Computational Fluids Mechanics

Part 1 : Numerical methods
Part 2 : Turbulence models
Part 3 : Practice of numerical simulation

N.Oshima A5-32 oshima@eng.hokudai.ac.jp
M.Tsubokura A5-33 mtsubo@eng.hokudai.ac.jp
Division of Mechanical and Space Engineering
Computational Fluid Mechanics Laboratory
http://www.eng.hokudai.ac.jp/labo/fluid/index_e.html

Computational Fluid Mechanics
Part1： Numerical Methods

Objective：

Numerical methods for fluids mechanics and their accuracy

1. Introduction
2. Numerical methods for fluid mechanics (1) ~ Basic equations
3. Numerical methods for fluid mechanics (2) ~Discretizing schemes
4. Numerical methods for fluid mechanics (3) ~Coupling algorism
5. Numerical methods for fluid mechanics (4) ~Additional problems
6. Reliability of numerical simulation

Summary

Prof. Oshima A5-32 oshima@eng.hokudai.ac.jp

Computational Fluid Mechanics

Part1：Numerical Methods (2a)

1. Introduction

2. Numerical methods for fluid mechanics (1) ~ governing equations
   – Governing equations of fluid flow
   – Typical solutions of fluid flow
   – Additional models for complex flow phenomena

3. Numerical methods for fluid mechanics (2) ~Discretizing schemes
4. Numerical methods for fluid mechanics (3) ~Coupling algorism
5. Numerical methods for fluid mechanics (4) ~Additional problems
6. Reliability of numerical simulation

Governing Eqs. of Fluid mechanics

Continuity Eq.
(mass conservation)

$$\frac{D\rho}{Dt} = -\rho I$$

Momentum eq.

$$\rho \frac{Du_i}{Dt} = -\frac{\partial p}{\partial x_i} + \frac{\mu}{3}\frac{\partial I}{\partial x_i} + \mu \nabla^2 u_i + \rho f_i$$

Energy Eq.

$$\rho c_v \frac{DT}{Dt} = -pI + \lambda \nabla^2 T + \Phi + \dot{q}$$

Eq. of state

$$p = \rho R T$$

$$; \frac{D}{Dt} \equiv \frac{\partial}{\partial t} + u_j \frac{\partial}{\partial x_j} \quad ; \nabla^2 \equiv \frac{\partial^2}{\partial x_k \partial x_k}$$

$$; I = \frac{\partial u_k}{\partial x_k} \qquad ; \Phi = \frac{\partial u_i}{\partial x_j}\left(\frac{\mu}{3} I \delta_{ij} + \mu \frac{\partial u_i}{\partial x_j} \right)$$

Governing Eqs. of Fluid Flow

Non-dimensional Parameters

– **Re**ynolds no.

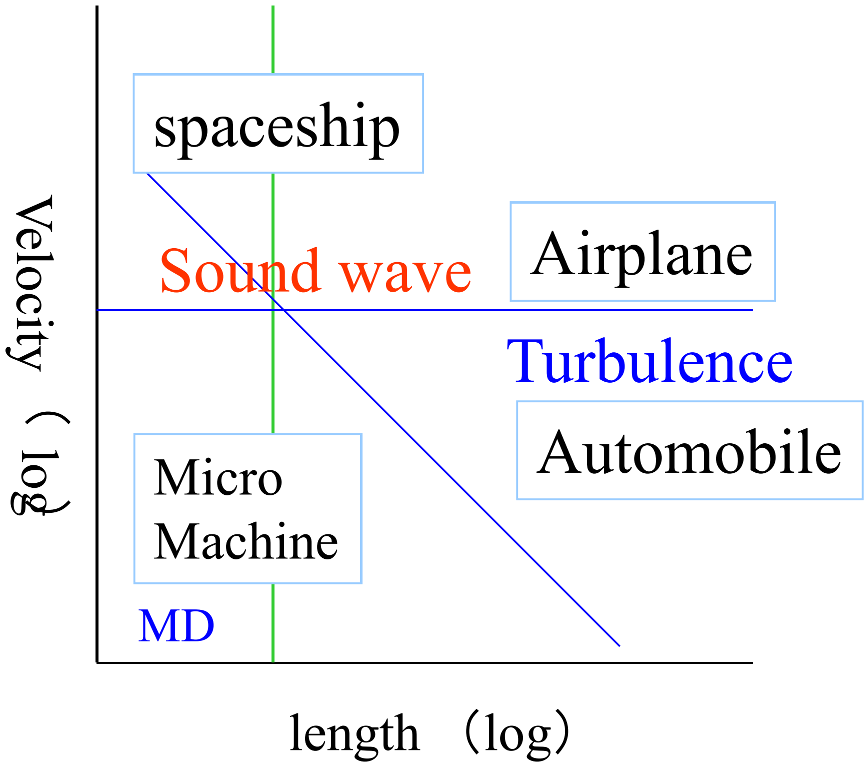
$$\frac{(\text{length}) \times (\text{velocity})}{(\text{viscosity})}$$

– **M**ach no.

(velocity) ／ (Sound speed)

– **Kn**ussen no.

(free pass) / (length)



Non-dimensional Parameters
- in the governing eq.-

$$\left[\frac{L}{t_0 U}\right]\frac{\partial \rho^*}{\partial t^*} + u_j^* \frac{\partial \rho^*}{\partial x_j^*} = -\rho^* \frac{\partial u_j^*}{\partial x_j^*} \qquad p^* = \rho^* T^* \qquad \frac{p_0}{\rho_0 T_0} = R$$

$$\left[\frac{L}{t_0 U}\right]\rho^* \frac{\partial u_i^*}{\partial t^*} + \rho^* u_j^* \frac{\partial u_i^*}{\partial x_j^*} = -\left[\frac{p_0}{\rho_0 U^2}\right]\frac{\partial p^*}{\partial x_i^*} + \left[\frac{\mu}{\rho_0 U L}\right]\left(\frac{1}{3}\frac{\partial I^*}{\partial x_i^*} + \frac{\partial^2 u_i^*}{\partial x_j^{*2}}\right) + \left[\frac{F}{U^2 L}\right]\rho^* f_i^*$$

$$\left[\frac{L}{t_0 U}\right]\rho^* \frac{\partial T^*}{\partial t^*} + \rho^* u_j^* \frac{\partial T^*}{\partial x_j^*}$$

$$= -\left[\frac{p_0}{\rho_0 c_v T_0}\right] p^* I^* + \left[\frac{\lambda}{\rho_0 c_v U L}\right]\frac{\partial^2 T^*}{\partial x_j^{*2}} + \left[\frac{\mu}{\rho_0 U L}\right]\left[\frac{U^2}{c_v T_0}\right]\Phi^* + \left[\frac{LQ}{\rho_0 c_v U}\right]\dot{q}^*$$

$$t = t^* t_0, \quad x_j = x_j^* L, \quad u_i = u_i^* U, \quad p = p^* p_0, \quad T = T^* T_0, \quad \rho = \rho^* \rho_0$$

$$f = F f^*, \quad \dot{q} = Q \dot{q}^*$$

Non-dimensional Parameters
- in the governing eq.-

Parameter of fluid flow

$$\left[\frac{L}{t_0 U}\right] = St \quad \text{(Strouhal no.)}$$

$$\left[\frac{p_0}{\rho_0 c_v T_0}\right] = \frac{\rho_0 R T_0}{\rho_0 c_v T_0} = \gamma - 1$$

