Stability Analysis of PDEs

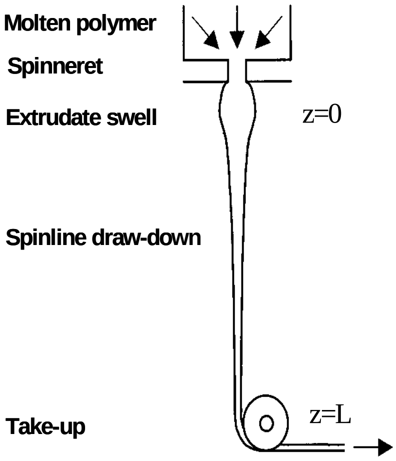
Part I. Fiber Spinning Process

Stability analysis of Newtonian fluids in spinning process

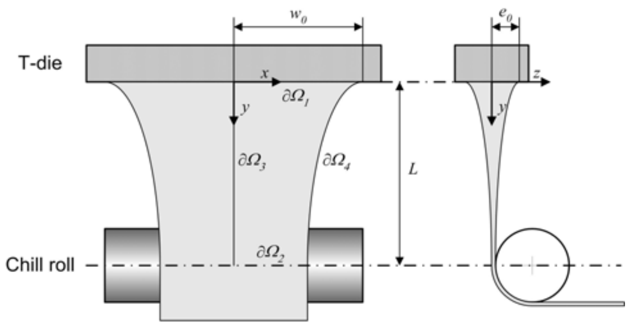
1. Characteristics of spinning processes

- **Typical extensional deformation processes:** spinning, film casting, tubular film blowing, coating, etc.
- **Schematic diagrams of several processes:**

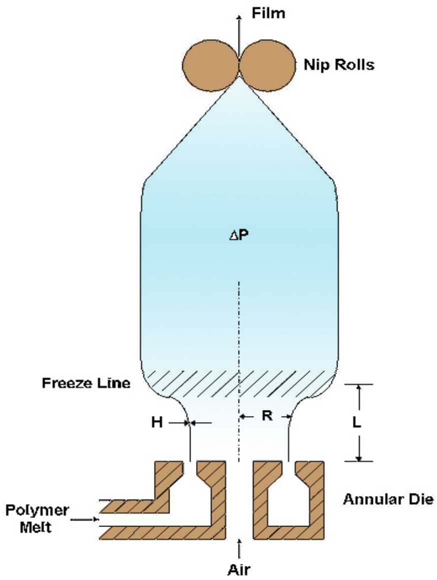
Fiber spinning process



Film casting process



Tubular film blowing process



Spinline variables:
spinline velocity, spinline radius, temperature, stress, strain rate, apparent extensional viscosity, crystallinity, orientation (Birefringence), etc

- **Phenomena occurring in the spinline**

  Rheological deformations (mostly extensional but some shear also)
  Cooling/solidification (coagulation)
  Orientation
  Crystallization

- **Important subjects in the dynamics of spinning**

  Spinnability ; Stability ; Sensitivity ; Productivity

① Spinnability: the ability to pull a melt out into a long thread
pre-requisite for fiber spinning / melt fracture
ductile fracture (=necking), cohesive fracture (=brittle fracture)
capillary jet stability (surface tension versus extensional viscosity)

② Stability: the most important factor of productivity (including product quality)
Draw resonance - a unique instability phenomenon / even for Newtonian fluids
self sustained periodic oscillation of spinline variables
(spinline cross-sectional area, spinline tension, etc.)

③ Sensitivity: propagation of processing disturbances
effects of the various process and material variables
empirical approach
simulation studies (steady/transient responses, frequency response)

④ Productivity: high spinning speed, fiber quality control, stable operation

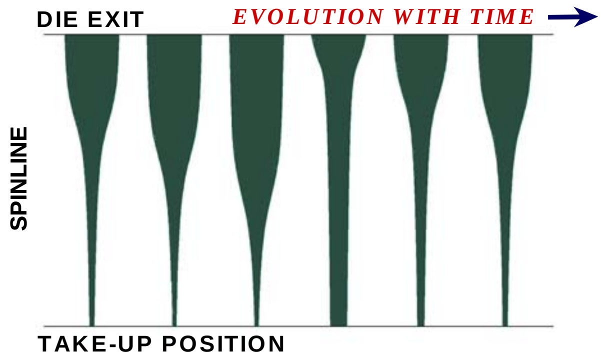
- **Typical instabilities occurring in the spinning**

