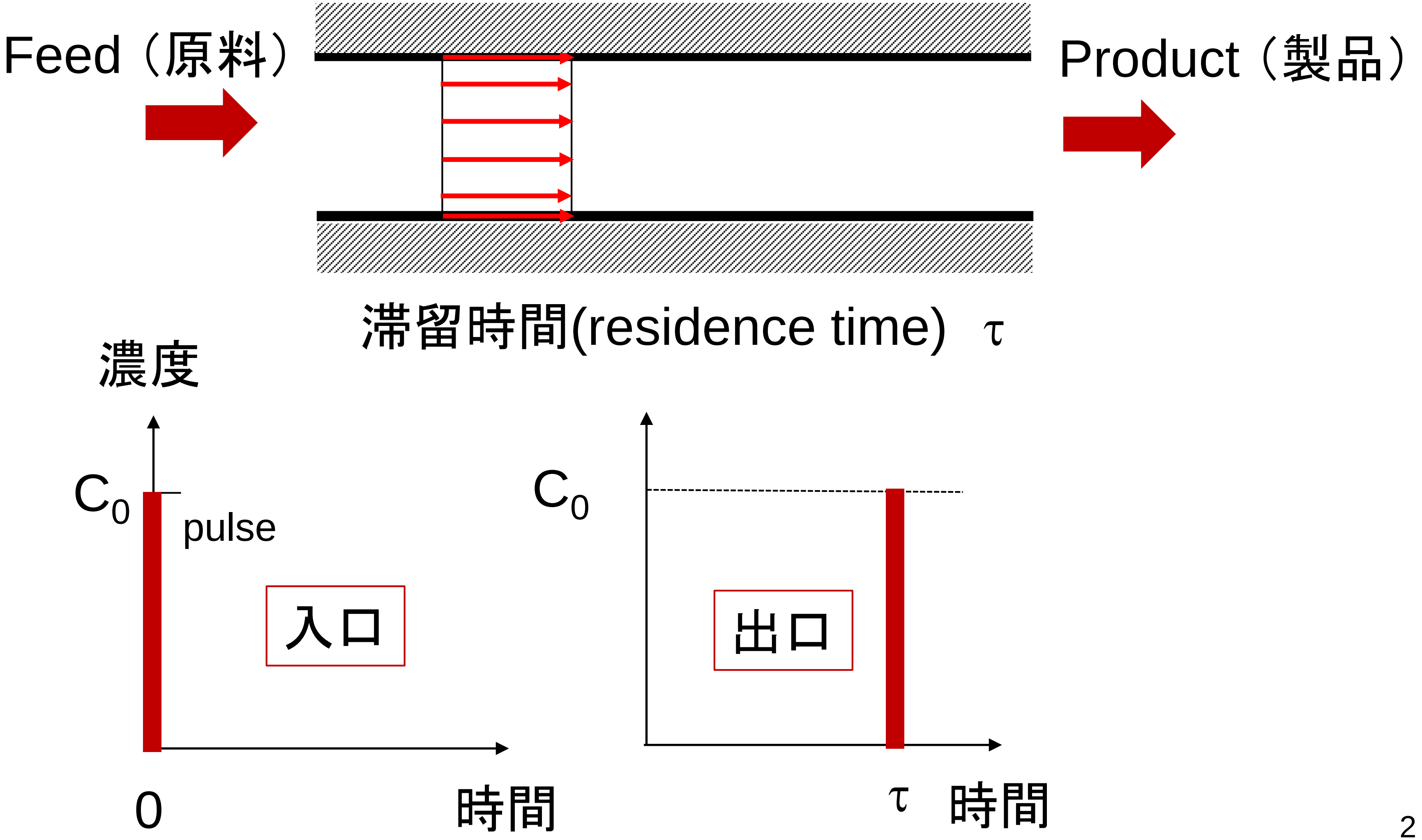
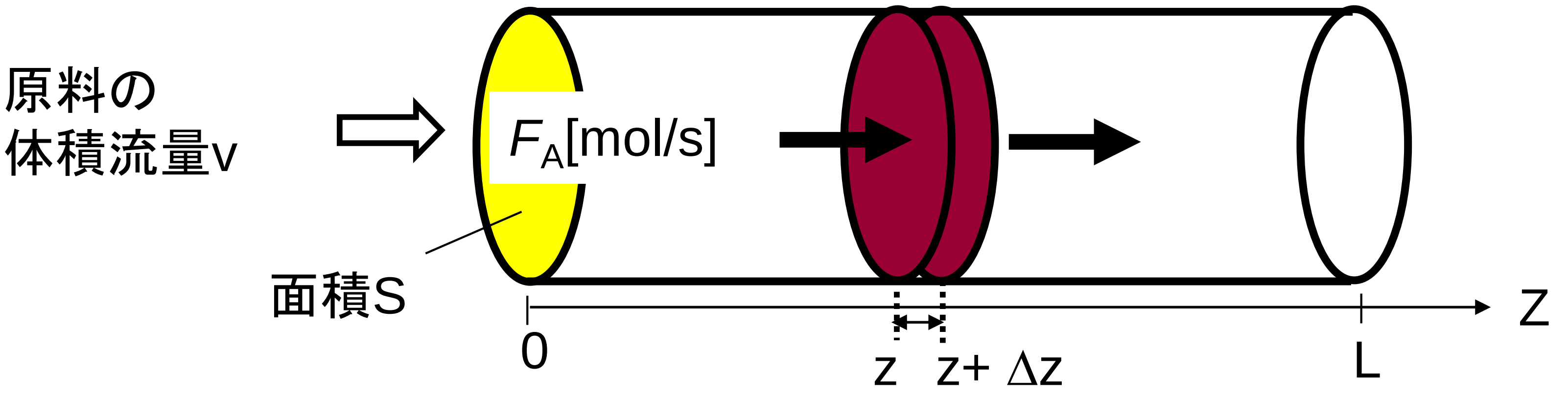
工業反応装置特論