(γ: specific heat ratio)

$$\left[\frac{p_0}{\rho_0 U^2}\right] = \frac{a_0^2}{\gamma U^2} = \frac{1}{\gamma M^2}$$

(M:Mach No)

$$\left[\frac{\lambda}{\rho_0 c_v U L}\right] = \mathrm{Pe} = \mathrm{Re} \cdot \mathrm{Pr}$$

（Pe:Peclet No.、Pr:Prandtl No.)

$$\left[\frac{\mu}{\rho_0 U L}\right] = \frac{1}{\mathrm{Re}} \quad \text{(Reynolds No.)}$$

$$\left[\frac{U^2}{c_v T_0}\right] = (\gamma - 1) M^2$$

Lagrangean vs. Eularian formulations

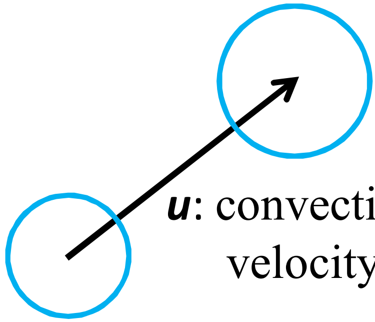
Lagrangean

$$\frac{D\phi}{Dt} \equiv \left(\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi \right)$$

on unit mass [*/kg]

$$\int \phi dV$$

V(t) :
Volume per unit mass



Eularian

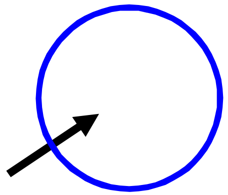
$$\frac{\partial \rho \phi}{\partial t} + \nabla \cdot \rho \mathbf{u} \phi$$

$$\equiv \rho \frac{D\phi}{Dt} + \phi \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} \right)$$

=0 (Mass conservation)

on unit volume [*/m^3]

$$\int \rho \phi dV$$



ρ(**x**,t):
Mass per unit volume

Conservation low

Mass flux vector

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u})$$

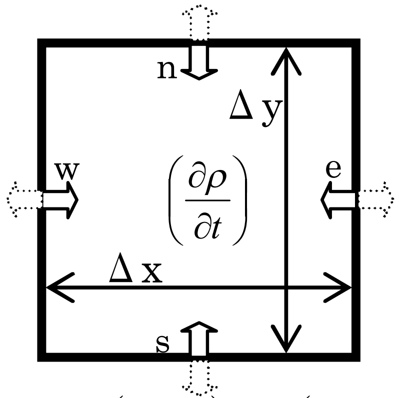
$$\frac{\partial \rho}{\partial t} = -\left(\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} \right)$$

$$\int \frac{\partial \rho}{\partial t} dV = -\int (\rho \mathbf{u}) \cdot \mathbf{n} dS$$

$$\left(\frac{\partial \rho}{\partial t} \right) \Delta x \Delta y \cong (\rho u_w - \rho u_e) \Delta y + (\rho v_s - \rho v_n) \Delta x$$

$$-(\rho \mathbf{u} \cdot \mathbf{n})_n = -(\rho u, \rho v) \cdot (0,1) = -\rho v_n$$

$$-(\rho \mathbf{u} \cdot \mathbf{n})_w = -(\rho u, \rho v) \cdot (-1,0) = \rho u_w$$



$$-(\rho \mathbf{u} \cdot \mathbf{n})_e = -(\rho u, \rho v) \cdot (1,0) = -\rho u_e$$

$$-(\rho \mathbf{u} \cdot \mathbf{n})_s = -(\rho u, \rho v) \cdot (0,-1) = \rho v_s$$

Conservation low

Flux vector vs. Stress tensor

$$\frac{\partial \rho \mathbf{u}^t}{\partial t} = -\nabla \cdot \left(\rho \mathbf{u}\mathbf{u}^t\right) - \nabla \cdot \mathbf{T} - \nabla \cdot \mathbf{P} + \mathbf{f}^t \quad \Rightarrow \quad \frac{\partial \rho u}{\partial t} = -\nabla \cdot (\rho \mathbf{u} u) - \nabla \cdot \boldsymbol{\tau}_x - \nabla \cdot \mathbf{p}_x + f_x$$

$$\rho \mathbf{u}^t = [\rho u \quad \rho v], \quad \mathbf{f}^t = [f_x \quad f_x] \qquad \rho \mathbf{u}\mathbf{u}^t = [\rho \mathbf{u} u \quad \rho \mathbf{u} v] = \begin{bmatrix} \rho u u & \rho u v \\ \rho v u & \rho v v \end{bmatrix},$$

$$\mathbf{P} = \left[\mathbf{p}_x \quad \mathbf{p}_y\right] = \begin{bmatrix} p & 0 \\ 0 & p \end{bmatrix} \left(= p\mathbf{I} = p\delta_{ij}\right) \qquad \therefore \nabla \cdot \mathbf{P} = (\nabla p)^t = \begin{bmatrix} \dfrac{\partial p}{\partial x} & \dfrac{\partial p}{\partial y} \end{bmatrix}$$

$$\mathbf{T} = \left[\boldsymbol{\tau}_x \quad \boldsymbol{\tau}_y\right] = \begin{bmatrix} -2\mu \dfrac{\partial u}{\partial x} & -\mu\left(\dfrac{\partial u}{\partial y} + \dfrac{\partial v}{\partial x}\right) \\ -\mu\left(\dfrac{\partial u}{\partial y} + \dfrac{\partial v}{\partial x}\right) & -2\mu \dfrac{\partial v}{\partial y} \end{bmatrix} \left(= 2\mu \mathbf{S}\right)$$

