

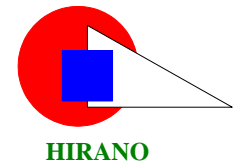


# REACTING FLUID DYNAMICS (2)

## PHENOMENA IN THE HYDROGEN-AIR BOUNDARY OR MIXING LAYER

**Toshisuke Hirano**

Chiba Institute of Science





# Topics

- **HEAT AND MASS TRANSFER**

Transfer Based on Molecular Exchange

*Heat Transfer; Mass Transfer; Explanation of Transfer Phenomena on the Basis of Gas Dynamics;*

Transfer Based on Turbulent Exchange

*Characteristics of Turbulent Flow; Mixing Length  $T^{k-\varepsilon}$ ; (Two Equations) Model*

Thermophoresis, Soret Effect, and Dufour Effect

*Thermophoresis; Soret Effect; Dufour Effect*

- **TEMPERATURE AND CONCENTRATION PROFILES**

Variation of Temperature and Species Concentration in a Quiescent Atmosphere

*Variation of Temperature Profile; Variation of Species Concentration Profile*



# Topics (Continued)

## Variation of Temperature and Species Concentration in a Laminar Flow

*Temperature and Species Concentration Profiles in the Boundary Layer; Temperature and Species Concentration Profiles in a Jet; Temperature and Species Concentration Profiles in Parallel Flows of Different Velocities*

## Temperature and Species Concentration Profiles in Turbulent Flows

*Turbulent Diffusion at the Site with Temperature or Species Concentration Difference; Temperature and Species Concentration Profiles across a Turbulent Jet; Temperature and Species Concentration Profiles across a Shear Flow*

- **STRUCTURE OF REACTION SITES**

### Surface Reaction

*Catalytic Reaction; Combustion Reaction;*

### Reaction in a Gas Flow

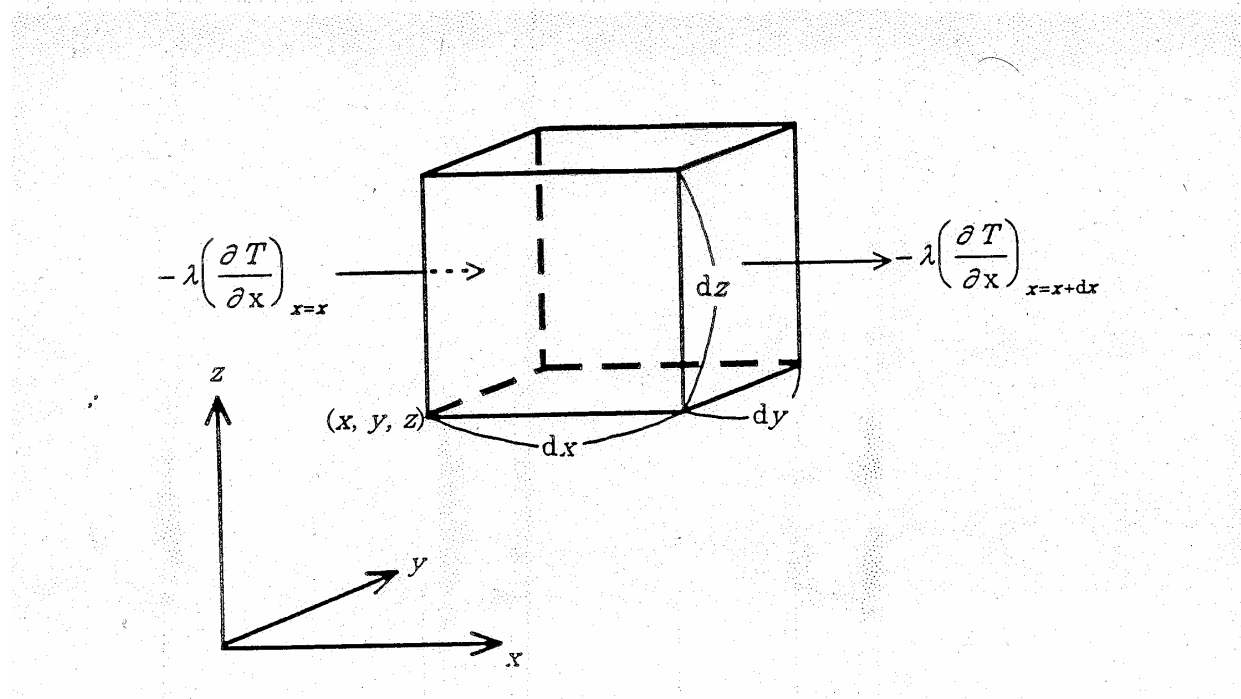
*Steady Premixed Flame; Diffusion Flame in a Boundary Layer; Analysis of a Boundary Layer with Large Density Gradient;*

# HEAT AND MASS TRANSFER

## Transfer Based on Molecular Exchange

### *Heat Transfer*

$$\dot{q}'' = -\lambda \nabla T$$



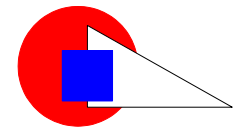


$$\lambda \left\{ \left( \frac{\partial^2 T}{\partial x^2} \right)_{x=x} + \left( \frac{\partial^2 T}{\partial y^2} \right)_{y=y} + \left( \frac{\partial^2 T}{\partial z^2} \right)_{z=z} \right\} dx dy dz dt$$

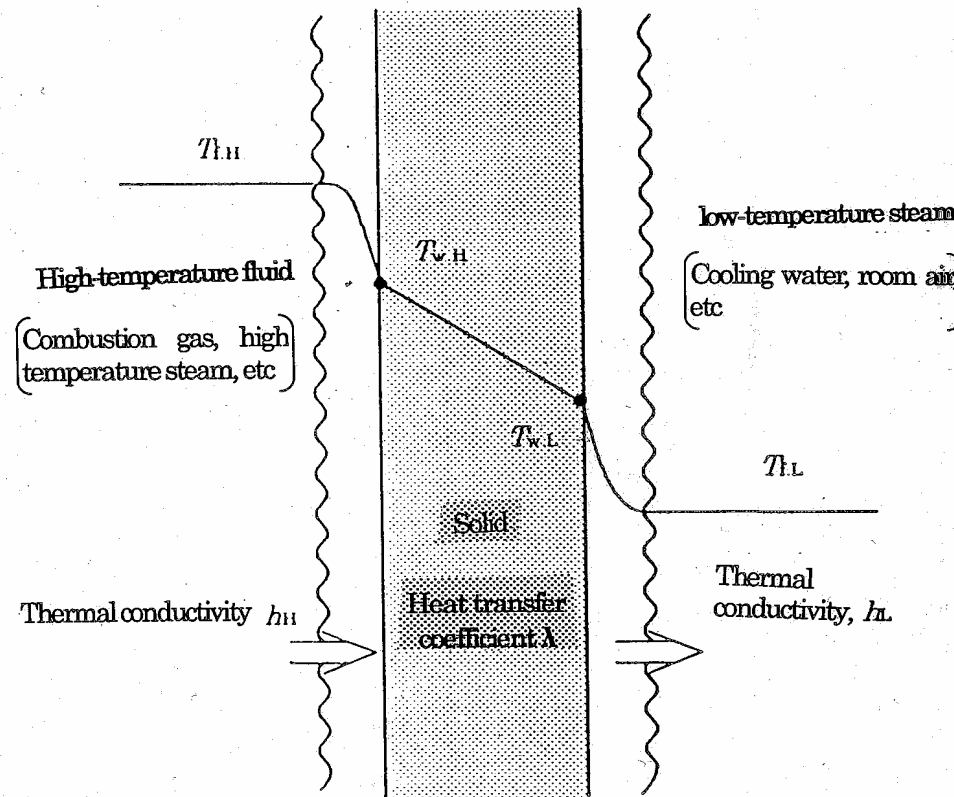
$$\rho c \{T(t + dt) - T(t)\} dx dy dz \equiv \rho c \left( \frac{\partial T}{\partial t} \right) dt dx dy dz$$

$$\rho c \frac{\partial T}{\partial t} = \lambda \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right)$$

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$



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$$\dot{q}'' = h(T_f - T_w)$$



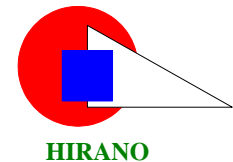
## *Mass Transfer*

$$\dot{m}''_A = \rho_A (v_A - v) = -\rho D_{AB} \nabla Y_A$$

$$j_A^* = C_A (v_A^* - v^*) = -c D_{AB} \nabla X_A$$

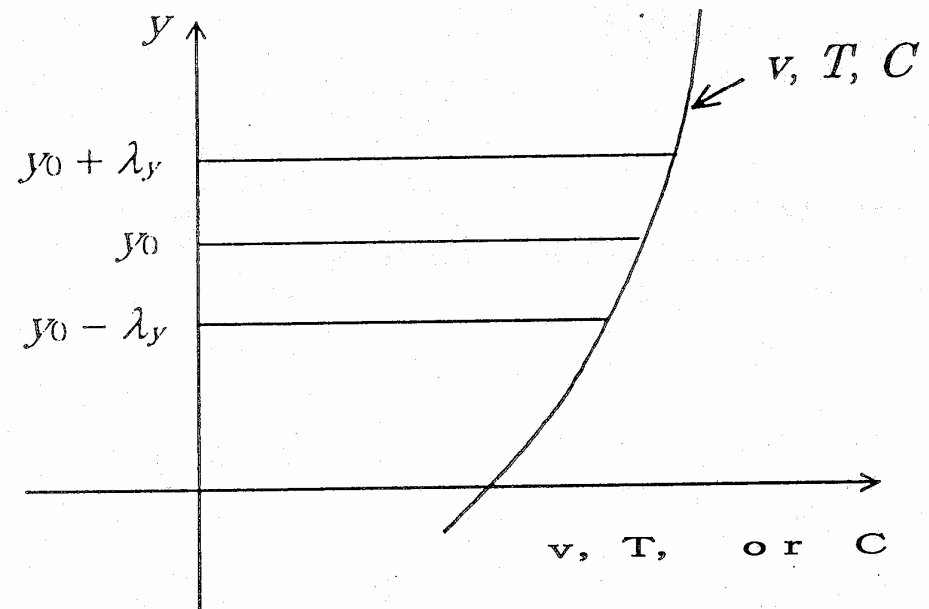
$$\dot{m}''_i = \rho_A (v_A - v) = -\rho D_i \nabla Y_i$$

$$\frac{\partial Y_i}{\partial t} = D_i \nabla^2 Y_i$$

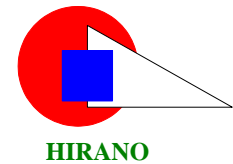




## *Explanation of Transfer Phenomena on the Basis of Gas Dynamics*



$$N = \frac{1}{4} n \bar{c}$$







$$G = N\{g(y_0 - \lambda_y) - g(y_0 + \lambda_y)\} = -\frac{1}{2}n\bar{c}\bar{\lambda}_y\left(\frac{dg}{dy}\right)_{y_0}$$

$$G = -\frac{1}{4}n\bar{c}\lambda_m\left(\frac{dng}{dy}\right)_{y_0}$$

$$\tau = -\frac{1}{4}\rho\bar{c}\lambda_m\frac{dv_x}{dy} \quad \tau = \mu\frac{dv_x}{dy} \quad \nu = -\frac{1}{4}\bar{c}\lambda_m$$

$$\dot{q}'' = -\frac{1}{4}\rho c_p\bar{c}\lambda_m\frac{dT}{dy} \quad \dot{m}'' = -\frac{1}{4}\rho\bar{c}\lambda_m\frac{dY_i}{dy}$$

$$\alpha = D_i = \frac{1}{4}\bar{c}\lambda_m$$





## Transfer Based on Turbulent Exchange

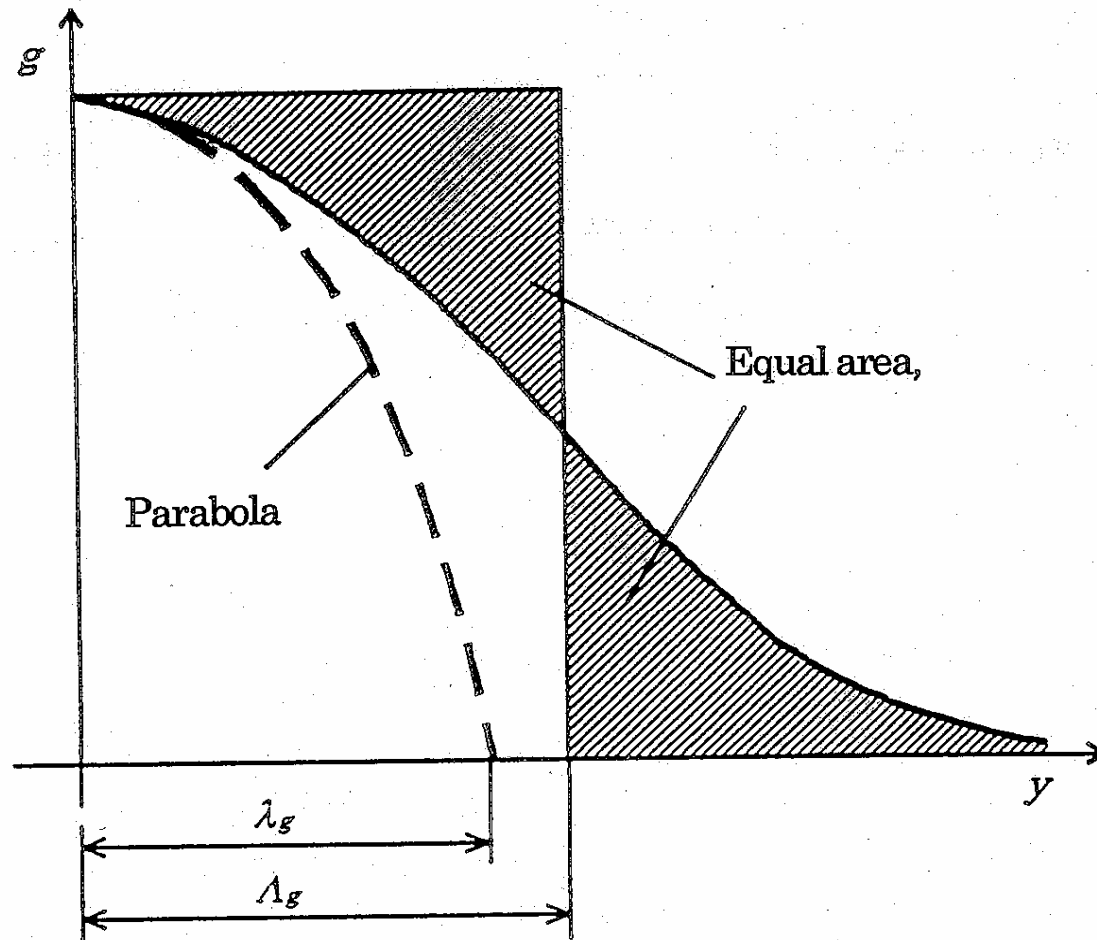
### *Characteristics of Turbulent Flow*

$$u = \bar{u} + u' \qquad \hat{u} = \sqrt{\overline{u'^2}}$$

$$c = \frac{\overline{u'(\tau)u'(\tau+t)}}{\{u'(\tau)\}^2} \qquad f = \frac{\overline{u'(r)u'(r+x)}}{\{u'(r)\}^2} \qquad g = \frac{\overline{u'(r)u'(r+y)}}{\{u'(r)\}^2}$$

$$g = 1 - \frac{y^2}{\lambda_g^2} \qquad A_g = \int_0^\infty g dy \qquad \eta = \left( \frac{v^3}{\varepsilon} \right)^{\frac{1}{4}}$$







