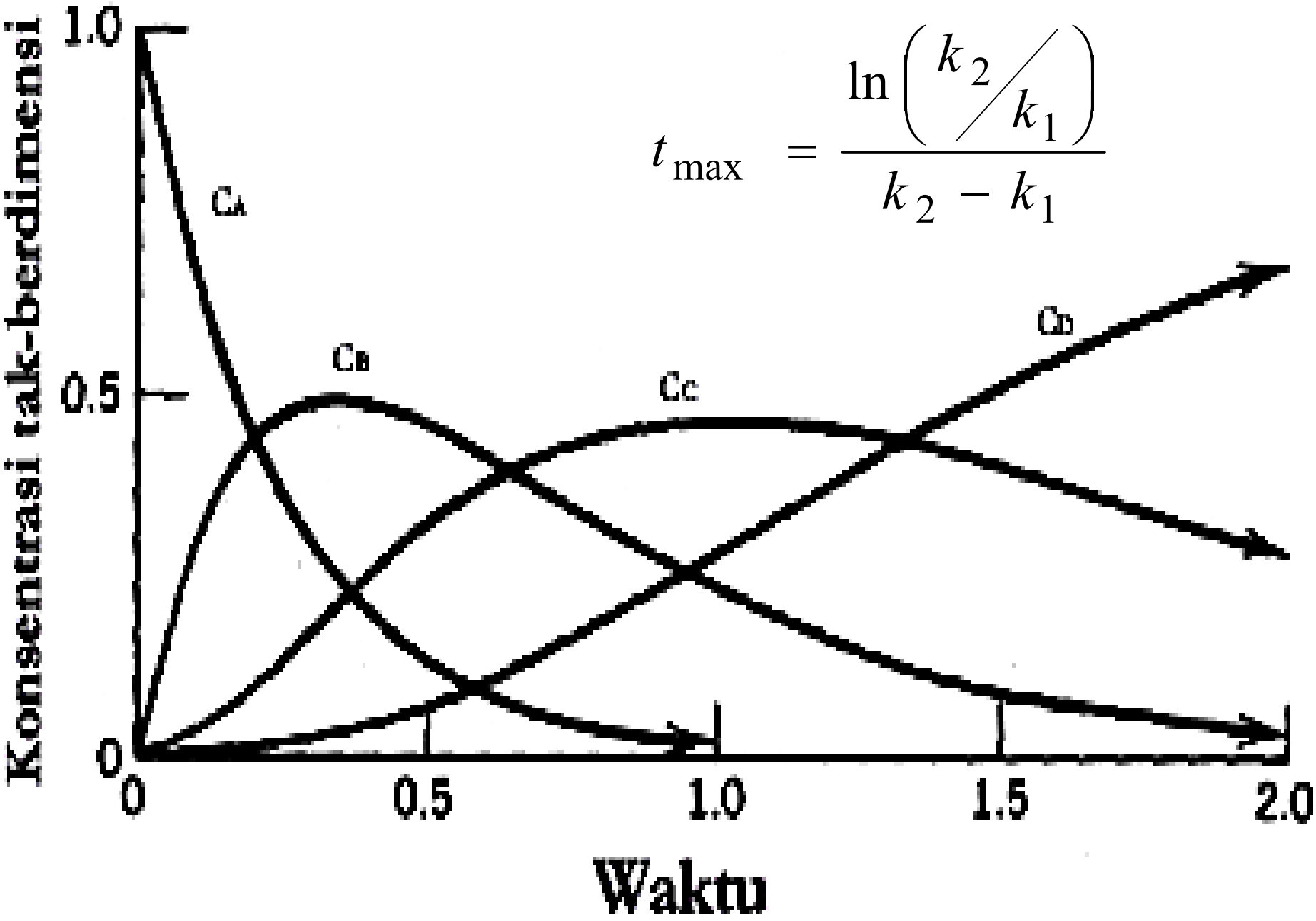
$$C_B = \left[C_{Bo} - \frac{C_{Ao} k_1}{k_2 - k_1} \right] e^{-k_2 t} + \left[\frac{C_{Ao} k_1}{k_2 - k_1} \right] e^{-k_1 t}$$

$$C_C = \left[C_{Co} - \frac{C_{Bo} k_2}{k_3 - k_2} + \frac{C_{Ao} k_1 k_2}{(k_3 - k_1)(k_3 - k_2)} \right] e^{-k_3 t}$$

$$+ \left[\frac{C_{Bo} k_2}{k_3 - k_2} - \frac{C_{Ao} k_1 k_2}{(k_3 - k_2)(k_2 - k_1)} \right] e^{-k_2 t}$$

$$+ \left[\frac{C_{Ao} k_1 k_2}{(k_3 - k_1)(k_2 - k_1)} \right] e^{-k_1 t}$$

$$C_D = C_{Do} + (C_{Ao} - C_A) + (C_{Bo} - C_B) + (C_{Co} - C_C)$$



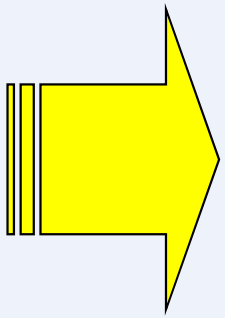
$$t_{\max} = \frac{\ln\left(k_2 / k_1\right)}{k_2 - k_1}$$