Conservation low

Momentum flux vector

$$\frac{\partial \rho u}{\partial t} = -\nabla \cdot \left(\mathbf{J}_{conv.} + \mathbf{J}_{diff.} + \mathbf{J}_{pres.} \right) + f_x$$

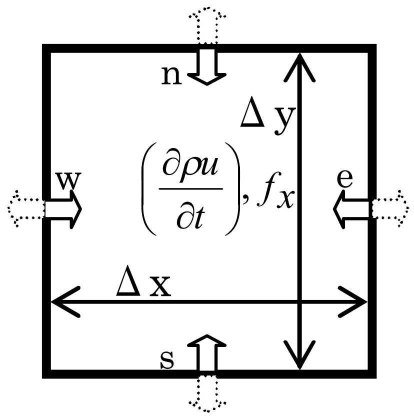
$$\mathbf{J}_{conv.} = \rho \mathbf{u}\, u = \begin{bmatrix} \rho u\, u \\ \rho v\, u \end{bmatrix}, \quad \mathbf{J}_{diff.} = \begin{bmatrix} -2\mu(\partial u/\partial x) \\ -\mu(\partial u/\partial y + \partial v/\partial x) \end{bmatrix}, \quad \mathbf{J}_{pres.} = \begin{bmatrix} p \\ 0 \end{bmatrix}$$

$$\int \frac{\partial \rho u}{\partial t} dV = -\int \left(\mathbf{J}_{conv.} + \mathbf{J}_{diff.} + \mathbf{J}_{pres.} \right) \cdot \mathbf{n} dS + \int f_x dV$$

$$-\left(\mathbf{J}_{conv.} \cdot \mathbf{n} \right)_w = J_{conv.} = \left(\rho u u \right)_w$$

$$-\left(\mathbf{J}_{diff.} \cdot \mathbf{n} \right)_w = J_{diff.} = -2\mu \frac{\partial u}{\partial x}_w$$

$$-\left(\mathbf{J}_{pres.} \cdot \mathbf{n} \right)_w = J_{pres.} = p_w$$



$$-\left(\mathbf{J}_{conv.} \cdot \mathbf{n} \right)_e = -J_{conv.} = -\left(\rho u u \right)_e$$

$$-\left(\mathbf{J}_{diff.} \cdot \mathbf{n} \right)_e = -J_{diff.} = 2\mu \frac{\partial u}{\partial x}_e$$

$$-\left(\mathbf{J}_{pres.} \cdot \mathbf{n} \right)_e = -J_{pres.} = -p_e$$

Exercise 2a

Calculate each component of momentum flux through the vertical surface (n & s in fig.) of considering volume.
Derive the conservation law for y-direction component of momentum (ρv)

Computational Fluid Mechanics

Part1： Numerical Methods (2b)

1. Introduction

2. Numerical methods for fluid mechanics (1) ~ governing equations
   - Governing equations of fluid flow
   - Typical solutions of fluid flow
   - Additional models for complex flow phenomena

3. Numerical methods for fluid mechanics (2) ~Discretizing schemes
4. Numerical methods for fluid mechanics (3) ~Coupling algorism
5. Numerical methods for fluid mechanics (4) ~Additional problems
6. Reliability of numerical simulation

Typical solutions of fluid flow

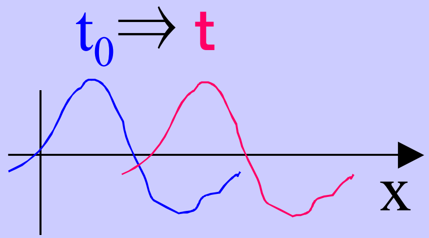
	convection	**interaction** (volume source)	**diffusion** (surface flux)
$\frac{\partial \rho}{\partial t} =$	$-u_j \frac{\partial \rho}{\partial x_j}$	$-\rho \frac{\partial u_k}{\partial x_k}$	
$\rho \frac{\partial u_i}{\partial t} =$	$-\rho u_j \frac{\partial u_j}{\partial x_j}$	$-\frac{\partial p}{\partial x_i} + F_i$	$+\frac{\partial}{\partial x_j}\left(\frac{\mu}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} + 2\mu S_{ij} \right)$
$\rho c_v \frac{\partial T}{\partial t} =$	$-\rho c_v u_j \frac{\partial T}{\partial x_j}$	$-p \frac{\partial u_k}{\partial x_k} + Q + \Phi$	$+\frac{\partial}{\partial x_j}\left(k \frac{\partial T}{\partial x_j} \right)$
		$p = \rho R T$	

Solution of convection

- Model of scalar convection

(linear eq.)

$$\frac{\partial \phi}{\partial t} = -u \frac{\partial \phi}{\partial x} \Rightarrow \phi(x,t) = \phi_0(x - ut)$$

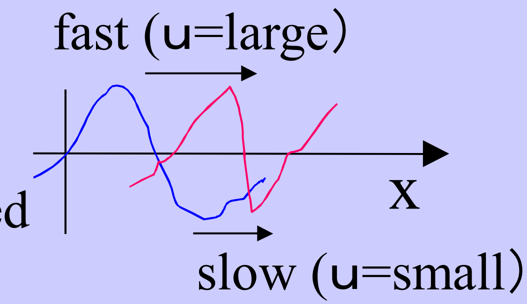


- Model of momentum convection

(Burger's Eq.)

$$\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x}$$

- shape deformed
- high frequency produced



⇒

- **keep linear solution**
- **adaptive to steep variation**

Solution of diffusion and external force

Diffusion of scalar (Linear)

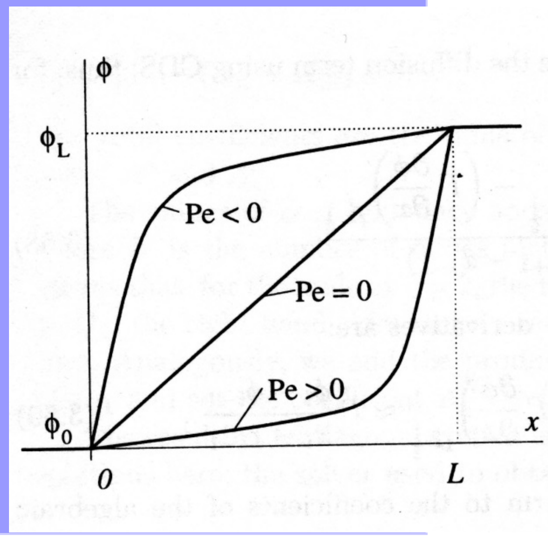
time dependent heat transfer problem

$$\frac{\partial \phi}{\partial t} = \Gamma \frac{\partial^2 \phi}{\partial x^2} \quad \Rightarrow \quad \phi = \phi_n \exp\left(inx - \frac{t}{\Gamma} \right)$$

steady convective – diffusion problem

$$u \frac{\partial \phi}{\partial x} = \Gamma \frac{\partial^2 \phi}{\partial x^2} \quad \Rightarrow \quad \left(u\phi - \Gamma \frac{\partial \phi}{\partial x} \right) = \text{const}$$

