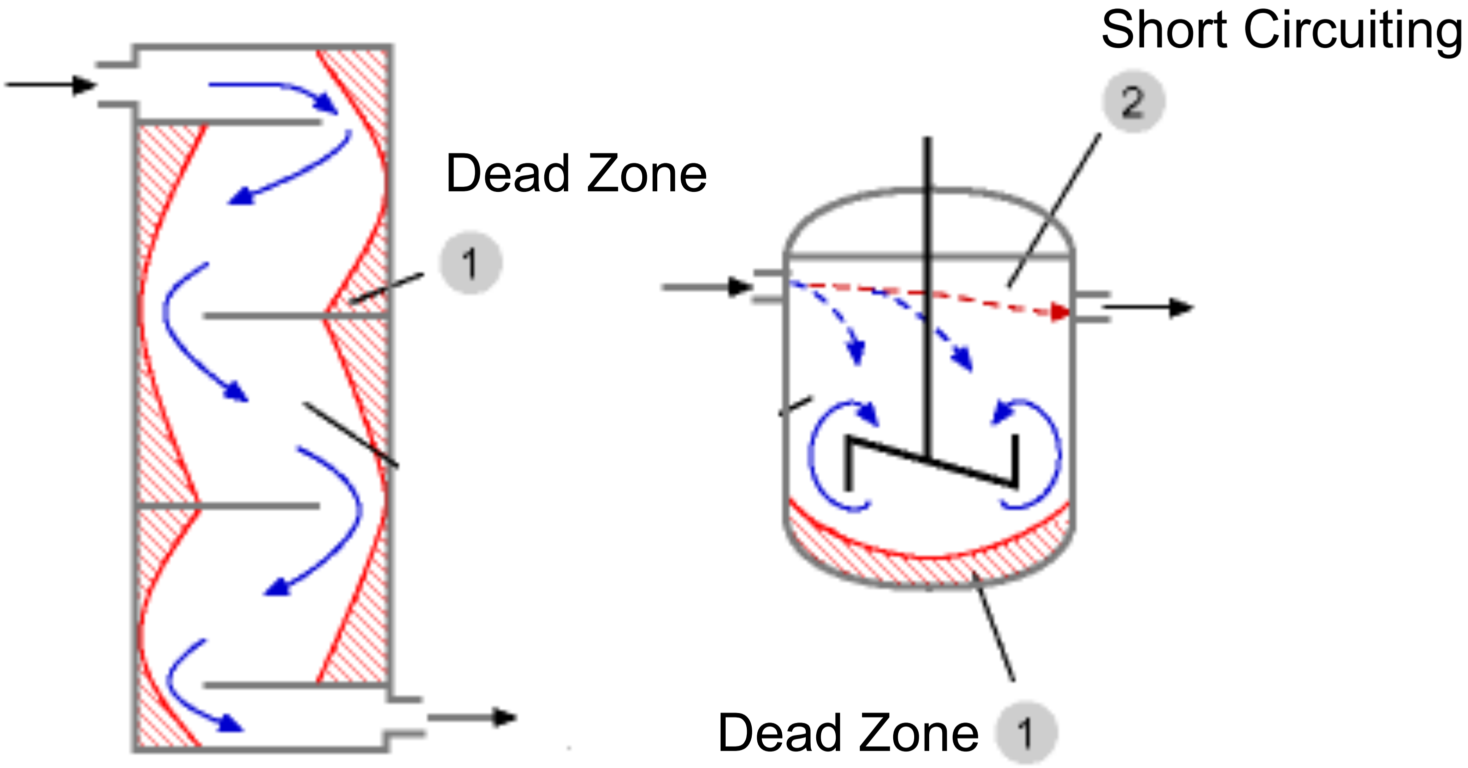
Review: Nonideal Flow in a CSTR

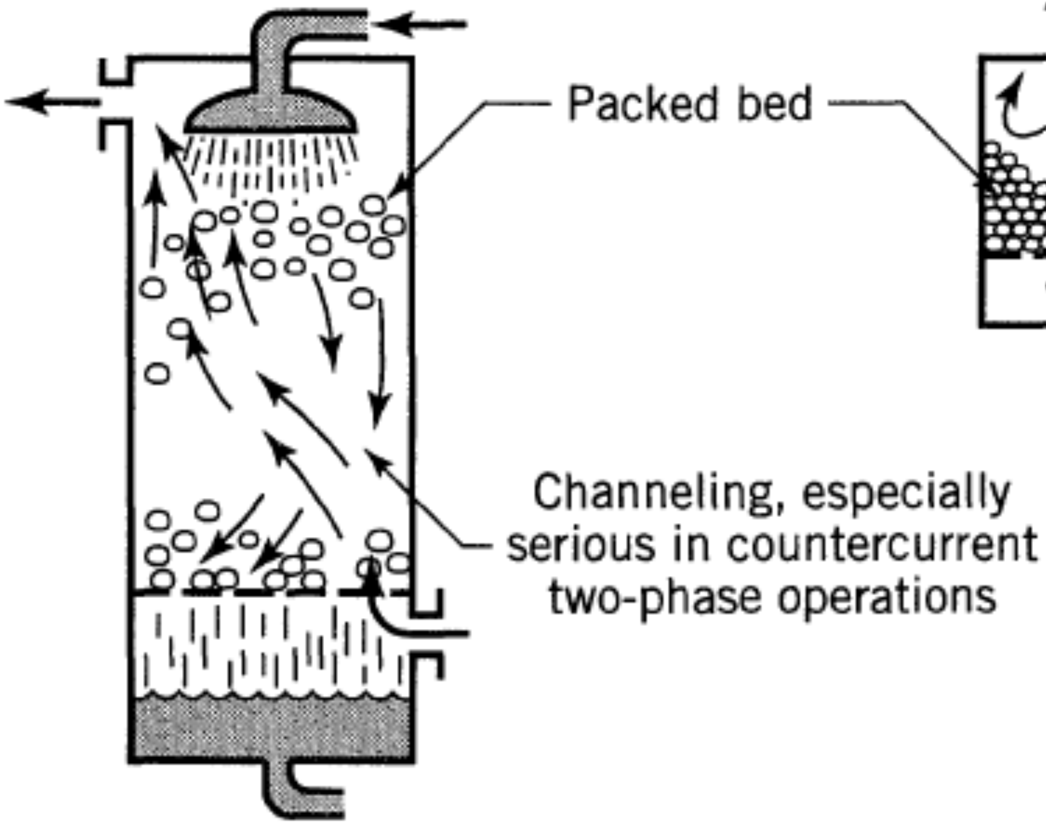
- Ideal CSTR: uniform reactant concentration throughout the vessel
- Real stirred tank
  - Relatively high reactant concentration at the feed entrance
  - Relatively low concentration in the stagnant regions, called dead zones (usually corners and behind baffles)

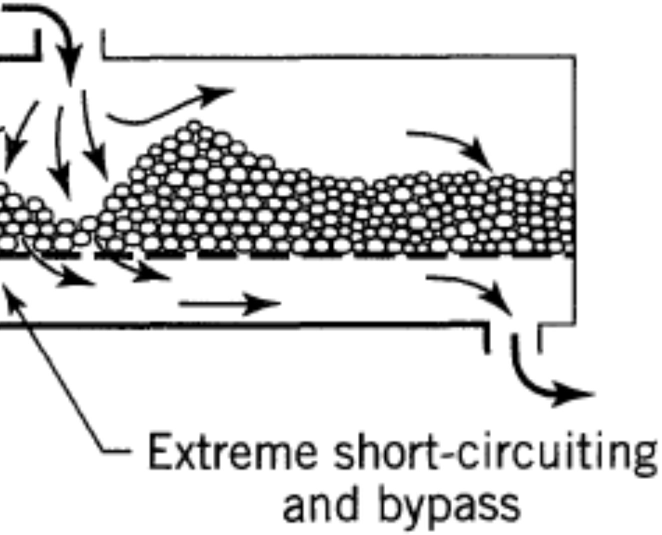


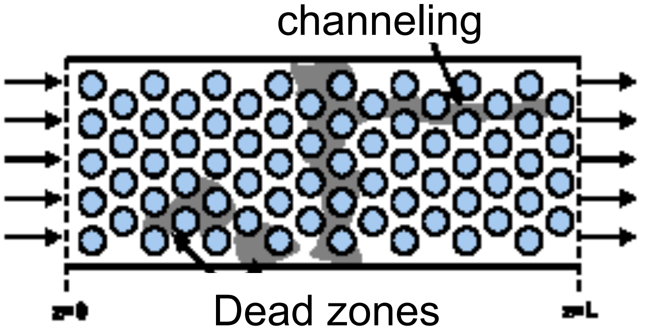
Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Review: Nonideal Flow in a PBR

- Ideal plug flow reactor: all reactant and product molecules at any given axial position move at same rate in the direction of the bulk fluid flow
- Real plug flow reactor: fluid velocity profiles, turbulent mixing, & molecular diffusion cause molecules to move with changing speeds and in different directions







Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, n.

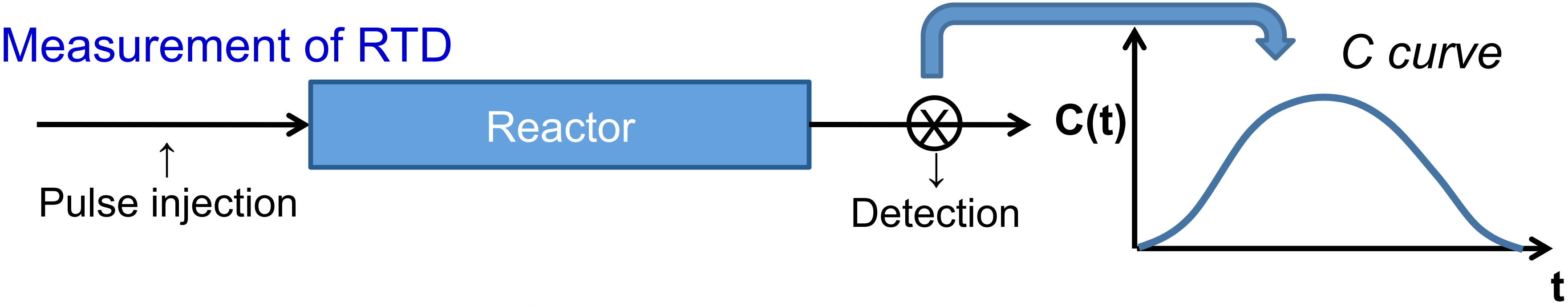
Review: Residence Time Distribution

RTD ≡ E(t) ≡ “residence time distribution” function

RTD describes the amount of time molecules have spent in the reactor

RTD is experimentally determined by injecting an inert “tracer” at t=0 and measuring the tracer concentration C(t) at exit as a function of time

Measurement of RTD



$$\mathrm{RTD} = E(t) = \frac{C(t)}{\int_0^\infty C(t)\,dt} = \frac{\text{tracer conc at exit between } t \text{ \& } t+\Delta t}{\text{sum of tracer conc at exit for infinite time}}$$

$$\int_0^\infty E(t)\,dt = 1$$

E(t)=0 for t<0 since no tracer can exit before it enters

E(t)≥0 for t>0 since mass fractions are always positive

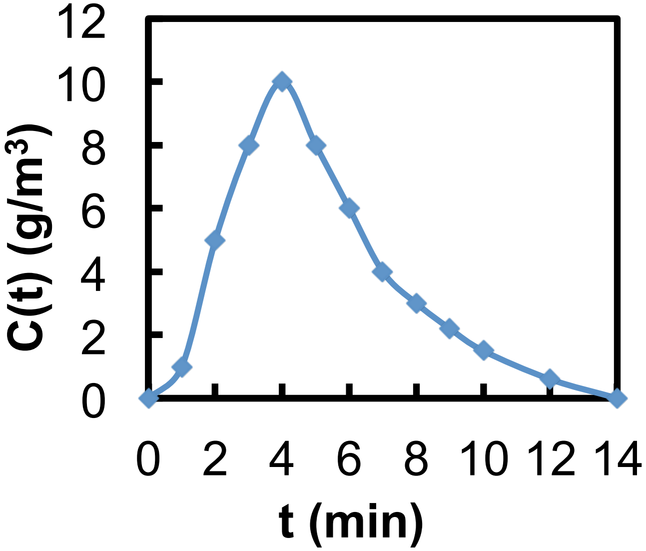
Fraction of material leaving reactor that has been inside reactor for a time between t_1 & t_2 $= \int_{t_1}^{t_2} E(t)\,dt$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

A pulse of tracer was injected into a reactor, and the effluent concentration as a function of time is in the graph below. Construct a figure of C(t) & E(t) and calculate the fraction of material that spent between 3 & 6 min in the reactor

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

Plot C vs time:



To tabulate E(t): divide C(t) by the total area under the C(t) curve, which must be numerically evaluated as shown below:

$$\int_0^\infty C(t)dt = \int_0^{10} C(t)dt + \int_{10}^{14} C(t)dt$$

$$\int_{X_0}^{X_N} f(x)dx = \frac{\Delta t}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 \ldots + 4f_{N-1} + f_N\right)$$

$$\int_{X_0}^{X_2} f(x)dx = \frac{\Delta t}{3}\left(f_0 + 4f_1 + f_2\right)$$

$$\rightarrow\rightarrow \int_0^\infty C(t)dt = 47.4\frac{g\cdot min}{m^3} + 2.6\frac{g\cdot min}{m^3} = 50\frac{g\cdot min}{m^3}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

A pulse of tracer was injected into a reactor, and the effluent concentration as a function of time is in the graph below. Construct a figure of C(t) & E(t) and calculate the fraction of material that spent between 3 & 6 min in the reactor

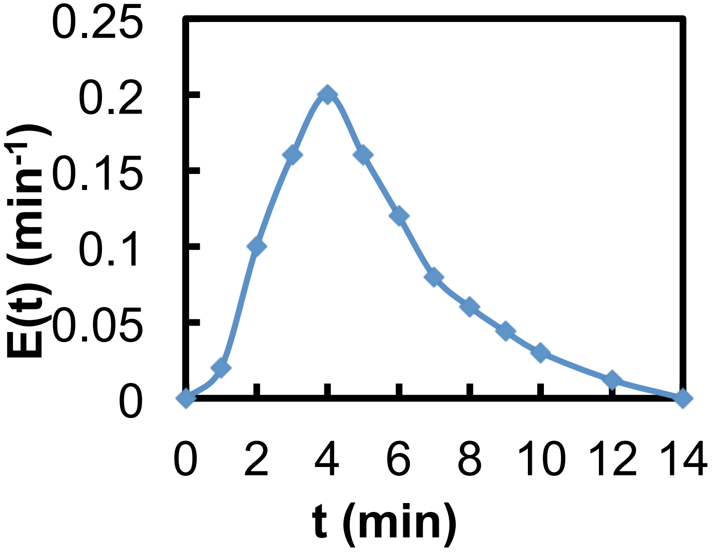
t min	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**12**	**14**
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

$$\int_0^\infty C(t)dt = 50\frac{g\cdot min}{m^3}$$

Tabulate E(t): divide C(t) by the total area under the C(t) curve:

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt}$$

Plot E(t):

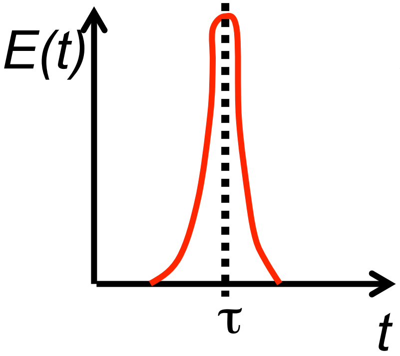


$$E(t_0) = \frac{0}{50} = 0 \qquad E(t_1) = \frac{1}{50} = 0.02$$

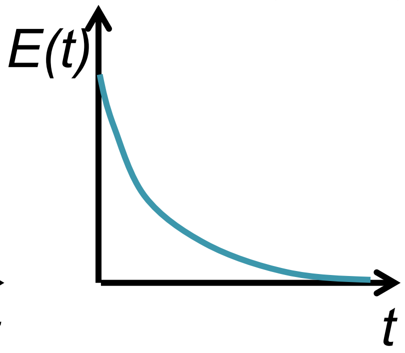
$$E(t_2) = \frac{5}{50} = 0.1 \qquad E(t_3) = \frac{8}{50} = 0.16$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

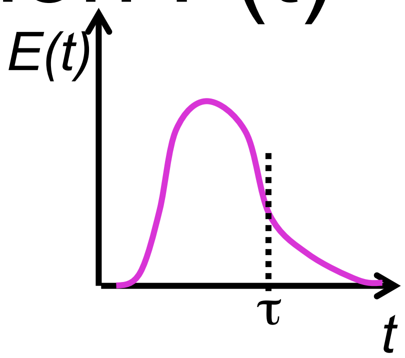
Review: RTD Profiles & Cum RTD Function F(t)



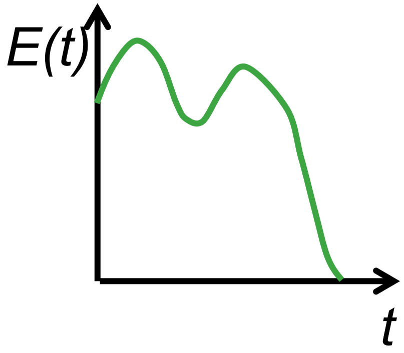
Nearly ideal PFR



Nearly ideal CSTR



PBR with channeling & dead zones



CSTR with dead zones

$$F(t)=\int_0^t E(t)\,dt$$

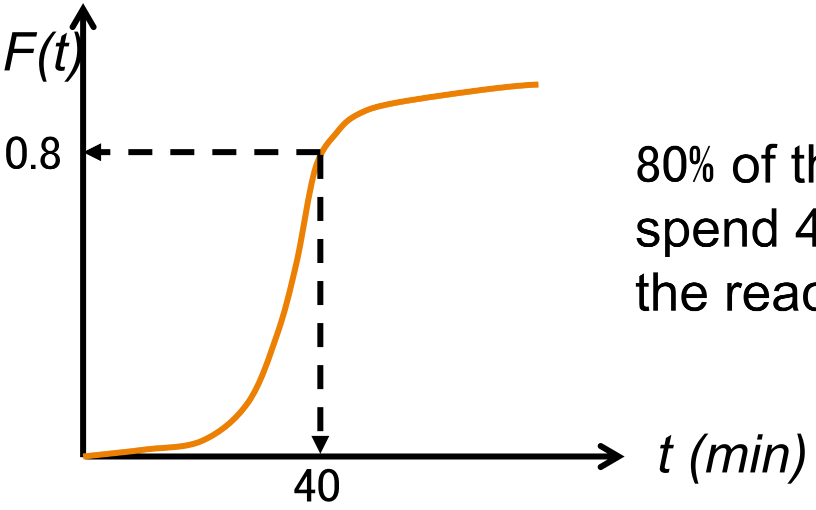
F(t)=fraction of effluent in the reactor less for than time t

$$F(t)=0 \text{ when } t<0$$

$$F(t)\geq 0 \text{ when } t\geq 0$$

$$F(\infty)=1$$

$$1-F(t)=\int_t^\infty E(t)\,dt$$

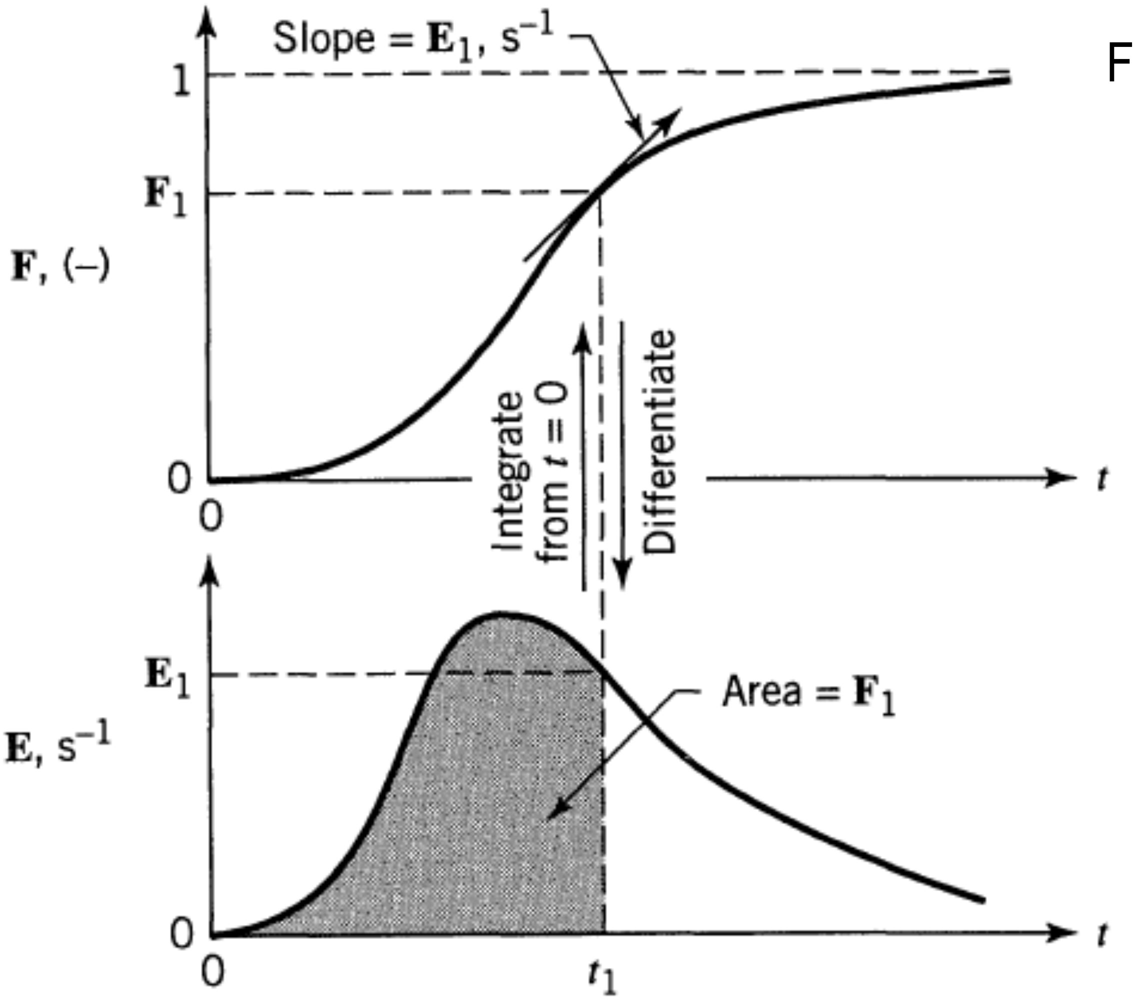


80% of the molecules spend 40 min or less in the reactor

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Review: Relationship between E & F

F(t) = fraction of effluent that has been in the reactor for less than time t



$$F(t) = \int_0^t E(t)\,dt$$

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)\,dt}$$

E(t)= Fraction of material leaving reactor that was inside for a time between t_1 & t_2

Review: Mean Residence Time, t_m

- For an ideal reactor, the space time τ is defined as V/υ_0
- The mean residence time t_m is equal to τ in either ideal or nonideal reactors

$$t_m = \frac{\int_0^\infty tE(t)dt}{\int_0^\infty E(t)dt} = \int_0^\infty tE(t)dt = \tau \qquad \frac{V}{\upsilon_0} = \tau = t_m$$

By calculating t_m, the reactor V can be determined from a tracer experiment

The spread of the distribution (variance): $\sigma^2 = \int_0^\infty (t - t_m)^2 E(t)dt$

Space time τ and mean residence time t_m would be equal if the following two conditions are satisfied:

- No density change
- No backmixing

In practical reactors the above two may not be valid, hence there will be a difference between them

Significance of Mixing

- RTD provides information on how long material has been in the reactor
- RTD does not provide information about the exchange of matter within the reactor (i.e., mixing)!
  - For a 1st order reaction: $$\frac{dX}{dt} = k(1 - X)$$
  - Concentration does not affect the rate of conversion, so RTD is sufficient to predict conversion
  - But concentration does affect conversion in higher order reactions, so we need to know the degree of mixing in the reactor
  - Macromixing: produces a distribution of residence times without specifying how molecules of different age encounter each other and are distributed inside of the reactor
  - Micromixing: describes how molecules of different residence time encounter each other in the reactor

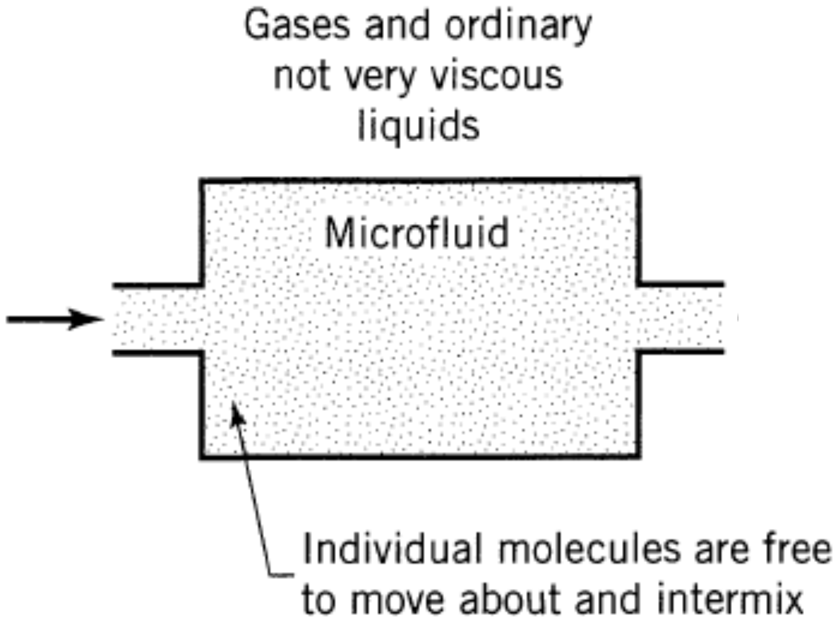
Quality of Mixing

- RTDs alone are not sufficient to determine reactor performance
- Quality of mixing is also required

Goal: use RTD and micromixing models to predict conversion in real reactors

2 Extremes of Fluid Mixing

Maximum mixedness: molecules are free to move anywhere, like a microfluid. This is the extreme case of early mixing



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Quality of Mixing

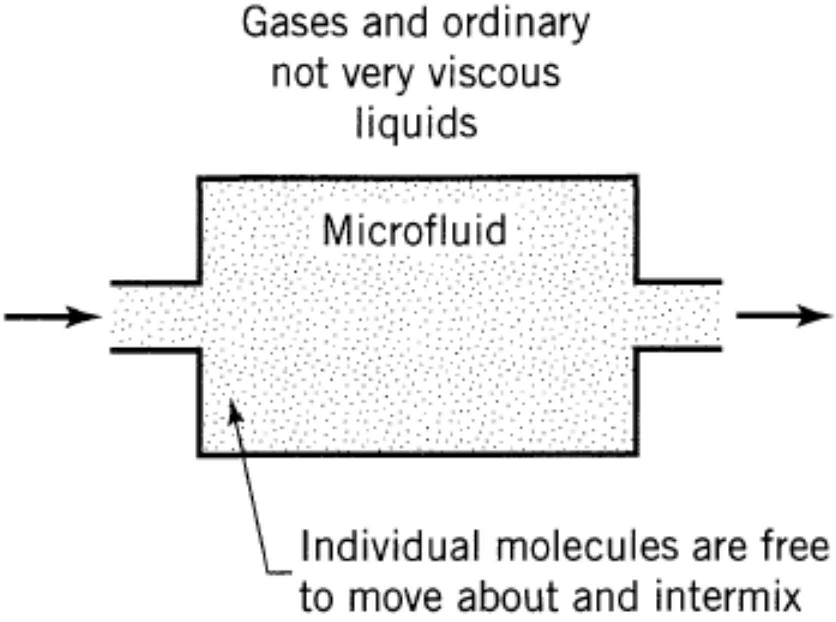
- RTDs alone are not sufficient to determine reactor performance
- Quality of mixing is also required

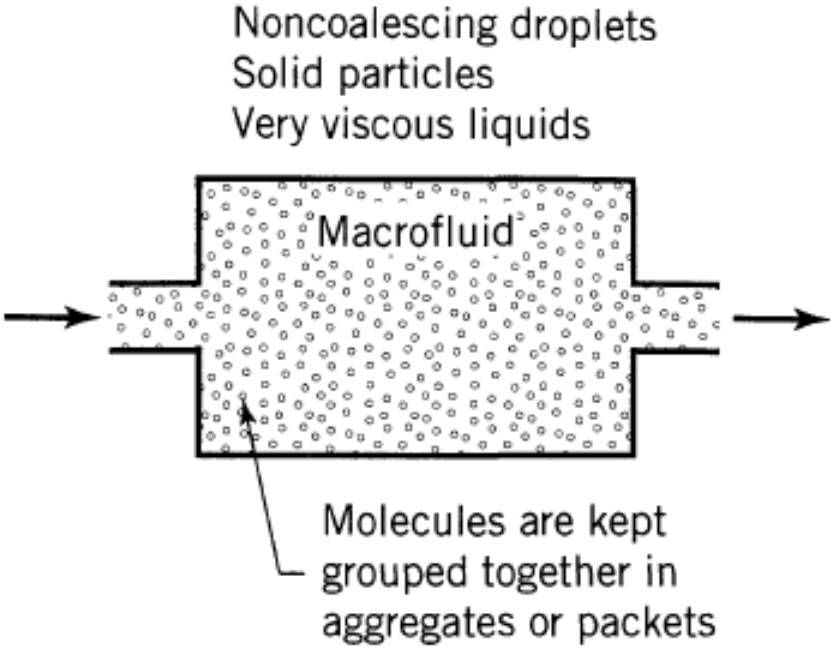
Goal: use RTD and micromixing models to predict conversion in real reactors