Reaktor Tangki Ideal Kontinyu :

$$\frac{dC_A}{d\tau} = -r_1 = -k_1 C_A$$

$$\frac{dC_B}{d\tau} = r_1 - r_2 = k_1 C_A - k_2 C_B$$

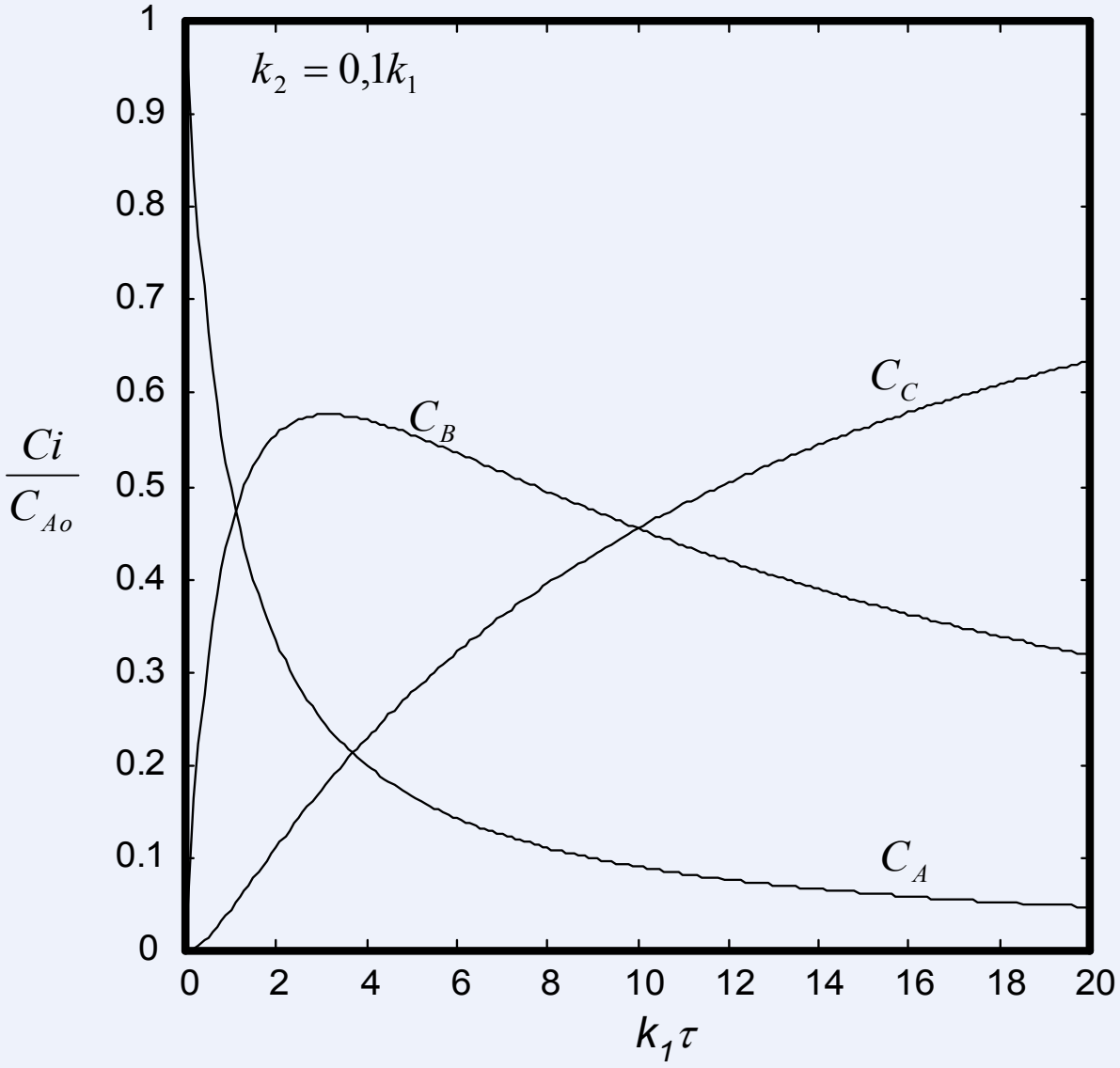
$$\frac{dC_C}{d\tau} = r_2 = k_2 C_B$$



$$C_A = \frac{C_{Ao}}{1 + k_1 \tau}$$

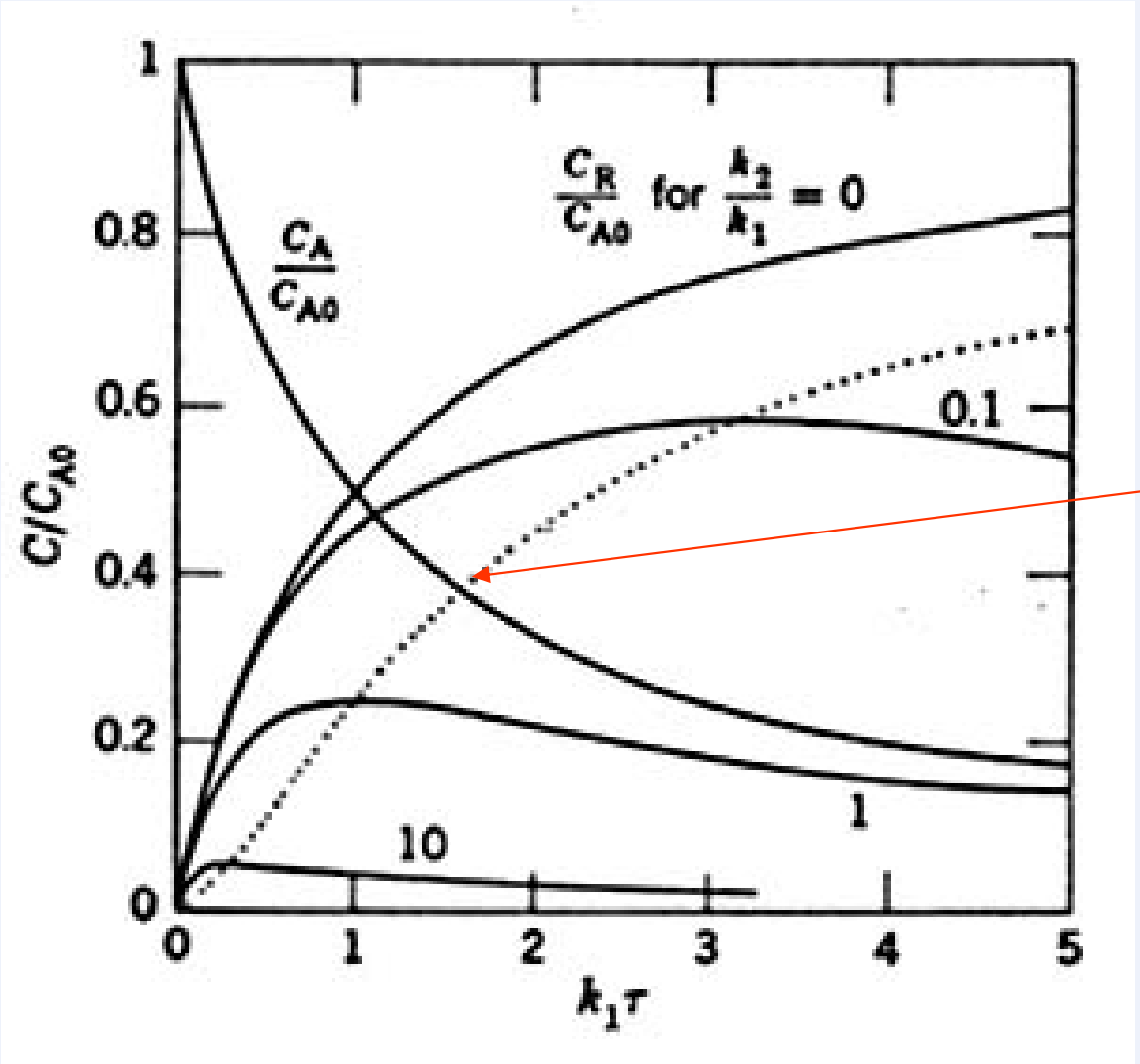
$$C_B = \frac{k_1 C_{Ao} \tau}{(1 + k_1 \tau)(1 + k_2 \tau)}$$

$$C_C = \frac{k_1 k_2 C_{Ao} \tau^2}{(1 + k_1 \tau)(1 + k_2 \tau)}$$


$k_2 = 0{,}1k_1$
C_C
C_B
C_A
$\frac{Ci}{C_{Ao}}$
$k_1\tau$
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
2
4
6
8
10
12
14
16
18
20