Pecret No.: Pe=uL/Γ



Source term (Linear)

$$\frac{\partial \phi}{\partial t} = -S\phi \quad \Rightarrow \quad \phi = \phi_0 \exp(-St)$$

Solution of Interaction step

Compressible （sound wave）

$$\frac{\partial \rho}{\partial t} = -\rho \frac{\partial u}{\partial x}$$

$$\rho \frac{\partial u}{\partial t} = -\frac{\partial p}{\partial x}$$

$$\frac{p}{\rho^{\kappa}} = \text{const}$$

（S＝const. ）

$$\Rightarrow$$

$$\frac{\partial \rho}{\partial t} = -\rho \frac{\partial u}{\partial x}$$

$$\rho \frac{\partial u}{\partial t} = -a^2 \frac{\partial \rho}{\partial x}$$

$$a^2 \equiv \left(\frac{dp}{d\rho}\right)_s = \sqrt{\kappa \frac{p}{\rho}}$$

Mach No. ：Ma = U / a
a： sound speed
U： flow velocity

$$\frac{\partial^2 u}{\partial t^2} = a^2 \frac{\partial^2 u}{\partial x^2}$$ Sound wave

$$\Rightarrow u = f(x - at) + g(x + at)$$

Solution of Interaction step

Incompressible flow

if Ma→0

a (sound speed)→∞

$$\nabla \cdot \mathbf{u} = \frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + F_i$$

$$(F_i = -u_j \frac{\partial u_i}{\partial x_i} + \cdots)$$

$$\rho = \text{const}$$

$$\frac{1}{\rho}\nabla \cdot \nabla p = -\frac{\partial}{\partial t}(\nabla \cdot \mathbf{u}) + \nabla \cdot \mathbf{F}$$

Pressure poison eq.

Solution of Interaction step

Compressible （1D nozzle）

$$\frac{d\rho}{\rho}+\frac{du}{u}+\frac{dA}{A}=0$$

$$udu+\frac{dp}{\rho}=0$$

$$\frac{dp}{p}-\kappa\frac{d\rho}{\rho}=0$$

$$\frac{dp}{p}=\frac{d\rho}{\rho}+\frac{dT}{T}$$

$$\frac{d\rho}{\rho}=-\frac{M^2}{M^2-1}\frac{dA}{A}$$

$$\frac{du}{u}=+\frac{1}{M^2-1}\frac{dA}{A}$$

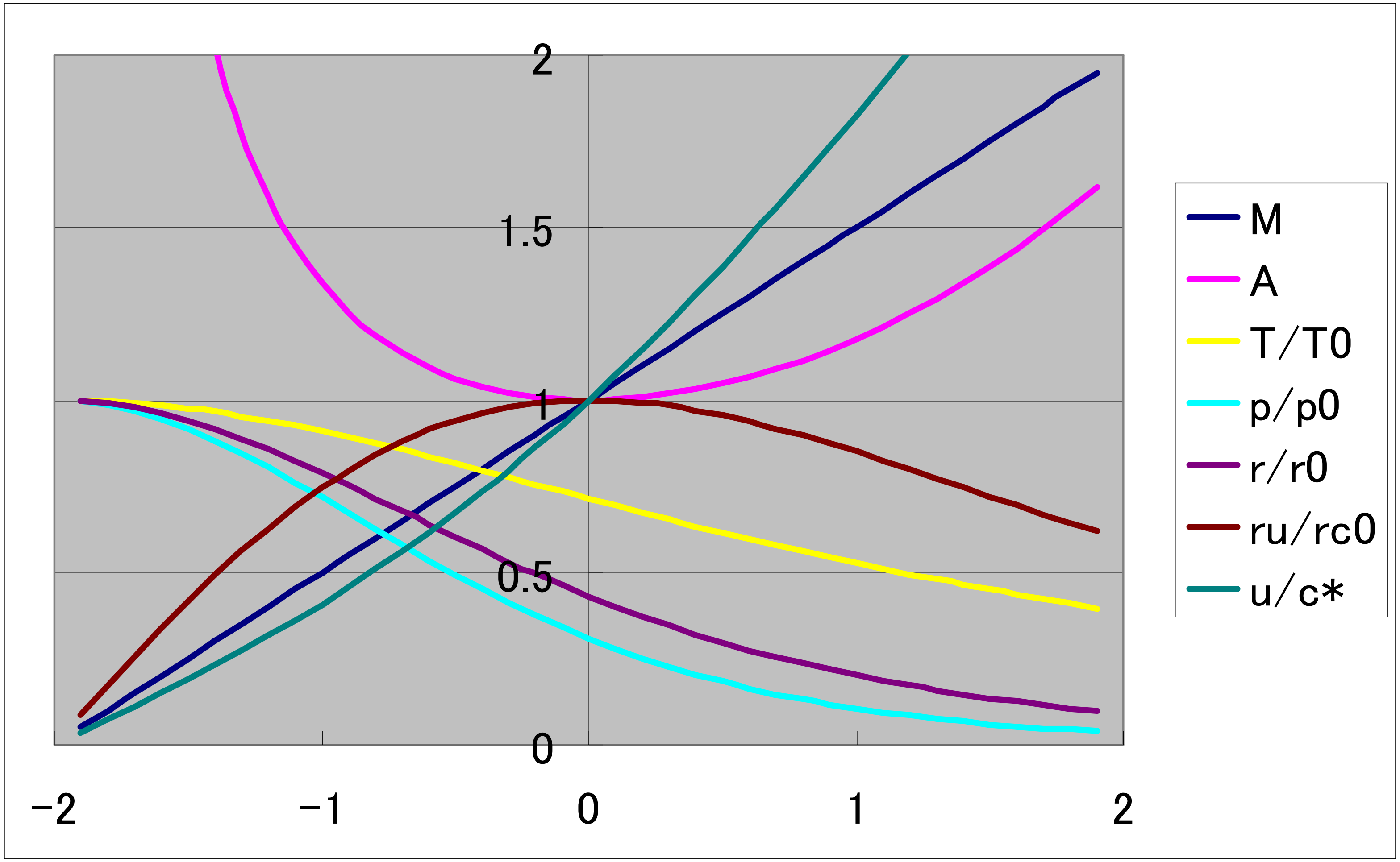
$$\frac{dp}{p}=-\frac{\kappa M^2}{M^2-1}\frac{dA}{A}$$

