

# Introduction to Laminar Flame Theory

## 层流燃烧理论导论

(英文版)

田振华(Jenn-Hwa Tien) 编著



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### 代表论文:

Combustion and Flame 3 篇(2002,1996,1991)。

Combustion Science and Technology 3 篇(1993,1992,1990)。

SCI 记录了 50 篇论文曾引用作者的论文,其中:

Journal of Fluid Mechanics 2 篇,

Combustion and Flame 16 篇,

Combustion Science and Technology 10 篇,

Proceedings of The Combustion Institute 5 篇,

Combustion Theory and Modeling 2 篇。

## Preface

This book originated from the author's note taken from the class of Prof. Moshe Matalon (my Ph. D. supervisor) at Northwestern U. The main part of it came from the book **Theory of Laminar Flames** by Buckmaster and Ludford (M. Matalon's Ph. D. supervisor and already passed away). Contents of the book **Combustion Theory** and the author's published research results (in Combustion and Flame) are also presented here.

The difference between this book and the above two well written and highly compact and accurate books is that the details of most of the derivations are shown here. Thus this book can be the beginner's handbook to prepare to read the above two books. The reasons to write it in English (although the author's manuscripts are still criticized by the reviewers of Combustion and Flame or Combustion Science and Technology for poor English) are two fold. First of all the author is not familiar with Chinese terminology in the field of combustion. Second graduate students here in China should practice their English also, because the best journals in the field of combustion are all in English. In the following the important books and best journals to the author's knowledge in this field are listed.

### Books:

**Theory of Laminar Flames** by Buckmaster, J. D. (U. of Illinois, Urbana-Champaign) and Ludford, G. S. S. (Cornell U.), Cambridge University press (1982).

**Combustion Theory** by Williams, F. A. (UC San. Diego), Benjamin Cummings (1985).

**Combustion Dynamics** by Toong, T. Y. (MIT), McGraw Hill (1983).

**Combustion Fundamentals** by Strehlow, R. A. (U. of Illinois, Urbana-Champaign), Kreiger (1984).

**Combustion Flames and Explosions of Gases** by Lewis, B. and von Elbe, G., Academic press (1961).

**Turbulent reacting flows** by Libby, P. A. (UC San. Diego) and Williams, F. A. , Academic press (1994).

Periodicals:

**Combustion and Flame**

(<http://elsevier.lib.tsinghua.edu.cn/>) currently editors in chief: Driscoll, J. F. (U. Of Michigan, Ann Arbor) and Hayhurst, A. N. (U. Of Cambridge)

**Combustion Science and Technology**

(<http://www.tandf.co.uk/journals/titles/00102202.html>) currently editors in chief: Irvin Glassman (Princeton U.) and Richard Yetter (Pennsylvania State U.)

**Combustion theory and modeling**

(<http://www.iop.org/EJ/journal/1364-7830>) currently editors in chief: Moshe Matalon, (Northwestern U.) and Mitchell Smooke (Yale U.)

**Proceedings of the Combustion Institute**

(<http://www.combustioninstitute.org>)

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# I . Fundamentals in Reacting Flow

## I – 1 The equations of gas dynamics

### Assumptions:

Fluid is continuous and homogeneous. Where continuous means the mean free path of the gas molecular in the problem is far smaller than the smallest scale in the problem. And homogeneous means there is only one phase in the problem.

### Fluid motion:

(1) Lagrangian: follow the fluid particles

$$t=0 \quad (x, y, z) = (a, b, c)$$

$$t>0 \quad [x(t, a, b, c), y(t, a, b, c), z(t, a, b, c)]$$

$$\text{velocity} \quad u = \frac{\partial x}{\partial t}, v = \frac{\partial y}{\partial t}, w = \frac{\partial z}{\partial t}$$

$$\text{acceleration} \quad \frac{\partial^2 x}{\partial t^2}, \frac{\partial^2 y}{\partial t^2}, \frac{\partial^2 z}{\partial t^2}$$

$$\text{temperature} \quad T = T(t, a, b, c)$$

(2) Eulerian: look at the behavior of certain fixed position at different time

$$\left. \begin{aligned} u &= u(x, y, z, t) \\ v &= v(x, y, z, t) \\ w &= w(x, y, z, t) \\ T &= T(x, y, z, t) \end{aligned} \right\} \mathbf{v} = (u, v, w)$$

Streamline: the line tangent to the velocity vector at all positions at

any point. On the stream line we have  $\frac{dx}{u} = \frac{dy}{v} = \frac{dz}{w}$



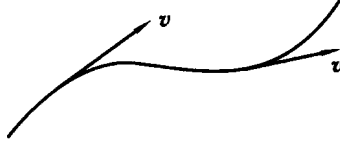


Fig. I - 1 Stream line and velocity vector

For steady flow, velocity does not depend on time (ie.  $\frac{\partial}{\partial t}=0$ ).

