Lecture 12

Chemical Reaction Engineering (CRE) is the field that studies the rates and mechanisms of chemical reactions and the design of the reactors in which they take place.

Lecture 12 – Tuesday

- Multiple Reactions
  - Selectivity and Yield
    $$A \xrightarrow{k_D} D$$
    $$A \xrightarrow{k_U} U$$
  - Series Reactions
    $$A \rightarrow B \rightarrow C$$
  - Complex Reactions
    $$A + B \rightarrow C + D$$
    $$A + C \rightarrow E$$

4 Types of Multiple Reactions

- Series: $A \rightarrow B \rightarrow C$
- Parallel: $A \rightarrow D$

  $A \rightarrow U$
- Independent: $A \rightarrow B$

  $C \rightarrow D$
- Complex: $A + B \rightarrow C + D$

  $A + C \rightarrow E$

With multiple reactors, either molar flow or number of moles must be used (no conversion!)

Selectivity and Yield

There are two types of selectivity and yield: Instantaneous and Overall.

	Instantaneous	Overall
Selectivity	$S_{DU} = \frac{r_D}{r_U}$	$\tilde{S}_{DU} = \frac{F_D}{F_U}$
Yield	$Y_D = \frac{r_D}{-r_A}$	$\tilde{Y}_D = \frac{F_D}{F_{A0} - F_A}$

Selectivity and Yield

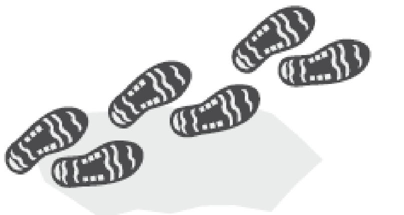
Example: $A + B \xrightarrow{k_1} D$ Desired Product: $r_D = k_1 C_A^2 C_B$

$A + B \xrightarrow{k_2} U$ Undesired Product: $r_U = k_2 C_A C_B$

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

To maximize the selectivity of D with respect to U run at high concentration of A and use PFR.

Gas Phase
Multiple Reactions



Number all reactions

Mole balances:

Mole balance on each and every species

PFR $\frac{dF_j}{dV} = r_j$

CSTR $F_{j0} - F_j = -r_j V$

Batch $\frac{dN_j}{dt} = r_j V$

Membrane ("i" diffuses in) $\frac{dF_i}{dV} = r_i + R_i$

Liquid-semibatch $\frac{dC_j}{dt} = r_j + \frac{v_0(C_{j0} - C_j)}{V}$

Rates:

Laws $r_{ij} = k_{ij} f_i(C_j, C_n)$

Relative rates $\frac{r_{iA}}{-a_i} = \frac{r_{iB}}{-b_i} = \frac{r_{iC}}{c_i} = \frac{r_{iD}}{d_i}$

Net rates $r_j = \sum_{i=1}^{q} r_{ij}$

Stoichiometry:

Gas phase $C_j = C_{T0} \frac{F_j}{F_T} \frac{P}{P_0} \frac{T_0}{T} = C_{T0} \frac{F_j}{F_T} \frac{T_0}{T} y$

$$y = \frac{P}{P_0}$$

$$F_T = \sum_{j=1}^{n} F_j$$

$$\frac{dy}{dW} = -\frac{\alpha}{2y}\left(\frac{F_T}{F_{T0}}\right)\frac{T}{T_0}$$

Liquid phase $v = v_0$

$$C_A, C_B, \ldots$$

Combine:

Polymath will combine all the equations for you. Thank you,

Multiple Reactions

A) **Mole Balance** of each and every species

Flow

Batch

$$\frac{dF_A}{dV} = r_A \qquad \frac{dN_A}{dt} = r_A V$$

$$\frac{dF_B}{dV} = r_B \qquad \frac{dN_B}{dt} = r_B V$$

Multiple Reactions

B) Rates

a) **Rate Law** for each reaction:

$$-r_{1A} = k_{1A} C_A C_B$$

$$-r_{2A} = k_{2A} C_C C_A$$

b) Net **Rates**:

$$r_A = \sum_{i=1} r_{iA} = r_{1A} + r_{2A}$$

c) Relative **Rates**:

$$\frac{r_{iA}}{-a_i} = \frac{r_{iB}}{-b_i} = \frac{r_{iC}}{c_i} = \frac{r_{iD}}{d_i}$$

Multiple Reactions

C) Stoichiometry

Gas:

$$C_A = C_{T0} \frac{F_A}{F_{A0}} \left(\frac{P}{P_0} \right) \left(\frac{T_0}{T} \right)$$