① Filament breakage (or spinnability): Capillarity
Ductile fracture (=necking)
Cohesive fracture (=brittle fracture)

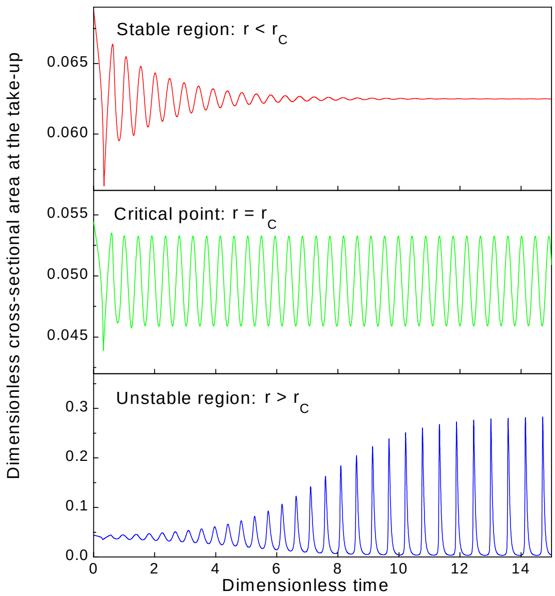
② Melt fracture

③ Draw resonance: Periodic variations of process variables (most notably extrudate cross-sectional area) with respect to time, occur and critically affect the process productivity as the drawdown ratio is increased beyond certain critical values. This intriguing instability phenomenon frequently arises in many extension deformation processes such as fiber spinning, film casting, and film blowing.

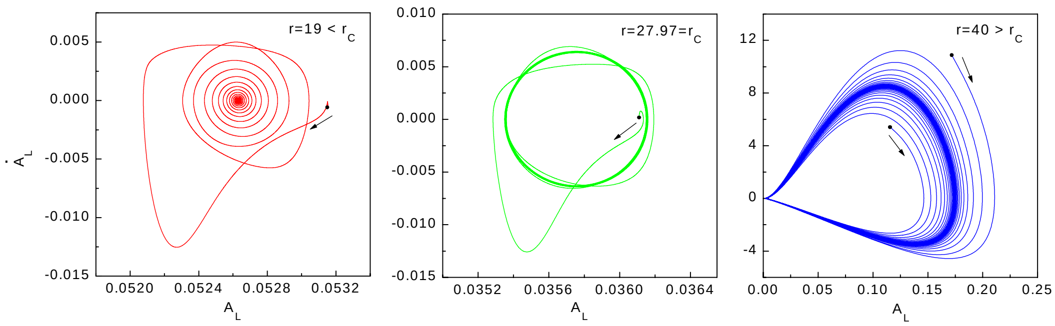
Schematic diagram describing draw resonance phenomenon



Transient responses of cross-sectional area



Phase planes

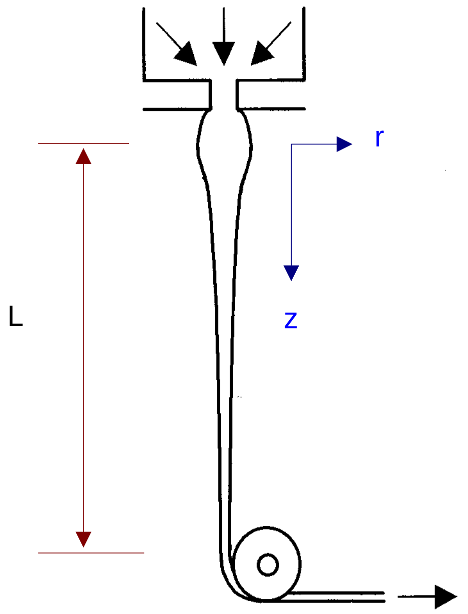


2. Linear stability analysis of Newtonian fluids

- **선형안정성 분석방법**: 지배방정식의 정상상태 해에 외란(normal modes)을 도입하여 외란이 수렴 또는 발산하는지를 eigenvalues의 부호로 판정. 즉, 가장 큰 eigenvalue의 실수부분이 양수이면 해가 발산하여 공정은 불안정해지고 음수이면 해가 수렴하여 공정은 안정하게 된다. 이 때 가장 큰 실수부분이 0일 때의 연신비(권취속도와 압출속도의 비)를 임계연신비라 하여 안정성을 판별하는 기준이 된다.