$$k_2 / k_1 = 0{,}1$$

Reaktor Tangki Ideal kontinyu :



$$A \xrightarrow{k_1} R \xrightarrow{k_2} S$$

Orde-1,

Tempat kedudukan $C_R$max

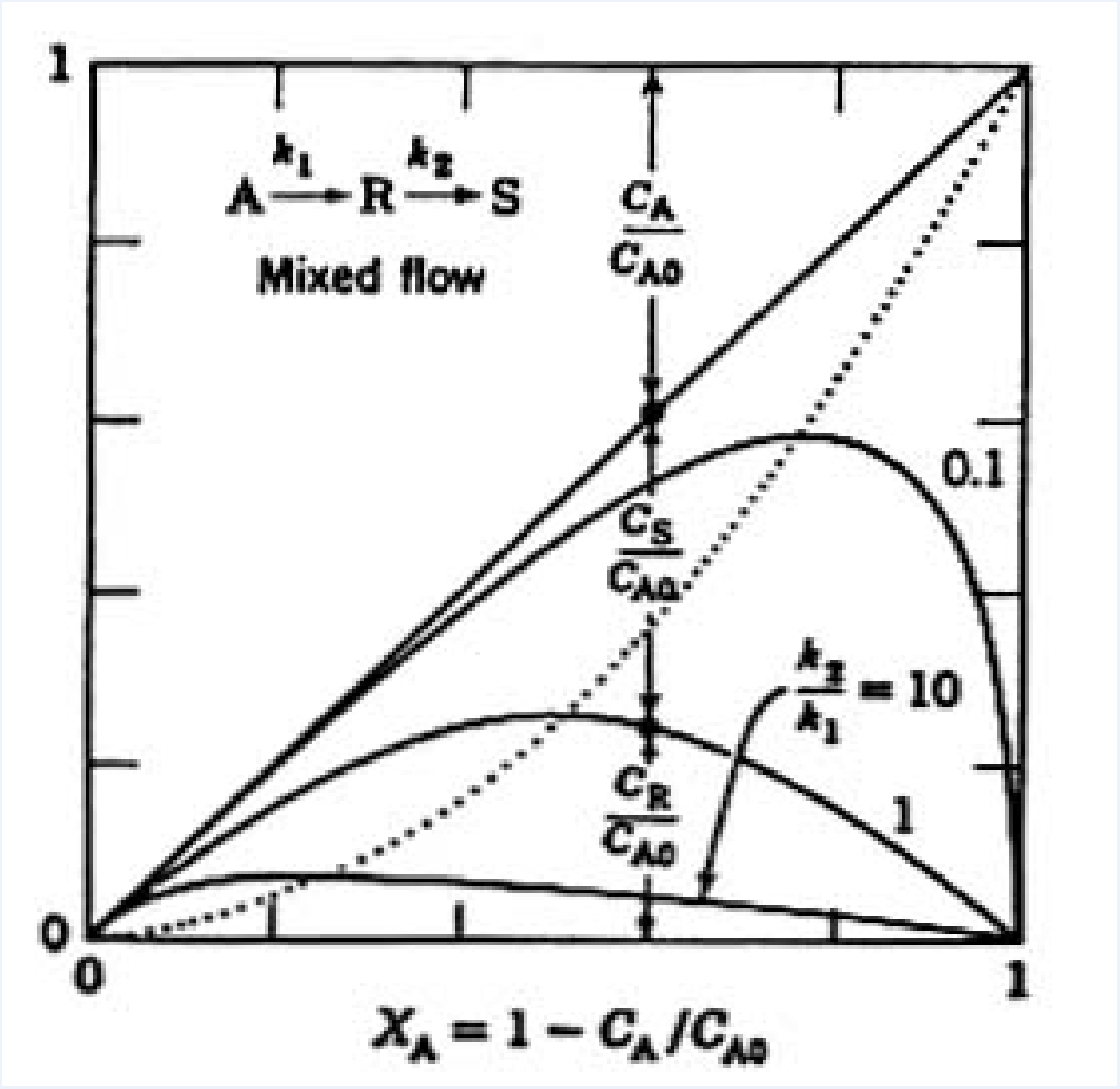
$$\frac{C_A}{C_{A0}} = \frac{1}{1+k_1\tau}$$