Liquid:

$$C_A = F_A / \upsilon_0$$

Example: $A \rightarrow B \rightarrow C$

(1) $A \rightarrow B$ k_1

(2) $B \rightarrow C$ k_2

Batch Series Reactions

1) **Mole Balances**

$$\frac{dN_A}{dt} = r_A V$$

$$\frac{dN_B}{dt} = r_B V$$

$$\frac{dN_C}{dt} = r_C V$$

$V=V_0$ (constant batch)

$$\frac{dC_A}{dt} = r_A \qquad \frac{dC_B}{dt} = r_A \qquad \frac{dC_C}{dt} = r_A$$

Batch Series Reactions

2) **Rate Laws**

$$-r_{1A} = k_{1A}C_A$$

$$-r_{1B} = k_{1B}C_B$$

Laws

$$r_A = r_{1A}$$

$$r_B = r_{1B} + r_{2B}$$

Net rates

$$\frac{r_{1A}}{-1} = \frac{r_{1B}}{1}$$

$$\frac{r_{2B}}{-1} = \frac{r_{2C}}{1}$$

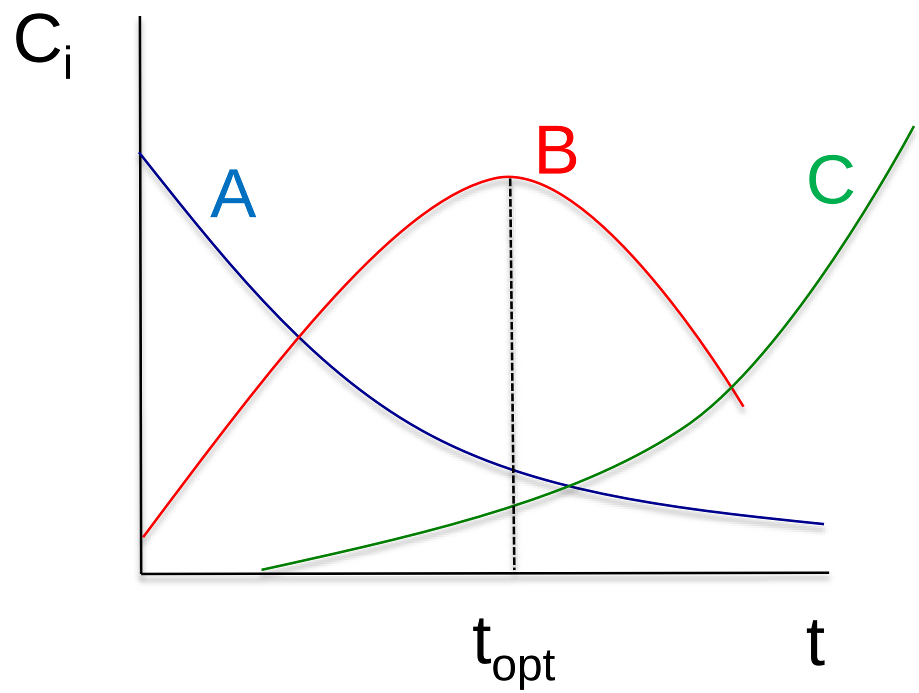
Relative rates

Example: Batch Series Reactions

$A \rightarrow B \rightarrow C$

(1) $A \rightarrow B$

(2) $B \rightarrow C$



1) Mole Balances $V = V_O$

$$\frac{dC_A}{dt} = r_A \qquad \frac{dC_B}{dt} = r_B \qquad \frac{dC_C}{dt} = r_C$$

Example: Batch Series Reactions

2) Rate Laws

Laws:

$$r_{1A} = -k_1 C_A$$

$$r_{2B} = -k_2 C_B$$

Relative:

$$\frac{r_{1A}}{-1} = \frac{r_{1B}}{1} \qquad \frac{r_{2B}}{-1} = \frac{r_{2C}}{1}$$

Example: Batch Series Reactions

3) Combine

Species A:

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

$$C_A = C_{A0} \exp\left(-k_1 t\right)$$

Species B:

$$\frac{dC_B}{dt} = r_B$$

$$r_B = r_{B\,NET} = r_{1B} + r_{2B} = k_1 C_A - k_2 C_B$$

$$\frac{dC_B}{dt} + k_2 C_B = k_1 C_{A0} \exp\left(-k_1 t\right)$$

Example: Batch Series Reactions

Using the integrating factor, $I.F. = \exp\left(\int k_2 dt\right) = \exp(k_2 t)$

$$d\frac{[C_B \exp(k_2 t)]}{dt} = k_1 C_{A0} \exp(k_2 - k_1)t$$

at t = 0, C_B=0

$$C_B = \frac{k_1 C_{A0}}{k_2 - k_1}\left[\exp(-k_1 t) - \exp(-k_2 t)\right]$$

$$C_C = C_{A0} - C_A - C_B$$

$$C_C = \frac{C_{A0}}{k_2 - k_1}\left[k_2\left(1 - e^{-k_1 t}\right) - k_1\left(1 - e^{-k_2 t}\right)\right]$$

Example: CSTR Series Reactions

A→B→C

What is the optimal τ?