(1) Governing equations

- **Assumptions**: one-dimensional flow, isothermal, no secondary forces included, starting point: max. extrudate swell



Area: A_o
velocity: V_o
Temperature: T_o

Area: A_L
velocity: V_L
Temperature: T_L

Eqn. of continuity: $\dfrac{\partial A}{\partial \tilde{t}} + \dfrac{\partial (A V)}{\partial z} = 0$

Eqn. of motion: $\dfrac{\partial (A[\sigma_{zz} - \sigma_{rr}])}{\partial z} = 0$

Constitutive eqn.: $\sigma_{zz} = 2\eta \dfrac{\partial V}{\partial z}, \quad \sigma_{rr} = -\eta \dfrac{\partial V}{\partial z}$

Boundary conditions: $A = A_o$, $V = V_o$ at z=0

$V = V_L = rV_o$ at z=L

(2) Dimensionless variables

$$a = \frac{A}{A_o}, \quad v = \frac{V}{V_o}, \quad t = \frac{\tilde{t} V_o}{L}, \quad x = \frac{z}{L}, \quad \tau = \frac{(\sigma_{zz} - \sigma_{rr}) L}{3 \eta V_o}$$

(3) Dimensionless governing equations

Eqn. of continuity: $\frac{\partial a}{\partial t} + \frac{\partial (a\,v)}{\partial x} = 0$

Eqn. of motion + Constitutive eqn: $\frac{\partial}{\partial x}\left(a\,\frac{\partial v}{\partial x}\right) = 0$

Boundary conditions: a=v=1 at x=0

v=r at x=1

(4) Steady state

$v=r^{x}$ or $a=r^{-x}$

(5) Linear stability analysis

Governing PDE System
Transient response

→

ODE System
$\underline{R}(\underline{y}, \dot{\underline{y}}, \underline{p}) = \underline{0}$

$\underline{y}$ = state variables ($\underline{v}$, $\underline{a}$, $\underline{\sigma}$, …)

p = parameters (*Dr*, *De*,…)

↓

Linearization
Small perturbation on steady states

$\underline{\underline{R}}_{y}\,\Delta\underline{y} + \underline{\underline{R}}_{\dot{y}}\,\Delta\dot{\underline{y}} + \underline{R}_{p}\,\Delta p = \underline{0}$

$\underline{\underline{R}}_{y} \equiv \partial\underline{R}/\partial\underline{y}$, etc.

Linearized Transient
General disturbances

$\underline{\underline{J}}\,\Delta\underline{y} + \underline{\underline{M}}\,\Delta\dot{\underline{y}} + \underline{F}\,\Delta p = \underline{0}$

$\underline{\underline{J}} \equiv \underline{\underline{R}}_{y}$, $\underline{\underline{M}} \equiv \underline{\underline{R}}_{\dot{y}}$, $\underline{F} \equiv \underline{R}_{p}$

Frequency Response
Ongoing disturbances sinusoidal

$(\underline{\underline{J}} + i\omega\underline{\underline{M}})\,\underline{z} = \underline{F}$

$\Delta\underline{y} = \underline{z}\exp(i\omega t)$

$\Delta p = \exp(i\omega t)$

ω = Frequency

Linear Stability
Initial disturbances normal modes

$-\underline{\underline{J}}\,\underline{\phi} = \lambda\,\underline{\underline{M}}\,\underline{\phi}$

$\Delta\underline{y} = \underline{\phi}\exp(\lambda t)$

$\Delta p = 0$

λ = Eigenvalue

$\underline{\phi}$ = Eigenfunction

a. Perturbation variables:

$$a(t,z) = a_s(z) + \alpha(z)e^{\Omega t}, \quad v(t,z) = v_s(z) + \beta(z)e^{\Omega t}$$

or $$a(t,z) = a_s(z)(1+\alpha(z)e^{\Omega t}), \quad v(t,z) = v_s(z)(1+\beta(z)e^{\Omega t})$$

b. Linearized governing equations: → homogeneous ODE

$$\Omega\alpha = -[v_s]\alpha' - [v_s']\alpha + \left[-\frac{v_s'}{v_s^2}\right]\beta - \left[\frac{1}{v_s}\right]\beta'$$