2 Extremes of Fluid Mixing

Maximum mixedness: molecules are free to move anywhere, like a microfluid. This is the extreme case of early mixing

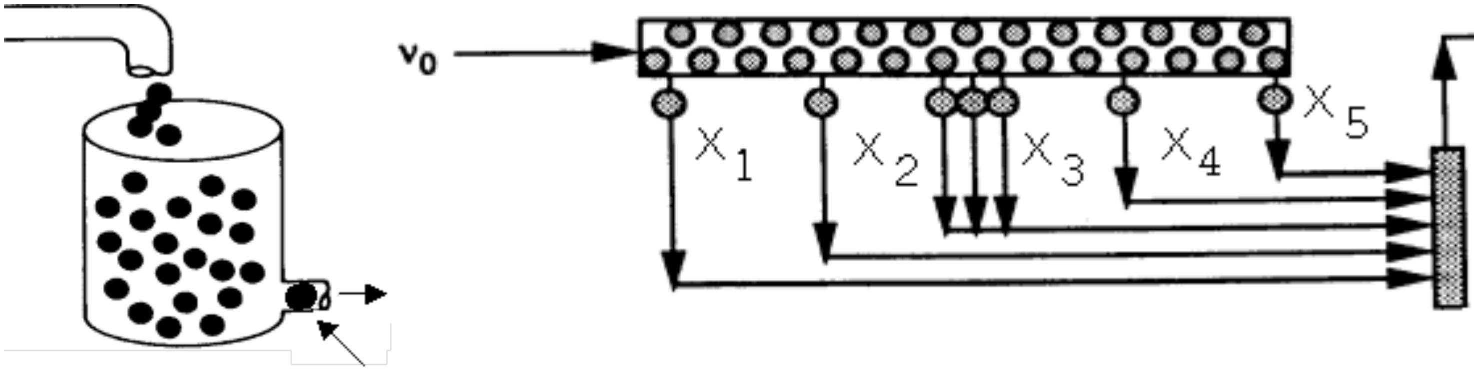
Complete segregation: molecules of a given age do not mix with other globules. This is the extreme case of late mixing





Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Complete Segregation Model



Mixing of different 'age groups' at the last possible moment

- Flow is visualized in the form of globules
- Each globule consists of molecules of the same residence time
- Different globules have different residence times
- No interaction/mixing between different globules

The mean conversion is the average conversion of the various globules in the exit stream:

$$\bar{X}_A = \sum_j \boxed{X_A\left(t_j\right)}\boxed{E\left(t_j\right)}\Delta t$$

Conversion achieved after spending time t_j in the reactor

Fraction of globules that spend between t_j and $t_j + \Delta t$ in the reactor

$$\xrightarrow{\Delta t \to 0} \bar{X}_A = \int_0^\infty X_A(t)E(t)dt$$

$X_A(t)$ is from the ***batch reactor*** design equation

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Complete Segregation Example

First order reaction, A→Products

Batch reactor design equation:

$$N_{A0}\frac{dX_A}{dt}=-r_AV \quad \rightarrow N_{A0}\frac{dX_A}{dt}=kC_AV$$

$$\rightarrow N_{A0}\frac{dX_A}{dt}=kC_{A0}\left(1-X_A\right)V \quad \rightarrow N_{A0}\frac{dX_A}{dt}=kN_{A0}\left(1-X_A\right)$$

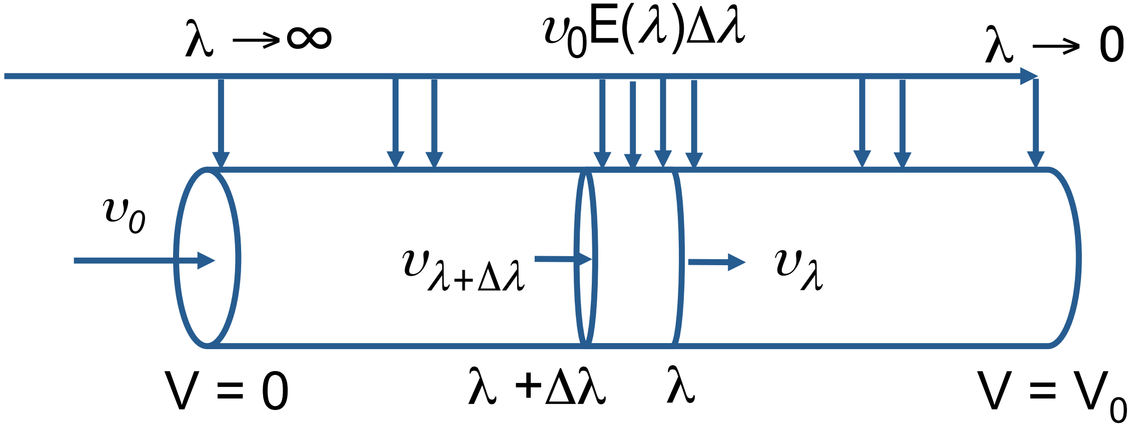
$$\rightarrow \frac{dX_A}{dt}=k\left(1-X_A\right) \quad \rightarrow \boxed{X_A\left(t\right)=1-e^{-kt}}$$

To compute conversion for a reaction with a 1st order rxn and complete segregation, insert E(t) from tracer experiment and $X_A(t)$ from batch reactor design equation into:

$$\overline{X}_A=\int_0^\infty X_A\left(t\right)E\left(t\right)dt \qquad \text{\& integrate}$$

Maximum Mixedness Model

In a PFR: as soon as the fluid enters the reactor, it is completely mixed radially with the other fluid already in the reactor. Like a PFR with side entrances, where each entrance port creates a new residence time:



λ: time it takes for fluid to move from a particular point to end of the reactor

$\upsilon(\lambda)$: volumetric flow rate at λ, = flow that entered at $\lambda+\Delta\lambda$ plus what entered through the sides

$\upsilon_0 E(\lambda)\Delta\lambda$: Volumetric flow rate of fluid fed into side ports of reactor in interval between $\lambda + \Delta\lambda$ & λ

Volumetric flow rate of fluid fed to reactor at λ: $\upsilon(\lambda) = \upsilon_0 \int_\lambda^\infty E(\lambda)d\lambda = \upsilon_0\left[1-\boxed{F(\lambda)}\right]$

fraction of effluent in reactor for less than time t

Volume of fluid with life expectancy between $\lambda + \Delta\lambda$ & λ: $\Delta V = \upsilon_0\left[1-F(\lambda)\right]\Delta\lambda$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Maximum Mixedness & Polymath

Mole balance on A gives:

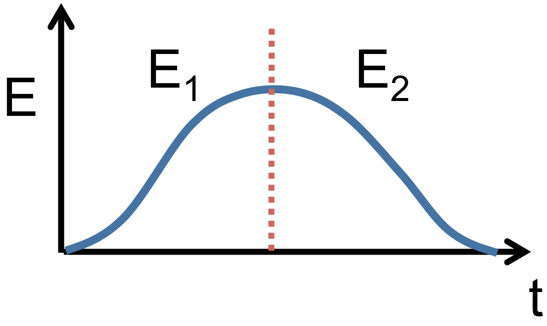
$$\frac{dX_A}{d\lambda} = \frac{r_A}{C_{A0}} + \frac{\boxed{E(\lambda)}}{1-\boxed{F(\lambda)}} X_A$$

residence time distribution function

fraction of effluent in reactor for less than time t

- E(t) must be specified
  - Often it is an expression that fits the experimental data
  - 2 curves, one on the increasing side, and a second for the decreasing side
  - Use the IF function to specify which E is used when

See section 13.8 in book



Also need to replace λ because Polymath cannot calculate as λ gets smaller

$z = \bar{T} - \lambda$ where $\bar{T}$ is the longest time measured

$$\frac{dX_A}{dz} = -\frac{r_A}{C_{A0}} - \frac{E(\bar{T}-z)}{1-F(\bar{T}-z)} X_A$$

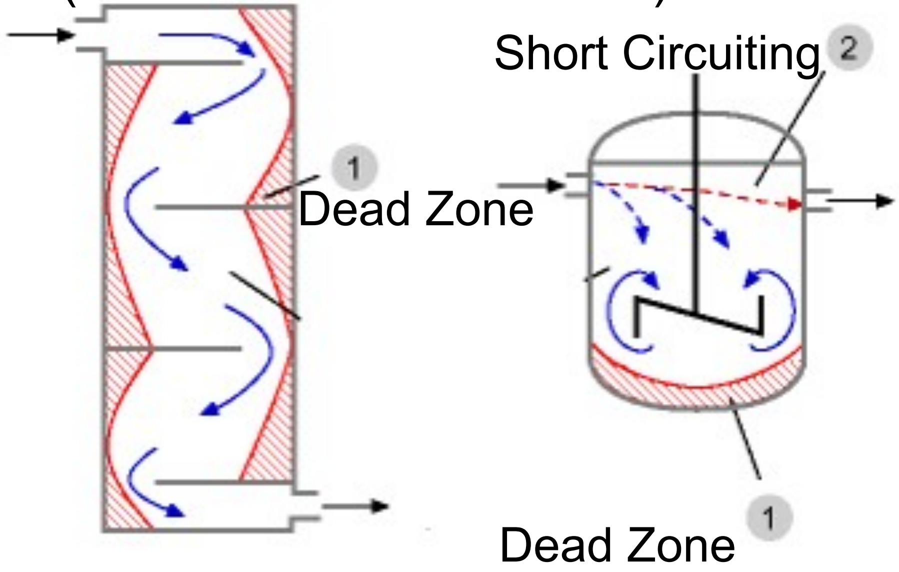
Note that the sign on each term changes

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Review: Nonideal Flow & Reactor Design

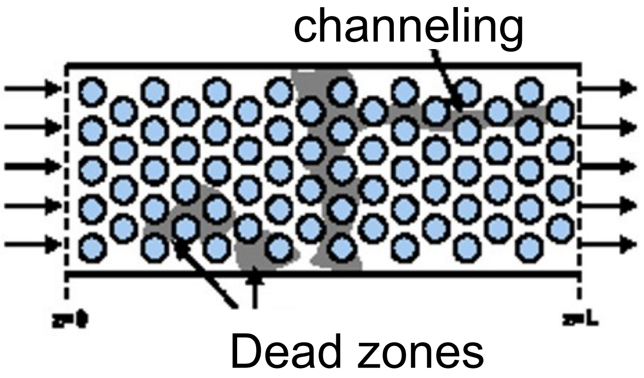
Real CSTRs

- Relatively high reactant conc at entrance
- Relatively low conc in stagnant regions, called dead zones (corners & behind baffles)



Real PBRs

- fluid velocity profiles, turbulent mixing, & molecular diffusion cause molecules to move at varying speeds & directions



Goal: mathematically describe non-ideal flow and solve design problems for reactors with nonideal flow

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

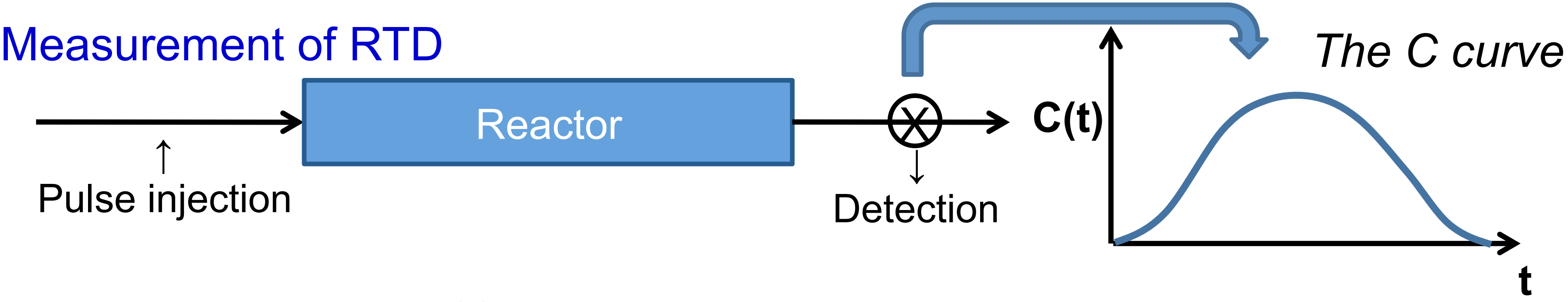
Residence Time Distribution (RTD)

RTD ≡ E(t) ≡ “residence time distribution” function

RTD describes the amount of time molecules have spent in the reactor

RTD is experimentally determined by injecting an inert “tracer” at t=0 and measuring the tracer concentration C(t) at exit as a function of time

Measurement of RTD



The C curve

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)\,dt} = \frac{\text{tracer conc at exit between t \& t+}\Delta\text{t}}{\text{sum of tracer conc at exit for infinite time}}$$

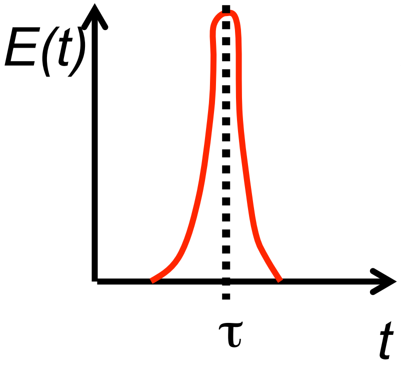
$$\int_0^\infty E(t)\,dt = 1$$

E(t)=0 for t<0 since no fluid can exit before it enters

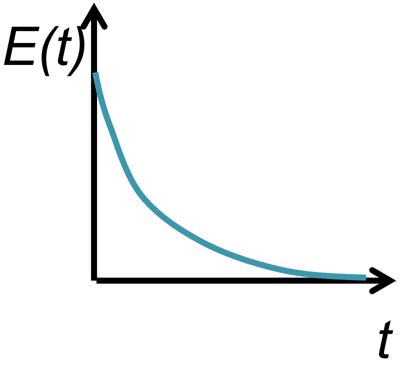
E(t)≥0 for t>0 since mass fractions are always positive

Fraction of material leaving reactor that has been inside reactor for a time between t_1 & t_2 $= \int_{t_1}^{t_2} E(t)\,dt$

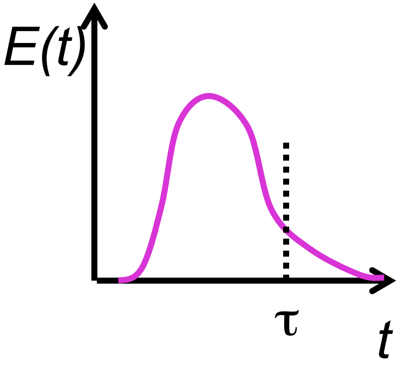
Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.