1) Mole Balances

A:

$$F_{A0} - F_A + r_A V = 0$$

$$C_{A0} v_0 - C_A v_0 + r_A V = 0$$

$$\boxed{C_{A0} - C_A + r_A \tau = 0}$$

B:

$$0 - v_0 C_B + r_B V = 0$$

$$\boxed{-C_B + r_B \tau = 0}$$

Example: CSTR Series Reactions

A→B→C

2) Rate Laws

Laws:

$$r_{1A} = -k_1 C_A$$

$$r_{2B} = -k_2 C_B$$

Relative:

$$\frac{r_{1A}}{-1} = \frac{r_{1B}}{1} \qquad \frac{r_{2B}}{-1} = \frac{r_{2C}}{1}$$

Net:

$$r_A = r_{1A} + 0 = -k_1 C_A$$

$$r_B = -r_{1A} + r_{2B} = k_1 C_A - k_2 C_B$$

Example: CSTR Series Reactions

A→B→C

3) Combine

$$C_{A0} - C_A - k_1 C_A t = 0$$

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

$$-C_B + \left(k_1 C_A - k_2 C_B\right) t = 0$$

$$C_B = \frac{k_1 C_A t}{1 + k_2 t}$$

$$C_B = \frac{k_1 C_{A0} t}{\left(1 + k_2 t\right)\left(1 + k_1 t\right)}$$

Example: CSTR Series Reactions

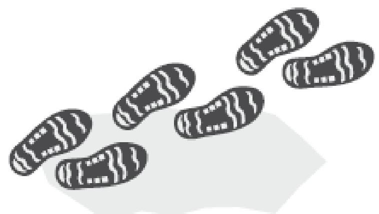
A→B→C

Find τ that gives maximum concentration of B

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

$$\frac{dC_B}{d\tau} = 0$$

$$\tau_{\max} = \frac{1}{\sqrt{k_1 k_2}}$$



Following the Algorithm

Number all reactions

Mole balances:

Mole balance on each and every species

PFR	$\frac{dF_j}{dV} = r_j$
CSTR	$F_{j0} - F_j = -r_j V$
Batch	$\frac{dN_j}{dt} = r_j V$
Membrane ("i" diffuses in)	$\frac{dF_i}{dV} = r_i + R_i$
Liquid-semibatch	$\frac{dC_j}{dt} = r_j + \frac{v_0 (C_{j0} - C_j)}{V}$

Rates:

Laws	$r_{ij} = k_{ij} f_i(C_j, C_n)$
Relative rates	$\frac{r_{iA}}{-a_i} = \frac{r_{iB}}{-b_i} = \frac{r_{iC}}{c_i} = \frac{r_{iD}}{d_i}$
Net rates	$r_j = \sum_{i=1}^{q} r_{ij}$

Stoichiometry:

Gas phase

$$C_j = C_{T0} \frac{F_j}{F_T} \frac{P}{P_0} \frac{T_0}{T} = C_{T0} \frac{F_j}{F_T} \frac{T_0}{T} y$$

$$y = \frac{P}{P_0}$$

$$F_T = \sum_{j=1}^{n} F_j$$

$$\frac{dy}{dW} = -\frac{\alpha}{2y} \left(\frac{F_T}{F_{T0}} \right) \frac{T}{T_0}$$

Liquid phase

$$v = v_0$$

$$C_A, C_B, \ldots$$

Combine:

Polymath will combine all the equations for you. Thank you,

End of Lecture 12

Supplementary Slides

Blood Coagulation

$$TF + VII \underset{k_2}{\overset{k_1}{\longleftrightarrow}} TF = VII$$

$$TF + VIIa \underset{k_4}{\overset{k_3}{\longleftrightarrow}} TF = VIIa$$

$$TF = VIIa + VII \overset{k_5}{\longrightarrow} TF = VIIa + VIIa$$

$$Xa + VII \overset{k_6}{\longrightarrow} Xa + VIIa$$

$$IIa + VII \overset{k_7}{\longrightarrow} IIa + VIIa$$

$$TF = VIIa + X \underset{k_9}{\overset{k_8}{\longleftrightarrow}} TF = VIIa = X \overset{k_{10}}{\longrightarrow} TF = VIIa = Xa$$