講義時間：6限
場所　　：8-1A
担当　　：山村

管型反応器(Plug Flow Reactor)



管型反応器の設計方程式(1)



Z=z～z+Δzの微小区間で成分Aの物質収支をとる

モル数の変化Δn_A = 反応による生成量$r_A S \Delta z\ \Delta t$
+反応器への流入量$F_A \big|_z \Delta t$
- 反応器からの流出量$F_A \big|_{z+\Delta z} \Delta t$

管型反応器の設計方程式（2）

両辺をΔtで除すと

$$\frac{\Delta n_A}{\Delta t} = r_A S\Delta z + F_A\Big|_z - F_A\Big|_{z+\Delta z}$$

$\Delta t \to 0$の極限をとれば

$$\frac{dn_A}{dt} = r_A S\Delta z + F_A\Big|_z - F_A\Big|_{z+\Delta z}$$

微小区間のモル濃度は$C_A=n_A/\Delta V$であることに注意して
両辺を$\Delta V=S\Delta z$で除すと

$$\frac{dC_A}{dt} = r_A + \frac{F_A\Big|_z - F_A\Big|_{z+\Delta z}}{S\Delta z}$$

管型反応器の設計方程式(3)

Δzを十分小さくとれば

$$\frac{F_A\big|_{z+\Delta z} - F_A\big|_z}{\Delta z} = \left.\frac{dF_A}{dz}\right|_z$$

従って

$$\frac{dC_A}{dt} = r_A - \frac{1}{S}\left.\frac{dF_A}{dz}\right|_z$$

$$= r_A - \left.\frac{dF_A}{dV}\right|_z$$

定常状態を考えると、$dC_A/dt=0$なので

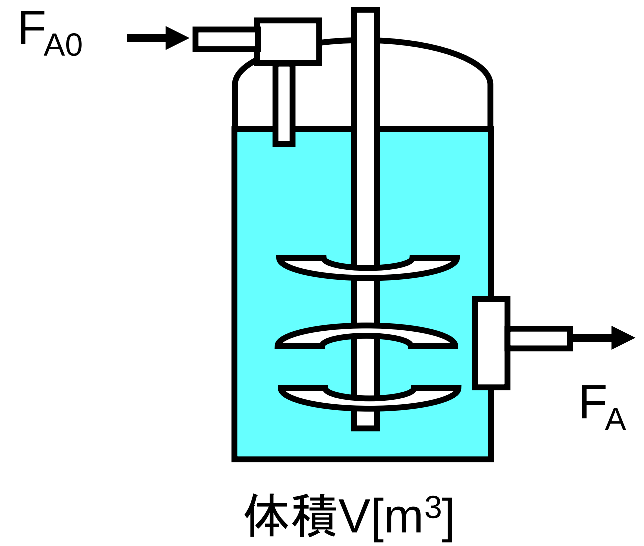
$$0 = r_A - \frac{dF_A}{dV}$$

管型反応器の設計方程式(4)