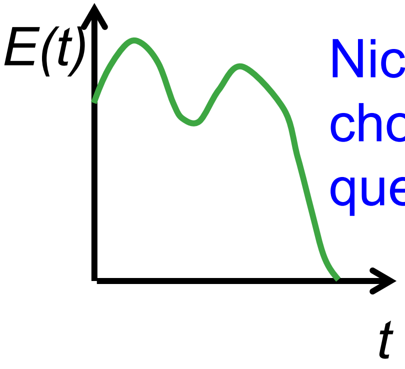
Nearly ideal PFR



Nearly ideal CSTR



PBR with dead zones



CSTR with dead zones

Nice multiple choice question

The fraction of the exit stream that has resided in the reactor for a period of time shorter than a given value *t*:

F(t) is a cumulative distribution function

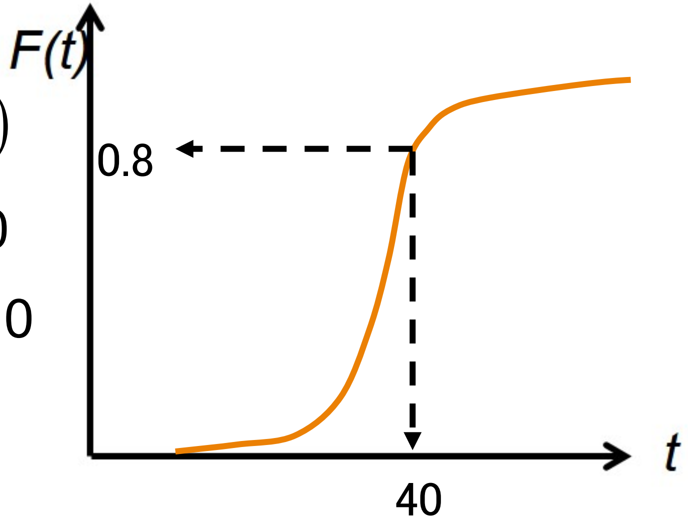
$$\int_0^t E(t)dt = F(t)$$

$$\int_t^\infty E(t)dt = 1 - F(t)$$

$$F(t) = 0 \text{ when } t<0$$

$$F(t) \geq 0 \text{ when } t \geq 0$$

$$F(\infty) = 1$$



80% of the molecules spend 40 min or less in the reactor

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

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By calculating t_m, the reactor V can be determined from a tracer experiment

The spread of the distribution (variance): $\sigma^2 = \int_0^\infty (t - t_m)^2 E(t)dt$

Space time τ and mean residence time t_m would be equal if the following two conditions are satisfied:

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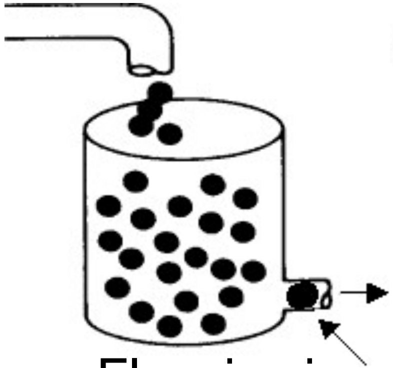
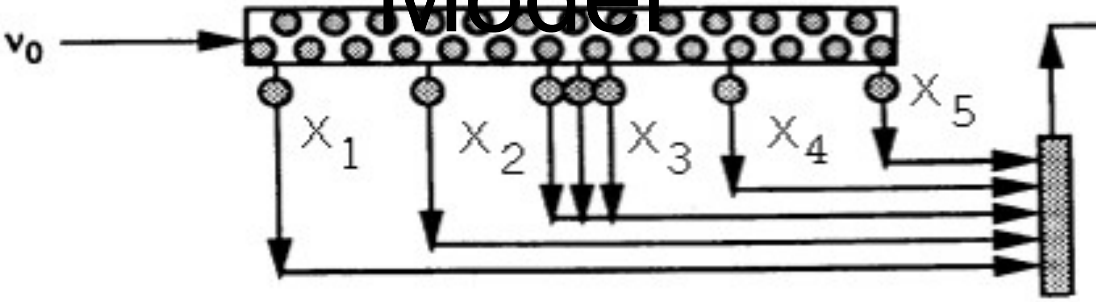
Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Review: Complete Segregation Model





Mixing of different ‘age groups’ at the last possible moment

- Flow is visualized in the form of globules
- Each globule consists of molecules of the same residence time
- Different globules have different residence times
- No interaction/mixing between different globules

The mean conversion is the average conversion of the various globules in the exit stream:

$$\bar{X}_A = \sum_j \boxed{X_A(t_j)}\boxed{E(t_j)}\Delta t$$

Conversion achieved after spending time t_j in the reactor

Fraction of globules that spend between t_j and $t_j + \Delta t$ in the reactor

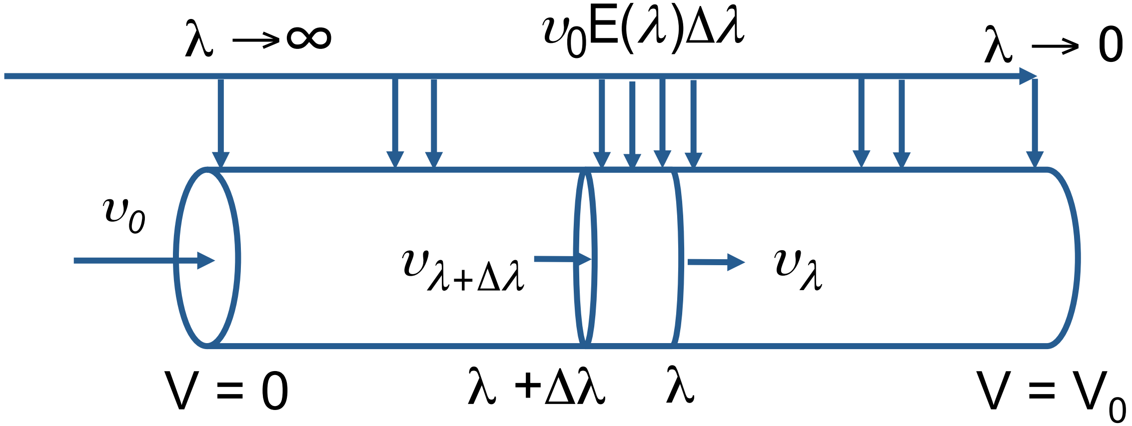
$$\xrightarrow{\Delta t \to 0} \bar{X}_A = \int_0^\infty X_A(t)E(t)\,dt$$

$X_A(t)$ is from the ***batch reactor*** design equation

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Review: Maximum Mixedness Model

In a PFR: as soon as the fluid enters the reactor, it is completely mixed radially with the other fluid already in the reactor. Like a PFR with side entrances, where each entrance port creates a new residence time:



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Volumetric flow rate of fluid fed to reactor at λ: $\upsilon(\lambda) = \upsilon_0 \int_\lambda^\infty E(\lambda)d\lambda = \upsilon_0 \left[1 - \boxed{F(\lambda)}\right]$

fraction of effluent that in reactor for less than time t

Volume of fluid with life expectancy between $\lambda + \Delta\lambda$ & λ: $\Delta V = \upsilon_0 \left[1 - F(\lambda)\right]\Delta\lambda$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, nonelementary rxn $A+B\rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for (1) an ideal PFR and (2) for the complete segregation model.

$C_{A0}=C_{B0}=0.0313$ mol/L & $k=176$ L^2/mol$^2\cdot$min at 320K

t min	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**12**	**14**
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

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E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Start with PFR design eq & see how far can we get:

$$\frac{dX_A}{dV}=\frac{-r_A}{F_{A0}} \rightarrow \frac{dX_A}{dV}=\frac{kC_AC_B^2}{C_{A0}\upsilon_0} \qquad C_A=C_{A0}(1-X_A) \qquad C_B=C_{B0}(1-X_A)$$

$$\rightarrow \frac{dX_A}{dV}=\frac{k\cancel{C_{A0}}C_{B0}^2(1-X_A)^3}{\cancel{C_{A0}}\upsilon_0}$$

Get like terms together & integrate

$$\rightarrow \int_0^{X_A}\frac{dX_A}{(1-X_A)^3}=\int_0^V\frac{kC_{B0}^2}{\upsilon_0}dV$$

$$\rightarrow \frac{1}{2(1-X_A)^2}\Bigg]_0^{X_A}=\frac{kC_{B0}^2}{\upsilon_0}V \rightarrow \frac{1}{(1-X_A)^2}-1=2kC_{B0}^2\tau \rightarrow X_A=1-\sqrt{\frac{1}{2kC_{B0}^2\tau+1}}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, nonelementary rxn $A+B \rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for (1) an ideal PFR and (2) for the complete segregation model.

$C_{A0}=C_{B0}=0.0313$ mol/L & $k=176\ L^2/mol^2\cdot min$ at 320K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0
t*E(t)	0	0.02	0.2	0.48	0.8	0.8	0.72	0.56	0.48	0.396	0.3	0.144	0

$$\boxed{X_A = 1-\sqrt{\frac{1}{2kC_{B0}^2\tau+1}}}$$

How do we determine τ?

For an ideal reactor, $\tau = t_m$

$$t_m = \int_0^\infty tE(t)dt$$

Use numerical method to determine t_m:

$$t_m = \int_0^\infty tE(t)dt = \int_0^{10} tE(t)dt + \int_{10}^{14} tE(t)dt$$

$$\int_0^{10} tE(t)dt = \frac{1}{3}\begin{bmatrix} 0+4(0.02)+2(0.2)+4(0.48)+2(0.8)+4(0.8) \\ +2(0.72)+4(0.56)+2(0.48)+4(0.396)+0.3 \end{bmatrix} = 4.57$$

$$\int_{10}^{14} tE(t)dt = \frac{2}{3}\left[0.3+4(0.144)+0\right] = 0.584 \quad \rightarrow t_m = 4.57+0.584 = 5.15\,\text{min}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, nonelementary rxn A+B→C+D, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for (1) an ideal PFR and (2) for the complete segregation model.

$C_{A0}=C_{B0}=0.0313$ mol/L & k=176 $L^2/mol^2\cdot min$ at 320K

t min	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**12**	**14**
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0
t*E(t)	0	0.02	0.2	0.48	0.8	0.8	0.72	0.56	0.48	0.396	0.3	0.144	0

$$\boxed{X_A = 1-\sqrt{\frac{1}{2kC_{B0}{}^2\tau + 1}}}$$

For an ideal PFR reactor, $\tau = t_m$

$$t_m = \int_0^\infty tE(t)dt$$

$$t_m = 5.15\,\text{min} = \tau$$

$$X_{A,PFR} = 1-\sqrt{\frac{1}{2\left(176\frac{L^2}{mol^2\cdot min}\right)\left(0.0313\frac{mol}{L}\right)^2(5.15\,\text{min})+1}}$$

$$X_{A,PFR} = 0.40$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, nonelementary rxn $A+B \rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for an ideal PFR, the complete segregation model and maximum mixedness model. $C_{A0}=C_{B0}=0.0313$ mol/L & $k=176\ L^2/mol^2{\cdot}min$ at 320K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Segregation model: $\bar{X}_A = \int_0^\infty X_A(t)E(t)dt$ $X_A(t)$ is from ***batch reactor*** design eq

Numerical method

1. Solve batch reactor design equation to determine eq for X_A
2. Determine X_A for each time
3. Use numerical methods to determine $\bar{X}_A$

Polymath Method

1. Use batch reactor design equation to find eq for X_A
2. Use Polymath polynomial curve fitting to find equation for E(t)
3. Use Polymath to determine $\bar{X}_A$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, nonelementary rxn $A+B \rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for an ideal PFR, the complete segregation model and maximum mixedness model. $C_{A0}=C_{B0}=0.0313$ mol/L & $k=176$ $L^2/mol^2 \cdot min$ at 320K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
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E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Segregation model: $\bar{X}_A = \int_0^\infty X_A(t)E(t)dt$ $X_A(t)$ is from ***batch reactor*** design eq

Batch design eq:

$N_{A0} = C_{A0}V$

$$N_{A0}\frac{dX_A}{dt} = -r_A V \rightarrow N_{A0}\frac{dX_A}{dt} = kC_{A0}C_{B0}^2(1-X_A)^3 V \rightarrow \frac{dX_A}{dt} = kC_{B0}^2(1-X_A)^3$$

Stoichiometry:

$-r_A = kC_AC_B^2$

$C_A = C_{A0}(1-X_A)$

$C_B = C_{B0}(1-X_A)$

$$\rightarrow \int_0^{X_A}\frac{dX_A}{(1-X_A)^3} = \int_0^t kC_{B0}^2dt \rightarrow \frac{1}{2(1-X_A)^2}\Bigg]_0^{X_A} = kC_{B0}^2t$$

$$\rightarrow \frac{1}{(1-X_A)^2} - 1 = 2kC_{B0}^2t \rightarrow X_A = 1-\sqrt{\frac{1}{1+2kC_{B0}^2t}}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, nonelementary rxn A+B→C+D, $-r_A = kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for an ideal PFR, the complete segregation model and maximum mixedness model. $C_{A0} = C_{B0} = 0.0313$ mol/L & $k = 176$ $L^2/mol^2 \cdot min$ at 320K

t min	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**12**	**14**
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0
X_A													

Segregation model:

$$\bar{X}_A = \int_0^\infty X_A(t)E(t)dt \qquad X_A = 1 - \sqrt{\frac{1}{1 + 2kC_{B0}{}^2 t}} = 1 - \sqrt{\frac{1}{1 + 0.3429\,\text{min}^{-1}\,t}}$$

Plug in each t & solve

Numerical method

$$X_{A(0)} = 1 - \sqrt{\frac{1}{1 + 0.3429\,\text{min}^{-1}(0)}} = 0$$

$$X_{A(1)} = 1 - \sqrt{\frac{1}{1 + 0.3429\,\text{min}^{-1}(1\,\text{min})}} = 0.137$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

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t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0
X_A	0	0.137	0.23	0.298	0.35	0.39	0.428	0.458	0.483	0.505	0.525	0.558	0.585

Segregation model:

$$\bar{X}_A=\int_0^\infty X_A(t)E(t)dt \qquad X_A=1-\sqrt{\frac{1}{1+2kC_{B0}{}^2t}}=1-\sqrt{\frac{1}{1+0.3429\,\text{min}^{-1}t}}$$

Numerical method

$$\bar{X}_A=\int_0^\infty X_A(t)E(t)dt=\int_0^{10} X_A(t)E(t)dt+\int_{10}^{14} X_A(t)E(t)dt$$

$$\int_0^{10} X_A(t)E(t)dt=\frac{1}{3}\begin{bmatrix}0+4(0.137)(0.02)+2(0.23)(0.1)+4(0.298)(0.16)\\+2(0.35)(0.2)+4(0.39)(0.16)+2(0.428)(0.12)+4(0.458)(0.08)\\+2(0.483)(0.06)+4(0.505)(0.044)+0.525(0.03)\end{bmatrix}$$

$$\int_0^{10} X_A(t)E(t)dt=0.35$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