$$TF = VIIa + Xa \underset{k_{12}}{\overset{k_{11}}{\longleftrightarrow}} TF = VIIa = Xa$$

$$TF = VIIa + IX \underset{k_{14}}{\overset{k_{13}}{\longleftrightarrow}} TF = VIIa = IX \overset{k_{15}}{\longrightarrow} TF = VIIa + IXa$$

$$Xa + II \overset{k_{16}}{\longrightarrow} Xa + IIa$$

$$IIa + VIII \overset{k_{17}}{\longrightarrow} IIa + VIIIa$$

$$VIIIa + IXa \underset{k_{19}}{\overset{k_{18}}{\longleftrightarrow}} IXa = VIIIa$$

$$IXa = VIIIa + X \underset{k_{21}}{\overset{k_{20}}{\longleftrightarrow}} IXa = VIIIa = X \overset{k_{22}}{\longrightarrow} IXa = VIIIa + Xa$$

$$VIIIa \underset{k_{24}}{\overset{k_{23}}{\longleftrightarrow}} VIIIa_1 \cdot L + VIIIa_2$$

$$IXa = VIIIa = X \overset{k_{25}}{\longrightarrow} VIIIa_1 \cdot L + VIIIa_2 + IXa$$

$$IIa + V \underset{k_{27}}{\overset{k_{26}}{\longleftrightarrow}} IIa + Va$$

$$Xa + Va \underset{k_{28}}{\overset{k_{27}}{\longleftrightarrow}} Xa = Va$$

$$Xa = Va + II \underset{k_{30}}{\overset{k_{29}}{\longleftrightarrow}} Xa = Va = II \overset{k_{31}}{\longrightarrow} Xa = Va + mIIa$$

$$mIIa + Xa = Va \overset{k_{32}}{\longrightarrow} Xa = Va + IIa$$

$$Xa + TPFI \underset{k_{34}}{\overset{k_{33}}{\longleftrightarrow}} Xa = TFPI$$

$$TF = VIIa = Xa + TFPI \underset{k_{36}}{\overset{k_{35}}{\longleftrightarrow}} TF = VIIa = Xa = TFPI$$

$$TF = VIIa + Xa = TFPI \overset{k_{37}}{\longrightarrow} TF = VIIa = Xa = TFPI$$

$$Xa + ATIII \overset{k_{38}}{\longrightarrow} Xa = ATIII$$

$$mIIa + ATIII \overset{k_{39}}{\longrightarrow} mIIa = ATIII$$

$$IXa + ATIII \overset{k_{40}}{\longrightarrow} IXa = ATIII$$

$$IIa + ATIII \overset{k_{41}}{\longrightarrow} IIa = ATIII$$

$$TF = VIIa + ATIII \overset{k_{42}}{\longrightarrow} TF = VIIa = ATIII$$

Courtesy of Hockin, M.F., Jones, K.C., Everse, S.J. and Mann, K.G. (2002). A model for the stoichiometric regulation of blood coagulation. *The Journal of Biological Chemistry* **277** (21), 18322-18333.

Notations

Species symbol	Nomenclature
TF	Tissue factor
VII	proconvertin
TF=VIIa	factor TF=VIIa
VIIa	factor novoseven
TF=VIIa	factor TF=VIIa complex
Xa	Stuart prower factor activated
IIa	thrombin
X	Stuart Prower factor
TF=VIIa=X	TF=VIIa=X complex
TF=VIIa=X	TF=VIIa=X complex
IX	Plasma Thromboplastin Component
TF=VIIa=IX	TF=VIIa=IX complex
IXa	factor IXa
II	prothrombin
VIII	antihemophilic factor
VIIIa	antihemophilic factor activated
IXa=VIIIa	IXa=VIIIa complex
IXa=VIIIa=X	IXa=VIIIa=X complex

Notations

$VIIIa_1L$	factor $VIIIa_1L$
$VIIIa_2$	factor $VIIIa_2$
V	proaccelerin
Va	factor Va
Xa=Va	Xa=Va complex
Xa=Va=II	Xa=Va=II complex
mIIa	meizothrombin
TFPI	tissue factor pathway inhibitor
Xa=TFPI	Xa=TFPI complex
TF=VIIa=Xa=TFPI	TF=VIIa=Xa=TFPI complex
ATIII	antithrombin
Xa=ATIII	Xa=ATIII complex
mIIa=ATIII	mIIa=ATIII complex
IXa=ATIII	IXa=ATIII complex
TF=VIIIa=ATIII	TF=VIIIa=ATIII complex
IIa=ATIII	IIa=ATIII complex