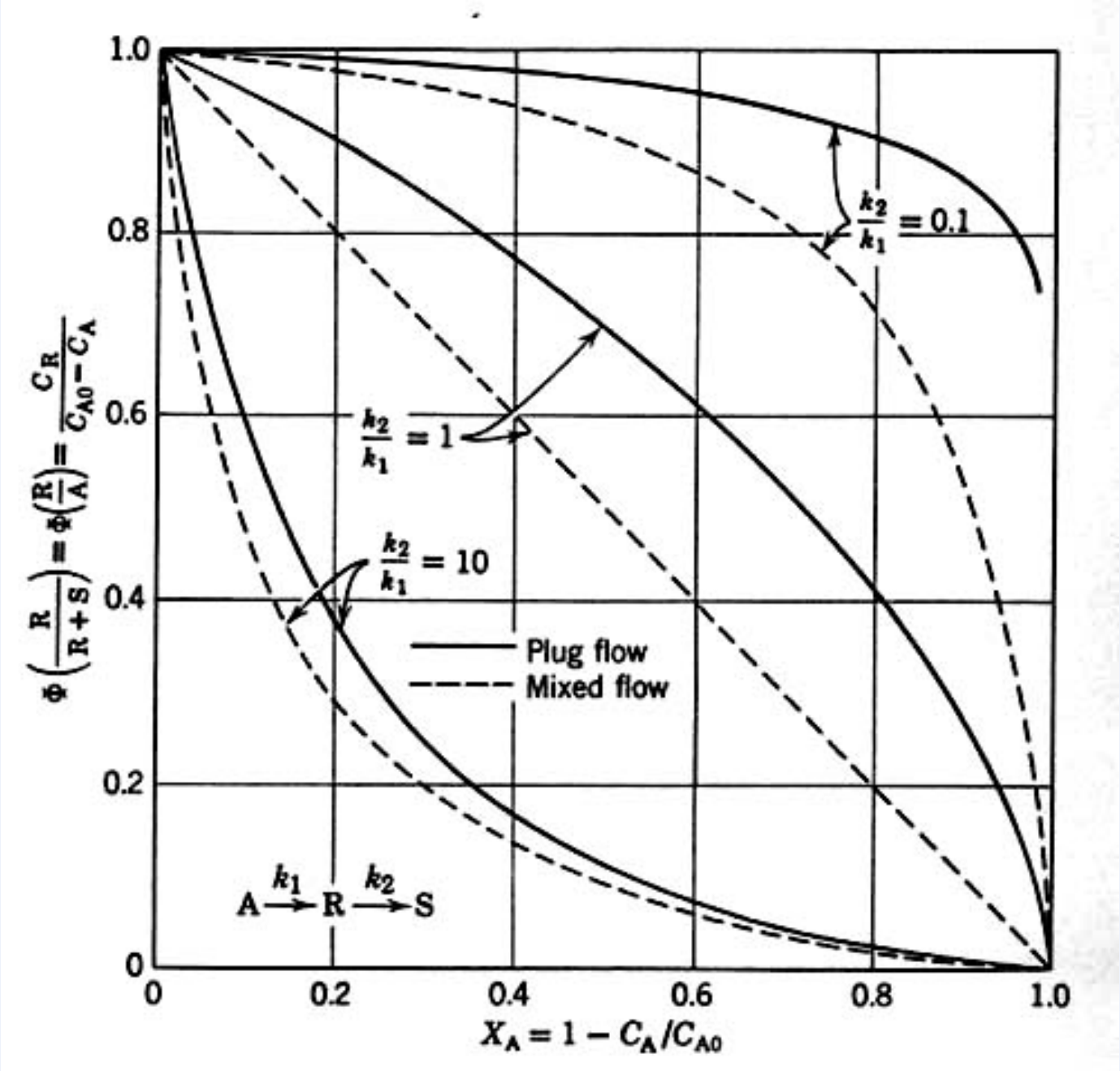
$$\frac{C_R}{C_{A0}} = \frac{k_1\tau}{(1+k_1\tau)(1+k_2\tau)}$$

$$\frac{C_S}{C_{A0}} = \frac{k_1k_2\tau^2}{(1+k_1\tau)(1+k_2\tau)}$$

Perbandingan C_A , C_R , dan C_S

Pada RTIK





Perbandingan Fractional yield R Dalam RTIK dan RAS

Soal 3 :

$2A \xrightarrow{k_1} B$ $\qquad r_1 = k_1 C_A^2$

$B + C \xrightarrow{k_2} P$ $\qquad r_2 = k_2 C_B C_C$

Reaktor Batch, vol. konstan :

$$\frac{dC_A}{dt} = r_A = -2k_1 C_A^2$$

$$\frac{dC_B}{dt} = r_B = k_1 C_A^2 - k_2 C_B C_C$$

$$\frac{dC_C}{dt} = r_C = -k_2 C_B C_C$$

$$\frac{dC_P}{dt} = r_P = k_2 C_B C_C$$

Jika :

$C_{A0} = C_{C0} = 30$ mol/m^3

$k_1 = 0{,}01 \qquad k2 = 0{,}02$

C_A, C_B, C_C, dan C_P = f(t) ??