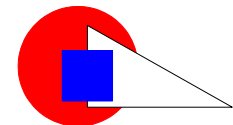
## Mixing Length Theory

$$\tau_1 = \mu \frac{\partial u}{\partial y} \quad \tau_t = -\rho \overline{u'v'} = A_\tau \frac{\partial \bar{u}}{\partial y} \quad \varepsilon_E = \frac{A_\tau}{\rho}$$

$$|\overline{v'}| = C_1 |\overline{u'}| = C_1 l \left| \frac{d\bar{u}}{dy} \right| \quad \overline{u'v'} = -C_3 l^2 \left( \frac{d\bar{u}}{dy} \right)^2$$

$$\overline{u'v'} = -l^2 \left( \frac{d\bar{u}}{dy} \right)^2 \quad \tau_t = -\rho \cdot l^2 \left( \frac{d\bar{u}}{dy} \right)^2 \quad \tau_t = -\rho \cdot l^2 \left| \frac{d\bar{u}}{dy} \right| \frac{d\bar{u}}{dy}$$

$$A_\tau = -\rho \cdot l^2 \left| \frac{d\bar{u}}{dy} \right| \quad \varepsilon_E = l^2 \left| \frac{d\bar{u}}{dy} \right|$$



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## $k - \varepsilon$ (Two Equations) Model

$$\mu_t = C_\mu \bar{\rho} \frac{k^2}{\varepsilon}$$

$$\bar{\rho} \cdot \bar{v}_y \frac{\partial k}{\partial y} = \frac{\partial}{\partial y} \left[ \left( \frac{\mu_t}{\sigma_k} + \mu \right) \frac{\partial k}{\partial y} \right] - \bar{\rho} \overline{v_x'' v_y''} \frac{\partial v_z}{\partial y} - \frac{\mu_t}{\bar{\rho}^2} \frac{\partial \bar{\rho}}{\partial x} \frac{\partial \bar{p}}{\partial x} - \bar{\rho} \varepsilon$$

$$\bar{\rho} \cdot \bar{v}_y \frac{\partial \varepsilon}{\partial y} = \frac{\partial}{\partial y} \left[ \left( \frac{\mu_t}{\sigma_k} + \mu \right) \frac{\partial \varepsilon}{\partial y} \right] - C_{\varepsilon 1} \frac{\varepsilon}{k} \left( \bar{\rho} \cdot \overline{v_x'' v_y''} \frac{\partial v_x}{\partial y} - \frac{\mu_t}{\bar{\rho}^2} \frac{\partial \bar{\rho}}{\partial x} \frac{\partial \bar{p}}{\partial x} \right) - C_{\varepsilon 2} \bar{\rho} \frac{\varepsilon^2}{k}$$

$$C_\mu = 0.09, \quad C_{\varepsilon 1} = 1.44, \quad C_{\varepsilon 2} = 1.92, \quad \sigma_k = 1.0, \quad \sigma_\varepsilon = 1.30, \quad \sigma_t = 0.7$$

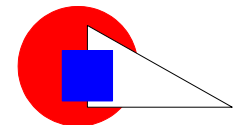


## Thermophoresis, Soret Effect, and Dufour Effect

### *Thermophoresis*

$$F_T = -\frac{32}{15} \cdot \frac{R^2}{\bar{c}} k_g (\nabla T)_x = -2\pi\mu\nu \frac{R^2}{\lambda_m} \cdot \frac{(\nabla T)_x}{T_0}$$

$$F_T = -\frac{12\pi\mu\nu R C_s \left( \frac{k_g}{k_p} + C_t \frac{\lambda_m}{R} \right) \frac{(\nabla T)_x}{T_0}}{\left( 1 + 3C_m \frac{\lambda_m}{R} \right) \left( 1 + 2 \frac{k_g}{k_p} + 2C_t \frac{\lambda_m}{R} \right)}$$





### *Soret Effect*

$$\Delta \dot{m}_{Ti}'' = -D_i^T \frac{\nabla T}{T} \quad k_T(T) = \frac{X_1 X_2}{\rho Y_1 Y_2} \frac{D_1^T}{D_{12}} = -\frac{\Delta X_1}{\ln\left(\frac{T'}{T}\right)}$$

$$\bar{T} = \left(\frac{TT'}{T' - T}\right) \ln\left(\frac{T'}{T}\right)$$

### *Dufour Effect*

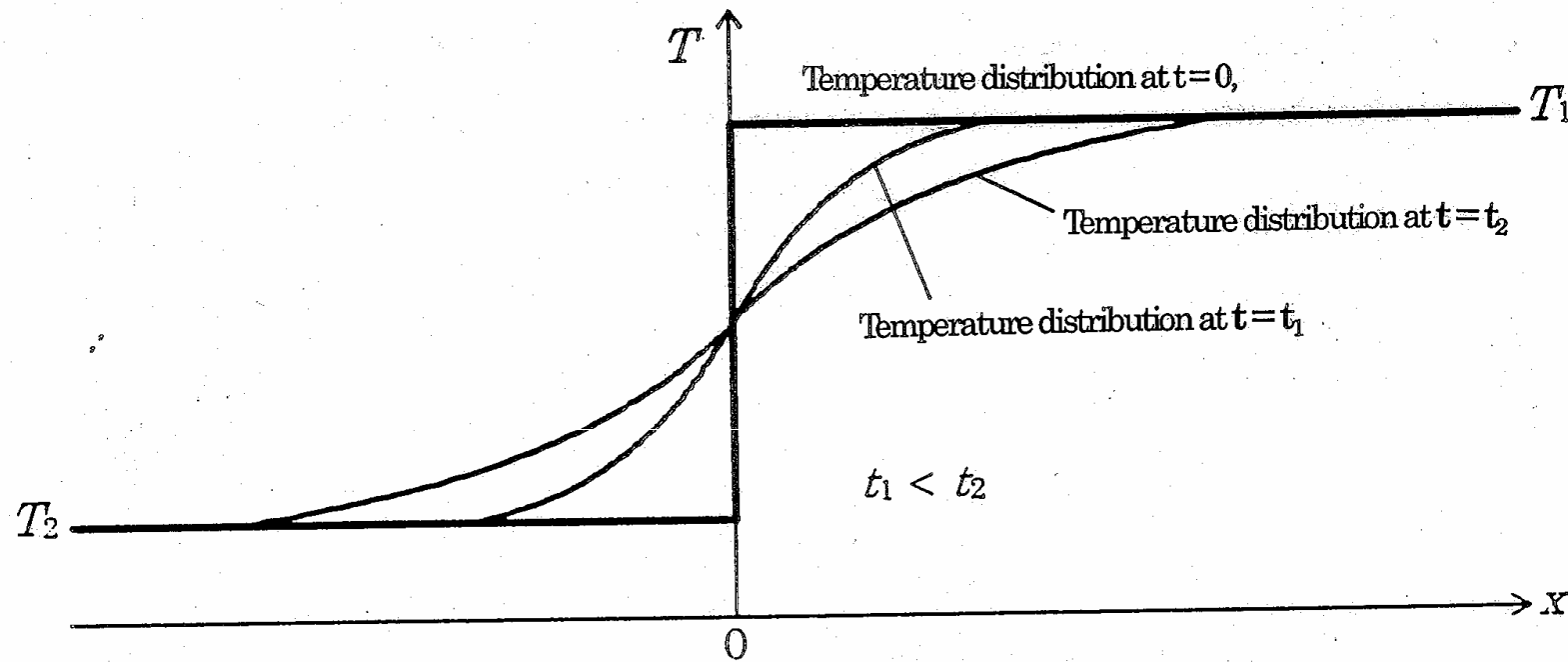
$$\Delta \dot{q}_i'' = RT \sum_{i=1}^N \sum_{j=1}^N \left( \frac{X_j D_{ij}}{W_i D_{ij}} \right) (\bar{V}_i - \bar{V}_j)$$





# TEMPERATURE AND CONCENTRATION PROFILES

## Variation of Temperature and Species Concentration in a Quiescent Atmosphere







$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

$$\Theta = \frac{T - T_2}{T_1 - T_2}$$

$$\frac{\partial \Theta}{\partial t} = \alpha \frac{\partial^2 \Theta}{\partial x^2}$$

$$\Theta = \frac{1}{2} \left\{ 1 + \operatorname{erf} \left( \frac{x}{2\sqrt{\alpha t}} \right) \right\}$$

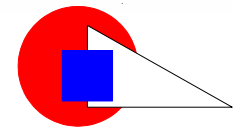
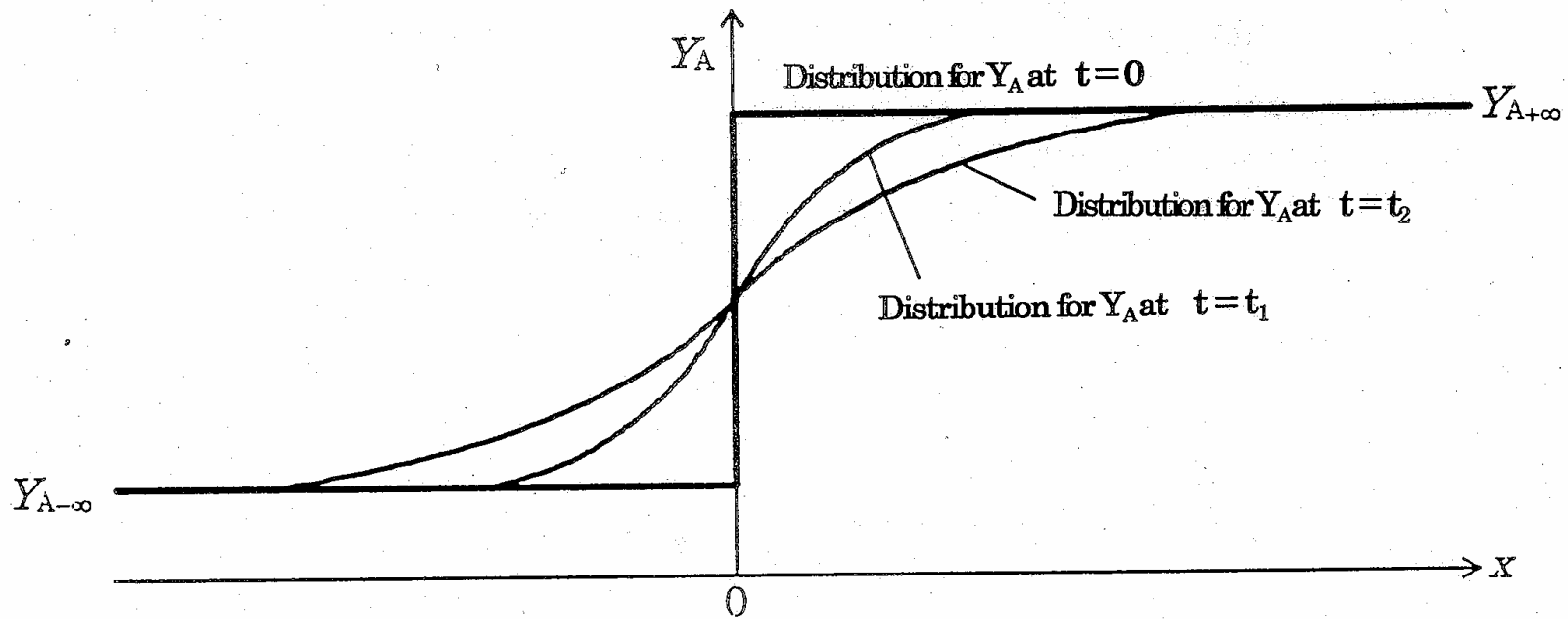
$$\left. \begin{array}{l} t = 0: \quad T = T_1 \quad \text{at} \quad x \geq 0 \\ \quad \quad T = T_2 \quad \text{at} \quad x < 0 \\ t > 0: \quad T = T_1 \quad \text{for} \quad x = \infty \\ \quad \quad T = T_2 \quad \text{for} \quad x = -\infty \end{array} \right\}$$

$$\left. \begin{array}{l} t = 0: \quad \Theta = 1 \quad \text{at} \quad x \geq 0 \\ \quad \quad \Theta = 0 \quad \text{at} \quad x < 0 \\ t > 0: \quad \Theta = 1 \quad \text{for} \quad x = \infty \\ \quad \quad \Theta = 0 \quad \text{for} \quad x = -\infty \end{array} \right\}$$