Mole Balances

$$\frac{dC_{TF}}{dT} = k_2 \cdot C_{TFVII} - k_1 \cdot C_{TF} \cdot C_{VII} - k_3 \cdot C_{TF} \cdot C_{VIIa} + k_4 \cdot C_{TFVIIa}$$

$$\frac{dC_{VII}}{dt} = k_2 \cdot C_{TFVII} - k_1 \cdot C_{TF} \cdot C_{VII} - k_6 \cdot C_{Xa} \cdot C_{VII} - k_7 \cdot C_{IIa} \cdot C_{VII} - k_5 \cdot C_{TFVIIa} \cdot C_{VII}$$

$$\frac{dC_{TFVII}}{dt} = -k_2 \cdot C_{TFVII} + k_1 \cdot C_{TF} \cdot C_{VII}$$

$$\frac{dC_{VIIa}}{dt} = k_4 \cdot C_{TFVIIa} - k_3 \cdot C_{TF} \cdot C_{VIIa} + k_5 \cdot C_{TFVIIa} \cdot C_{VII} + k_6 \cdot C_{Xa} \cdot C_{VII} + k_7 \cdot C_{IIa} \cdot C_{VII}$$

$$\frac{dC_{TFVIIa}}{dt} = -k_4 \cdot C_{TFVIIa} + k_3 \cdot C_{TF} \cdot C_{VIIa} + k_9 \cdot C_{TFVIIaX} - k_8 \cdot C_{TFVIIa} \cdot C_X - k_{11} \cdot C_{TFVIIa} \cdot C_{Xa} +$$
$$k_{12} \cdot C_{TFVIIaXa} - k_{13} \cdot C_{TFVIIa} \cdot C_{IX} + k_{14} \cdot C_{TFVIIaIX} + k_{15} \cdot C_{TFVIIaIX} - k_{37} \cdot C_{TFVIIa} \cdot C_{XaTFPI} -$$
$$k_{42} \cdot C_{TFVIIa} \cdot C_{ATIII}$$

$$\frac{dC_{Xa}}{dt} = k_{11} \cdot C_{TFVIIa} \cdot C_{Xa} + k_{12} \cdot C_{TFVIIaXa} + k_{22} \cdot C_{IXaVIIIaX} + k_{28} \cdot C_{XaVa} - k_{27} \cdot C_{Xa} \cdot C_{Va} +$$
$$k_{34} \cdot C_{XaTFPI} - k_{33} \cdot C_{Xa} \cdot C_{TFPI} - k_{38} \cdot C_{Xa} \cdot C_{ATIII}$$

$$\frac{dC_{IIa}}{dt} = k_{16} \cdot C_{Xa} \cdot C_{II} + k_{32} \cdot C_{mIIa} \cdot C_{XaVa} - k_{41} \cdot C_{IIa} \cdot C_{ATIII}$$

$$\frac{dC_X}{dt} = -k_8 \cdot C_{TFVIIa} \cdot C_X + k_9 \cdot C_{TFVIIaX} - k_{20} \cdot C_{IXaVIIIa} \cdot C_X + k_{21} \cdot C_{IXaVIIIaX} + k_{25} \cdot C_{IXaVIIIaX}$$

$$\frac{dC_{TFVIIaX}}{dt} = k_8 \cdot C_{TFVIIa} \cdot C_X - k_9 \cdot C_{TFVIIaX} - k_{10} \cdot C_{TFVIIaX}$$

Mole Balances

$$\frac{dC_{TFVIIaXa}}{dt} = k_{10} \cdot C_{TFVIIaX} + k_{11} \cdot C_{TFVIIa} \cdot C_{Xa} - k_{12} \cdot C_{TFVIIaXa} + k_{36} \cdot C_{TFVIIaXaTFPI} - k_{35} \cdot C_{TFVIIaXa} C_{TFPI}$$

$$\frac{dC_{IX}}{dt} = k_{14} \cdot C_{TFVIIaIX} - k_{13} \cdot C_{TFVIIa} \cdot C_{IX}$$

$$\frac{dC_{TFVIIaIX}}{dt} = -k_{14} \cdot C_{TFVIIaIX} + k_{13} \cdot C_{TFVIIa} \cdot C_{IX} - k_{15} \cdot C_{TFVIIaIX}$$

$$\frac{dC_{IXa}}{dt} = k_{15} \cdot C_{TFVIIaIX} - k_{18} \cdot C_{VIIIa} \cdot C_{IXa} + k_{19} \cdot C_{IXaVIIIa} + k_{25} \cdot C_{IXaVIIIaX} - k_{40} \cdot C_{IXa} \cdot C_{ATIII}$$