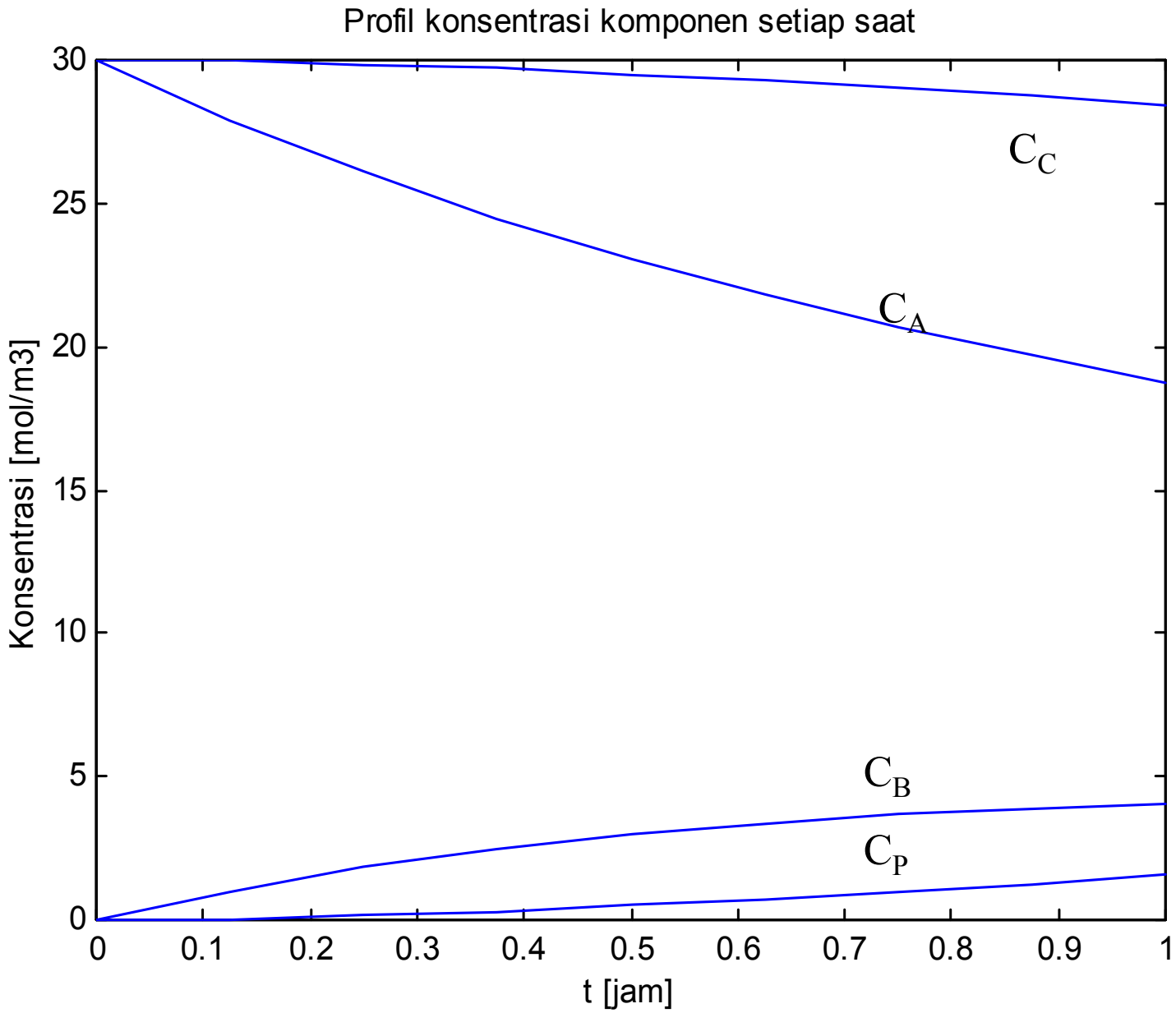
Rutin u/ fungsi pers diferensial :

```
function dCdt = contoh2(t,C)

% Ca = C(1)
% Cb = C(2)
% Cc = C(3)
% Cp = C(4)
% nilai awal dari sistem persamaan diferensial ini
adalah:
% C = [30  0  30  0]
% tspan = [0:0.125:1]

k1 = 0.01;
k2 = 0.02;
dCdt = [ -2.*k1.*C(1).^2
   k1.*C(1).^2 - k2.*C(2).*C(3)
   -k2.*C(2).*C(3)
   k2.*C(2).*C(3)];
```