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-\xi^2) d\xi$$



## Variation of Species Concentration Profile



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$$\frac{\partial Y_A}{\partial t} = D_A \nabla^2 Y_A$$

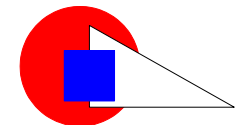
$$\Phi = \frac{Y_A - Y_{A-\infty}}{Y_{A+\infty} - Y_{A-\infty}}$$

$$\frac{\partial \Phi}{\partial t} = D_A \frac{\partial^2 \Phi}{\partial x^2}$$

$$\Phi = \frac{1}{2} \left\{ 1 + \operatorname{erf} \left( \frac{x}{2\sqrt{D_A t}} \right) \right\}$$

$$\left. \begin{array}{l} t = 0: Y_A = Y_{A+\infty} \quad \text{at } x \geq 0 \\ Y_A = Y_{A-\infty} \quad \text{at } x < 0 \\ t > 0: Y_A = Y_{A+\infty} \quad \text{for } x = \infty \\ Y_A = Y_{A-\infty} \quad \text{for } x = -\infty \end{array} \right\}$$

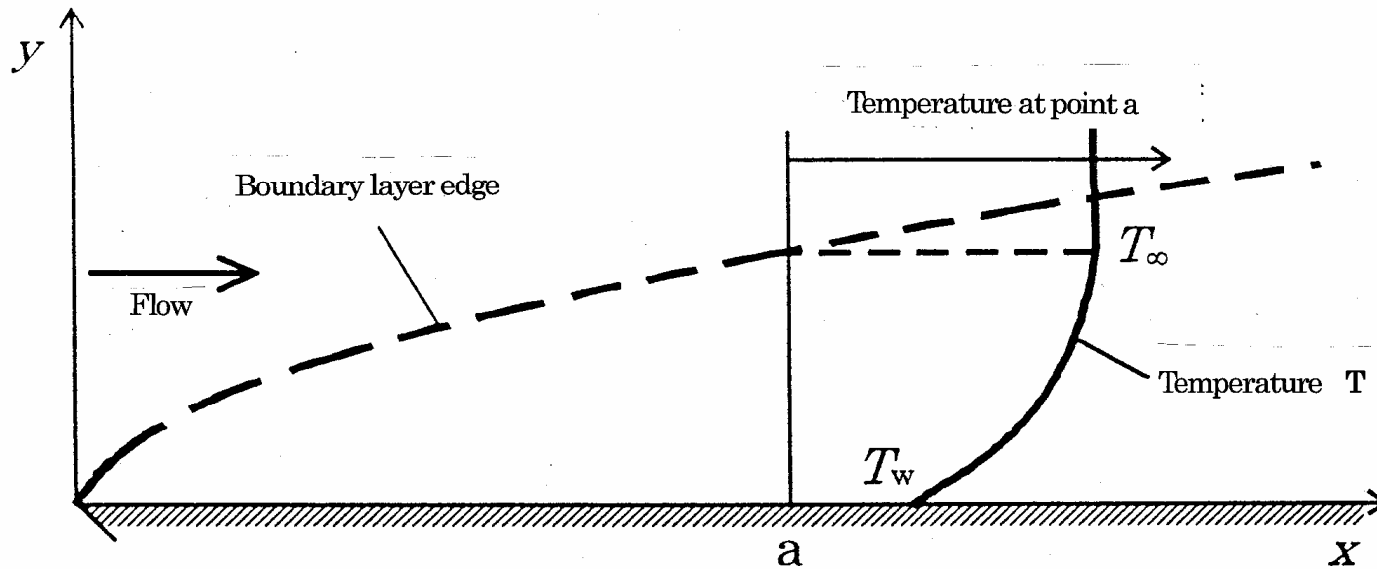
$$\left. \begin{array}{l} t = 0: \Phi = 1 \quad \text{at } x \geq 0 \\ \Phi = 0 \quad \text{at } x < 0 \\ t > 0: \Phi = 1 \quad \text{for } x = \infty \\ \Phi = 0 \quad \text{for } x = -\infty \end{array} \right\}$$



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## Variation of Temperature and Species Concentration in a Laminar Flow

### *Temperature and Species Concentration Profiles in the Boundary Layer*





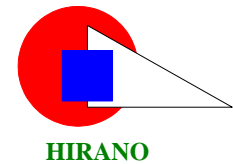
$$\frac{DT}{Dt} = \alpha \nabla^2 T$$

$$v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} = \alpha \frac{\partial^2 T}{\partial y^2}$$

$$v_x = \frac{\partial \Psi}{\partial y}, \quad v_y = -\frac{\partial \Psi}{\partial x} \quad \Psi(x, y) = (vUx)^{\frac{1}{2}} f(\eta)$$

$$\eta \equiv y \left( \frac{U}{v x} \right)^{\frac{1}{2}} \quad \Theta = \frac{T - T_w}{T_\infty - T_w}$$

$$2\Theta'' + \text{Pr} f\Theta' = 0 \quad \left. \begin{array}{l} \eta = 0: \quad \Theta = 0 \\ \eta = \infty: \quad \Theta = 1 \end{array} \right\}$$



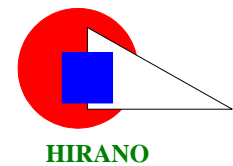


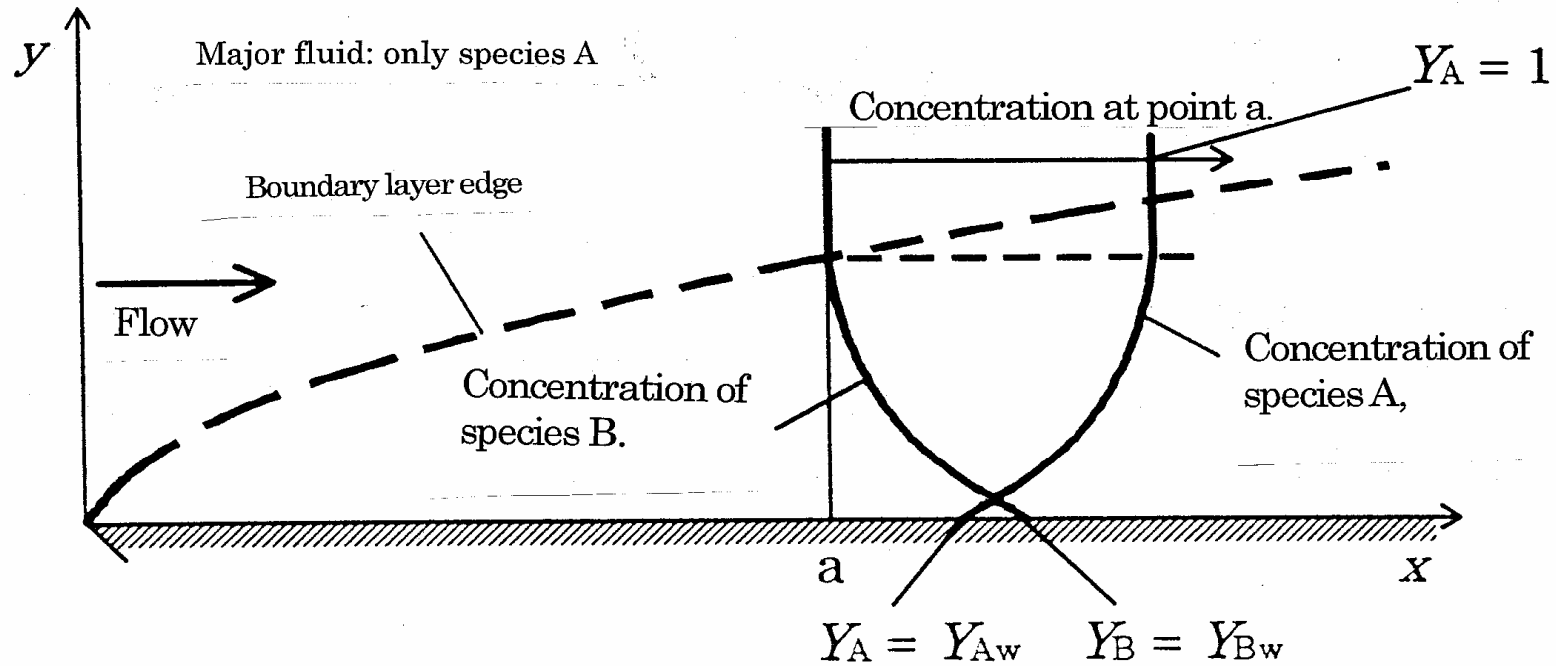
$$\Theta = \frac{\int_0^{\eta} \exp\left(-\frac{1}{2} \int_0^{\eta} (\text{Pr } f) d\eta\right) d\eta}{\int_0^{\infty} \exp\left(-\frac{1}{2} \int_0^{\eta} (\text{Pr } f) d\eta\right) d\eta}$$

$$2f''' + ff'' = 0$$

$$\left. \begin{array}{l} \eta = 0: \quad f' = f = 0 \\ \eta = \infty: \quad f' = 1 \end{array} \right\}$$

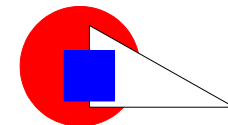
$$\Theta = f'$$





$$\frac{DY_A}{Dt} = D_A \nabla^2 Y_A$$

$$v_x \frac{\partial Y_A}{\partial x} + v_y \frac{\partial Y_A}{\partial y} = D_A \frac{\partial^2 Y_A}{\partial y^2}$$



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$$\Phi(\eta) = \frac{Y_A - Y_{Aw}}{1 - Y_{Aw}}$$

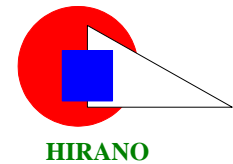
$$2\Phi'' + Scf\Phi' = 0$$

$$\left. \begin{array}{l} \eta = 0: \Phi = 0 \\ \eta = \infty: \Phi = 1 \end{array} \right\}$$

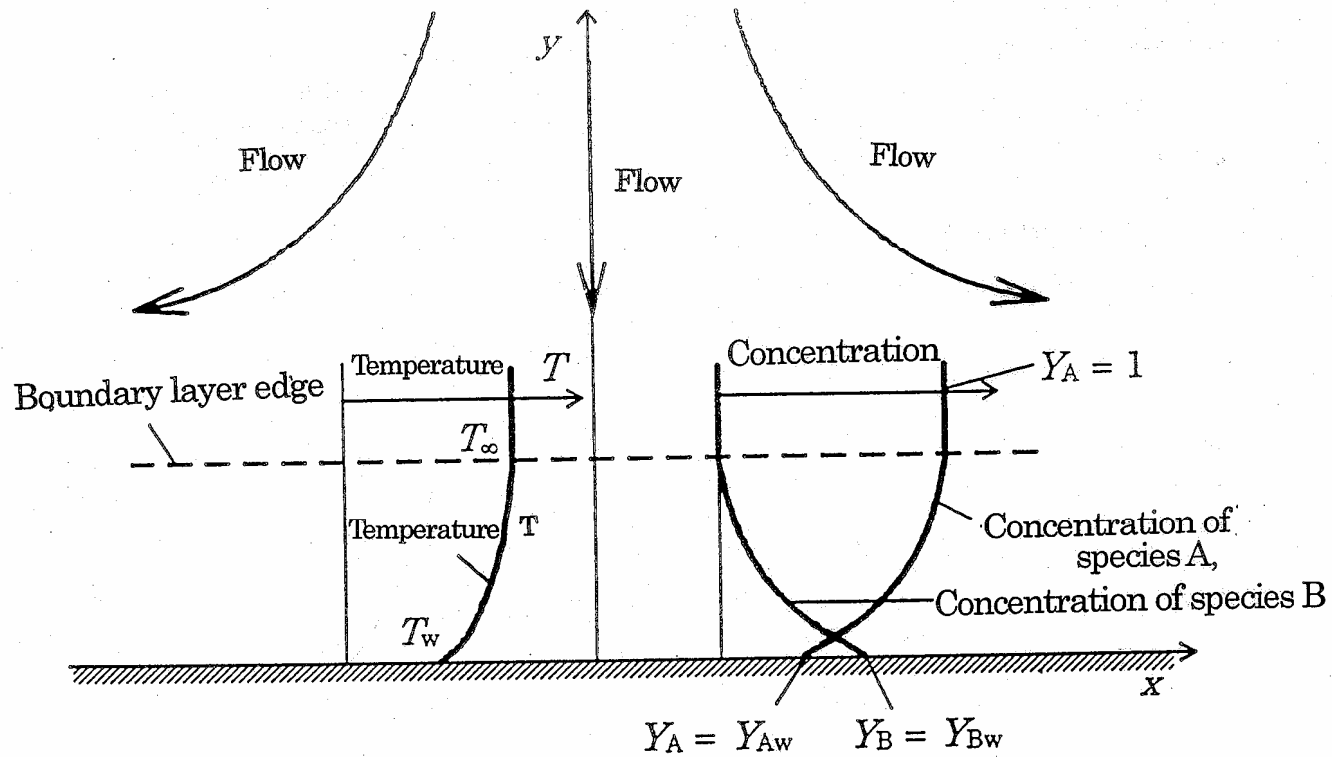
$$\Phi = \frac{\int_0^\eta \exp\left(-\frac{1}{2} \int_0^\eta (Scf) d\eta\right) d\eta}{\int_0^\infty \exp\left(-\frac{1}{2} \int_0^\eta (Scf) d\eta\right) d\eta}$$