The streamline of steady flow does not change with time.

For any property say  $T=T(x,y,z,t)$  we have:

$$\begin{aligned}dT &= \frac{\partial T}{\partial x}dx + \frac{\partial T}{\partial y}dy + \frac{\partial T}{\partial z}dz + \frac{\partial T}{\partial t}dt \\ &= \nabla T \cdot d\mathbf{r} + \frac{\partial T}{\partial t}dt\end{aligned}$$

for a given particle

$$dx=u dt, dy=v dt, dz=w dt \text{ (dx, dy, dz are independent)}$$

$$\therefore d\mathbf{r} = \mathbf{v} \cdot dt \Rightarrow \frac{dT}{dt} = \mathbf{v} \cdot \nabla T + \frac{\partial T}{\partial t}$$

which is the rate of change of say  $T$  ( $T$  is a scalar property).

Convective derivative (material derivative) a linear operator:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$$

for instance: acceleration of a particle is :

$$\frac{D\mathbf{v}}{Dt} = \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = \frac{\partial \mathbf{v}}{\partial t} + \nabla \left( \frac{\mathbf{v} \cdot \mathbf{v}}{2} \right) - \mathbf{v} \times (\nabla \times \mathbf{v})$$

note: form **Advanced Calculus** by Hildebrand equation 74 e

$$\nabla (\mathbf{u} \cdot \mathbf{v}) = (\mathbf{u} \cdot \nabla) \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{u} + \mathbf{u} \times (\nabla \times \mathbf{v}) + \mathbf{v} \times (\nabla \times \mathbf{u})$$

$$\begin{aligned}\therefore \nabla \left( \frac{\mathbf{v} \cdot \mathbf{v}}{2} \right) &= \frac{1}{2} [(\mathbf{v} \cdot \nabla) \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \mathbf{v} \times (\nabla \times \mathbf{v}) + \\ &\quad \mathbf{v} \times (\nabla \times \mathbf{v})] \\ &= (\mathbf{v} \cdot \nabla) \mathbf{v} + \mathbf{v} \times (\nabla \times \mathbf{v})\end{aligned}$$

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (\text{continuity equation}) \quad (\text{I} - 1)$$

$\nabla \cdot (\rho \mathbf{v}) \rightarrow$  change of mass flux through a unite control volume.

$\frac{\partial \rho}{\partial t} \rightarrow$  rate of change of mass inside the unite control volume of (I - 1).

$$\frac{\partial \rho}{\partial t} + \rho \nabla \cdot \mathbf{v} + \mathbf{v} \cdot \nabla \rho = 0$$

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0$$

So  $\frac{1}{\rho} \frac{D\rho}{Dt} + \nabla \cdot \mathbf{v} = 0 \quad (\text{I} - 2)$

(1) Incompressible flow  $\frac{1}{\rho} \frac{D\rho}{Dt} \ll 1$  as the result  $\nabla \cdot \mathbf{v} = 0$ .

(2) Steady flow  $\frac{\partial \rho}{\partial t} = 0$  as the result  $\nabla \cdot (\rho \mathbf{v}) = 0$ .

Stream tube: a tube formed by stream lines, so no fluid can cross the wall.

Thus  $\rho |\mathbf{v}| A$  is a constant along the tube. Where  $|\mathbf{v}|$  is the length of the velocity vector  $\mathbf{v}$ .

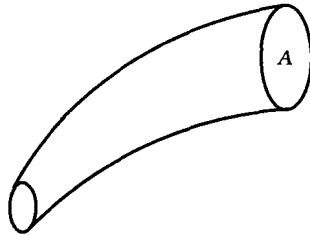


Fig. I - 2 stream tube

### Momentum Conservation:

#### External forces:

- (1) Body forces: acting throughout the fluid element for example, gravitational force; electromagnetical force.
- (2) Surface forces: acting on the surface of an element for example, pressure (the normal stress), friction (the tangential stress).