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t min	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**12**	**14**
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0
X_A	0	0.137	0.23	0.298	0.35	0.39	0.428	0.458	0.483	0.505	0.525	0.558	0.585

Segregation model:

$$\bar{X}_A = \int_0^\infty X_A(t)E(t)dt \qquad X_A = 1-\sqrt{\frac{1}{1+2kC_{B0}{}^2t}} = 1-\sqrt{\frac{1}{1+0.3429\,\text{min}^{-1}t}}$$

Numerical method $$\bar{X}_A = \int_0^\infty X_A(t)E(t)dt = 0.35 + \int_{10}^{14} X_A(t)E(t)dt$$

$$\int_{10}^{14} X_A(t)E(t)dt = \frac{2}{3}\left[(0.525)(0.03)+4(0.558)(0.012)+(0.585)0\right] = 0.0425$$

$$\bar{X}_A = \int_0^\infty X_A(t)E(t)dt = 0.35 + 0.04 \rightarrow \bar{X}_A = 0.39$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, nonelementary rxn A+B→C+D, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for an ideal PFR, the complete segregation model and maximum mixedness model. $C_{A0}=C_{B0}=0.0313$ mol/L & k=176 $L^2/mol^2\cdot min$ at 320K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0
X_A	0	0.137	0.23	0.298	0.35	0.39	0.428	0.458	0.483	0.505	0.525	0.558	0.585

Alternative approach: segregation model by Polymath:

$$\bar{X}_A=\int_0^\infty X_A(t)E(t)dt$$

$$\boxed{\frac{d\bar{X}_A}{dt}=X_A(t)E(t)}$$

$$\boxed{X_A=1-\sqrt{\frac{1}{1+2kC_{B0}{}^2t}}}$$

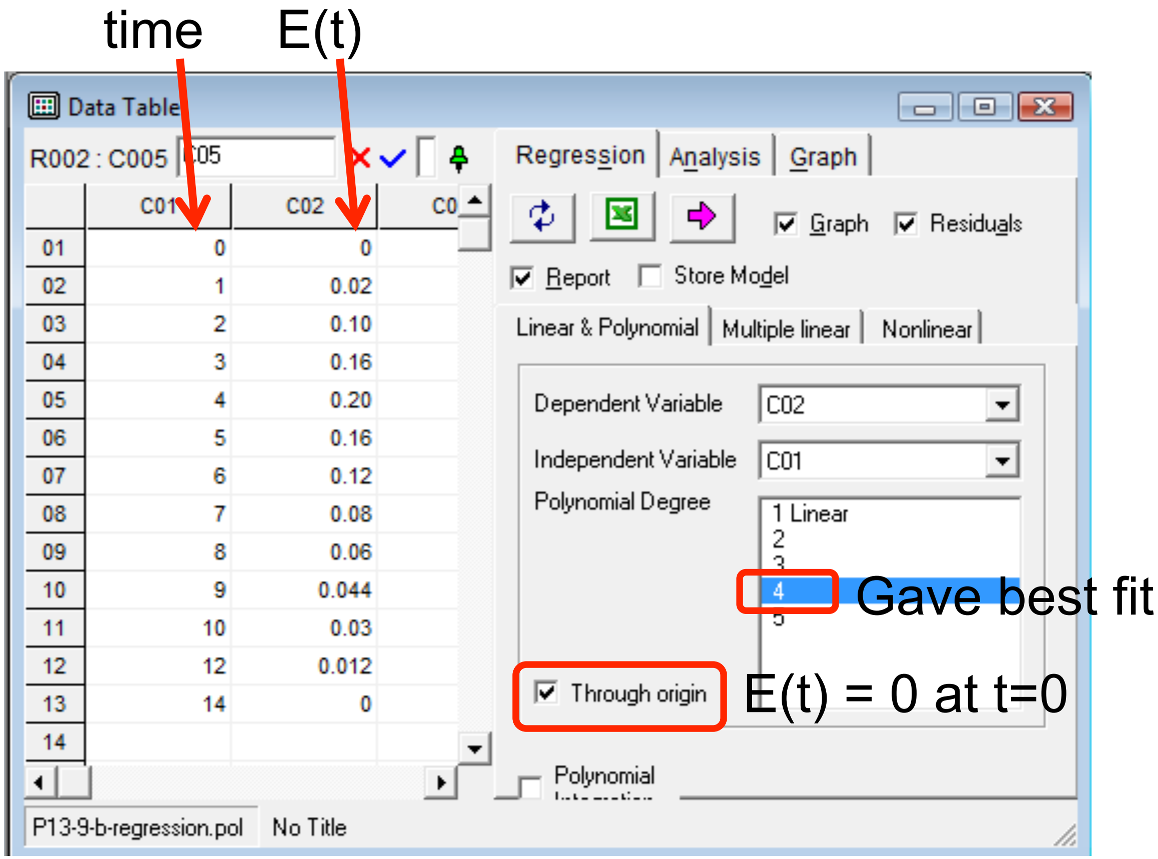
Need an equation for E(t)

$\boxed{k=176}$

$\boxed{C_{B0}=0.0313}$

Use Polymath to fit the E(t) vs t data in the table to a polynomial

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.



time E(t)

R002 : C005 C05

	C01	C02
01	0	0
02	1	0.02
03	2	0.10
04	3	0.16
05	4	0.20
06	5	0.16
07	6	0.12
08	7	0.08
09	8	0.06
10	9	0.044
11	10	0.03
12	12	0.012
13	14	0
14		

☑ Graph ☑ Residuals

☑ Report ☐ Store Model

Dependent Variable C02

Independent Variable C01

Polynomial Degree 4

Gave best fit

☑ Through origin

E(t) = 0 at t=0

☐ Polynomial Integration

P13-9-b-regression.pol No Title

For the irreversible, liquid-phase, nonelementary rxn $A+B\rightarrow C+D$, $-r_A=kC_AC_B^2$ Calculate the X_A using the complete segregation model using Polymath

Model: C02= a1*C01 + a2*C01^2 + a3*C01^3 + a4*C01^4

a1=0.0889237
a2= -0.0157181
a3= 0.0007926
a4= -8.63E-06

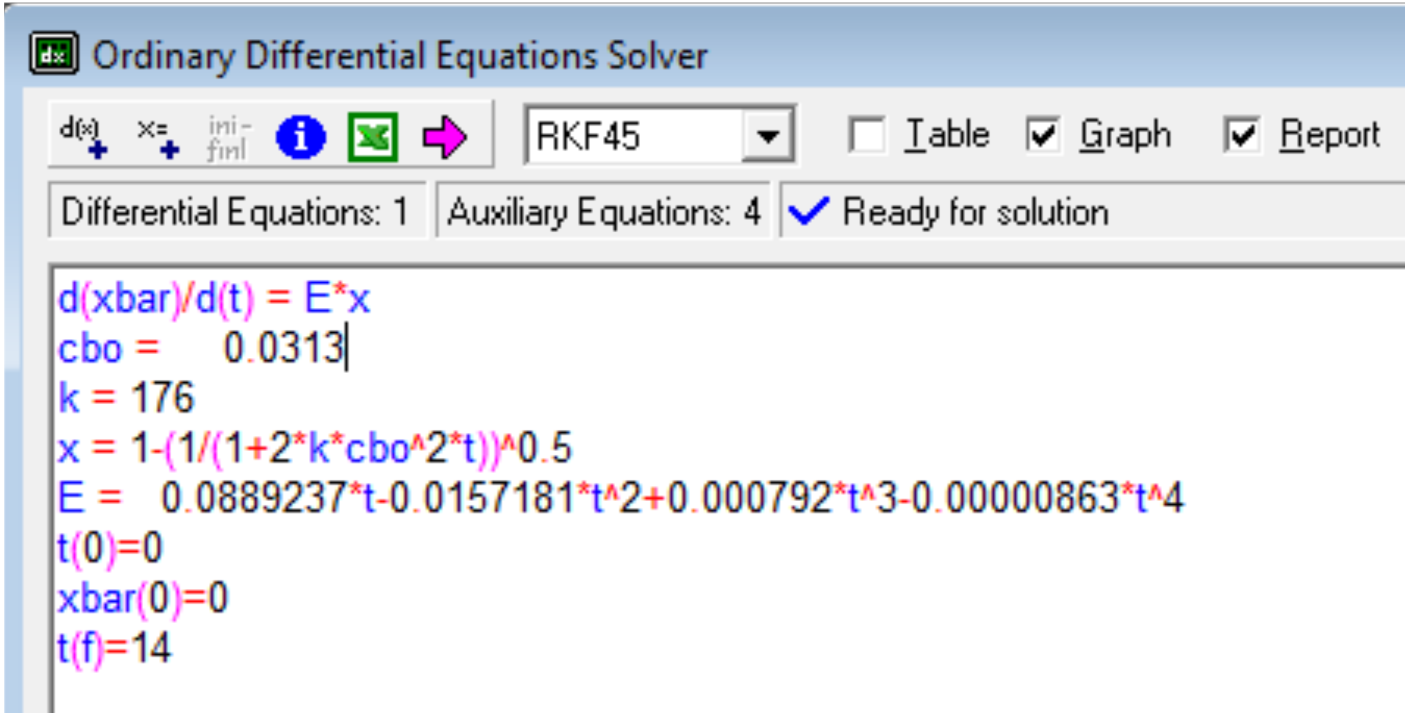
Final Equation: $\boxed{E= 0.0889237*t -0.0157181*t^2 + 0.0007926*t^3 - 8.63E\text{-}6*t^4}$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Complete segregation model by Polymath

$A+B\rightarrow C+D$

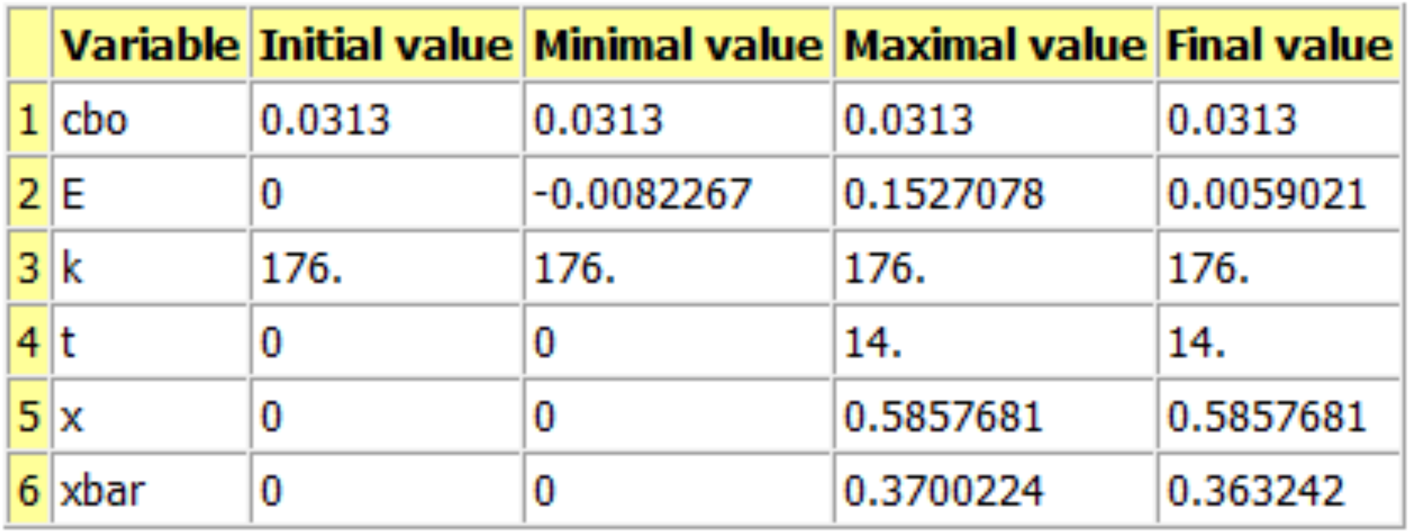
$-r_A=kC_AC_B^2$



RKF45 ☐ Table ☑ Graph ☑ Report

Differential Equations: 1 Auxiliary Equations: 4 ✓ Ready for solution

```
d(xbar)/d(t) = E*x
cbo =     0.0313
k = 176
x = 1-(1/(1+2*k*cbo^2*t))^0.5
E =   0.0889237*t-0.0157181*t^2+0.000792*t^3-0.00000863*t^4
t(0)=0
xbar(0)=0
t(f)=14
```



	Variable	Initial value	Minimal value	Maximal value	Final value
1	cbo	0.0313	0.0313	0.0313	0.0313
2	E	0	-0.0082267	0.1527078	0.0059021
3	k	176.	176.	176.	176.
4	t	0	0	14.	14.
5	x	0	0	0.5857681	0.5857681
6	xbar	0	0	0.3700224	0.363242

Segregation model by Polymath: $\bar{X}_A = 0.36$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, nonelementary rxn A+B→C+D, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for an ideal PFR, the complete segregation model and maximum mixedness model. $C_{A0}=C_{B0}=0.0313$ mol/L & k=176 $L^2/mol^2\cdot min$ at 320K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Maximum mixedness model: $$\frac{dX_A}{d\lambda} = \frac{r_A}{C_{A0}} + \frac{E(\lambda)}{1-F(\lambda)}X_A$$ λ=time $$\frac{dF}{d\lambda} = E$$

F(λ) is a cumulative distribution function

$$\boxed{-r_A = kC_{A0}C_{B0}^2(1-X_A)^3}$$

$$\boxed{C_{A0} = C_{B0} = 0.0313\,\mathrm{mol/L}}$$

$$\boxed{k = 176\frac{L^2}{mol^2\cdot min}}$$

Polymath cannot solve because λ→0 (needs to increase)

Substitute λ for z, where $z=\bar{T}-\lambda$ where $\bar{T}$=longest time interval (14 min)

$$\boxed{\frac{dX_A}{dz} = -\left(\frac{r_A}{C_{A0}} + \frac{E(\bar{T}-z)}{1-F(\bar{T}-z)}X_A\right)}$$