$$\Phi = f'$$

$$Y_A = (1 - Y_{Aw})\Phi + Y_{Aw}$$

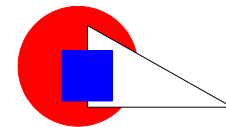






$$f(\eta) = \frac{\Psi(x, y)}{(vU_\infty x)^{\frac{1}{2}}} = \frac{\Psi(x, y)}{x(av)^{\frac{1}{2}}}$$

$$\eta \equiv \left(\frac{a}{v}\right)^{\frac{1}{2}} y$$





$$\Phi'' + Scf\Phi' = 0$$

$$\Theta'' + Prf\Theta' = 0$$

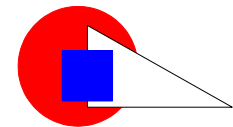
$$\left. \begin{array}{l} \eta = 0: \Phi = \Theta = 0 \\ \eta = \infty: \Phi = \Theta = 1 \end{array} \right\}$$

$$\Phi = \frac{\int_0^\eta \exp\left(-\int_0^\eta (Scf) d\eta\right) d\eta}{\int_0^\infty \exp\left(-\int_0^\eta (Scf) d\eta\right) d\eta}$$

$$\Theta = \frac{\int_0^\eta \exp\left(-\int_0^\eta (Prf) d\eta\right) d\eta}{\int_0^\infty \exp\left(-\int_0^\eta (Prf) d\eta\right) d\eta}$$

$$f''' + ff'' - (f')^2 + 1 = 0$$

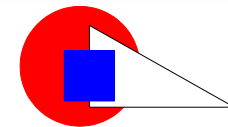
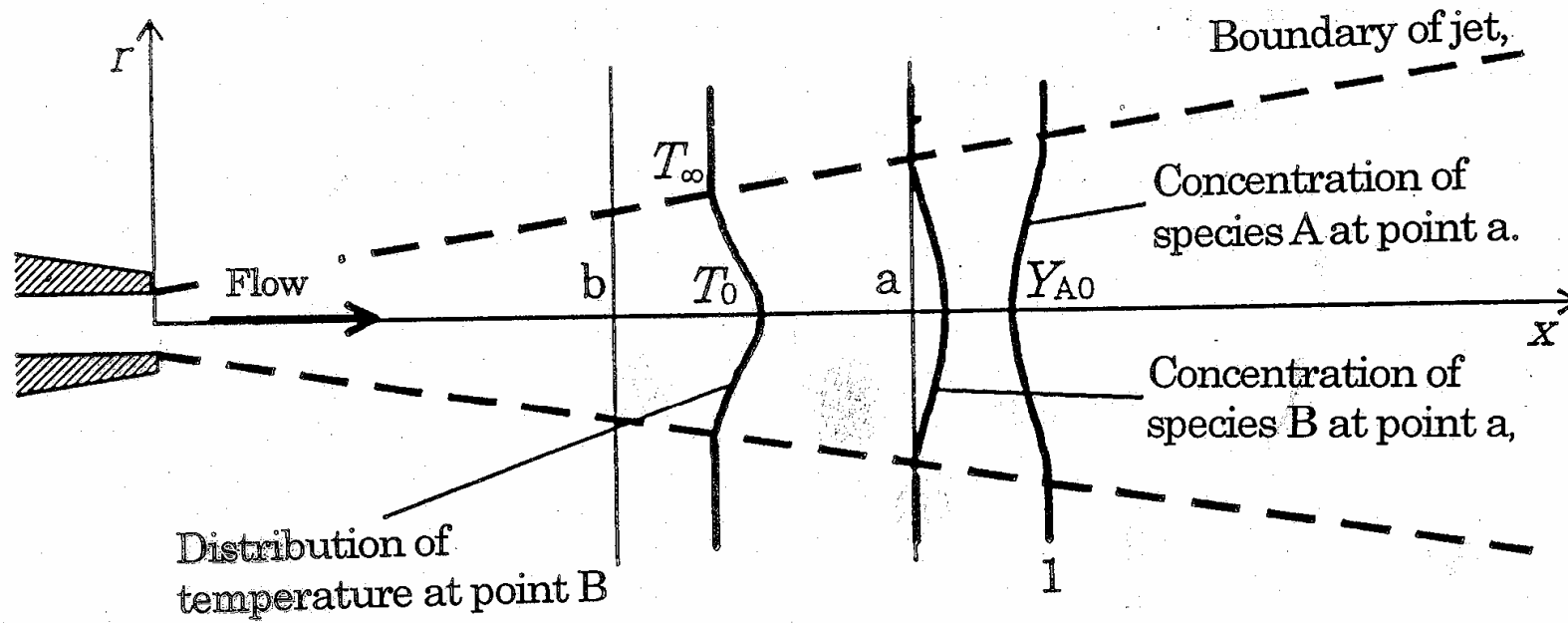
$$\left. \begin{array}{l} \eta = 0: f' = f = 0 \\ \eta = \infty: f' = 1 \end{array} \right\}$$



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## *Temperature and Species Concentration Profiles in a Jet*



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$$v_x \frac{\partial T}{\partial x} + v_r \frac{\partial T}{\partial r} = \alpha \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) \right\}$$

$$\eta \equiv \frac{r}{x} \quad r v_x = \frac{\partial \Psi}{\partial r}, \quad r v_r = -\frac{\partial \Psi}{\partial x}, \quad \Psi = v_x F(\eta)$$

$$\Theta = \frac{T_0 - T}{T_0 - T_w}$$

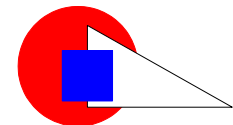
$$\eta \Theta'' + \Theta' + \text{Pr} F \Theta' = 0$$

$$\left. \begin{aligned} \eta = 0: \quad \Theta = 0 \\ \eta = \infty: \quad \Theta = 1 \end{aligned} \right\}$$

$$\Theta = \frac{\int_0^\eta \exp\left(-\int_0^\eta (\text{Pr} F + 1) d\eta\right) d\eta}{\int_0^\infty \exp\left(-\int_0^\eta (\text{Pr} F + 1) d\eta\right) d\eta}$$

$$\eta F'' + FF' - F' = 0$$

$$\eta = 0: \quad F(0) = F'(0) = 0$$





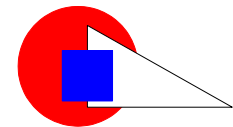
$$v_x \frac{\partial Y_A}{\partial x} + v_r \frac{\partial Y_A}{\partial r} = D_A \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial Y_A}{\partial r} \right) \right\}$$

$$\Phi = \frac{Y_A - Y_{A0}}{1 - Y_{A0}}$$

$$\eta \Phi'' + \Phi' + ScF \Phi' = 0$$

$$\left. \begin{array}{l} \eta = 0: \quad \Phi = 0 \\ \eta = \infty: \quad \Phi = 1 \end{array} \right\}$$

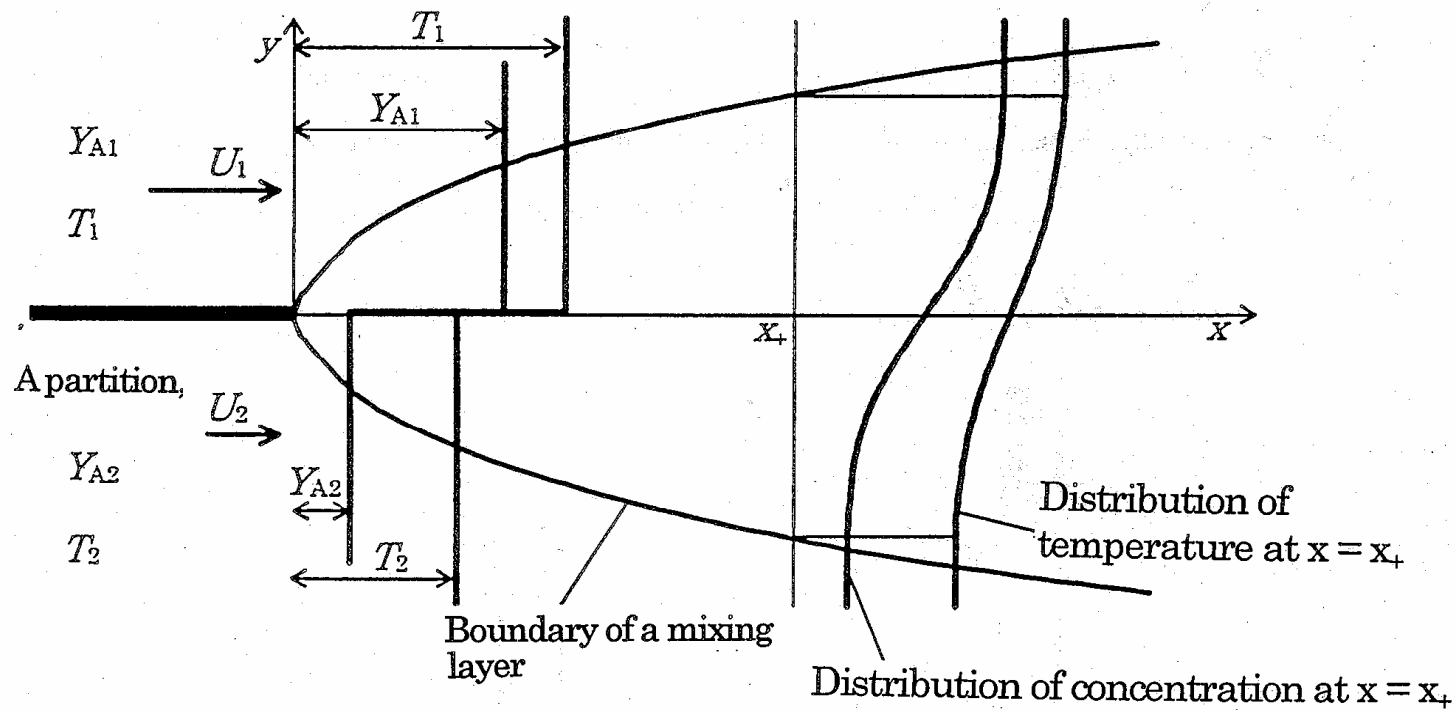
$$\Phi = \frac{\int_0^\eta \exp\left(-\int_0^\eta (ScF + 1)d\eta\right) d\eta}{\int_0^\infty \exp\left(-\int_0^\eta (ScF + 1)d\eta\right) d\eta}$$



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## *Temperature and Species Concentration Profiles in Parallel Flows of Different Velocities*





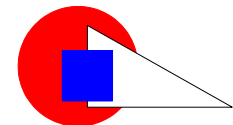
$$v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} = \alpha \frac{\partial^2 T}{\partial y^2}$$

$$\eta = \left( \frac{U_1}{\nu x} \right)^{\frac{1}{2}} y \quad \Psi = (\nu \cdot U_1 x)^{\frac{1}{2}} f \quad \Theta = \frac{2T - T_1 - T_2}{T_1 - T_2}$$

$$2\Theta'' + \text{Pr} f\Theta' = 0$$

$$\left. \begin{array}{l} \eta = -\infty : \Theta = -1 \\ \eta = \infty : \Theta = 1 \end{array} \right\}$$

$$\Theta = \frac{\int_0^\eta \exp\left(-\frac{1}{2} \int_0^\eta (\text{Pr} f) d\eta\right) d\eta}{\int_0^\infty \exp\left(-\frac{1}{2} \int_0^\eta (\text{Pr} f) d\eta\right) d\eta}$$



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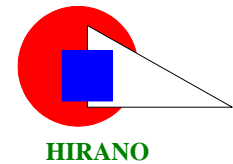


$$v_x \frac{\partial Y_A}{\partial x} + v_y \frac{\partial Y_A}{\partial r} = D_A \frac{\partial^2 Y_A}{\partial y^2}$$

$$\Phi = \frac{2Y_A - Y_{A2} - Y_{A1}}{Y_{A1} - Y_{A2}}$$

$$2\Phi'' + Scf\Phi' = 0 \quad \left. \begin{array}{l} \eta = -\infty : \Phi = -1 \\ \eta = \infty : \Phi = 1 \end{array} \right\}$$

$$\Phi = \frac{\int_0^\eta \exp\left(-\frac{1}{2} \int_0^\eta (Scf) d\eta\right) d\eta}{\int_0^\infty \exp\left(-\frac{1}{2} \int_0^\eta (Scf) d\eta\right) d\eta}$$