$$\frac{dT}{T}=-\frac{(\kappa-1)M^2}{M^2-1}\frac{dA}{A}$$

$$\frac{da}{a}=-\frac{(\kappa-1)M^2}{2(M^2-1)}\frac{dA}{A}$$

$$\frac{dM}{M}=+\frac{2+(\kappa-1)M^2}{M^2-1}\frac{dA}{A}$$

Solution of 1D compressible flow



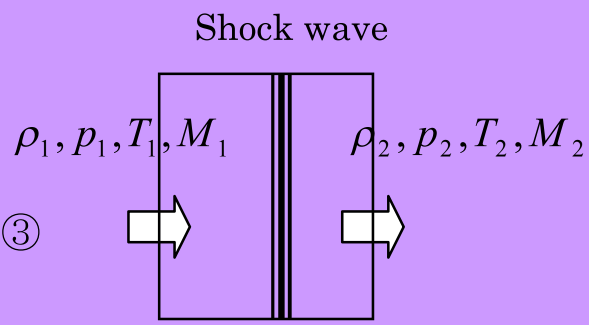
Solution of Interaction step

Compressible （1D shock wave）

Mass : $\rho_1 u_1 = \rho_2 u_2$ ①

Momentum : $p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2$ ②

Energy : $\frac{\kappa}{\kappa - 1}\frac{p_1}{\rho_1} + \frac{1}{2}u_1^2 = \frac{\kappa}{\kappa - 1}\frac{p_2}{\rho_2} + \frac{1}{2}u_2^2$ ③

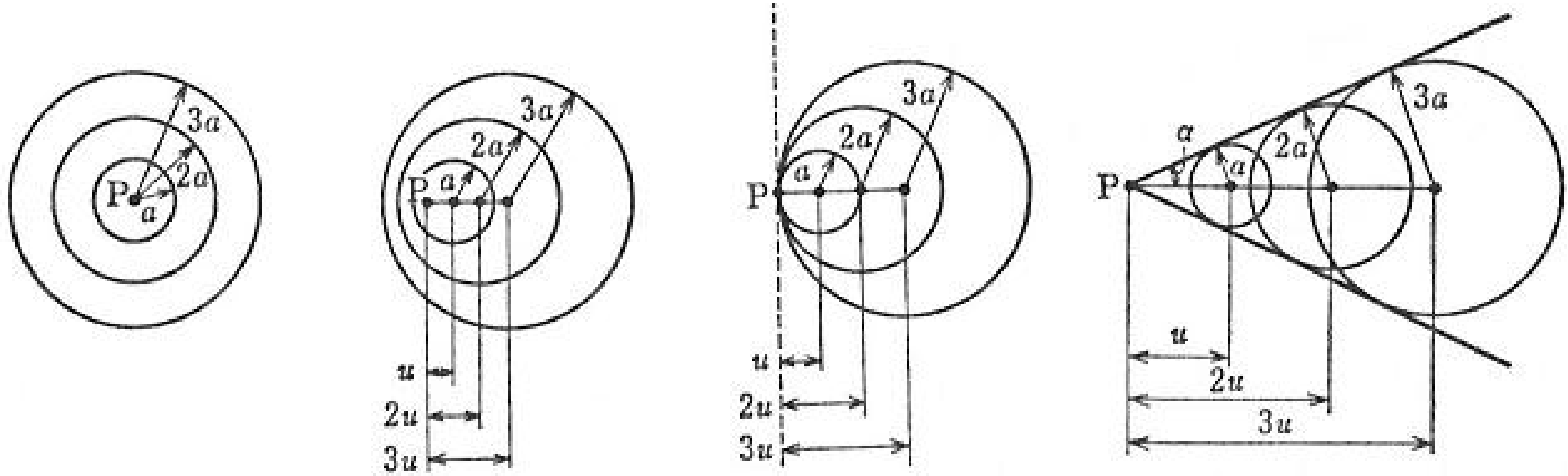


$$\therefore \frac{\rho_2}{\rho_1} = \frac{\left(\frac{\kappa+1}{\kappa-1}\frac{p_2}{p_1} + 1\right)}{\left(\frac{p_2}{p_1} + \frac{\kappa+1}{\kappa-1}\right)} = \frac{u_1}{u_2} > 1$$

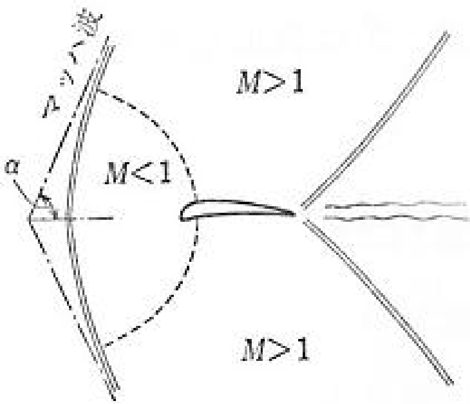
Rankine－Hugoniot eq.

$$\therefore \frac{T_2}{T_1} = \frac{p_2}{p_1}\frac{\rho_1}{\rho_2} = \frac{\frac{p_2}{p_1}\left(\frac{\kappa+1}{\kappa-1}\frac{p_2}{p_1} + 1\right)}{\left(\frac{p_2}{p_1} + \frac{\kappa+1}{\kappa-1}\right)} = \frac{\left(\frac{p_2}{p_1} + \frac{\kappa+1}{\kappa-1}\right)}{\left(\frac{p_1}{p_2} + \frac{\kappa+1}{\kappa-1}\right)} > 1$$

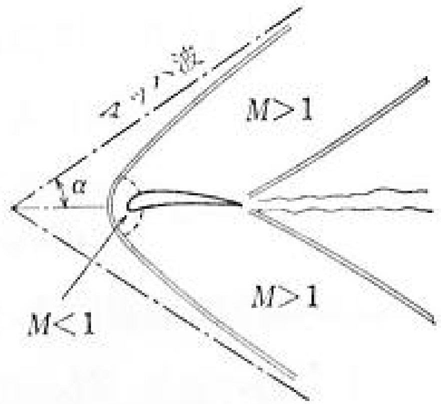
Profiles of shock wave



(a) $u=0$, $M=0$ (b) $u<a$, $0<M<1$ (c) $u=a$, $M=1$ (d) $u>a$, $M>1$



(d) M_∞ medium



(e) M_∞ large

Exercise 2b

Solve the following equations of $\phi(x)$ and draw the profiles for different parameter values.