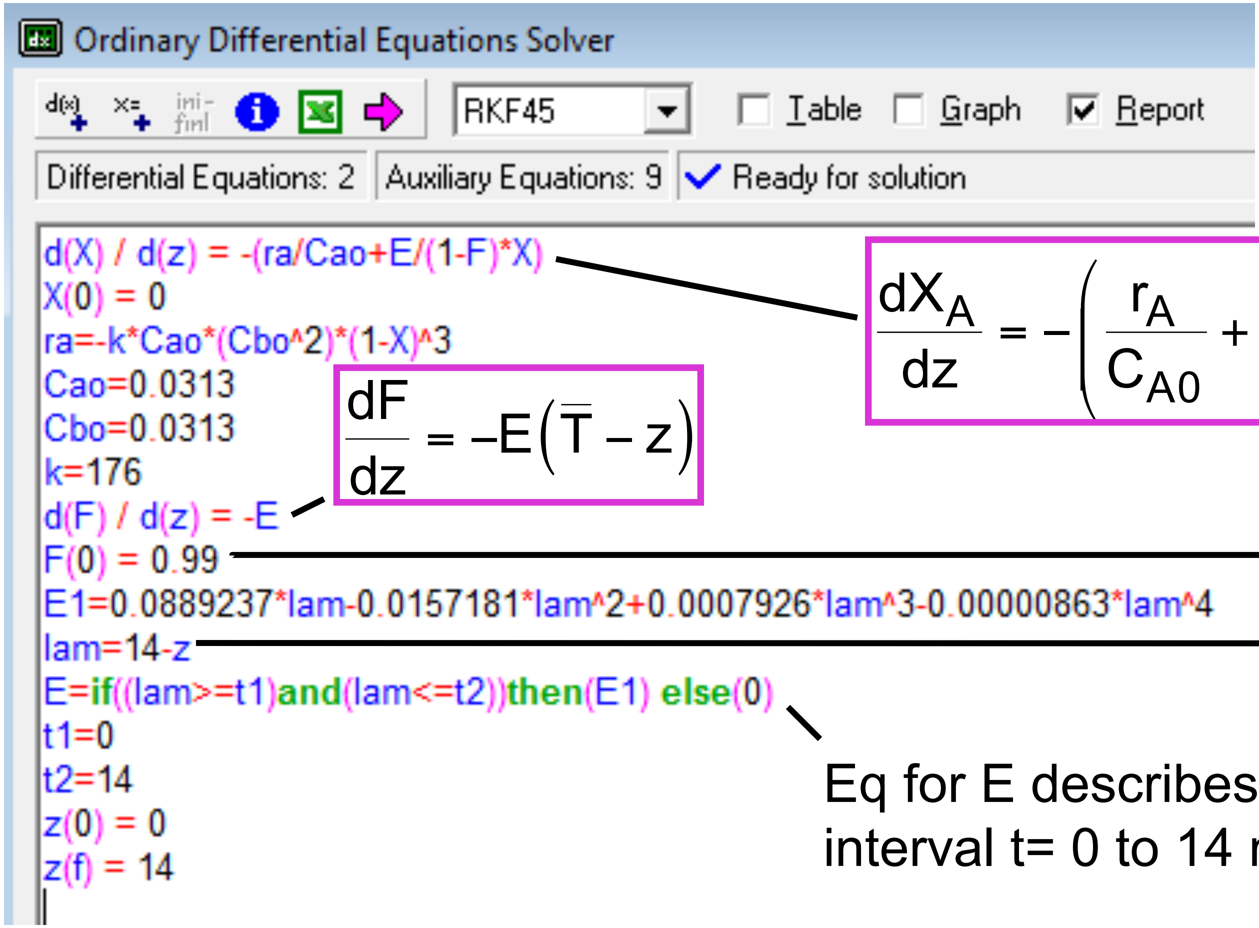
$$\boxed{\frac{dF}{dz} = -E(\bar{T}-z)}$$

E must be in terms of $\bar{T}$-z. Since $\bar{T}$-z=λ & λ=t, simply substitute λ for t

$$\boxed{E(\lambda)= 0.0889237*\lambda-0.0157181*\lambda^2 + 0.0007926*\lambda^3 - 8.63E\text{-}6*\lambda^4}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Maximum Mixedness Model, nonelementary reaction A+B→C+D



Differential Equations: 2 Auxiliary Equations: 9 ✓ Ready for solution

```
d(X) / d(z) = -(ra/Cao+E/(1-F)*X)
X(0) = 0
ra=-k*Cao*(Cbo^2)*(1-X)^3
Cao=0.0313
Cbo=0.0313
k=176
d(F) / d(z) = -E
F(0) = 0.99
E1=0.0889237*lam-0.0157181*lam^2+0.0007926*lam^3-0.00000863*lam^4
lam=14-z
E=if((lam>=t1)and(lam<=t2))then(E1) else(0)
t1=0
t2=14
z(0) = 0
z(f) = 14
```

$$\frac{dX_A}{dz} = -\left(\frac{r_A}{C_{A0}} + \frac{E(\bar{T}-z)}{1-F(\bar{T}-z)}X_A\right)$$

$$\frac{dF}{dz} = -E(\bar{T}-z)$$

Denominator cannot = 0

$$z = \bar{T} - \lambda \rightarrow \lambda = \bar{T} - z$$

Eq for E describes RTD function only on interval t= 0 to 14 minutes, otherwise E=0

$$X_{A,\text{ maximum mixedness}} = 0.347$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, C(t) & E(t) are given in the table below. The irreversible, liquid-phase, nonelementary rxn $A+B \rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out in this reactor. Calculate the conversion for the complete segregation model under adiabatic conditions with T_0= 288K, $C_{A0}=C_{B0}$=0.0313 mol/L, k=176 $L^2/mol^2 \cdot min$ at 320K, $\Delta H°_{RX}$=-40000 cal/mol, E/R =3600K, $C_{PA}=C_{PB}$=20cal/mol·K & $C_{PC}=C_{PD}$=30 cal/mol·K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Polymath eqs for segregation model:

$$\boxed{\frac{d\bar{X}_A}{dt} = X_A(t)E(t)}$$

$$\boxed{\frac{dX_A}{dt} = kC_{B0}^2(1-X_A)^3}$$

E(t)= 0.0889237*t -0.0157181*t² + 0.0007926*t³ – 8.63E-6*t⁴

Express k as function of T:

$$\boxed{k(T) = 176\frac{L^2}{mol^2 \cdot min}\exp\left[3600K\left(\frac{1}{320K}-\frac{1}{T}\right)\right]}$$

Need equations from energy balance. For adiabatic operation:

$$T = \frac{\left[-\Delta H^o_{RX}(T_R)\right]X_A + \sum_{i=1}^{n}\Theta_i C_{p_i}T_0 + X_A\Delta C_P T_R}{\left[\sum_{i=1}^{n}\Theta_i C_{p_i} + X_A\Delta C_P\right]}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, C(t) & E(t) are given in the table below. The irreversible, liquid-phase, nonelementary rxn A+B→C+D, $-r_A=kC_AC_B^2$ will be carried out in this reactor. Calculate the conversion for the complete segregation model under adiabatic conditions with T_0= 288K, $C_{A0}=C_{B0}$=0.0313 mol/L, k=176 L²/mol²·min at 320K, ΔH°_{RX}=-40000 cal/mol, E/R =3600K, $C_{PA}=C_{PB}$=20cal/mol·K & $C_{PC}=C_{PD}$=30 cal/mol·K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Energy balance for adiabatic operation:

$$T = \frac{\left[-\Delta H^o_{RX}\left(T_R\right)\right]X_A + \sum_{i=1}^{n}\Theta_i C_{p_i} T_0 + X_A \Delta C_P T_R}{\left[\sum_{i=1}^{n}\Theta_i C_{p_i} + X_A \Delta C_P\right]}$$

Not zero!

$$\sum_{i=1}^{n}\Theta_i C_{p_i} = C_{p_A} + C_{p_B} = 40\frac{\text{cal}}{\text{mol}\cdot\text{K}} \qquad \Delta C_p = \left(30+30-20-20\right)\frac{\text{cal}}{\text{mol}\cdot\text{K}} = 20\frac{\text{cal}}{\text{mol}\cdot\text{K}}$$

$$\rightarrow \boxed{T = \frac{1702\frac{\text{cal}}{\text{mol}}X_A + 576\frac{\text{cal}}{\text{mol}}}{2\frac{\text{cal}}{\text{mol}\cdot\text{K}} + X_A\left(\frac{\text{cal}}{\text{mol}\cdot\text{K}}\right)}}$$

$$\boxed{\frac{d\bar{X}_A}{dt} = X_A\left(t\right)E\left(t\right)} \qquad \boxed{\frac{dX_A}{dt} = kC_{B0}^2\left(1-X_A\right)^3}$$

$$\boxed{k\left(T\right) = 176\frac{L^2}{\text{mol}^2\cdot\text{min}}\exp\left[3600K\left(\frac{1}{320K}-\frac{1}{T}\right)\right]}$$

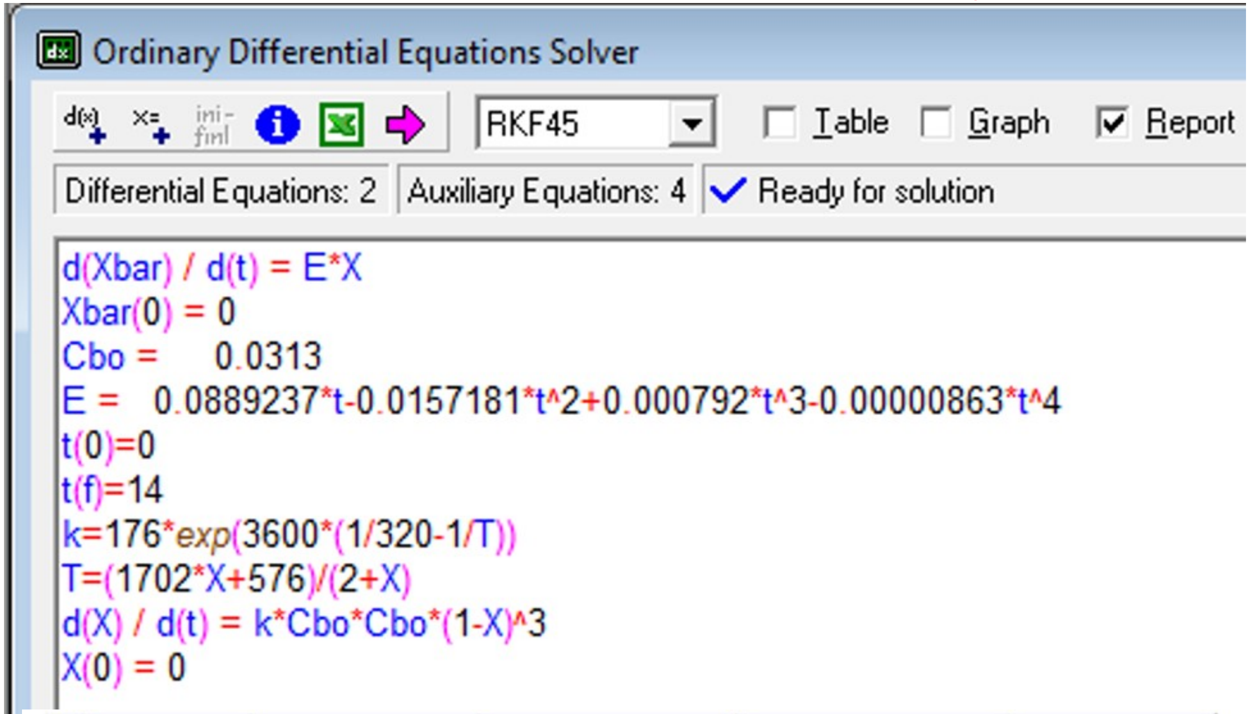
$$\boxed{E(t) = 0.0889237{*}t - 0.0157181{*}t^2 + 0.0007926{*}t^3 - 8.63E\text{-}6{*}t^4}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Segregation model, adiabatic operation, nonelementary reaction kinetics

$A+B \rightarrow C+D$

$-r_A = kC_AC_B^2$



RKF45

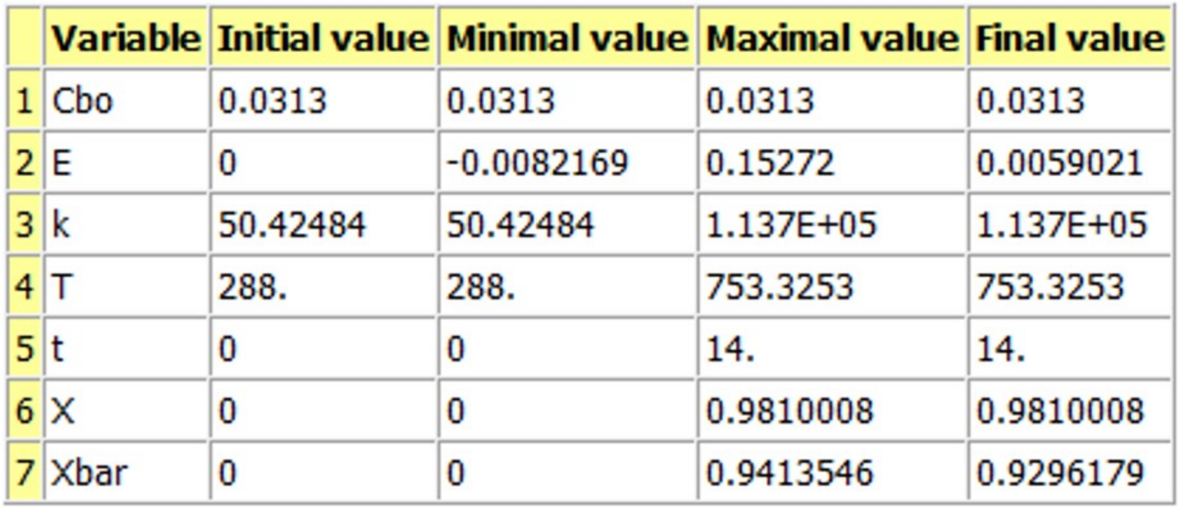
☐ Table ☐ Graph ☑ Report

Differential Equations: 2

Auxiliary Equations: 4

✓ Ready for solution

```
d(Xbar) / d(t) = E*X
Xbar(0) = 0
Cbo =      0.0313
E =   0.0889237*t-0.0157181*t^2+0.000792*t^3-0.00000863*t^4
t(0)=0
t(f)=14
k=176*exp(3600*(1/320-1/T))
T=(1702*X+576)/(2+X)
d(X) / d(t) = k*Cbo*Cbo*(1-X)^3
X(0) = 0
```



	Variable	Initial value	Minimal value	Maximal value	Final value
1	Cbo	0.0313	0.0313	0.0313	0.0313
2	E	0	-0.0082169	0.15272	0.0059021
3	k	50.42484	50.42484	1.137E+05	1.137E+05
4	T	288.	288.	753.3253	753.3253
5	t	0	0	14.	14.
6	X	0	0	0.9810008	0.9810008
7	Xbar	0	0	0.9413546	0.9296179

$$\bar{X}_A = 0.93$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

The following slides show how the same problem would be solved and the solutions would differ if the reaction rate was still $-r_A=kC_AC_B^2$ but the reaction was instead elementary: $A+\underline{2B}\rightarrow C+D$

These slides may be provided as an extra example problem that the students may study on there own if time does not permit doing it in class.