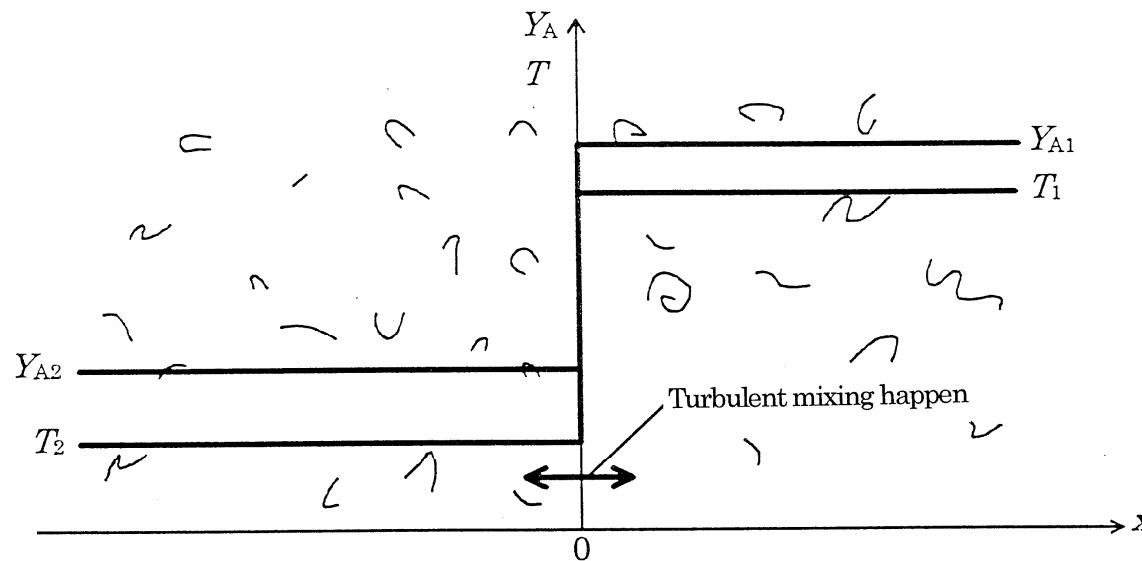






# Temperature and Species Concentration Profiles in Turbulent Flows

*Turbulent Diffusion  
at the Site with Temperature or Species Concentration Difference*





$$t \leq 0: \quad \left. \begin{array}{l} \bar{T} = T_1 \quad \text{for } x \geq 0 \\ \bar{T} = T_2 \quad \text{for } x < 0 \end{array} \right\}$$

$$\frac{D\bar{T}}{Dt} = \varepsilon_T \nabla^2 \bar{T}$$

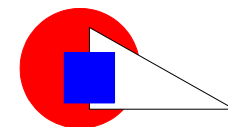
$$\frac{\partial \bar{T}}{\partial t} = \varepsilon_T \frac{\partial^2 \bar{T}}{\partial x^2}$$

$$\Theta = \frac{\bar{T} - T_2}{T_1 - T_2}$$

$$\frac{\partial \Theta}{\partial t} = \varepsilon_T \frac{\partial^2 \Theta}{\partial x^2}$$

$$\left. \begin{array}{l} t = 0: \quad \Theta = 1 \quad \text{for } x \geq 0 \\ \quad \quad \Theta = 0 \quad \text{for } x < 0 \\ t > 0: \quad \Theta = 1 \quad \text{for } x = \infty \\ \quad \quad \Theta = 0 \quad \text{for } x = -\infty \end{array} \right\}$$

$$\Theta = \frac{1}{2} \left\{ 1 + \operatorname{erf} \left( \frac{x}{2\sqrt{\varepsilon_T t}} \right) \right\}$$



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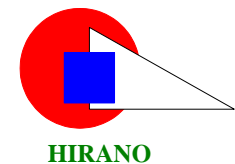
$$\varepsilon_T = \lambda t \quad \tau = t^2/2$$

$$\frac{\partial \Theta}{\partial \tau} = \lambda \frac{\partial^2 \Theta}{\partial x^2}$$

$$\left. \begin{array}{l} \tau = 0: \quad \Theta = 1 \quad \text{for } x \geq 0 \\ \quad \quad \Theta = 0 \quad \text{for } x < 0 \\ \tau > 0: \quad \Theta = 1 \quad \text{for } x = \infty \\ \quad \quad \Theta = 0 \quad \text{for } x = -\infty \end{array} \right\}$$

$$\Theta = \frac{1}{2} \left\{ 1 + \operatorname{erf} \left( \frac{x}{2\sqrt{\lambda \tau}} \right) \right\} = \frac{1}{2} \left\{ 1 + \operatorname{erf} \left( \frac{x}{\sqrt{2\varepsilon_T t}} \right) \right\}$$

The temperature profile change in the case  
when the turbulent heat transfer coefficient increases with time





$$t \leq 0: \quad \left. \begin{array}{l} \bar{Y}_A = Y_{A1} \quad \text{for } x \geq 0 \\ \bar{Y}_A = Y_{A2} \quad \text{for } x < 0 \end{array} \right\}$$

$$\frac{D\bar{Y}_A}{Dt} = \varepsilon_{DA} \nabla^2 \bar{Y}_A \quad \frac{\partial \bar{Y}_A}{\partial t} = \varepsilon_{DA} \frac{\partial^2 \bar{Y}_A}{\partial x^2}$$

$$\Phi = \frac{\bar{Y}_A - \bar{Y}_{A2}}{\bar{Y}_{A1} - \bar{Y}_{A2}} \quad \frac{\partial \Phi}{\partial t} = \varepsilon_{DA} \frac{\partial^2 \Phi}{\partial x^2}$$

$$\left. \begin{array}{l} t = 0: \quad \Phi = 1 \quad \text{for } x \geq 0 \\ \quad \quad \Phi = 0 \quad \text{for } x < 0 \\ t > 0: \quad \Phi = 1 \quad \text{for } x = \infty \\ \quad \quad \Phi = 0 \quad \text{for } x = -\infty \end{array} \right\}$$

$$\Phi = \frac{1}{2} \left\{ 1 + \operatorname{erf} \left( \frac{x}{2\sqrt{\varepsilon_{DA} t}} \right) \right\}$$



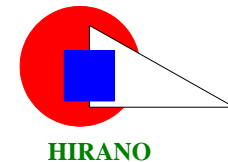
$$\varepsilon_{DA} = \kappa t \quad \tau = t^2/2$$

$$\frac{\partial \Phi}{\partial \tau} = \kappa \frac{\partial^2 \Phi}{\partial x^2}$$

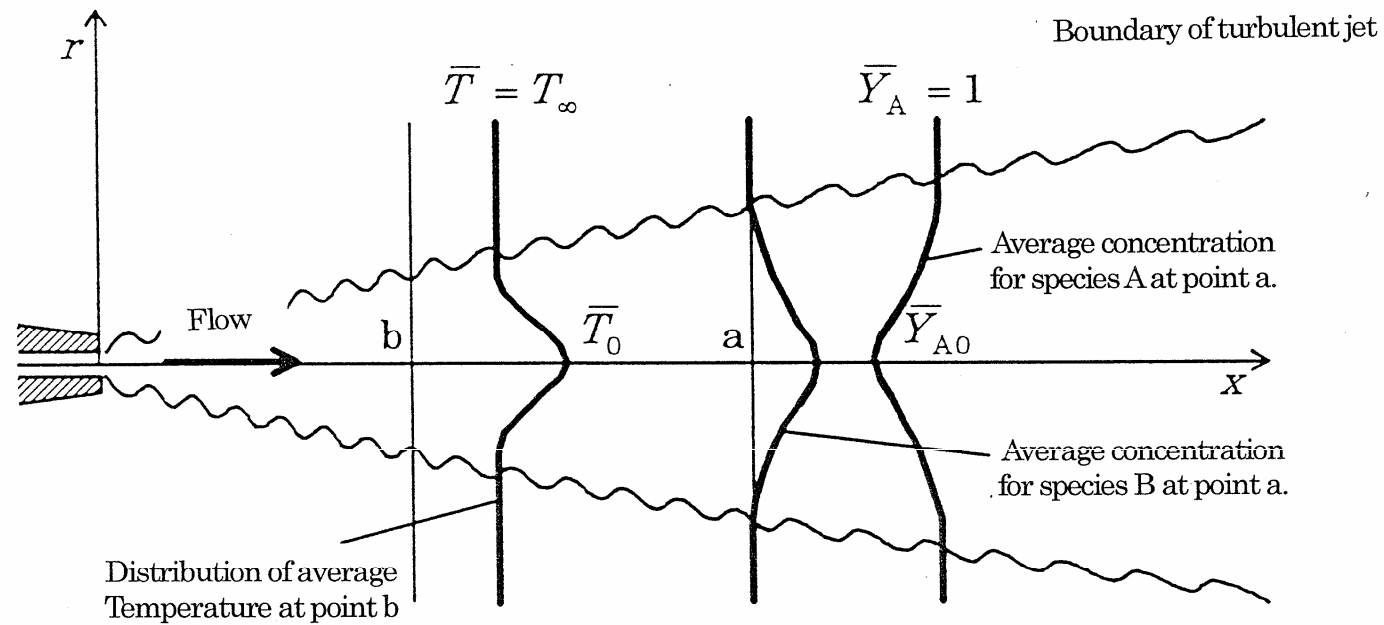
$$\left. \begin{array}{l} \tau = 0: \quad \Phi = 1 \quad \text{for } x \geq 0 \\ \quad \quad \Phi = 0 \quad \text{for } x < 0 \\ \tau > 0: \quad \Phi = 1 \quad \text{for } x = \infty \\ \quad \quad \Phi = 0 \quad \text{for } x = -\infty \end{array} \right\}$$

$$\Phi = \frac{1}{2} \left\{ 1 + \operatorname{erf} \left( \frac{x}{2\sqrt{\kappa\tau}} \right) \right\} = \frac{1}{2} \left\{ 1 + \operatorname{erf} \left( \frac{x}{\sqrt{2\varepsilon_{DA}t}} \right) \right\}$$

The species concentration profile change in the case when the turbulent mass transfer coefficient increases with time



## *Temperature and Species Concentration Profiles across a Turbulent Jet*





$$v_x \frac{\partial \bar{T}}{\partial x} + v_r \frac{\partial \bar{T}}{\partial r} = \varepsilon_T \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \bar{T}}{\partial r} \right) \right\}$$

$$\xi \equiv \frac{r}{x} \quad r\bar{v}_x = \frac{\partial \Psi}{\partial r}, \quad r\bar{v}_r = -\frac{\partial \Psi}{\partial x}, \quad \Psi = \varepsilon_T x F(\xi) \quad \Theta = \frac{\bar{T}_0 - \bar{T}}{\bar{T}_0 - T_w}$$

$$\xi \Theta'' + \Theta' + \text{Pr}_t F \Theta' = 0 \quad \left. \begin{array}{l} \xi = 0: \Theta = 0 \\ \xi = \infty: \Theta = 1 \end{array} \right\}$$

$$\Theta = \frac{\int_0^\xi \exp\left(-\int_0^\xi (\text{Pr}_t F + 1) d\xi\right) d\xi}{\int_0^\infty \exp\left(-\int_0^\xi (\text{Pr}_t F + 1) d\xi\right) d\xi}$$





$$\bar{v}_x \frac{\partial \bar{Y}_A}{\partial x} + \bar{v}_r \frac{\partial \bar{Y}_A}{\partial r} = \epsilon_{DA} \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \bar{Y}_A}{\partial r} \right) \right\}$$

$$\Phi = \frac{\bar{Y}_A - \bar{Y}_{A0}}{1 - \bar{Y}_{A0}}$$

$$\xi \Phi'' + \Phi' + Sc_t F \Phi' = 0 \quad \left. \begin{array}{l} \xi = 0: \quad \Phi = 0 \\ \xi = \infty: \quad \Phi = 1 \end{array} \right\}$$

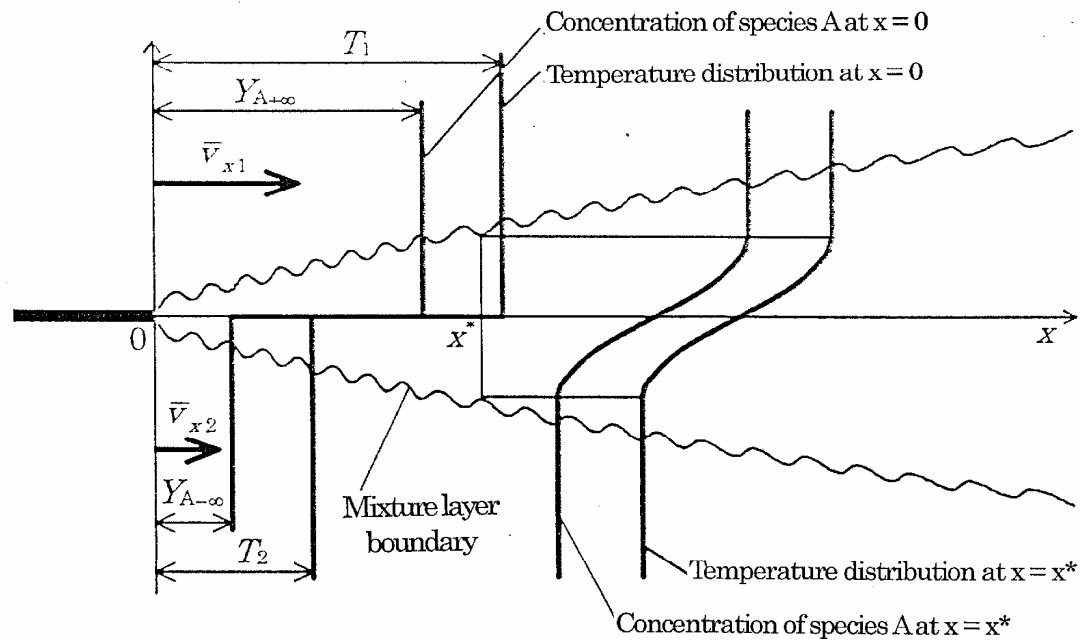
$$\Phi = \frac{\int_0^\xi \exp\left(-\int_0^\xi (Sc_t F + 1) d\xi\right) d\xi}{\int_0^\infty \exp\left(-\int_0^\xi (Sc_t F + 1) d\xi\right) d\xi}$$