$$u\frac{\partial \phi}{\partial x} = \Gamma \frac{\partial^2 \phi}{\partial x^2}$$

$u,\ \Gamma$ are constant parameter

$$0 \le x \le L \qquad \phi = 0 \quad at\, x = 0$$

$$\phi = 1 \quad at\, x = L$$

Computational Fluid Mechanics

Part1：Numerical Methods (2a)

1. Introduction

2. Numerical methods for fluid mechanics (1) ~ governing equations
   – Governing equations of fluid flow
   – Typical solutions of fluid flow
   – Additional models for complex flow phenomena

3. Numerical methods for fluid mechanics (2) ~Discretizing schemes
4. Numerical methods for fluid mechanics (3) ~Coupling algorism
5. Numerical methods for fluid mechanics (4) ~Additional problems
6. Reliability of numerical simulation

Complexity of system

Strong coupling

	convection	interaction	diffusion	external-force	
$\frac{\partial \rho}{\partial t} =$	$-u_j \frac{\partial \rho}{\partial x_j}$	$-\rho \frac{\partial u_k}{\partial x_k}$		$+M$	mass
$\rho \frac{\partial u_i}{\partial t} =$	$-\rho u_j \frac{\partial u_j}{\partial x_j}$	$-\frac{\partial p}{\partial x_i}$	$+\frac{\partial}{\partial x_j}\left(\frac{\mu}{3} I\delta_{ij} + 2\mu S_{ij}\right)$	$+F_i$	momentum
$\rho c_v \frac{\partial T}{\partial t} =$	$-\rho c_v u_j \frac{\partial T}{\partial x_j}$	$-p \frac{\partial u_k}{\partial x_k}$	$+\frac{\partial}{\partial x_j}\left(k \frac{\partial T}{\partial x_j}\right)$	$+\Phi + Q$	energy
		$p = \rho RT$			

1) hyperbolic (compressible) Ma>1

2) harmonic (sound wave)

3) parabolic (incompressible) } Ma<1

Combined solution Is needed

Complexity of system

Weak coupling

convction | interaction | diffusion | production

mass:

$$\frac{\partial \rho}{\partial t} = -u_j \frac{\partial \rho}{\partial x_j} - \rho \frac{\partial u_k}{\partial x_k} + M$$

momentum:

$$\rho \frac{\partial u_i}{\partial t} = -\rho u_j \frac{\partial u_j}{\partial x_j} - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\frac{\mu}{3} I\delta_{ij} + 2\mu S_{ij} \right) + F_i$$

energy:

$$\rho c_v \frac{\partial T}{\partial t} = -\rho c_v u_j \frac{\partial T}{\partial x_j} - p \frac{\partial u_k}{\partial x_k} + \frac{\partial}{\partial x_j}\left(k \frac{\partial T}{\partial x_j} \right) + \Phi + Q$$

$$p = \rho R T$$

Alternative solution Is available

Additional eqs.

- Turbulence model
- NonNewtonian fluid

- Buoyancy force
- Multi-phase model
- Chemical reaction

Model of Combustion Flow

- Basic eqs. of reactive flow-

Mass: $$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j\right) = 0$$

Momentum: $$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_i u_j\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\mu S_{ij}\right) + \frac{\partial}{\partial x_j}\left\{\left(\mu_V - \frac{2}{3}\mu\right)\frac{\partial u_k}{\partial x_k}\delta_{ij}\right\}$$

Energy: $$\rho Cp\frac{\partial T}{\partial t} + \rho Cp u_j \frac{\partial T}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\frac{\mu}{\Pr}\frac{\partial T}{\partial x_j}\right] + \frac{\partial p}{\partial t} + \left[\sum_{\alpha=1}^{N} Cp_\alpha \frac{\mu}{Sc_\alpha}\frac{\partial Y_\alpha}{\partial x_j}\right]\frac{\partial T}{\partial x_j} - \sum_{\alpha=1}^{N} h_{0\alpha}\omega_\alpha$$

Eq.of gas state: $$p = \rho R_o T \sum_{\alpha=1}^{N} Y_\alpha / M_\alpha$$

+

Chemical spices $$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho Y_\alpha u_j\right) = \frac{\partial}{\partial x_j}\left[\frac{\mu}{Sc_\alpha}\frac{\partial Y_\alpha}{\partial x_j}\right] + \omega_\alpha$$

Chemical reaction

$$\nu_{Fu} Fu + \nu_{ox} Ox \rightarrow \nu_{pro} Pro$$

Arrhenius' law

$$\omega_{fu} = -B\exp\left(-\frac{E}{RT}\right)\left(\frac{\rho Y_{fu}}{M_{fu}}\right)^{\nu_{fu}}\left(\frac{\rho Y_{ox}}{M_{ox}}\right)^{\nu_{ox}}$$

Detail reactions of H2･O2 flame

Spices	N_2	O_2	H_2	H_2O	OH
Lewis No.	1	1.11	0.3	1.12	0.73
Spices	O	H	H_2O_2	HO_2	-
Lewis No.	0.7	0.18	1.12	1.1	-

$$
\left.\begin{array}{rcl rcl}
H + O_2 & \leftrightarrow & OH + O & H_2O_2 + M & \leftrightarrow & OH + OH + M \\
H_2 + O & \leftrightarrow & OH + H & H_2O_2 + OH & \leftrightarrow & H_2O + HO_2 \\
H_2O + O & \leftrightarrow & OH + OH & O + HO_2 & \leftrightarrow & OH + O_2 \\
H_2 + OH & \leftrightarrow & H_2O + H & H + HO_2 & \leftrightarrow & O + H_2O \\
H + O_2 + M^1 & \rightarrow & HO_2 + M^1 & H + O + M^2 & \leftrightarrow & OH + M^2 \\
H + HO_2 & \rightarrow & OH + OH & O + O + M & \leftrightarrow & O_2 + M \\
H + HO_2 & \rightarrow & H_2 + O_2 & H_2O_2 + H & \leftrightarrow & H_2O + OH \\
OH + HO_2 & \rightarrow & H_2O + O_2 & H_2O_2 + H & \leftrightarrow & HO_2 + H_2 \\
H + H + M^1 & \rightarrow & H_2 + M^1 & O + OH + M & \leftrightarrow & HO_2 + M \\
H + OH + M^1 & \rightarrow & H_2O + M^1 & H_2 + O_2 & \leftrightarrow & OH + OH \\
HO_2 + HO_2 & \rightarrow & H_2O_2 + O_2 & & &
\end{array}\right\} \quad H_2 + \frac{1}{2}O_2 \Leftrightarrow H_2O
$$