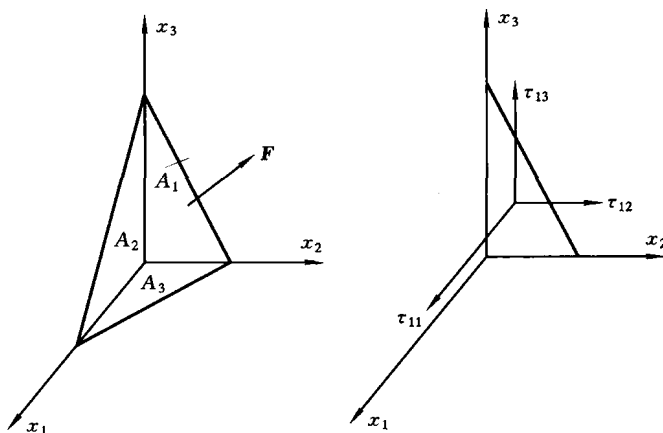


Fig. I-3 Stress tensor acting on a fluid element

$\tau_{ij}$  acting on the  $i$ th surface in the  $j$ th direction

note : force per unite area  $\rightarrow$  stress

$$\text{stress tensor} \quad \tilde{\pi} = \begin{pmatrix} \tau_{11} & \tau_{12} & \tau_{13} \\ \tau_{12} & \tau_{22} & \tau_{23} \\ \tau_{13} & \tau_{23} & \tau_{33} \end{pmatrix}$$

First of all it accounts only for three surfaces, because this is enough to describe all the surface forces acting on a cub. Second the tensor is symmetrical thus the fluid can be treated as continuum (the cub does not rotate about itself).

The balance of surface force is like;

so the net force is  $\frac{\partial \tau_{11}}{\partial x} dx$  and for a control volume with three sides

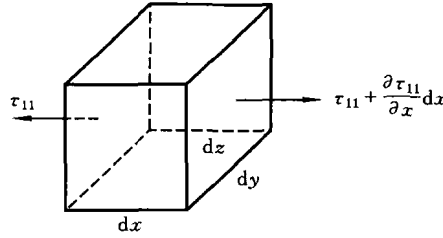


Fig. I - 4 Balance of surface force on a fluid element

$dx, dy, dz$ .

We have 
$$\rho \frac{D\mathbf{v}}{Dt} = \rho \mathbf{g} + (\nabla \cdot \tilde{\boldsymbol{\pi}}) \quad (\text{I} - 3)$$

$dx \times dy \times dz$  has been cancelled on both sides and  $\rho \frac{D\mathbf{v}}{Dt}$  is the mass of the fluid element of unite volume times acceleration while  $\rho \mathbf{g}$  is the body force where  $\nabla \cdot \tilde{\boldsymbol{\pi}}$  is the net surface force.

#### Energy Conservation:

Rate of change of the energy of a fluid element equals the rate of work done on the element plus the rate of heat transfer to the element.

Name:  $e_T$ : total energy of an element of unite mass

$\mathbf{q}$ : the heat flux vector (heat per unite area).

For energy balance of a small control volume we have :

$$\rho \frac{De_T}{Dt} = \rho \mathbf{g} \cdot \mathbf{v} + \nabla \cdot (\tilde{\boldsymbol{\pi}} \cdot \mathbf{v}) - \nabla \cdot \mathbf{q} \quad (\text{I} - 4)$$

Where the left hand side is the rate of increase of total energy of the cub,  $\rho \mathbf{g} \cdot \mathbf{v}$  is the rate of work done by the gravitational force (body force),  $\nabla \cdot (\tilde{\boldsymbol{\pi}} \cdot \mathbf{v})$  is the rate of work done by the surface force. (The divergence come from the same effect mentioned in Fig. I - 4). And  $\nabla \cdot \mathbf{q}$  is the net amount of heat flowing out of the control volume.

$\mathbf{v} \cdot (\text{I} - 3)$  gives us

$$\begin{aligned}\mathbf{v} \cdot \left[ \rho \frac{D\mathbf{v}}{Dt} = \rho \mathbf{g} + \nabla \cdot \tilde{\boldsymbol{\pi}} \right] \\ \rho \mathbf{v} \cdot \frac{D\mathbf{v}}{Dt} = \rho \mathbf{g} \cdot \mathbf{v} + (\nabla \cdot \tilde{\boldsymbol{\pi}}) \cdot \mathbf{v} \\ \rho \frac{D}{Dt} \left( \frac{v^2}{2} \right) = \rho \mathbf{g} \cdot \mathbf{v} + (\nabla \cdot \tilde{\boldsymbol{\pi}}) \cdot \mathbf{v}\end{aligned}$$