## *Temperature and Species Concentration Profiles across a Shear Flow*





$$\bar{v}_x \frac{\partial \bar{T}}{\partial x} + \bar{v}_y \frac{\partial \bar{T}}{\partial y} = \varepsilon_T \frac{\partial^2 \bar{T}}{\partial y^2}$$

$$\left. \begin{aligned} \Psi = xUF(\xi), \quad \xi = \frac{oy}{x}, \quad \sigma = (4\lambda\kappa_1 c)^{-\frac{1}{3}}, \quad \lambda = \frac{\bar{v}_{x1} - \bar{v}_{x2}}{\bar{v}_{x1} + \bar{v}_{x2}} \\ \Theta = \frac{2\bar{T} - T_1 - T_2}{T_1 - T_2}, \quad U = \frac{1}{2}(\bar{v}_{x1} - \bar{v}_{x2}), \quad \text{Pr}_t = \frac{\varepsilon_E}{\varepsilon_T} \end{aligned} \right\}$$

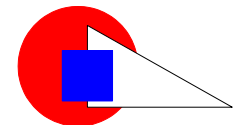
$$\Theta + 2\sigma^2 \text{Pr}_t F \Theta' = 0$$

$$\left. \begin{aligned} \xi = -\infty: \quad \Theta = -1 \\ \xi = +\infty: \quad \Theta = 1 \end{aligned} \right\}$$

$$\Theta = \frac{\int_0^\xi \exp\left(-2\sigma \int_0^\xi (\text{Pr}_t F) d\xi\right) d\xi}{\int_0^\infty \exp\left(-2\sigma \int_0^\xi (\text{Pr}_t F) d\xi\right) d\xi}$$

$$x\bar{v}_x / (2\varepsilon_E) = 2\sigma^2 \text{Pr}_t,$$

$$\Theta = F'$$



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$$\bar{v}_x \frac{\partial \bar{Y}_A}{\partial x} + \bar{v}_y \frac{\partial \bar{Y}_A}{\partial y} = \varepsilon_{DA} \frac{\partial^2 \bar{Y}_A}{\partial y^2}$$

$$\Phi = \frac{2\bar{Y}_A - Y_{A+\infty} - Y_{A-\infty}}{Y_{A+\infty} - Y_{A-\infty}}, \quad Sc_t = \frac{\varepsilon_E}{\varepsilon_{DA}}$$

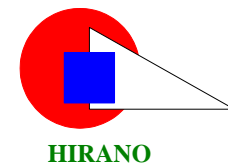
$$\Phi'' + 2\sigma^2 Sc_t F \Phi' = 0$$

$$\left. \begin{array}{l} \xi = -\infty : \Phi = -1 \\ \xi = +\infty : \Phi = 1 \end{array} \right\}$$

$$\Phi = \frac{\int_0^\xi \exp\left(-2\sigma \int_0^\xi (Sc_t F) d\xi\right) d\xi}{\int_0^{+\infty} \exp\left(-2\sigma \int_0^\xi (Sc_t F) d\xi\right) d\xi}$$

$$x\bar{v}_x / (2\varepsilon_E) = 2\sigma^2 Sc_t,$$

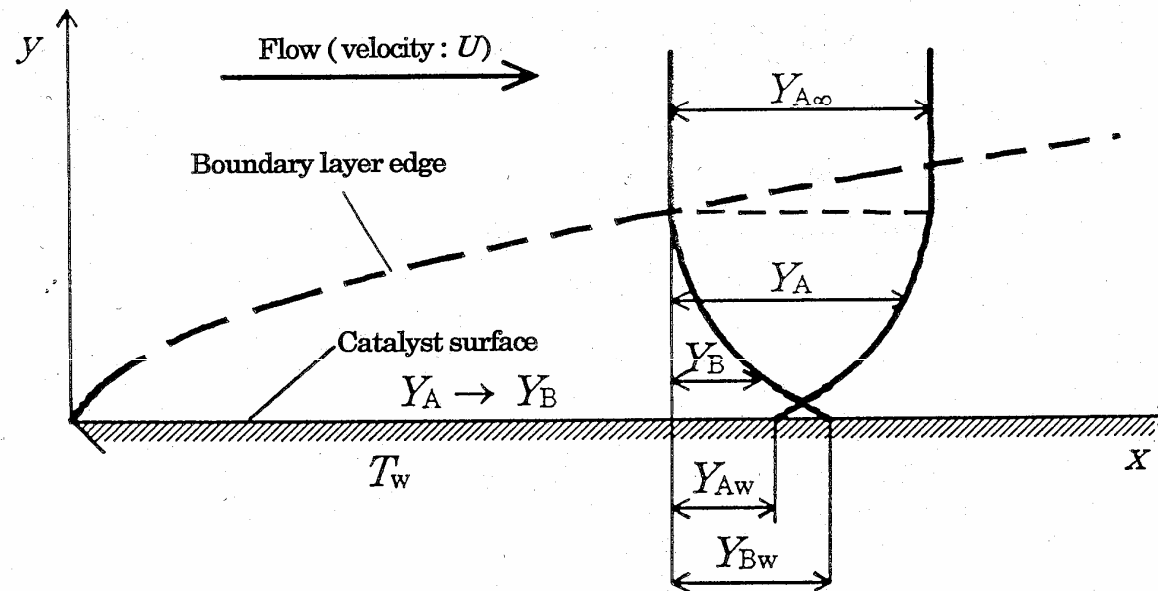
$$\Phi = F'$$



# STRUCTURE OF REACTION SITES

## Surface Reaction

### *Catalytic Reaction*





$$-\dot{m}''_{Aw} = \rho_w Y_{Aw} B \exp\left(-\frac{E}{RT_w}\right)$$

$$\rho_w Y_{Aw} B \exp\left(-\frac{E}{RT_w}\right) = \rho_w D_A \left(\frac{\partial Y_A}{\partial y}\right)_w$$

$$\Phi = \frac{Y_A - Y_{Aw}}{Y_{A\infty} - Y_{Aw}}$$

$$Y_{Aw} = \frac{D_A Y_{A\infty} \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_w}{B \exp\left(-\frac{E}{RT_w}\right) + D_A \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_w}$$

$$B \exp\left(-\frac{E}{RT_w}\right) \ll D_A \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_w$$

$$Y_{Aw} \cong Y_{A\infty}$$

$$-\dot{m}''_{Aw} = \rho_w Y_{A\infty} B \exp\left(-\frac{E}{RT_w}\right)$$

$$B \exp\left(-\frac{E}{RT_w}\right) \gg D_A \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_w$$

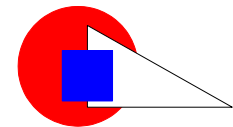
$$Y_{Aw} = \frac{D_A Y_{A\infty} \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_w}{B \exp\left(-\frac{E}{RT_w}\right)}$$



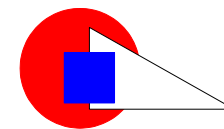
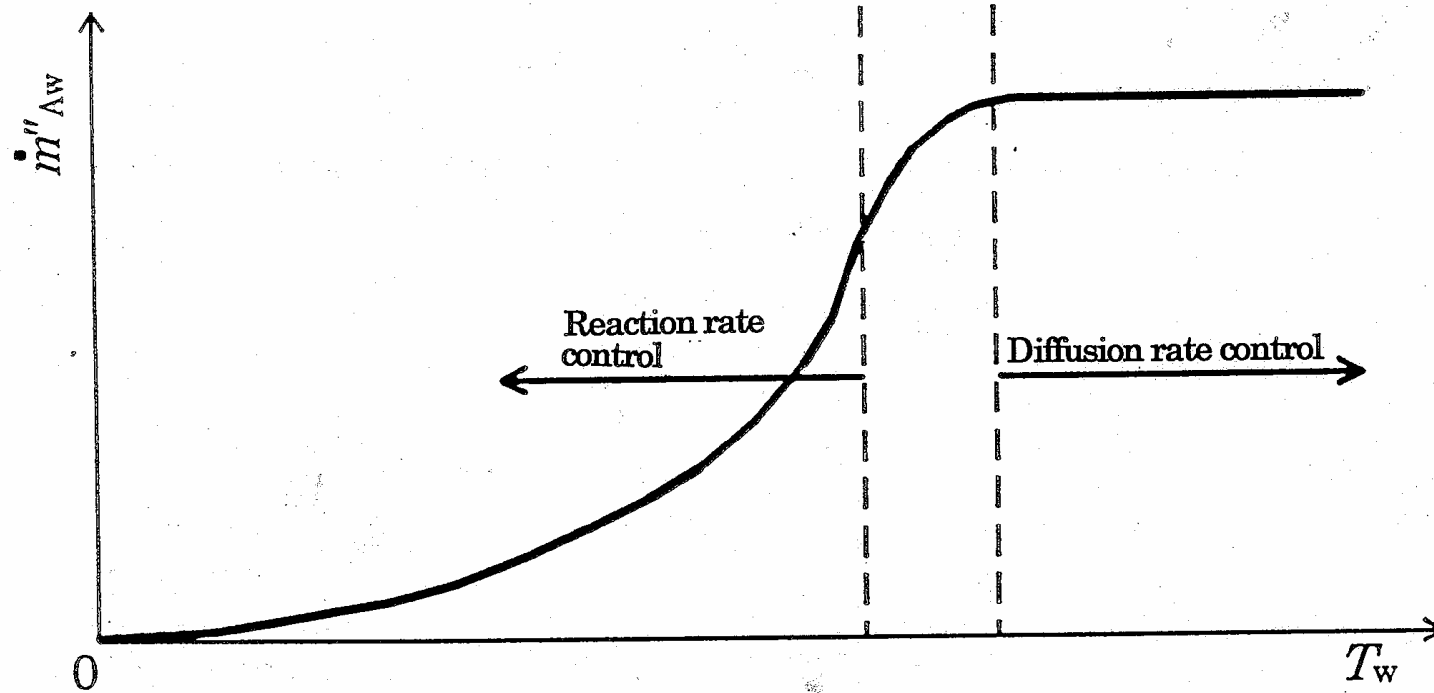
$$Y_{Aw} = \frac{D_A Y_{A\infty} \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_w}{B \exp\left(-\frac{E}{RT_w}\right)}$$

$$\frac{Y_{Aw}}{Y_{A\infty}} = \frac{D_A \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_w}{B \exp\left(-\frac{E}{RT_w}\right)} \quad \eta \equiv \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} y, \quad \Psi(x, y) = (\nu U x)^{\frac{1}{2}} f(\eta)$$

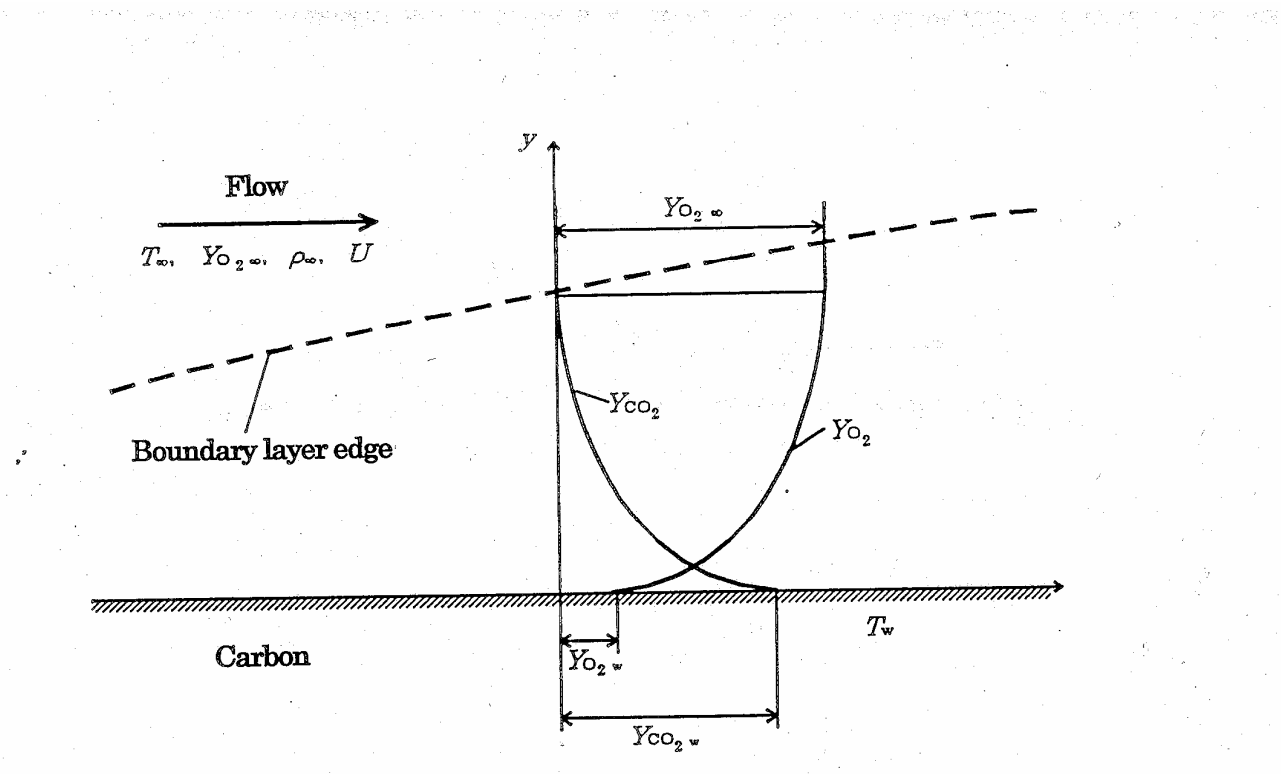
$$\begin{aligned} -\dot{m}''_{Aw} &= \rho_w D_A \left(\frac{\partial Y_A}{\partial y}\right)_w = \rho_w D_A (Y_{A\infty} - Y_{Aw}) \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_w \\ &\cong \rho_w D_A (Y_{A\infty}) \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_w \end{aligned}$$