Hasil simulasi : u/ $C_{A0} = C_{C0} = 30$ mol/m^3 , $C_{B0} = C_{P0} = 0$



$k_1 = 0{,}01$

$k_2 = 0{,}02$

REAKSI SERI - PARALEL

Contoh : $A + B \rightarrow R$

$R + B \rightarrow S$

Ditinjau dari A : $A \rightarrow R \rightarrow S$ (Seri)

Ditinjau dari B : $B \rightarrow R$ (paralel)

$B \rightarrow S$

Reaksi orde-1 : $r_A = - k_1 C_A C_B$

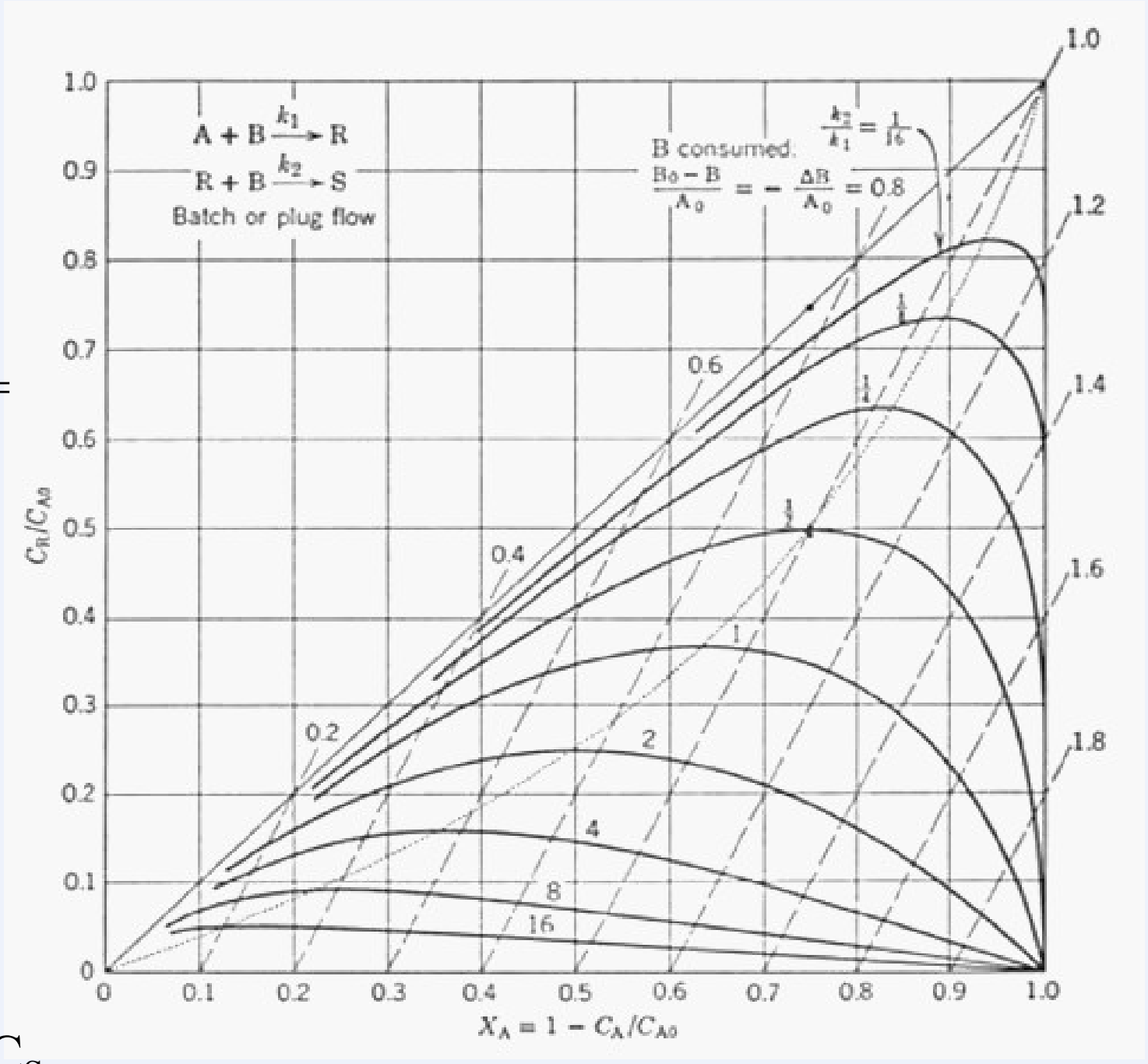
$r_B = - k_1 C_A C_B - k_2 C_R C_B$

$r_R = k_1 C_A C_B - k_2 C_R C_B$

$r_S = k_2 C_R C_B$

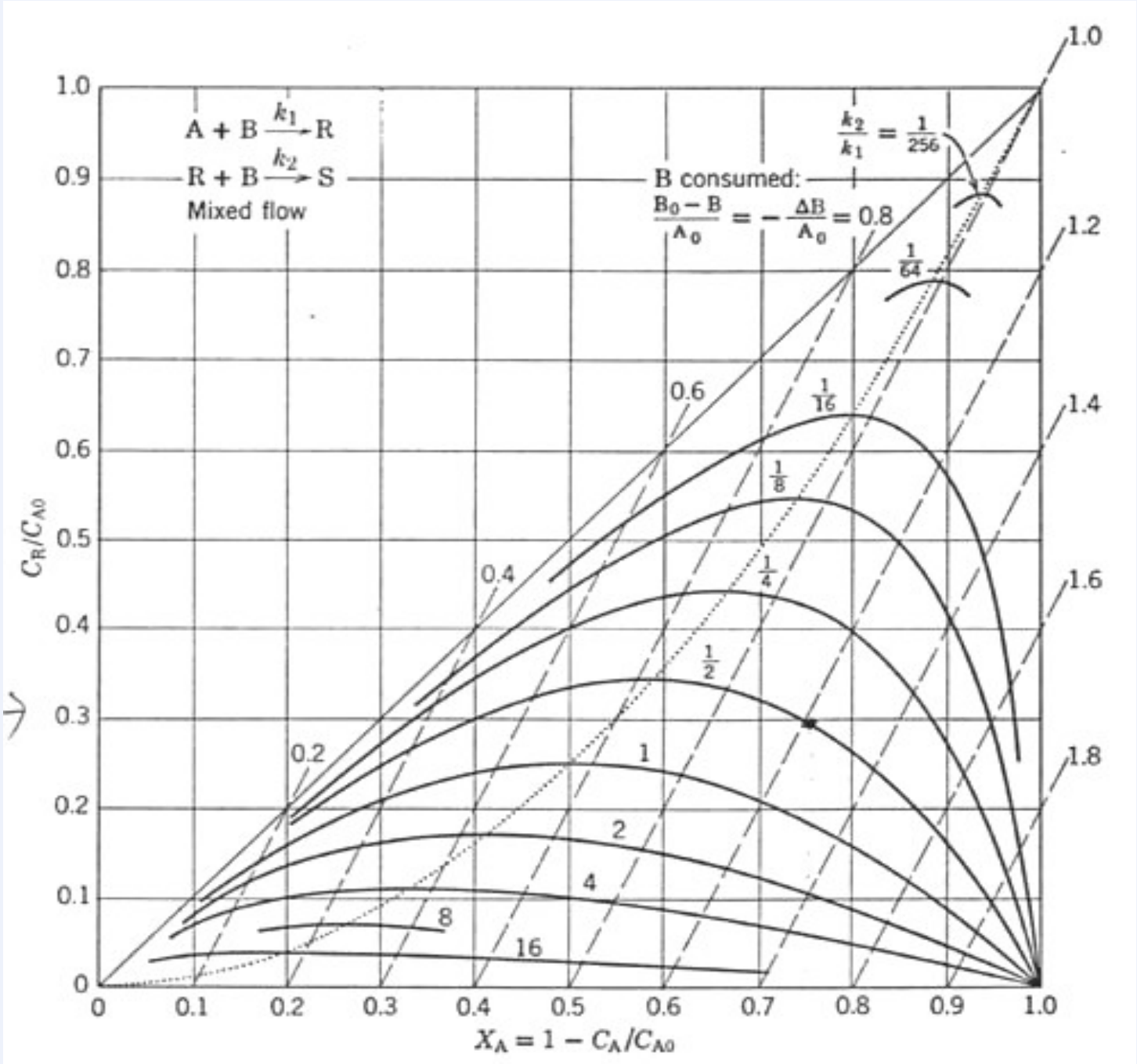
Untuk Reaktor Batch / RAS

$$C_{A0} + C_{R0} + C_{S0} = C_A + C_R + C_S$$



$$\Delta C_A = \Delta C_R = \Delta C_S$$

Untuk RTIK


A + B $\xrightarrow{k_1}$ R
R + B $\xrightarrow{k_2}$ S
Mixed flow
B consumed:
$\frac{B_0 - B}{A_0} = -\frac{\Delta B}{A_0} = 0.8$
$\frac{k_2}{k_1} = \frac{1}{256}$
$\frac{1}{64}$
$\frac{1}{16}$
$\frac{1}{8}$
$\frac{1}{4}$
$\frac{1}{2}$
1
2
4
8
16
0.2
0.4
0.6
1.0
1.2
1.4
1.6
1.8
C_R/C_{A0}
$X_A = 1 - C_A/C_{A0}$
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0