$$r_A = \frac{dF_A}{dV}$$

必要なPFRの体積V_{PFR}は$V_{PFR} = \int_{F_{A0}}^{F_{Af}} \frac{1}{r_A} dF_A$

CSTRのImpulse応答（1）



設計方程式

$$V\frac{dC_A}{dt}=r_AV+C_{A0}v_0-C_Av_0$$

$$t=0\text{で}C_A=C_A{}^0$$

$$t>0\text{で}C_{A0}=0,\quad r_A=0(\text{反応無})$$

$$V\frac{dC_A}{dt}=-C_Av_0$$

滞留時間$\tau\equiv V/v_0$より

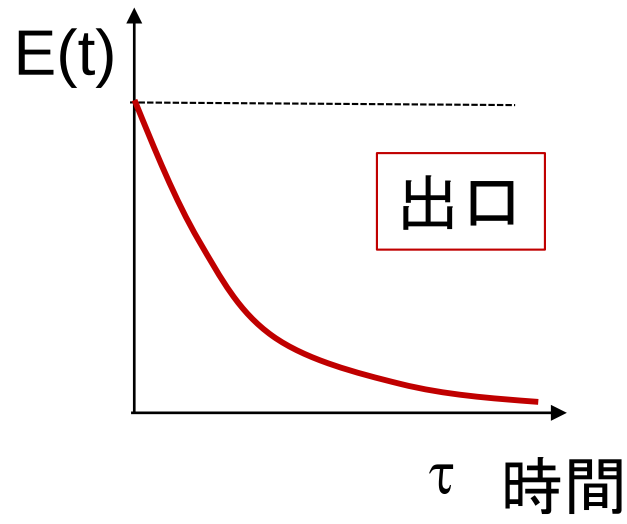
$$\tau\frac{dC_A}{dt}=-C_A$$

CSTRのImpulse応答（2）

積分すると

$$\int_0^t dt = -\tau \int_{C_{A0}}^{C_A} \frac{1}{C_A} dC_A = -\tau \ln \frac{C_A}{C_{A0}}$$

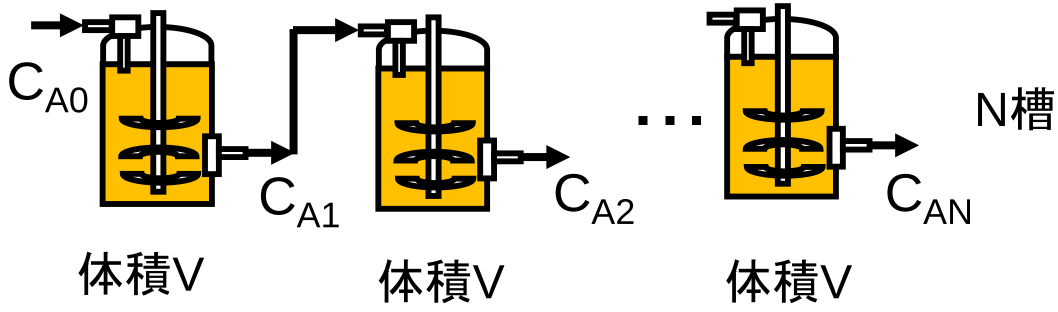
$$\therefore \frac{C_A}{C_{A0}} = \exp(-t/\tau)$$



$$residence\ time\ distribution\ \ function, E$$

$$E \equiv \frac{C_A(t)}{\int_0^\infty C_A(t)dt} = \frac{C_{A0}\exp(-t/\tau)}{C_{A0}\int_0^\infty \exp(-t/\tau)dt} = \frac{\exp(-t/\tau)}{\tau}$$