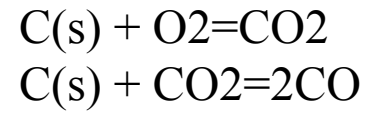
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## Combustion Reaction







$$\dot{m}''_{\text{CO}_2\text{w}} = \rho_w Y_{\text{O}_2\text{w}} B_1 \exp\left(-\frac{E_1}{RT_w}\right)$$

$$\dot{m}''_{\text{COw}} = \rho_w Y_{\text{CO}_2\text{w}} B_2 \exp\left(-\frac{E_2}{RT_w}\right)$$

$$\left(\dot{m}''_{\text{CO}_2\text{w}}\right)_{\text{Net}} = \dot{m}''_{\text{CO}_2\text{w}} - j\dot{m}''_{\text{COw}}$$

$$\rho_w Y_{\text{O}_2\text{w}} B_1 \exp\left(-\frac{E_1}{RT_w}\right) - j\rho_w Y_{\text{CO}_2\text{w}} B_2 \exp\left(-\frac{E_2}{RT_w}\right) = \rho_w D_{\text{CO}_2} \left(\frac{\partial Y_{\text{CO}_2}}{\partial y}\right)_w$$



$$\Phi_{\text{CO}_2} = \frac{Y_{\text{CO}_2\text{w}} - Y_{\text{CO}_2}}{Y_{\text{CO}_2\text{w}}}$$

$$Y_{\text{CO}_2\text{w}} = \frac{Y_{\text{O}_2\text{w}} B_1 \exp\left(-\frac{E_1}{RT_w}\right)}{jB_2 \exp\left(-\frac{E_2}{RT_w}\right) + D_{\text{CO}_2} \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_{\text{CO}_2\text{w}}}$$

Low Temperature

$$\frac{Y_{\text{CO}_2\text{w}}}{Y_{\text{O}_2\text{w}}} = \frac{B_1 \exp\left(-\frac{E_{C1}}{RT_w}\right)}{D_{\text{CO}_2} \left(\frac{U}{\nu x}\right)^{\frac{1}{2}} \Phi'_{\text{CO}_2\text{w}}}$$

$$\left(\dot{m}''_{\text{CO}_2\text{w}}\right)_{\text{Net}} = \dot{m}''_{\text{CO}_2\text{w}}$$

High Temperature

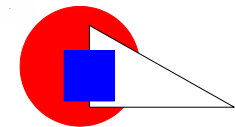
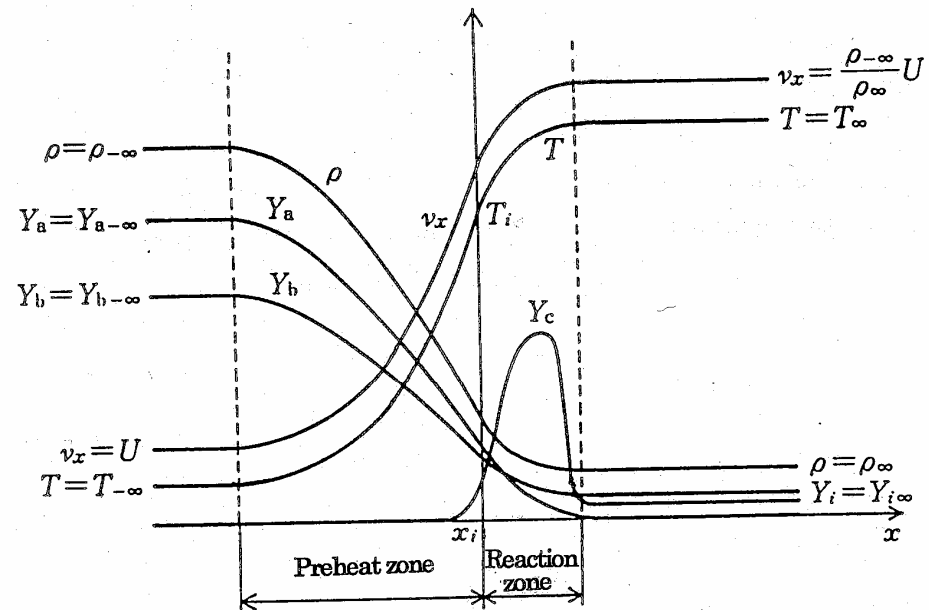
$$\frac{Y_{\text{CO}_2\text{w}}}{Y_{\text{O}_2\text{w}}} = \frac{B_1 \exp\left(-\frac{E_1}{RT_w}\right)}{jB_2 \exp\left(-\frac{E_2}{RT_w}\right)}$$

$$\left(\dot{m}''_{\text{CO}_2\text{w}}\right)_{\text{Net}} = \dot{m}''_{\text{CO}_2\text{w}} - j\dot{m}''_{\text{COw}} = 0$$



# Reaction in a Gas Flow

## *Steady Premixed Flame*



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$$\frac{d(\rho v_x)}{dx} = 0$$

$$\rho v_x \frac{dv_x}{dx} = -\frac{dp}{dx} + \frac{d}{dx} \left( \mu \frac{dv_x}{dx} \right)$$

$$\rho c_p v_x \frac{dT}{dx} = \frac{d}{dx} \left( \lambda \frac{dT}{dx} \right) + \dot{\omega}_F''' \Delta H$$

$$\rho v_x \frac{dY_i}{dx} = \frac{d}{dx} \left( \rho D_i \frac{dY_i}{dx} \right) + \dot{\omega}_i'''$$

$$\dot{\omega}_i''' = \sum_j A_{ij} B_{ij} \exp\left(-\frac{E_{ij}}{RT}\right)$$

$$pV = nRT$$

$$\left. \begin{array}{l} x = -\infty: \quad v_x = U, \quad T = T_{-\infty}, \quad Y_i = Y_{i-\infty}, \quad \rho = \rho_{-\infty} \\ x = \infty: \quad v_x = \frac{\rho_{-\infty}}{\rho_{\infty}} U, \quad T = T_{\infty}, \quad Y_i = Y_{i\infty}, \quad \rho = \rho_{\infty} \end{array} \right\}$$



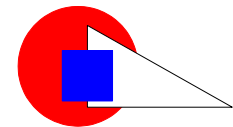
$$\rho_{-\infty} c_p U \frac{dT}{dx} = \lambda \frac{d^2 T}{dx^2} + \dot{\omega}_F''' \Delta H$$

$$\left( \frac{dT}{dx} \right)_i = \frac{\rho c_p U}{\lambda} (T_i - T_u)$$

$$\rho Y_F U = -\dot{\omega}_F''' \delta_r$$

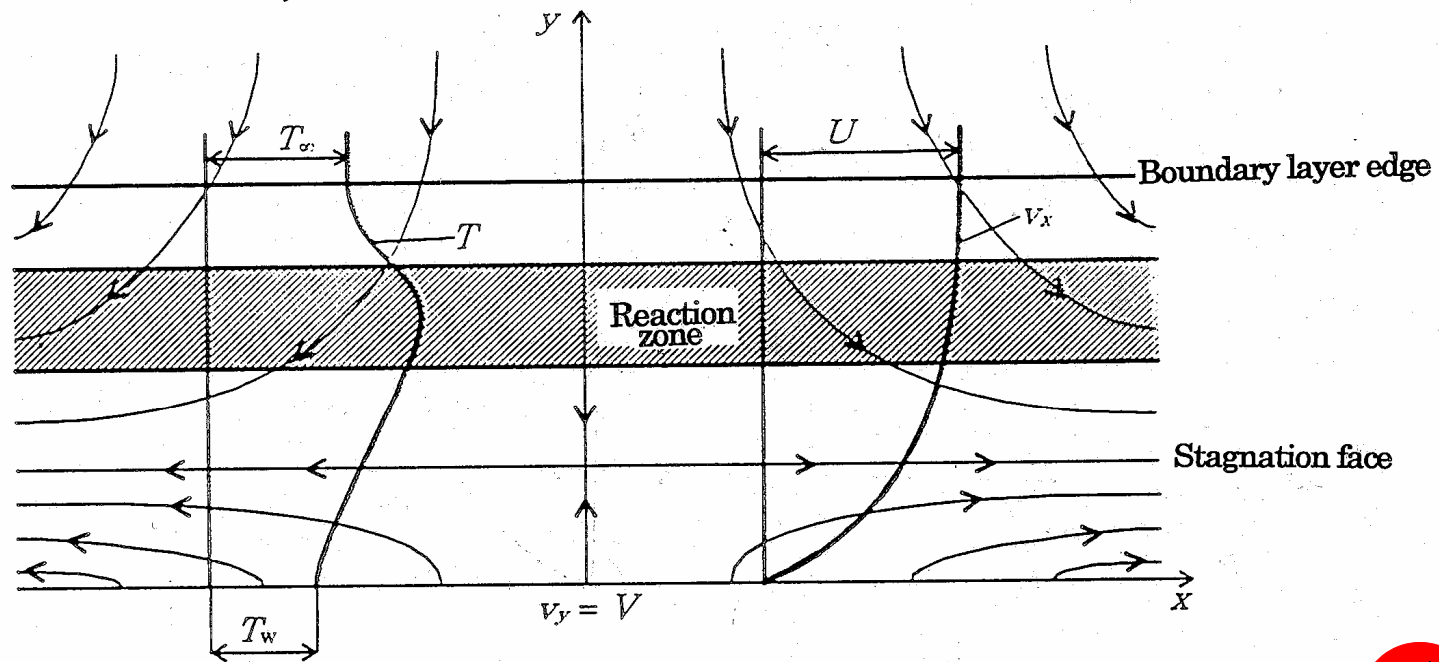
$$\left( \frac{dT}{dx} \right)_i = \left( \frac{R}{\delta_r} \right) (T_b - T_i)$$

$$\delta_r = \left\{ R \left( \frac{T_b - T_i}{T_i - T_u} \right) \left( \frac{\lambda}{\rho c_p} \right) \left( \frac{\rho Y_F}{-\dot{\omega}_F'''} \right) \right\}^{\frac{1}{2}}$$



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## *Diffusion Flame in a Boundary Layer*





$$v_F W_F + v_O W_O = v_P W_P$$

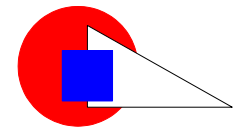
$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0$$

$$v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left( \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} \right)$$

$$v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} = \alpha \frac{\partial^2 T}{\partial y^2} - \sum_i \frac{\dot{\omega}_i''' h^{(0)}}{\rho c_p}$$

$$v_x \frac{\partial Y_i}{\partial x} + v_y \frac{\partial Y_i}{\partial y} = D_i \frac{\partial^2 Y_i}{\partial y^2} + \frac{\dot{\omega}_i'''}{\rho} \quad (i = F, O, P)$$

$$\dot{\omega}_F''' = -v_F W_F \left( \frac{\rho Y_F}{W_F} \right)^{v_F} \left( \frac{\rho Y_O}{W_O} \right)^{v_O} b \exp\left(-\frac{E}{RT}\right)$$



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$$\dot{\omega}_O''' = -\nu_O W_O \left( \frac{\rho Y_F}{W_F} \right)^{\nu_F} \left( \frac{\rho Y_O}{W_O} \right)^{\nu_O} b \exp\left(-\frac{E}{RT}\right)$$

$$\dot{\omega}_P''' = -\nu_P W_P \left( \frac{\rho Y_F}{W_F} \right)^{\nu_F} \left( \frac{\rho Y_O}{W_O} \right)^{\nu_O} b \exp\left(-\frac{E}{RT}\right)$$

$$\sum_i Y_i = 1$$

$$\left. \begin{aligned} y=0: \quad & \nu_x = 0, \quad \nu_y = V, \quad T = T_w, \quad Y_F = Y_{Fw}, \quad Y_N = Y_{Nw} \\ y=\infty: \quad & \nu_x = U, \quad T = T_\infty, \quad Y_O = Y_{O\infty}, \quad Y_N = Y_{N\infty} \end{aligned} \right\}$$

$$\Theta = \frac{T - T_w}{T_\infty - T_w} \quad U = ax, \quad \frac{dp}{dx} = -\rho a^2 x, \quad \eta \equiv \left(\frac{a}{\nu}\right)^{\frac{1}{2}}, \quad f(\eta) = \frac{\Psi(x, y)}{x(a\nu)^{\frac{1}{2}}}$$

$$\left. \begin{aligned} \Theta'' + \text{Pr} f\Theta' - \frac{\text{Pr}}{a(T_\infty - T_w)} \left( \sum_i \frac{\dot{\omega}_i''' h_i^{(0)}}{\rho c_p} \right) = 0 \\ \eta = 0: \quad \Theta = 0 \\ \eta = \infty: \quad \Theta = 1 \end{aligned} \right\}$$





$$\Phi_F = \frac{Y_F}{Y_{Fw}}, \quad \Phi_O = \frac{Y_O}{Y_{Ow}}, \quad \Phi_N = \frac{Y_N - Y_{Nw}}{Y_{N\infty} - Y_{Nw}}$$

$$\Phi'' + Sc_i f \Phi_i' + Sc_i \frac{W_i}{a(Y_{i\infty} - Y_{iw})} \frac{\dot{\omega}_i'''}{\rho} = 0 \quad (i = F, O, P)$$

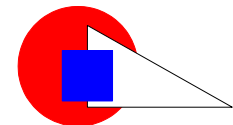
$$\left. \begin{array}{l} \eta = 0: \quad \Phi_F = 1, \quad \Phi_O = 0, \quad \Phi_N = 0 \\ \eta = \infty: \quad \Phi_F = 0, \quad \Phi_O = 1, \quad \Phi_N = 1 \end{array} \right\}$$

$$V = Y_F V - D_F \left( \frac{\partial Y_F}{\partial y} \right)_w \quad 0 = Y_{Nw} V - D_N \left( \frac{\partial Y_N}{\partial y} \right)_w \quad Y_C \equiv \frac{Y_F}{\nu_F W_F} - \frac{Y_O}{\nu_O W_O}$$