$$\beta'' - \left[-\frac{v_s'}{v_s}\right]\beta' = -[v_s v_s'']\alpha - [v_s v_s']\alpha'$$

$$\rightarrow \quad \Omega\alpha = -[r^x]\alpha' - [r^x(\ln r)]\alpha + \left[-\frac{(\ln r)}{r^x}\right]\beta - \left[\frac{1}{r^x}\right]\beta'$$

$$\beta'' - [\ln r]\beta' = -[r^{x2}(\ln r)^2]\alpha - [r^{x2}(\ln r)]\alpha'$$

B.C.'s: $\alpha(0) = \beta(0) = \beta(1) = 0$

c. Differentiation

Eqn. of continuity

i=1, Central differences)

$$\Omega\alpha_1 = -r^{x_1}\frac{(\alpha_2-\alpha_o)}{2dx} - r^{x_1}(\ln Dr)\alpha_1 + \frac{(\ln r)}{r^{x_1}}\beta_1 - \frac{1}{r^{x_1}}\frac{(\beta_2-\beta_o)}{2dx}$$

i=2, $$\Omega\alpha_2 = -r^{x_2}\frac{(\alpha_3-\alpha_1)}{2dx} - r^{x_2}(\ln r)\alpha_2 + \frac{(\ln r)}{r^{x_2}}\beta_2 - \frac{1}{r^{x_2}}\frac{(\beta_3-\beta_1)}{2dx}$$

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i=n-1, $$\Omega\alpha_{n-1} = -r^{x_{n-1}}\frac{(\alpha_n-\alpha_{n-2})}{2dx} - r^{x_{n-1}}(\ln r)\alpha_{n-1} + \frac{(\ln r)}{r^{x_{n-1}}}\beta_{n-1}$$

$$-\frac{1}{r^{x_{n-1}}}\frac{(\beta_n-\beta_{n-2})}{2dx}$$

i=n, (Backward differences)

$$\Omega\alpha_n = -r^{x_n}\frac{(3\alpha_n - 4\alpha_{n-1} + \alpha_{n-2})}{2dx} - r^{x_n}(\ln Dr)\alpha_n + \frac{(\ln r)}{r^{x_n}}\beta_n$$

$$-\frac{1}{r^{x_n}}\frac{(3\beta_n - 4\beta_{n-1} + \beta_{n-2})}{2dx}$$

Eqn. of motion + constitutive eqn.

i=1, (Central differences)

$$\frac{(\beta_2 - 2\beta_1 + \beta_o)}{dx^2} - (\ln r)\frac{(\beta_2 - \beta_o)}{2dx} = -r^{x_1^2}(\ln r)^2\alpha_1 - r^{x_1^2}(\ln r)\frac{(\alpha_2 - \alpha_o)}{2dx}$$

i=2, $$\frac{(\beta_3 - 2\beta_2 + \beta_1)}{dx^2} - (\ln r)\frac{(\beta_3 - \beta_1)}{2dx} = -r^{x_2^2}(\ln r)^2\alpha_2 - r^{x_2^2}(\ln r)\frac{(\alpha_3 - \alpha_1)}{2dx}$$

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i=n-1, $$\frac{(\beta_n - 2\beta_{n-1} + \beta_{n-2})}{dx^2} - (\ln r)\frac{(\beta_n - \beta_{n-2})}{2dx}$$

$$= -r^{x_{n-1}^2}(\ln r)^2\alpha_{n-1} - r^{x_{n-1}^2}(\ln r)\frac{(\alpha_n - \alpha_{n-2})}{2dx}$$

d. Matrix from

$$\lambda\underline{I}\alpha = \underline{B}(n,n)\alpha + \underline{C}(n,n-1)\beta$$

$$\underline{D}(n-1,n)\alpha = \underline{E}(n-1,n-1)\beta$$

where $\alpha = [\alpha_1, \alpha_2, \alpha_3, \cdots, \alpha_{n-1}, \alpha_n]^T$, $\beta = [\beta_1, \beta_2, \beta_3, \cdots, \beta_{n-1}]^T$