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, elementary rxn $A+\underline{2B}\rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for an ideal PFR, the complete segregation model and maximum mixedness model. $C_{A0}=C_{B0}=0.0313$ mol/L & $k=176$ $L^2/mol^2\cdot min$ at 320K

t min	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**12**	**14**
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Start with PFR design eq & see how far can we get:

$$\frac{dX_A}{dV}=\frac{-r_A}{F_{A0}}\rightarrow\frac{dX_A}{dV}=\frac{kC_AC_B^2}{C_{A0}\upsilon_0}\rightarrow\frac{dX_A}{d\tau}=\frac{kC_AC_B^2}{C_{A0}}$$

$$C_A=C_{A0}\left(1-X_A\right)\qquad \nu_b=\frac{b}{a}=\frac{2}{1}\rightarrow C_B=C_{B0}\left(1-2X_A\right)$$

$$\rightarrow\frac{dX_A}{d\tau}=\frac{k\cancel{C_{A0}}C_{B0}^2\left(1-X_A\right)\left(1-2X_A\right)^2}{\cancel{C_{A0}}}\rightarrow\boxed{\frac{dX_A}{d\tau}=kC_{B0}^2\left(1-X_A\right)\left(1-2X_A\right)^2}$$

$$\boxed{C_{B0}=0.0313}\qquad\boxed{k=0.0313}$$

Could solve with Polymath if we knew the value of τ

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, elementary rxn $A+2B \rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for an ideal PFR, the complete segregation model and maximum mixedness model. $C_{A0}=C_{B0}=0.0313$ mol/L & $k=176$ $L^2/mol^2 \cdot min$ at 320K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/ m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0
t*E(t)	0	0.02	0.2	0.48	0.8	0.8	0.72	0.56	0.48	0.396	0.3	0.144	0

$$\boxed{\frac{dX_A}{d\tau} = kC_{B0}^2(1-X_A)(1-2X_A)^2}$$

How do we determine τ?

For an ideal reactor, $\tau = t_m$

$$t_m = \int_0^\infty tE(t)dt$$

Use numerical method to determine t_m:

$$t_m = \int_0^\infty tE(t)dt = \int_0^{10} tE(t)dt + \int_{10}^{14} tE(t)dt$$

$$\int_0^{10} tE(t)dt = \frac{1}{3}\begin{bmatrix} 0+4(0.02)+2(0.2)+4(0.48)+2(0.8)+4(0.8) \\ +2(0.72)+4(0.56)+2(0.48)+4(0.396)+0.3 \end{bmatrix} = 4.57$$

$$\int_{10}^{14} tE(t)dt = \frac{2}{3}\left[0.3+4(0.144)+0\right] = 0.584 \qquad \rightarrow t_m = 4.57+0.584 = 5.15\,\text{min}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, elementary rxn $A+\underline{2}B \rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for an ideal PFR, the complete segregation model and maximum mixedness model. $C_{A0}=C_{B0}=0.0313$ mol/L & $k=176$ L^2/mol^2·min at 320K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0
t*E(t)	0	0.02	0.2	0.48	0.8	0.8	0.72	0.56	0.48	0.396	0.3	0.144	0

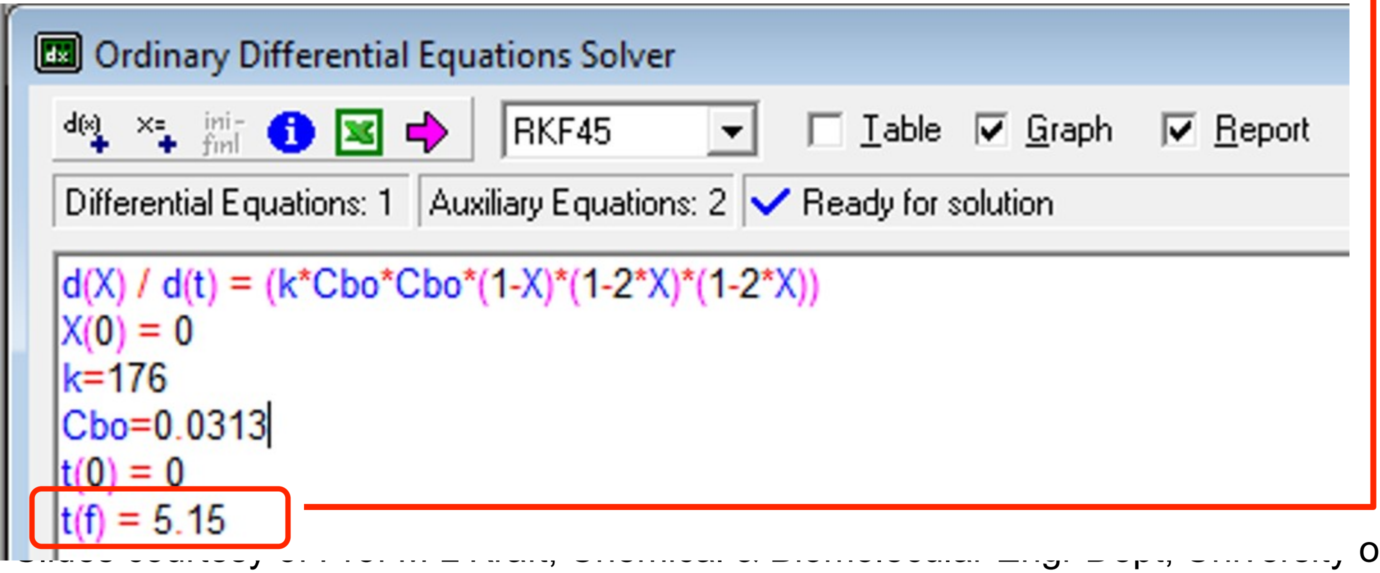
$$\boxed{\frac{dX_A}{d\tau} = kC_{B0}^2(1-X_A)(1-2X_A)^2}$$

For an ideal reactor, $\tau = t_m$

$$t_m = \int_0^\infty tE(t)dt$$

$$t_m = 5.15\,\text{min} = \tau$$

Final X_A corresponds to τ=5.15 min



Ordinary Differential Equations Solver

RKF45 ☐ Table ☑ Graph ☑ Report

Differential Equations: 1 Auxiliary Equations: 2 ✓ Ready for solution

```
d(X) / d(t) = (k*Cbo*Cbo*(1-X)*(1-2*X)*(1-2*X))
X(0) = 0
k=176
Cbo=0.0313
t(0) = 0
t(f) = 5.15
```

$$X_{A,PFR} = 0.29$$

Slides courtesy of Prof. M L Kraft, Chemical & Biomolecular Eng. Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, elementary rxn $A+\underline{2B}\rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for an ideal PFR, the complete segregation model and maximum mixedness model. $C_{A0}=C_{B0}=0.0313$ mol/L & $k=176$ L²/mol²·min at 320K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Segregation model with Polymath:

$$\bar{X}_A=\int_0^\infty X_A(t)E(t)dt \rightarrow \boxed{\frac{d\bar{X}_A}{dt}=X_A(t)E(t)}$$

$X_A(t)$ is from ***batch reactor*** design eq

Batch reactor design eq:

$$N_{A0}\frac{dX_A}{dt}=-r_AV \rightarrow \cancel{N_{A0}}\frac{dX_A}{dt}=k\cancel{C_{A0}}C_{B0}^2(1-X_A)(1-2X_A)^2\cancel{V}$$

$$N_{A0}=C_{A0}V$$

Stoichiometry:

$$-r_A=kC_AC_B^2$$

$$C_A=C_{A0}(1-X_A)$$

$$C_B=C_{B0}(1-2X_A)$$

$$\rightarrow \boxed{\frac{dX_A}{dt}=kC_{B0}^2(1-X_A)(1-2X_A)^2}$$

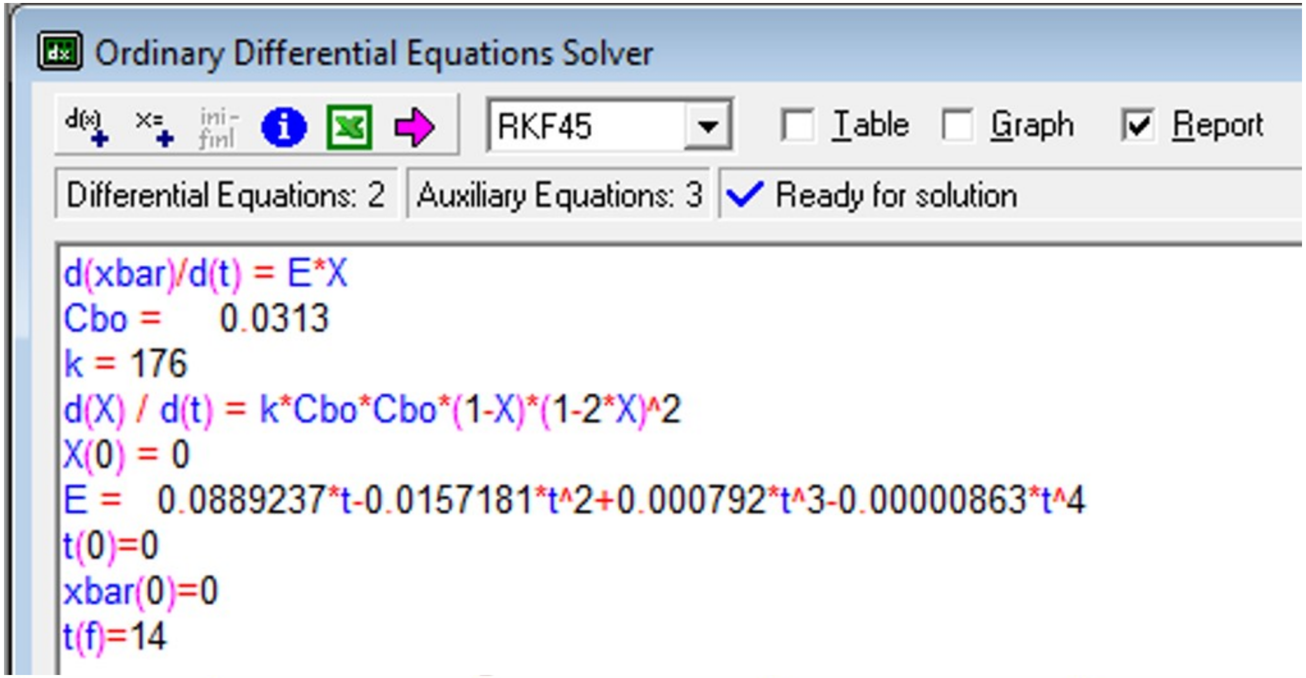
$\boxed{k=176}$ $\boxed{C_{B0}=0.0313}$

Best-fit polynomial line for E(t) vs t calculated by Polymath (slide 19)

$$\boxed{E(t)=0.0889237*t-0.0157181*t^2+0.0007926*t^3-8.63E\text{-}6*t^4}$$

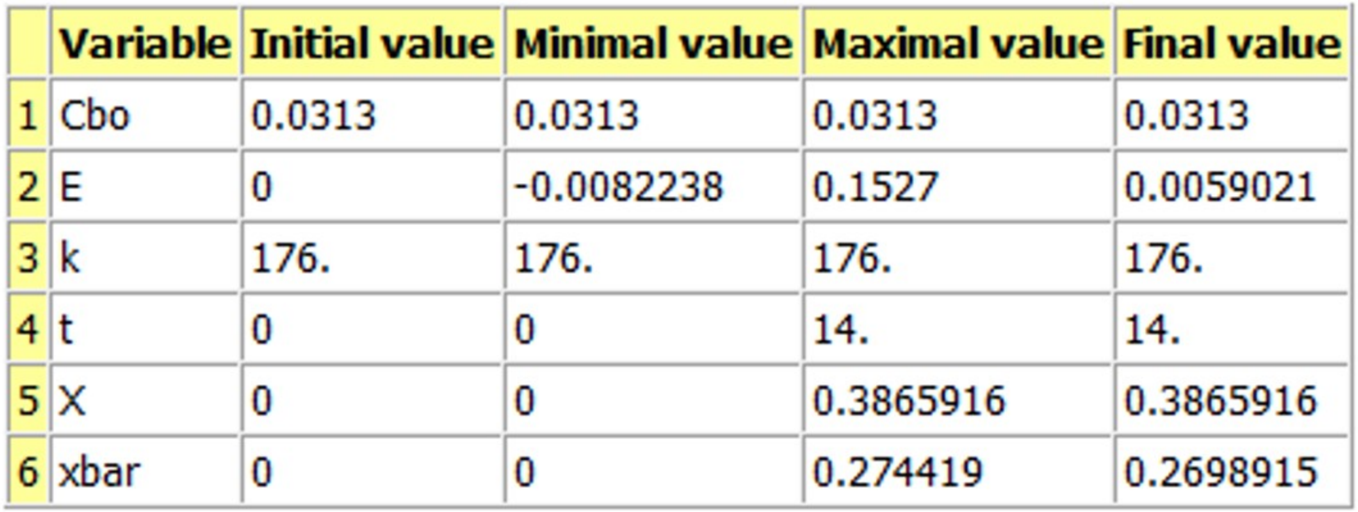
Slides courtesy of Prof M L Kra

Segregation model, isothermal operation, elementary rxn: $A+2B \rightarrow C+D$



Differential Equations: 2 | Auxiliary Equations: 3 | ✓ Ready for solution

```
d(xbar)/d(t) = E*X
Cbo =     0.0313
k = 176
d(X) / d(t) = k*Cbo*Cbo*(1-X)*(1-2*X)^2
X(0) = 0
E =   0.0889237*t-0.0157181*t^2+0.000792*t^3-0.00000863*t^4
t(0)=0
xbar(0)=0
t(f)=14
```



	Variable	Initial value	Minimal value	Maximal value	Final value
1	Cbo	0.0313	0.0313	0.0313	0.0313
2	E	0	-0.0082238	0.1527	0.0059021
3	k	176.	176.	176.	176.
4	t	0	0	14.	14.
5	X	0	0	0.3865916	0.3865916
6	xbar	0	0	0.274419	0.2698915

$$X_{A,seg} = 0.27$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, the effluent concentration C(t) & RTD function E(t) are given in the table below. The irreversible, liquid-phase, elementary rxn $A+\underline{2B} \rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out isothermally at 320K in this reactor. Calculate the conversion for an ideal PFR, the complete segregation model and maximum mixedness model. $C_{A0}=C_{B0}=0.0313$ mol/L & $k=176\ L^2/mol^2 \cdot min$ at 320K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Maximum mixedness model: $$\frac{dX_A}{d\lambda}=\frac{r_A}{C_{A0}}+\frac{E(\lambda)}{1-F(\lambda)}X_A \qquad \lambda=\text{time} \qquad \frac{dF}{d\lambda}=E$$

Polymath cannot solve because λ→0 (must increase)

$$\boxed{-r_A=kC_{A0}C_{B0}^2(1-X_A)(1-2X_A)^2}$$

$$\boxed{k=176\frac{L^2}{mol^2 \cdot min}}$$

$$\boxed{C_{A0}=C_{B0}=0.0313\,mol/L}$$

Substitute λ for z, where $z=\bar{T}-\lambda$ where $\bar{T}$=longest time interval (14 min)

$$\boxed{\frac{dX_A}{dz}=-\left(\frac{r_A}{C_{A0}}+\frac{E(\bar{T}-z)}{1-F(\bar{T}-z)}X_A\right)}$$