$$\frac{dC_{II}}{dt} = -k_{16} \cdot C_{Xa} \cdot C_{II} + k_{30} \cdot C_{XaVaII} - k_{29} \cdot C_{XaVa} \cdot C_{II}$$

$$\frac{dC_{VIII}}{dt} = -k_{17} \cdot C_{IIa} \cdot C_{VIII}$$

$$\frac{dC_{VIIIa}}{dt} = k_{17} \cdot C_{IIa} \cdot C_{VIII} - k_{18} \cdot C_{VIIIa} \cdot C_{IXa} + k_{19} \cdot C_{IXaVIIIa} - k_{23} \cdot C_{VIIIa} + k_{24} \cdot C_{VIIIa_1 \cdot L}$$

$$\frac{dC_{IXaVIIIa}}{dt} = k_{18} \cdot C_{VIIIa} \cdot C_{IXa} - k_{19} \cdot C_{IXaVIIIa} + k_{21} \cdot C_{IXaVIIIaX} - k_{20} \cdot C_{IXaVIIIa} \cdot C_{X} + k_{22} \cdot C_{IXaVIIIaX}$$

$$\frac{dC_{IXaVIIIaX}}{dt} = -k_{21} \cdot C_{IXaVIIIaX} + k_{20} \cdot C_{IXaVIIIa} \cdot C_{X} - k_{22} \cdot C_{IXaVIIIaX} - k_{25} \cdot C_{IXaVIIIaX}$$

$$\frac{dC_{VIIIa_1 \cdot L}}{dt} = k_{23} \cdot C_{VIIIa} - k_{24} \cdot C_{VIIIa_1 \cdot L} \cdot C_{VIIIa_2} + k_{25} \cdot C_{IXaVIIIaX}$$

$$\frac{dC_{VIIIa_2}}{dt} = k_{23} \cdot C_{VIIIa} - k_{24} \cdot C_{VIIIa_1 \cdot L} \cdot C_{VIIIa_2} + k_{25} \cdot C_{IXaVIIIaX}$$

Mole Balances

$$\frac{dC_V}{dt} = -k_{26} \cdot C_{IIa} \cdot C_V$$

$$\frac{dC_{Va}}{dt} = k_{26} \cdot C_{IIa} \cdot C_V + k_{28} \cdot C_{Xa} \cdot C_{Va} - k_{27} \cdot C_{Xa} \cdot C_{Va}$$

$$\frac{dC_{XaVa}}{dt} = -k_{28} \cdot C_{Xa} \cdot C_{Va} + k_{27} \cdot C_{Xa} \cdot C_{Va} - k_{29} \cdot C_{IIaVa} \cdot C_{II} + k_{30} \cdot C_{XaVaII} + k_{31} \cdot C_{XaVaII}$$

$$\frac{dC_{XaVaII}}{dt} = k_{29} \cdot C_{IIaVa} \cdot C_{II} - k_{30} \cdot C_{XaVaII} - k_{31} \cdot C_{XaVaII}$$

$$\frac{dC_{mIIa}}{dt} = k_{31} \cdot C_{XaVaII} - k_{32} \cdot C_{mIIa} \cdot C_{XaVa} - k_{39} \cdot C_{mIIa} \cdot C_{ATIII}$$

$$\frac{dC_{TFPI}}{dt} = k_{34} \cdot C_{XaTFPI} - k_{33} \cdot C_{Xa} \cdot C_{TFPI} + k_{36} \cdot C_{TFVIIaXaTFPI} - k_{35} \cdot C_{TFVIIaXa} \cdot C_{TFPI}$$

$$\frac{dC_{XaTFPI}}{dt} = -k_{34} \cdot C_{XaTFPI} + k_{37} \cdot C_{Xa} \cdot C_{TFPI} - k_{37} \cdot C_{TFVIIa} \cdot C_{XaTFPI}$$

$$\frac{dC_{TFVIIaXaTFPI}}{dt} = -k_{36} \cdot C_{TFVIIaXaTFPI} + k_{35} \cdot C_{TFVIIaXa} \cdot C_{TFPI} + k_{37} \cdot C_{TFVIIa} \cdot C_{XaTFPI}$$

$$\frac{dC_{ATIII}}{dt} = -k_{38} \cdot C_{Xa} \cdot C_{ATIII} - k_{39} \cdot C_{mIIa} \cdot C_{ATIII} - k_{40} \cdot C_{IXa} \cdot C_{ATIII} - k_{41} \cdot C_{IIa} \cdot C_{ATIII} - k_{42} \cdot C_{TFVIIa} \cdot C_{ATIII}$$