① $\underline{B}(n,n)$ =

$$\begin{bmatrix} -r^{z_1}(K) & \frac{-r^{z_1}}{2dx} & 0 & 0 & 0 & \cdots & 0 & 0 \\ \frac{r^{z_2}}{2dx} & -r^{z_2}(K) & \frac{-r^{z_2}}{2dx} & 0 & 0 & \cdots & 0 & 0 \\ 0 & \frac{r^{z_3}}{2dx} & -r^{z_3}(K) & \frac{-r^{z_3}}{2dx} & 0 & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \frac{r^{z_{n-1}}}{2dx} & -r^{z_{n-1}}(K) & \frac{-r^{z_{n-1}}}{2dx} \\ 0 & 0 & 0 & \cdots & 0 & \frac{-r^{z_n}}{2dx} & \frac{2r^{z_n}}{dx} & \frac{-3r^{z_n}}{2dx} - r^{z_n}(K) \end{bmatrix}$$

② C(n,n-1) =

$$
\begin{bmatrix}
\frac{K}{r^{z_1}} & -\frac{1}{r^{z_1}2dx} & 0 & 0 & 0 & \cdots & 0 & 0 \\
\frac{1}{r^{z_2}2dx} & \frac{K}{r^{z_2}} & -\frac{1}{r^{z_2}2dx} & 0 & 0 & \cdots & 0 & 0 \\
0 & \frac{1}{r^{z_3}2dx} & \frac{K}{r^{z_3}} & -\frac{1}{r^{z_3}2dx} & 0 & \cdots & 0 & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & 0 & \frac{1}{r^{z_{n-1}}2dx} & \frac{K}{r^{z_{n-1}}} \\
0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{r^{z_n}2dx} & \frac{2}{r^{z_n}dx}
\end{bmatrix}
$$

③ D(n-1,n) =

$$
\begin{bmatrix}
-(r^{z_1})^2K^2 & \frac{-K(r^{z_1})^2}{2dx} & 0 & 0 & 0 & \cdots & 0 \\
\frac{K(r^{z_2})^2}{2dx} & -(r^{z_2})^2K^2 & \frac{-K(r^{z_2})^2}{2dx} & 0 & 0 & \cdots & 0 \\
0 & \frac{K(r^{z_3})^2}{2dx} & -(r^{z_3})^2K^2 & \frac{-K(r^{z_3})^2}{2dx} & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & \frac{K(r^{z_{n-1}})^2}{2dx} & -(r^{z_{n-1}})^2K^2 & \frac{-K(r^{z_{n-1}})^2}{2dx}
\end{bmatrix}
$$

④ E(n-1,n-1) =

$$
\begin{bmatrix}
-\frac{2}{dx^2} & \frac{1}{dx^2}-\frac{K}{2dx} & 0 & 0 & 0 & \cdots & 0 \\
\frac{K}{2dx}+\frac{1}{dx^2} & -\frac{2}{dx^2} & \frac{1}{dx^2}-\frac{K}{2dx} & 0 & 0 & \cdots & 0 \\
0 & \frac{K}{2dx}+\frac{1}{dx^2} & -\frac{2}{dx^2} & \frac{1}{dx^2}-\frac{K}{2dx} & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & \frac{K}{2dx}+\frac{1}{dx^2} & -\frac{2}{dx^2} & \frac{1}{dx^2}-\frac{K}{2dx} \\
0 & 0 & 0 & \cdots & 0 & \frac{K}{2dx}+\frac{1}{dx^2} & \frac{-2}{dx^2}
\end{bmatrix}
$$

e. Methods for evaluating eigenvalues from eigensystems

① Shift-invert transformation method

- In general, the eigenvalues associated with the equations that are not time dependent are indefinitely large.
- These infinite eigenvalues have to be removed from the equation system. Otherwise, they will be the ones with largest real part.

$$\mathbf{A}\underline{y} = \Omega\mathbf{M}\underline{y}$$ (M: mass matrix. M is singular in this case.)

$$\Rightarrow \mathbf{A}\underline{y} - \sigma\mathbf{M}\underline{y} = \Omega\mathbf{M}\underline{y} - \sigma\mathbf{M}\underline{y} = (\Omega - \sigma)\mathbf{M}\underline{y}$$ (shift σ s real)

$$\Rightarrow \frac{1}{(\Omega - \sigma)}\underline{y} = (\mathbf{A} - \sigma\mathbf{M})^{-1}\mathbf{M}\underline{y} \Rightarrow \mu\underline{y} = \mathbf{B}\underline{y}$$

$$\therefore \text{eigenvalues: } \mu = \frac{1}{(\Omega - \sigma)}$$

- The infinite eigenvalues of the generalized problem are mapped into zero eigenvalues of the simple eigenvalue problem.