$\cdots$ 21 reactions

Model of Combustion Flow
- non-dimensional parameters of mass & heat transfer-

- Nusselt no. $Nu \equiv \dfrac{h\lambda}{L}$ h : heat transfer coefficient

  λ : Thermal conductivity

- Prandtl no. $\mathrm{Pr} \equiv \dfrac{\nu}{\alpha}$ ν : kinetic viscosity

- Schmidt no. $Sc \equiv \dfrac{\nu}{D}$ D : mass diffusion conductivity

- Lewis no. $Le \equiv \dfrac{\alpha}{D}$ α : temp. diffusion conductivity

Model of Combustion Flow
– non-dimensional parameters of reactive flow–

- (primal) Damköhler no. $D \equiv \frac{\tau_r}{\tau_c}$ τ_r: time scale of flow

  τ_c: time scale of reaction

- Karlovits no. $K \equiv \frac{\eta}{U}\frac{dU}{dy}$ Tickness of heating zone: $\eta = \frac{\lambda}{\rho c_p S} = \frac{\alpha}{S}$

  Combustion speed : S

- turbulent Damköhler no.

$$Da \equiv \frac{\tau_t}{\tau_c} = \frac{\ell}{u'}\frac{S}{\delta}$$

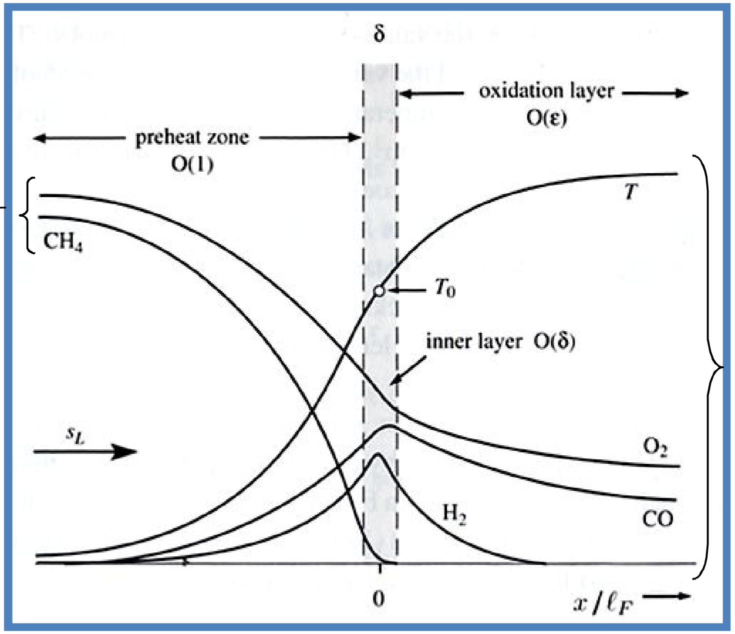
l : turbulent length scale

u' : velocity fractuation、δ: flame thickness

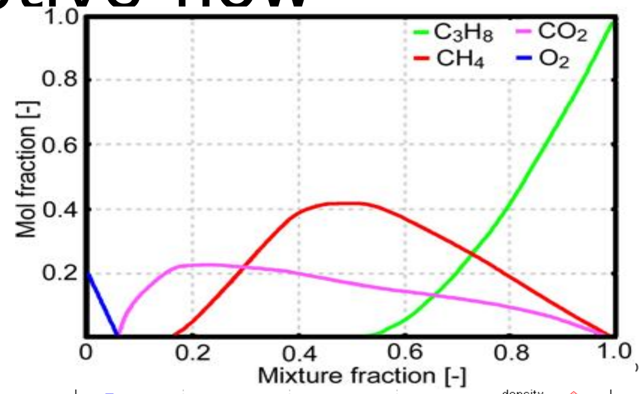
Model of Combustion
- mechanics of reactive flow-

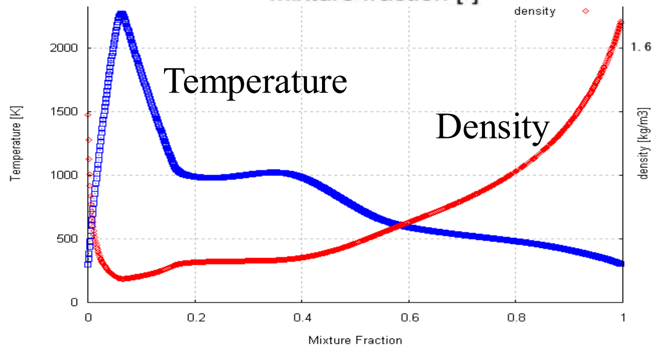
$$\xi = \frac{Y_{CH_4}}{Y_{CH_4} + Y_{O_2}}$$

Mixture fraction



→ time





Enthalpy: H＝E＋PV ⇒ dH＝(TdS－PdV)＋d(PV)＝ TdS＋VdP $\left(\frac{\partial H}{\partial S}\right)_p = T > 0$

Free energy: G＝H－TS ⇒ dG＝(TdS＋VdP)－d(TS) ＝ －SdT＋VdP $\left(\frac{\partial G}{\partial T}\right)_p = -S < 0$

Enthalpy components: $dH = \sum_\alpha h_\alpha^0 dn_\alpha + c_p dT$ $\left(\frac{\partial H}{\partial T}\right)_p = c_p$