直列CSTRのImpulse応答（1）

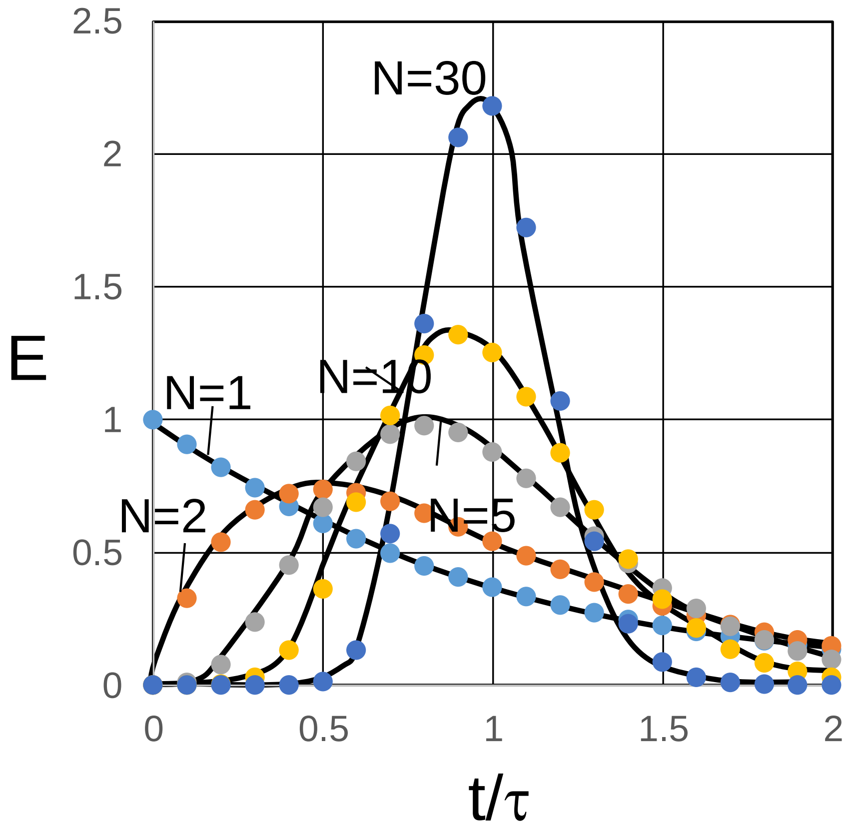


$$residence\ time\ distribution\ \ function, E$$

$$E \equiv \frac{N(Nt/\tau)^{N-1}}{(N-1)!}\exp(-Nt/\tau)$$

$$N = 1 では E \equiv \frac{N(t/\tau)^{N-1}}{\tau(N-1)!}\exp(-t/\tau)$$

直列CSTRのImpulse応答（2）



N=1では単槽CSTR
Nが増加するとPFRに漸近

実反応器でインパルス応答実験を行い、
上の曲線にfittingすれば槽数Nが決まる
（槽列モデルとも呼ばれる）

Report 11 Chemical Process Simulator – combination of CSTR and PFR 氏名

Design a chemical process with two reactors connected in series. We have single reaction, Methyl acetate + water →acetic acid + methanol, in each reactor. We supply the feed that contains 26.75 mol/s of water, 0.25 mol/s of Methyl acetate, and 0.025 mol/s of acetic acid into the first reactor. No methanol is included in the feed.

Q1.Show that the parameters below result in "Flow Methyl acetate" of 0.05 mol/s in stream 3.
This corresponds to the conversion of (0.25-0.05)/0.25=0.8, namely 80% of Methyl acetate in the feed is converted into products.

Q2. Determine pairs of volumes of the CSTR/PFR reactors that satisfy "Flow Methyl acetate" of 0.05 mol/s in stream 3. Calculate the total reactor volume (V_{CSTR}+V_{PFR}) against the volume of CSTR and show that the total volume shows a minimum at a critical V_{CSTR}.

Q3. Switch the CSTR and PFR at the same volumes and conditions in Q2. Show that the "Flow Methyl acetate" becomes larger than 0.05 mol/s in product stream, namely more unreacted ethyl acetate remains in the system when we use PFR first and then CSTR reactors.

1. Material selection
setting-property packages-add-TEA-select-New-Model set:Peng Robinson-add-filter-Methyl acetate-OK-add-filter-water-OK-add-filter-acetic acid-OK-add-filter-methanol-OK-OK-
2. Reactior/Reaction selection
Reaction packages-add-CORN Reaction Package Manager-select-New-New Reaction Packages-Edit-Compounds-Add-From material template-default-OK-check H2O-check filter-Methyl acetate-check acetic acid-OK-check methanol-OK-Reactions-Create-rxn1-OK-Stoich-"-1"(water)- "-1"(Methyl acetate)- "-1"(acetic acid)-"1"(methanol)-Rate-1.e-6*C("Methyl acetate")*C("Acetic acid)-Phase-Liquid-OK-
3. CSTR
Insert Unit Operations-Reactors-CSTR-select-Edit unit operation-Isotherml 298.15K-Reactor-Reactor volume 1.62 m^3-Reactions-add-rnx1
4. PFR
Insert Unit Operations-Reactors-PFR-select-Edit unit operation-Reactor-Reactor length 1 m- Reactor diameter 1.128 = $(4/\pi)^{1/2}$ m - Enthalpy-constant temperature 298.15K-Reactions-add-rnx1
5. Feed
Insert stream-Edit/view streams-0.1013 MPa-25 C-Compound flows-Water-26.75 mol/s-Methyl acetate-0.25 mol/s-Acetic acid 0.025 mol/s-Methanol 0 mol/s-
6. Stream 2 and 3
Insert stream-Edit/view streams 0.1013 MPa-25 C
7. solve(F5)