② Matrix transformation for the simplified eigenproblem

$$\beta = \underline{E}^{-1}\underline{D}\alpha$$

$$\rightarrow \lambda\underline{I}\alpha = \underline{B}\alpha + \underline{C}\,\underline{E}^{-1}\underline{D}\alpha$$

$$\rightarrow \lambda\underline{I}\alpha = \underline{F}\alpha \quad (\underline{F} = \underline{B} + \underline{C}\,\underline{E}^{-1}\underline{D})$$

Table 1. The largest real and imaginary parts of eigenvalues at various r.

r	real part	imaginary part
15	-0.628	13.075
20	-0.0237	13.975
20.218	0	14.009
22	0.181	14.273
25	0.459	14.674

Table 2. Critical drawdown ratio with the number of mesh.

Number of mesh	Critical draw ratio
100	20.2611
200	20.2286
300	20.2227
400	20.2206
500	20.2195
700	20.2188
1000	20.21841
1100	20.21834
1200	20.21828
2000	20.21809

Part II. Linear Stability Analysis of Catalytic Reaction

● **Governing equations**

- Chemical reaction A → B in a porous catalyst pellet

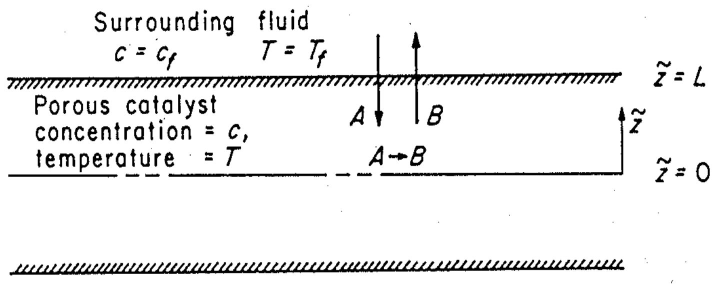

Figure: Schematic diagram of diffusion and reaction in a porous slab catalyst.

- Assumptions: 1st-order reaction.

  there is no surface resistance to the transport of mass or energy.

$$\frac{\partial c}{\partial \tilde{t}} = D\frac{\partial^2 c}{\partial \tilde{z}^2} - k e^{-E/RT} c$$

$$\frac{\partial T}{\partial \tilde{t}} = D_T\frac{\partial^2 T}{\partial \tilde{z}^2} + \frac{[-\Delta H]k}{\rho c_p} e^{-E/RT} c$$

B.C.: $c=c_f$, $T=T_f$ at $\tilde{z}=L$

$$\frac{\partial c}{\partial \tilde{z}} = 0, \quad \frac{\partial T}{\partial \tilde{z}} = 0 \quad \text{at } \tilde{z}=0$$

(D: effective mass diffusivity, D_T: effective thermal diffusivity)

● **Dimensionless governing equations**

- Dimensionless variables:

$$x = \frac{c}{c_f}, \quad y = \frac{T}{T_f}, \quad \alpha = \frac{L^2 k}{D}, \quad L = \frac{D}{D_T} \text{ (Lewis number)}$$

$$\gamma = \frac{E}{RT_f}, \quad \beta = \frac{[-\Delta H]c_f L}{\rho c_p T_f}, \quad t = \frac{D\tilde{t}}{L^2}, \quad z = \frac{\tilde{z}}{L}$$

- Dimensionless governing equations

$$\frac{\partial x}{\partial t} = \frac{\partial^2 x}{\partial z^2} - \alpha x e^{-\gamma/y}, \qquad L\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial z^2} + \alpha\beta x e^{-\gamma/y}$$

B.C.: $x = y = 1$ at $z=1$

$$\frac{\partial x}{\partial z} = \frac{\partial y}{\partial z} = 0 \quad \text{at } z=0$$

- define $F(y) = [\beta + 1 - y]e^{-\gamma/y}$

- **Steady-state catalyst particle**

$$x_s'' - \alpha x_s e^{-\gamma/y_s} = 0, \quad y_s'' + \alpha\beta x_s e^{-\gamma/y_s} = 0$$