$$\frac{dC_{XaATIII}}{dt} = k_{38} \cdot C_{Xa} \cdot C_{ATIII}$$

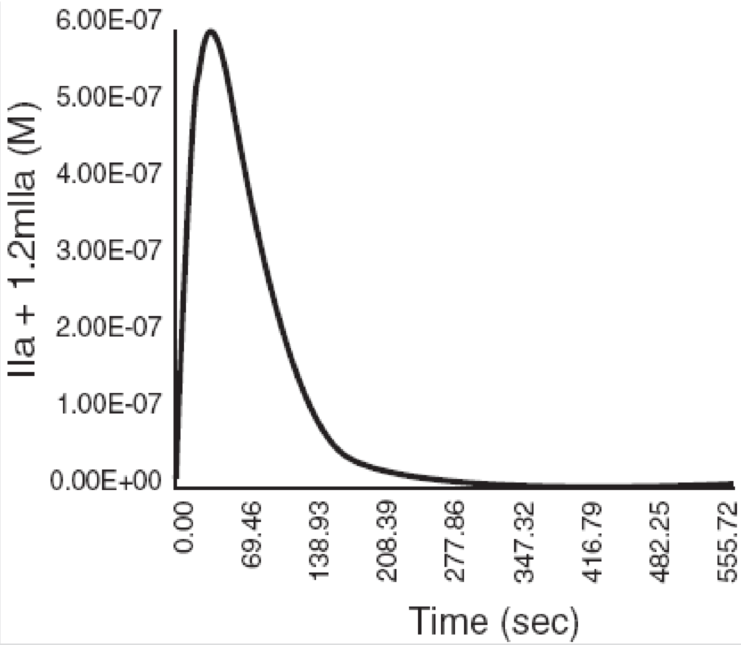
$$\frac{dC_{mIIaATIII}}{dt} = k_{39} \cdot C_{mIIa} \cdot C_{ATIII}$$

$$\frac{dC_{IXaATIII}}{dt} = k_{40} \cdot C_{IXa} \cdot C_{ATIII}$$

$$\frac{dC_{TFVIIaATIII}}{dt} = k_{42} \cdot C_{TFVIIa} \cdot C_{ATIII}$$

$$\frac{dC_{IIaATIII}}{dt} = k_{41} \cdot C_{IIa} \cdot C_{ATIII}$$

Results



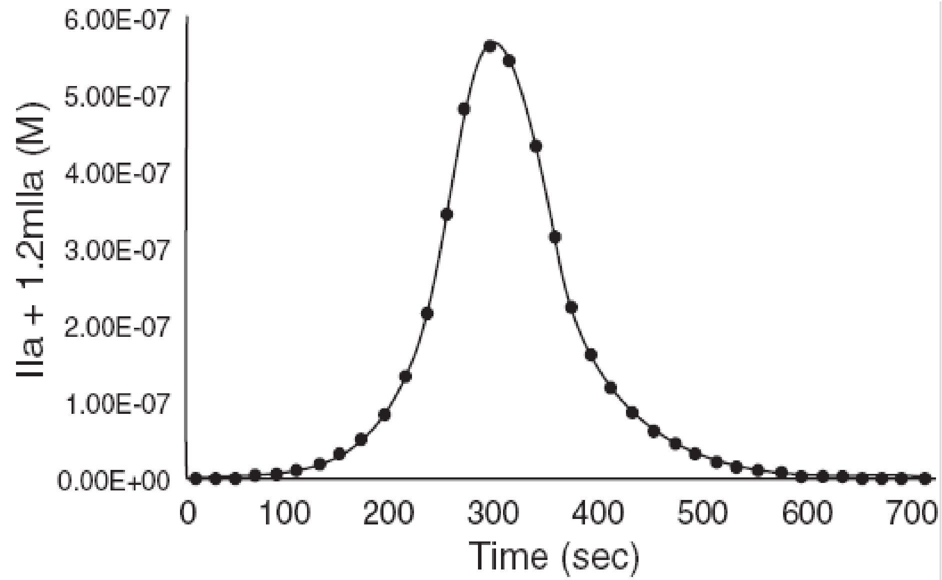


Figure D. Total thrombin as a function of time with an initiating TF concentration of 25 p*M* (after running Polymath) for the abbreviated blood clotting cascade.

Figure E. Total thrombin as a function of time with an initiating TF concentration of 25 p*M*. [Figure courtesy of M. F. Hockin et al., "A Model for the Stoichiometric Regulation of Blood Coagulation," *The Journal of Biological Chemistry,* 277[21], pp. 18322–18333 (2002)]. Full blood clotting cascade.