Chemical potential＋thermal energy

Mass transport

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{V}_\alpha) = \dot{\varpi}_\alpha$$

$$Y_\alpha = \rho_\alpha / \rho$$

$$\frac{\partial \rho Y_\alpha}{\partial t} + \nabla \cdot (\rho Y_\alpha \mathbf{V}_\alpha) = \dot{\varpi}_\alpha$$

$$\mathbf{v}_{d\alpha} = \mathbf{V}_\alpha - \mathbf{V} \qquad ; \mathbf{V} = \frac{\sum \rho \mathbf{V}_\alpha}{\rho}$$

$$\rho \frac{DY_\alpha}{Dt} \equiv \rho \frac{\partial Y_\alpha}{\partial t} + \underbrace{\rho \mathbf{V} \cdot \nabla Y_\alpha}_{\text{convection}} = \underbrace{-\nabla \cdot (\rho Y_\alpha \mathbf{v}_{d\alpha})}_{\text{diffusion}} + \dot{\varpi}_\alpha$$

$$\rho Y_\alpha \mathbf{v}_{d\alpha} \approx -\rho D_\alpha \nabla Y_\alpha \quad \text{Fick's law}$$

$$\rho \frac{DY_\alpha}{Dt} = \frac{\partial \rho Y_\alpha}{\partial t} + \nabla \cdot (\rho Y_\alpha \mathbf{V}) = \nabla \cdot (\rho D_\alpha \nabla Y_\alpha) + \dot{\varpi}_\alpha \qquad D_\alpha = \frac{\mu}{Sc_\alpha} \quad Le_\alpha = \frac{\Pr_\alpha}{Sc_\alpha}$$

$$\rho = \sum \rho_\alpha, \quad \sum \dot{\varpi}_\alpha = 0, \quad \sum Y_\alpha \mathbf{v}_{d\alpha} = 0 \quad \frac{D\rho}{Dt} \equiv \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

Mass transport

Distribution of mole fraction

$$\nabla X_\alpha = \sum_\beta \frac{X_\alpha Y_\beta}{D_{\alpha\beta}}\left(\mathbf{v}_\beta - \mathbf{v}_\alpha\right) + \left(Y_\alpha - X_\alpha\right)\frac{\nabla p}{p}$$

$$X_\alpha = \frac{Y_\alpha / W_\alpha}{\sum_\beta Y_\beta / W_\beta}$$

$$+\frac{\rho}{p}\sum_\beta Y_\alpha Y_\beta\left(\mathbf{f}_\alpha - \mathbf{f}_\chi\right) + \sum_\beta \frac{X_\alpha Y_\beta}{\rho D_{\alpha\beta}}\left(\frac{D_{T\beta}}{Y_\beta} - \frac{D_{T\alpha}}{Y_\alpha}\right)\frac{\nabla T}{T}$$

In case of two spices

$$Y_1 \mathbf{v}_1 = -D_{12}\left\{\nabla Y_1 + \frac{Y_1 Y_2}{X_1 X_2}\left(Y_1 - X_1\right)\frac{\nabla p}{p} + \frac{\left(Y_1 Y_2\right)^2}{X_1 X_2}\frac{\rho}{p}\left(\mathbf{f}_1 - \mathbf{f}_2\right) + \frac{D_{T,1}}{\rho D_{T,2}}\frac{\nabla T}{T}\right\}$$

Fick's law

$$Y_\alpha Y_\beta\left(\mathbf{v}_\beta - \mathbf{v}_\alpha\right) = Y_\alpha Y_\beta\left(\mathbf{V}_{d\beta} - \mathbf{V}_{d\alpha}\right) = Y_\alpha \underbrace{\left(Y_\beta \mathbf{V}_{d\beta}\right)}_{= -Y_\alpha \mathbf{V}_{d\alpha}} - Y_\beta\left(Y_\alpha \mathbf{V}_{d\alpha}\right) = \underbrace{\left(Y_\alpha + Y_\beta\right)}_{=1}\left(-Y_\alpha \mathbf{V}_{d\alpha}\right)$$

Energy transport

Theory. $$\rho dh = dp + \rho T ds$$

Enthalpy eq. $$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \nabla \cdot \lambda \nabla h - \sum \nabla \cdot \rho D \sum (1 - Le_\alpha) \nabla Y_\alpha + \Phi + Q_R$$

Temperature eq. $$\rho C_p \frac{DT}{Dt} = \frac{Dp}{Dt} + \nabla \cdot \lambda \nabla T + \sum c_{p_\alpha} \mathbf{j}_\alpha \cdot \nabla T + \Phi + Q_R + \dot{Q}_{reac}$$

Reactive heat

$$dh = \sum Y_\alpha h_\alpha = \sum \left(h_\alpha^\circ dY_\alpha + c_{p,\alpha} Y_\alpha dT \right), \quad h_\alpha = h_\alpha^\circ + \int_{T_0}^{T} c_{p,\alpha} dT$$

$\sum h_\alpha^\circ \dot{\varpi} = -\dot{Q}_{reac.}$: Reactive heat

$C_p = \sum Y_\alpha C_{p,\alpha}$ Specific heat

Heat flux (Fourier's law) $\mathbf{q} = -\lambda \nabla T$

$\alpha = \lambda / \rho C_p$ Thermal conductivity

Mass fux (Fick's law) $\mathbf{j}_\alpha = -\rho D_\alpha \nabla Y_\alpha$

$Le_\alpha = \lambda / (\rho C_p D_\alpha) = \alpha / D_\alpha$

Low Ma No. apprrox. $\nabla p \approx 0 \quad \therefore \frac{Dp}{Dt} \equiv \frac{\partial p}{\partial t} + \mathbf{v} \cdot \nabla p \approx \frac{dp}{dt}$

Solution of combustion flow

		convection	interaction	diffusion	external-force	
$\frac{\partial \rho}{\partial t}$	$=$	$-u_j \frac{\partial \rho}{\partial x_j}$	$-\rho \frac{\partial u_k}{\partial x_k}$		$+M$	mass
$\rho \frac{\partial u_i}{\partial t}$	$=$	$-\rho u_j \frac{\partial u_j}{\partial x_j}$	$-\frac{\partial p}{\partial x_i}$	$+\frac{\partial}{\partial x_j}\left(\frac{\mu}{3} I\delta_{ij} + 2\mu S_{ij}\right)$	$+F_i$	momentum
$\rho c_v \frac{\partial T}{\partial t}$	$=$	$-\rho c_v u_j \frac{\partial T}{\partial x_j}$	$-p \frac{\partial u_k}{\partial x_k}$	$+\frac{\partial}{\partial x_j}\left(k \frac{\partial T}{\partial x_j}\right)$	$+\Phi + Q$	energy
			$p = \rho RT$			

Weak relation by low Ma approx.

Heat source

Additional eqs.

$$\rho \frac{\partial Y_\alpha}{\partial t} = -\rho u_j \frac{\partial Y_\alpha}{\partial x_j} + \frac{\partial}{\partial x_j}\left(D \frac{\partial Y_\alpha}{\partial x_j}\right) \quad \dot{\omega} +$$

chemical spices

Exercise 2c

Consider a system of equations for complex flow phenomena and analyze its coupling process to fluid dynamics;

Ex. Multi-phase flow
Buoyancy flow
Magneto-hydrodynamics
Flow in porous media
Plasma flow etc.