B.C.: $x_s(1) = y_s(1) = 1$, $x'_s(0) = y'_s(0) = 0$

→ $\frac{d^2}{dz^2}[\beta x_s + y_s] = 0, \quad \beta x_s + y_s = 1 + \beta$ ($0 \le x_s \le 1$, $1 \le y_s \le 1+\beta$

(steady state is independent of the Lewis number)

- **Linear stability analysis**

(1) Case1: Adiabatic perturbation, *L*=1

- $\frac{\partial w}{\partial t} = \frac{\partial^2 w}{\partial z^2}$, $w = \beta x + y$ (w: residual enthalpy)

B.C.: $w = 1 + \beta$ at z=1

$\frac{\partial w}{\partial z} = 0$ at z=0

- Another expression of energy eq.: $\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial z^2} + \alpha[w - y]e^{-\gamma/y}$
- If the systems is initially perturbed from the steady state such that following relationship is preserved ($\beta x + y = 1 + \beta$ at t=0). w is a constant as $1+\beta$

$$\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial z^2} + \alpha F(y)$$

- Linearization of above equation by defining, $\eta = y - y_s$

$$\frac{\partial \eta}{\partial t} = \frac{\partial^2 \eta}{\partial z^2} + \alpha F'(y_s)\eta$$

B.C.: $\frac{\partial \eta}{\partial z} = 0$ at $z = 0$; $\eta = 0$ at $z = 1$

linear homogeneous PDE with linear homogeneous B.C.

- Method for solving the above linearized equation:

the method of separation of variables, $\eta = \theta(t)\,\phi(z)$, Φ Ɔ) = Φ .) = 0

$$\dot{\theta}\phi = \theta\phi'' + \alpha F'(y_s)\theta\phi$$

→ $\dot{\theta} - \lambda\theta = 0, \quad \phi'' + [-\lambda + \alpha F'(y_s)]\phi = 0$ (λ s a constant): $\theta = e^{\lambda t}$

The eigenvalues are all real, so an oscillatory response is impossible.

For the largest eigenvalue, $\lambda \le \alpha \max F'(y_s) - \frac{\pi^2}{4}$

(2) Case 2: *L*=1

- Adiabatic perturbation is the worst perturbation for the catalytic reaction with *L*=1.
- Define two deviation variables: $\eta = y - y_s, \quad \omega = w - w_s = w - 1 - \beta$

$$\frac{\partial \eta}{\partial t} = \frac{\partial^2 \eta}{\partial z^2} + \alpha F'(y_s)\eta + \alpha e^{-\gamma/y_s}\omega$$

$$\frac{\partial \omega}{\partial t} = \frac{\partial^2 \omega}{\partial z^2}$$

B.C.: $\frac{\partial \eta}{\partial z} = \frac{\partial \omega}{\partial z} = 0$ at $z = 0$, $\eta = \omega = 0$ at $z = 1$

- By separation of variables,

$$\eta = \theta_1(t)\,\phi(z)\ ,\quad \omega = \theta_2(t)\,\psi(z),\quad \phi'(0) = \psi'(0) = \phi(1) = \psi(1) = 0$$

$$\frac{\dot{\theta}_1}{\theta_1} = \frac{\phi'' + \alpha F'(y_s)\phi + \alpha e^{-\gamma/y_s}\psi[\theta_2/\theta_1]}{\phi} = \lambda$$

→ solution by separation of variables is possible if and only if $\theta_1 = \theta_2 = e^{\lambda}$

- Linearized equations: $\phi'' + [-\lambda + \alpha F'(y_s)]\phi + \alpha e^{-\gamma/y_s}\psi = 0$

$$\psi'' - \lambda\psi = 0$$

(3) Case 3: $L \neq$

$$\frac{\partial w}{\partial t} + [L-1]\frac{\partial y}{\partial t} = \frac{\partial^2 w}{\partial z^2}$$

$$L\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial z^2} + \alpha[w - y]e^{-\gamma/y}$$

- Using the deviation variables, $\eta = e^{\lambda t}\phi(z) = y - y_s$

$$\omega = e^{\lambda t}\psi(z) = w - 1 - \beta$$

- Linearized equations:

$$\psi'' - \lambda\psi - \lambda[L-1]\phi = 0$$

$$\phi'' + [-L\lambda + \alpha F'(y_s)]\phi + \alpha e^{-\gamma/y_s}\psi = 0$$

B.C.: $\psi'(0) = \phi'(0) = \psi(1) = \phi(1) = 0$