Blood Coagulation

Many metabolic reactions involve a large number of sequential reactions, such as those that occur in the coagulation of blood.

Cut → Blood → Clotting

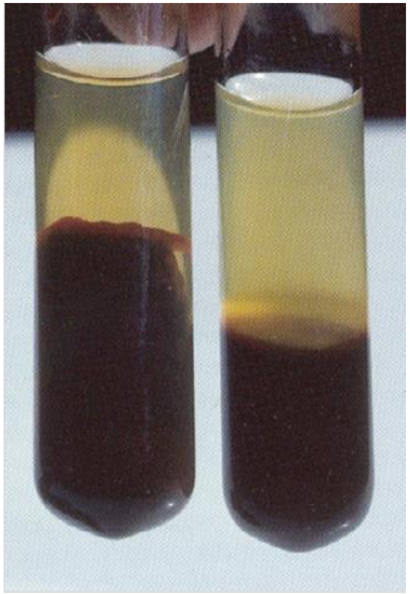


Figure A. Normal Clot Coagulation of blood

(picture courtesy of: Mebs, Venomous and Poisonous Animals, Medpharm, Stugart 2002, Page 305)

Schematic of Blood Coagulation

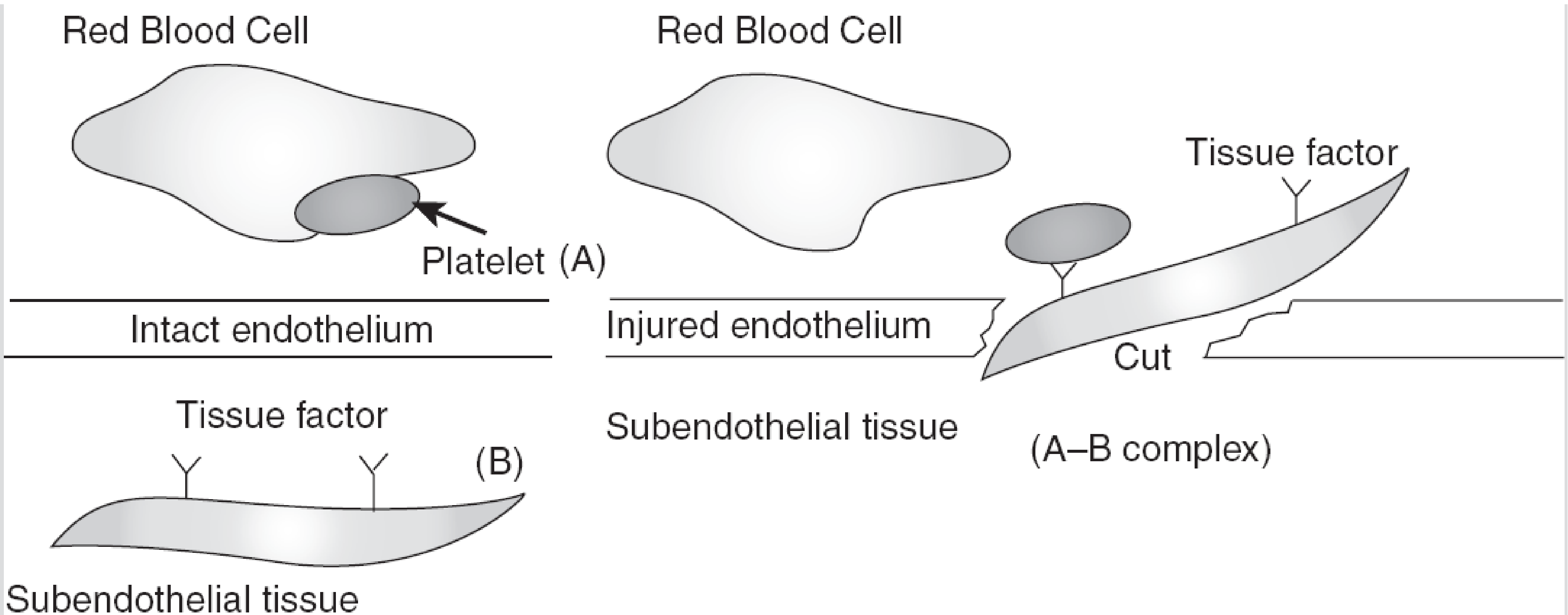


Figure B. Schematic of separation of TF (A) and plasma (B) before cut occurs.

Figure C. Cut allows contact of plasma to initiate coagulation. (A + B $\rightarrow$ Cascade)

Cut

↓

A + B

↓

C

↓

D

↓

E

↓

F

↓

Clot