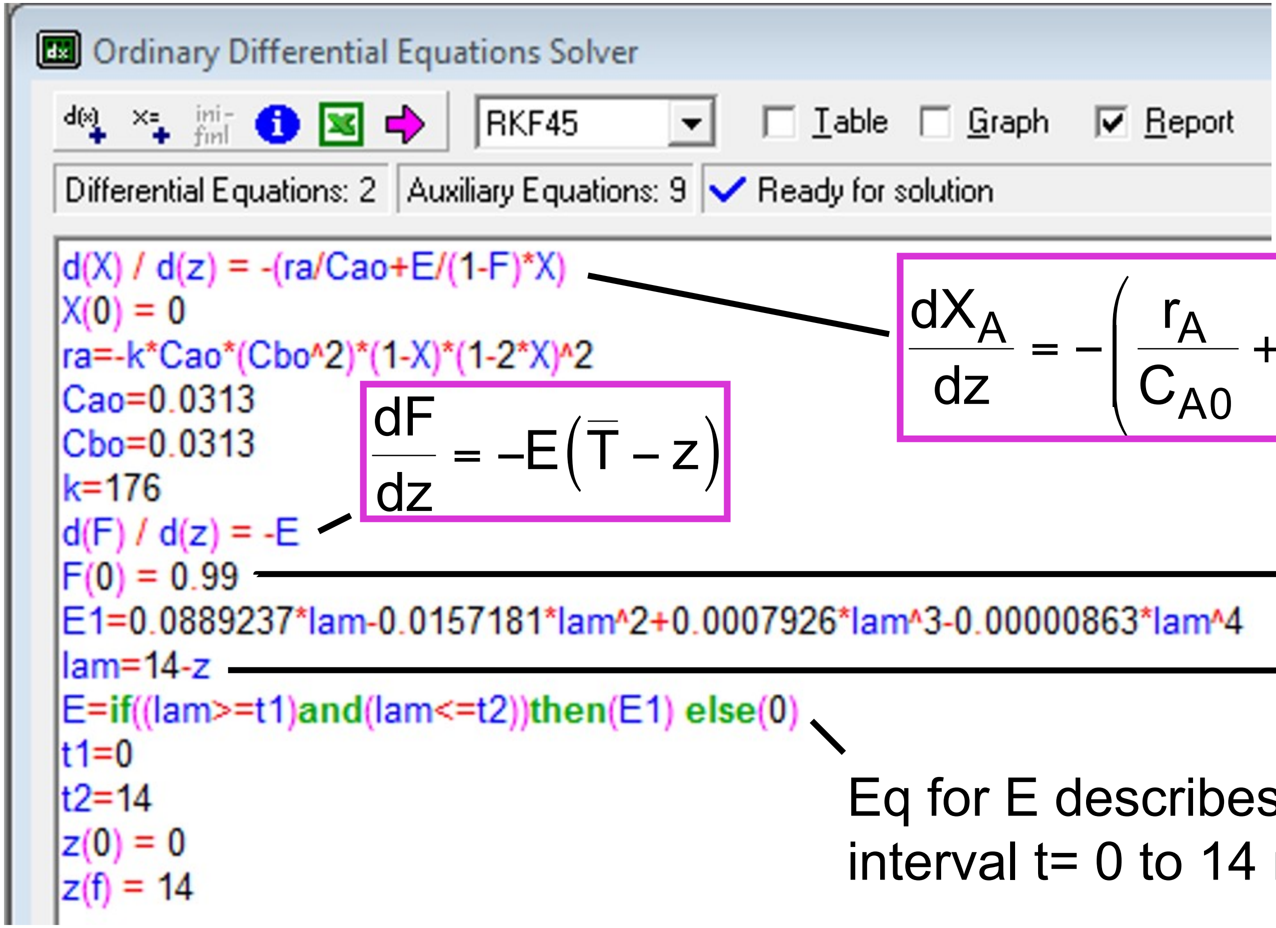
$$\boxed{\frac{dF}{dz}=-E(\bar{T}-z)}$$

E must be in terms of $\bar{T}$-z. Since $\bar{T}$-z=λ & λ=t, simply substitute λ for t

$$\boxed{E(\lambda)=0.0889237*\lambda-0.0157181*\lambda^2+0.0007926*\lambda^3-8.63E\text{-}6*\lambda^4}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Maximum Mixedness Model, elementary reaction $A+\underline{2B}\rightarrow C+D$, $-r_A=kC_AC_B^2$



Ordinary Differential Equations Solver

RKF45 ☐ Table ☐ Graph ☑ Report

Differential Equations: 2 | Auxiliary Equations: 9 | ✓ Ready for solution

```
d(X) / d(z) = -(ra/Cao+E/(1-F)*X)
X(0) = 0
ra=-k*Cao*(Cbo^2)*(1-X)*(1-2*X)^2
Cao=0.0313
Cbo=0.0313
k=176
d(F) / d(z) = -E
F(0) = 0.99
E1=0.0889237*lam-0.0157181*lam^2+0.0007926*lam^3-0.00000863*lam^4
lam=14-z
E=if((lam>=t1)and(lam<=t2))then(E1) else(0)
t1=0
t2=14
z(0) = 0
z(f) = 14
```

$$\frac{dX_A}{dz}=-\left(\frac{r_A}{C_{A0}}+\frac{E\left(\bar{T}-z\right)}{1-F\left(\bar{T}-z\right)}X_A\right)$$

$$\frac{dF}{dz}=-E\left(\bar{T}-z\right)$$

Denominator cannot = 0

$$z=\bar{T}-\lambda\rightarrow\lambda=\bar{T}-z$$

Eq for E describes RTD function only on interval t= 0 to 14 minutes, otherwise E=0

$$X_{A,\text{ maximum mixedness}}=0.25$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, C(t) & E(t) are given in the table below. The irreversible, liquid-phase, elementary rxn $A+\underline{2B}\rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out in this reactor. Calculate the conversion for the complete segregation model under adiabatic conditions with T_0= 288K, $C_{A0}=C_{B0}$=0.0313 mol/L, k=176 $L^2/mol^2\cdot min$ at 320K, $\Delta H°_{RX}$=-40000 cal/mol, E/R =3600K, $C_{PA}=C_{PB}$=20cal/mol·K & $C_{PC}=C_{PD}$=30 cal/mol·K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Polymath eqs for segregation model:

$$\boxed{\frac{d\bar{X}_A}{dt}=X_A(t)E(t)}$$

$$\boxed{\frac{dX_A}{dt}=kC_{B0}^2(1-X_A)(1-2X_A)^2}$$

E(t)= 0.0889237*t -0.0157181*t^2 + 0.0007926*t^3 – 8.63E-6*t^4

Express k as function of T:

$$\boxed{k(T)=176\frac{L^2}{mol^2\cdot min}\exp\left[3600K\left(\frac{1}{320K}-\frac{1}{T}\right)\right]}$$

Need equations from energy balance. For adiabatic operation:

$$T=\frac{\left[-\Delta H^o{}_{RX}(T_R)\right]X_A+\sum_{i=1}^{n}\Theta_iC_{p_i}T_0+X_A\Delta C_PT_R}{\left[\sum_{i=1}^{n}\Theta_iC_{p_i}+X_A\Delta C_P\right]}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

For a pulse tracer expt, C(t) & E(t) are given in the table below. The irreversible, liquid-phase, elementary rxn $A+\underline{2B}\rightarrow C+D$, $-r_A=kC_AC_B^2$ will be carried out in this reactor. Calculate the conversion for the complete segregation model under adiabatic conditions with T_0= 288K, $C_{A0}=C_{B0}$=0.0313 mol/L, k=176 $L^2/mol^2\cdot min$ at 320K, $\Delta H°_{RX}$=-40000 cal/mol, E/R =3600K, $C_{PA}=C_{PB}$=20cal/mol·K & $C_{PC}=C_{PD}$=30 cal/mol·K

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Adiabatic EB:

$$T=\frac{\left[-\Delta H^o_{RX}\left(T_R\right)\right]X_A+\sum_{i=1}^{n}\Theta_iC_{p_i}T_0+X_A\Delta C_PT_R}{\left[\sum_{i=1}^{n}\Theta_iC_{p_i}+X_A\Delta C_P\right]}$$

$$\Delta C_p=\left(30+30-2\left(20\right)-20\right)=0$$

$$\sum_{i=1}^{n}\Theta_iC_{p_i}=C_{pA}+C_{pB}=40\frac{cal}{mol\cdot K}$$

$$\boxed{T=288K+1000X_A}$$

$$\boxed{\frac{d\bar{X}_A}{dt}=X_A\left(t\right)E\left(t\right)}$$

$$\boxed{\frac{dX_A}{dt}=kC_{B0}^2\left(1-X_A\right)\left(1-2X_A\right)^2}$$

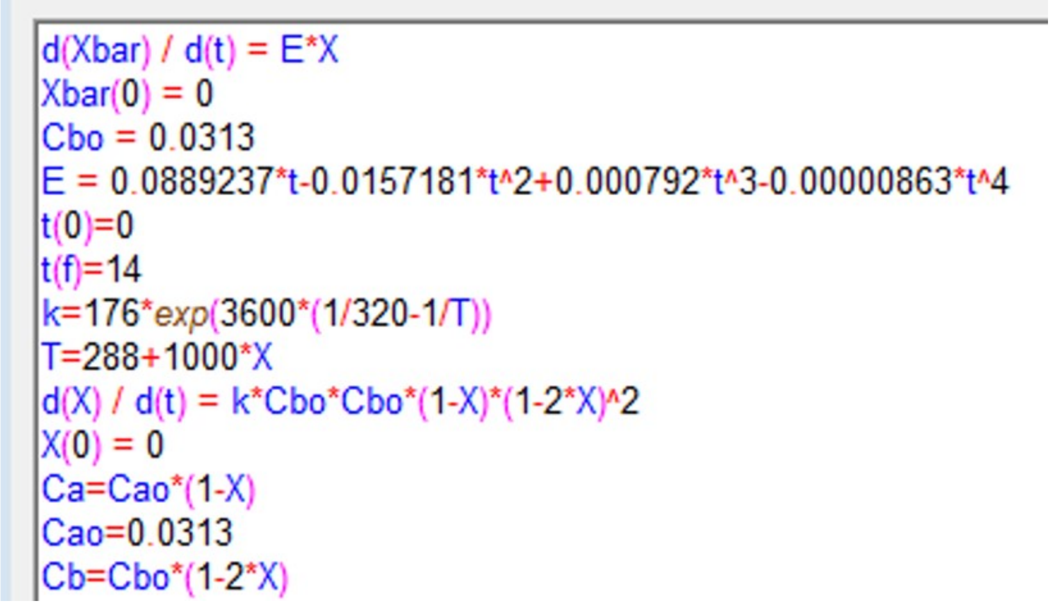
$$\boxed{k\left(T\right)=176\frac{L^2}{mol^2\cdot min}\exp\left[3600K\left(\frac{1}{320K}-\frac{1}{T}\right)\right]}$$

$$\boxed{E(t)=0.0889237*t-0.0157181*t^2+0.0007926*t^3-8.63E\text{-}6*t^4}$$

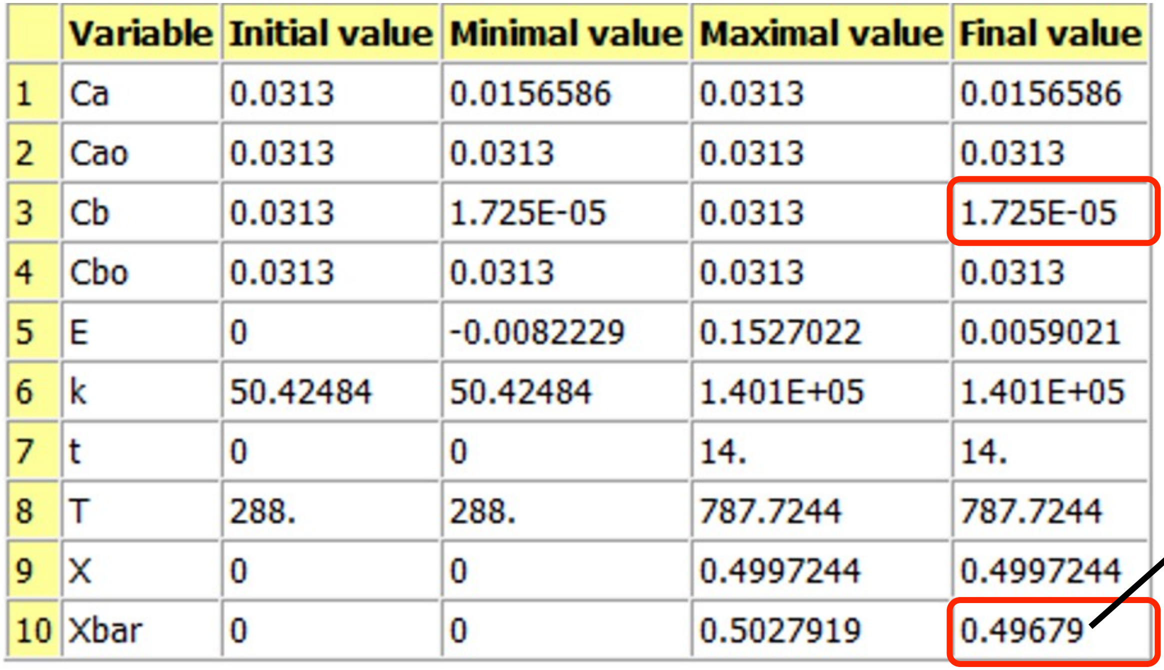
Segregation model, adiabatic operation, elementary reaction kinetics

$A+\underline{2B}\rightarrow C+D$

$-r_A=kC_AC_B^2$



```
d(Xbar) / d(t) = E*X
Xbar(0) = 0
Cbo = 0.0313
E = 0.0889237*t-0.0157181*t^2+0.000792*t^3-0.00000863*t^4
t(0)=0
t(f)=14
k=176*exp(3600*(1/320-1/T))
T=288+1000*X
d(X) / d(t) = k*Cbo*Cbo*(1-X)*(1-2*X)^2
X(0) = 0
Ca=Cao*(1-X)
Cao=0.0313
Cb=Cbo*(1-2*X)
```



	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	0.0313	0.0156586	0.0313	0.0156586
2	Cao	0.0313	0.0313	0.0313	0.0313
3	Cb	0.0313	1.725E-05	0.0313	1.725E-05
4	Cbo	0.0313	0.0313	0.0313	0.0313
5	E	0	-0.0082229	0.1527022	0.0059021
6	k	50.42484	50.42484	1.401E+05	1.401E+05
7	t	0	0	14.	14.
8	T	288.	288.	787.7244	787.7244
9	X	0	0	0.4997244	0.4997244
10	Xbar	0	0	0.5027919	0.49679

Because B is completely consumed by $X_A=0.5$

$\bar{X}_A = 0.50$

Why so much lower than before?

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.