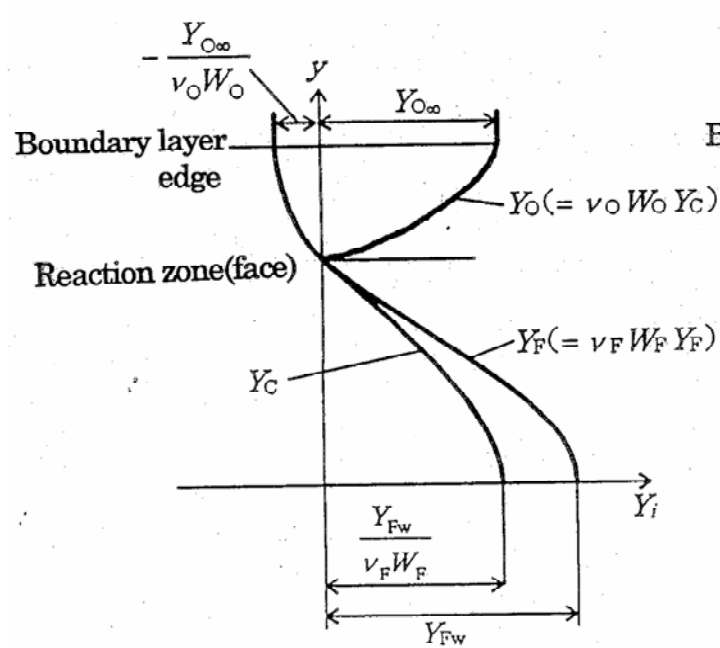
$$v_x \frac{\partial Y_C}{\partial x} + v_y \frac{\partial Y_C}{\partial y} = D \frac{\partial^2 Y_C}{\partial y^2} \quad \Phi_C = \frac{Y_C - Y_{Cw}}{Y_{C\infty} - Y_{Cw}}$$

$$\Phi_C'' + Sc_C f \Phi_C$$

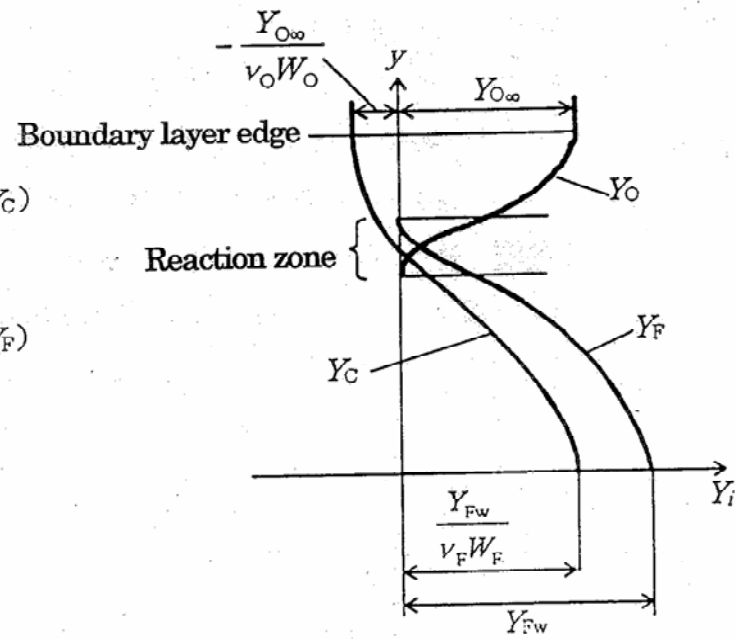
$$\left. \begin{array}{l} \eta = 0: \quad \Phi_C = 0 \\ \eta = \infty: \quad \Phi_C = 1 \end{array} \right\}$$



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(a)  $b$  is infinite,  $\infty$



(b)  $b$  is finite

$$Y_C = \frac{Y_F}{v_F W_F}$$

$$Y_C = -\frac{Y_O}{v_O W_O}$$

$$\Phi_C = \frac{-Y_{Cw}}{Y_{C\infty} - Y_{Cw}}$$



$$v_x \frac{\partial Y_F}{\partial x} + v_y \frac{\partial Y_F}{\partial y} = D_F \frac{\partial^2 Y_F}{\partial y^2}$$

$$\left. \begin{array}{l} y = 0: \quad V = Y_F V - D_F \frac{\partial^2 Y_F}{\partial y^2} \\ y = y^*: \quad Y_F = 0 \end{array} \right\}$$

$$v_x \frac{\partial Y_O}{\partial x} + v_y \frac{\partial Y_O}{\partial y} = D_O \frac{\partial^2 Y_O}{\partial y^2}$$

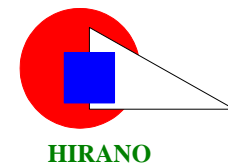
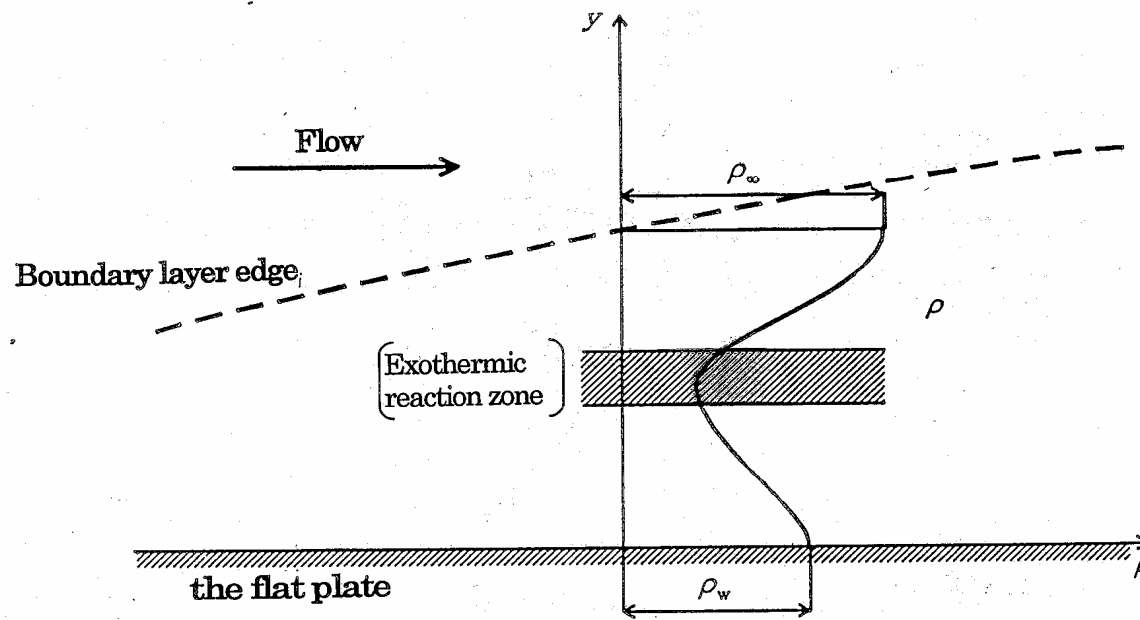
$$\left. \begin{array}{l} y = y^*: \quad Y_O = 0 \\ y = \infty: \quad Y_O = Y_{O\infty} \end{array} \right\}$$

$$y = y^*: \quad D_F \frac{\partial Y_F}{\partial y} = \left( \frac{\nu_F W_F}{\nu_O W_O} \right) D_O \frac{\partial Y_O}{\partial y}$$





## *Analysis of a Boundary Layer with Large Density Gradient*





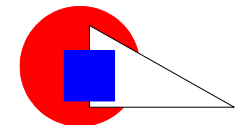
$$\frac{\partial(\rho v_x)}{\partial x} + \frac{\partial(\rho v_y)}{\partial y} = 0$$

$$\rho v_x \frac{\partial v_x}{\partial x} + \rho v_y \frac{\partial v_x}{\partial y} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial y} \left( \mu \frac{\partial v_x}{\partial y} \right)$$

$$\rho c_p v_x \frac{\partial T}{\partial x} + \rho c_p v_y \frac{\partial T}{\partial y} = \frac{\partial}{\partial y} \left( \lambda \frac{\partial T}{\partial y} \right) + \dot{\omega}_F''' \Delta H$$

$$\rho v_x \frac{\partial Y_i}{\partial x} + \rho v_y \frac{\partial Y_i}{\partial y} = \frac{\partial}{\partial y} \left( \rho D_i \frac{\partial Y_i}{\partial y} \right) + W_i \dot{\omega}_F'''$$

$$\left. \begin{array}{l} y = 0: \quad v_x = 0, \quad v_y = V, \quad T = T_w, \quad Y_i = Y_{iw} \\ y = \infty: \quad v_x = U, \quad T = T_\infty, \quad Y_i = Y_{i\infty} \end{array} \right\}$$



HIRANO

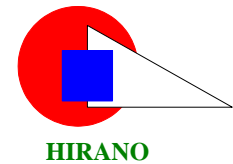


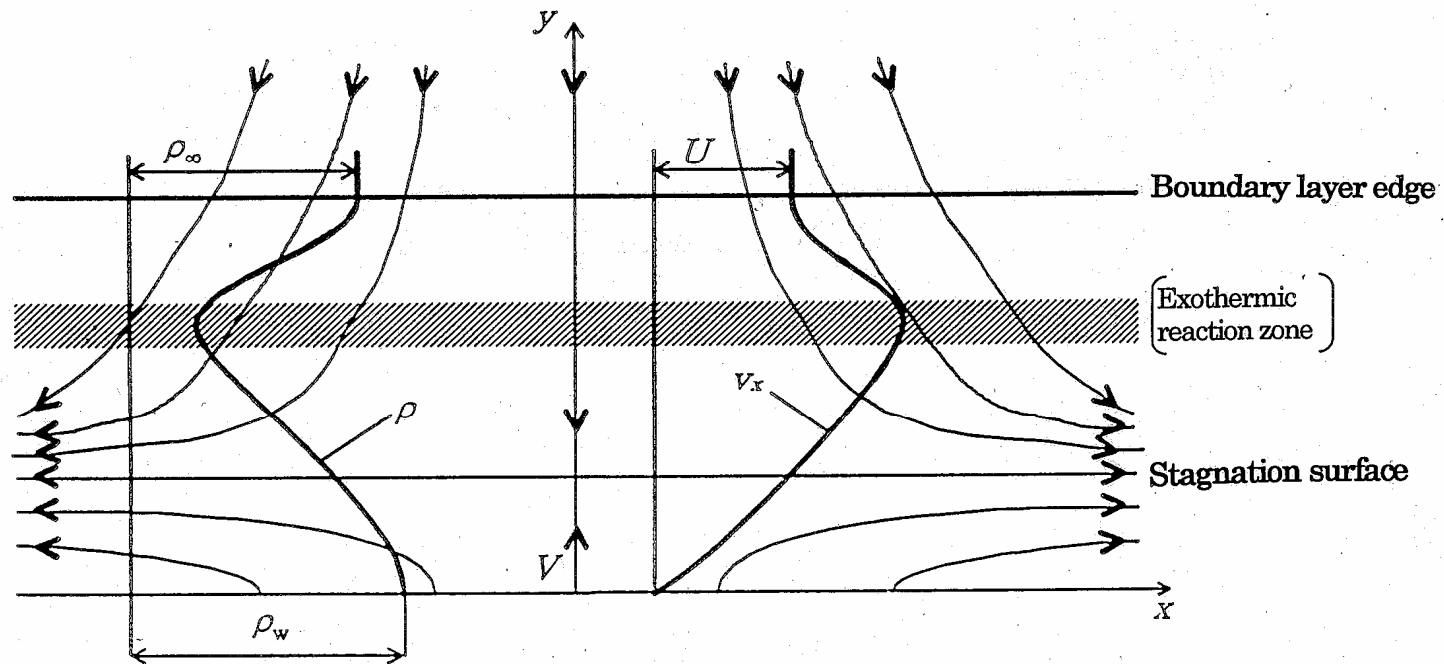
$$\left. \begin{aligned} \xi &= U\rho_\infty\mu_\infty x, & \eta &= \left(\frac{U}{\nu_\infty x}\right)^{\frac{1}{2}} \int_0^y \frac{\rho}{\rho_\infty} dy, \\ \Psi &= (U\rho_\infty\mu_\infty x)f(\eta), & \rho v_x &= \frac{\partial \Psi}{\partial y}, & \rho v_y &= -\frac{\partial \Psi}{\partial x} \end{aligned} \right\}$$

$$\rho\mu = \text{constant}$$

$$2f''' + ff'' = 0$$

$$\left. \begin{aligned} \eta = 0: & \quad f' = 0, \quad f = 0 \\ \eta = \infty: & \quad f' = 1 \end{aligned} \right\}$$



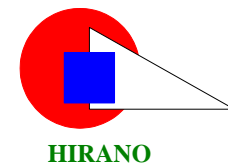




$$\left. \begin{aligned} \xi &= \int_0^x U \rho_\infty \mu_\infty dx, & \eta &= \frac{U \rho_\infty}{\xi^{\frac{1}{2}}} \int_0^y \frac{\rho}{\rho_\infty} dy, \\ \Psi &= \xi^{\frac{1}{2}} f(\eta), & \rho v_x &= \frac{\partial \Psi}{\partial y}, & \rho v_y &= -\frac{\partial \Psi}{\partial x} \end{aligned} \right\}$$

$$2f''' + ff'' - \frac{2}{U} \frac{\partial U}{\partial \xi} (f')^2 + \frac{2a\xi}{\rho^2 \mu_\infty U^2} = 0$$

$$\left. \begin{aligned} \eta = 0: & \quad f' = 0, \quad f = 0 \\ \eta = \infty: & \quad f' = 1 \end{aligned} \right\}$$







Thank you for your kind attention