Set internal energy for unite mass to be  $e = e_T - \frac{v^2}{2}$  me have:

$$\begin{aligned}\rho \frac{De}{Dt} + \rho \frac{D}{Dt} \left( \frac{v^2}{2} \right) = \rho \mathbf{g} \cdot \mathbf{v} + \nabla \cdot (\tilde{\boldsymbol{\pi}} \cdot \mathbf{v}) - \nabla \cdot \mathbf{q} \\ \rho \frac{De}{Dt} = \nabla \cdot (\tilde{\boldsymbol{\pi}} \cdot \mathbf{v}) - (\nabla \cdot \tilde{\boldsymbol{\pi}}) \cdot \mathbf{v} - \nabla \cdot \mathbf{q}\end{aligned}$$

for symmetrical tensor we have:

$$\nabla \cdot (\tilde{\boldsymbol{\pi}} \cdot \mathbf{v}) = \mathbf{v} \cdot (\nabla \cdot \tilde{\boldsymbol{\pi}}) + \tilde{\boldsymbol{\pi}} : \nabla \mathbf{v}$$

note:

$$\begin{aligned}\nabla \mathbf{v} &= \begin{bmatrix} \frac{\partial v_1}{\partial x_1} & \frac{\partial v_2}{\partial x_1} & \frac{\partial v_3}{\partial x_1} \\ \frac{\partial v_1}{\partial x_2} & \frac{\partial v_2}{\partial x_2} & \frac{\partial v_3}{\partial x_2} \\ \frac{\partial v_1}{\partial x_3} & \frac{\partial v_2}{\partial x_3} & \frac{\partial v_3}{\partial x_3} \end{bmatrix} \\ \tilde{\boldsymbol{\pi}} : \nabla \mathbf{v} &= \sum_i \sum_j \tau_{ij} \frac{\partial v_i}{\partial x_j}\end{aligned}$$

So the energy equation can be simplified as:

$$\rho \frac{De}{Dt} = \tilde{\boldsymbol{\pi}} : \nabla \mathbf{v} - \nabla \cdot \mathbf{q} \quad (\text{I-5})$$

where  $\tilde{\boldsymbol{\pi}} : \nabla \mathbf{v}$  is the friction generated heat and  $-\nabla \cdot \mathbf{q}$  is the heat transfer.

Stress and rate of strain:

$$(1) \text{ Fluid at rest } \tau_{ij} = -P\delta_{ij} \quad \delta_{ij} = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$$

(2) Fluid in motion

The pressure of moving fluid can be defined as

$$P = -\frac{1}{3} \sum_{i=1}^3 \tau_{ii}$$

Then the stress tensor can be separated into

$$\tilde{\pi} = -P\tilde{\mathbf{I}} + \tilde{\Sigma}$$

where  $\tilde{\mathbf{I}}$  is the identity tensor.

Assuming the fluid is Newtonian and then homogeneous then we can relate the stress tensor to the rate of strain as follow:

$$\tilde{\Sigma} = \mu(\nabla \mathbf{v} + (\nabla \mathbf{v})^T) + \left(\kappa - \frac{2}{3}\mu\right)(\nabla \cdot \mathbf{v})\tilde{\mathbf{I}}$$

where superscript T means transpose.

And  $\nabla \mathbf{v} + (\nabla \mathbf{v})^T$  is the rate of strain from shearing deformation while  $(\nabla \cdot \mathbf{v})\tilde{\mathbf{I}}$  is the rate of strain from dilatation (deformation in normal direction).

$\mu$  is the coefficient of viscosity and  $\kappa$  is the coefficient of bulk viscosity.

Thus

$$\tilde{\Sigma} = \mu \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \left( \kappa - \frac{2}{3}\mu \right) \sum_k \frac{\partial v_k}{\partial x_k} \delta_{ij}$$

now we have:

$$\tilde{\pi} : \nabla \mathbf{v} = -P\tilde{\mathbf{I}} : \nabla \mathbf{v} + \tilde{\Sigma} : \nabla \mathbf{v}$$

where

$$\tilde{\mathbf{I}} : \nabla \mathbf{v} = \nabla \cdot \mathbf{v}$$

thus

$$\tilde{\pi} : \nabla \mathbf{v} = -P \nabla \cdot \mathbf{v} + \Phi$$

while

$$\Phi = \tilde{\Sigma} : \nabla \mathbf{v}$$

$$\begin{aligned} &= \left( \mu \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \left( \kappa - \frac{2}{3}\mu \right) \sum_k \frac{\partial v_k}{\partial x_k} \delta_{ij} \right) : \frac{\partial v_i}{\partial x_j} \\ &= \mu \sum_{ij} \left( \frac{\partial v_i}{\partial x_j} \right)^2 + \mu \sum_{ij} \frac{\partial v_j}{\partial x_i} \frac{\partial v_i}{\partial x_j} + \left( \kappa - \frac{2}{3}\mu \right) (\nabla \cdot \mathbf{v})^2 \end{aligned}$$

$$= \frac{\mu}{2} \sum_{ij} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)^2 + \left( \kappa - \frac{2}{3} \mu \right) (\nabla \cdot \mathbf{v})^2$$

since 
$$\sum_{ij} \left( \frac{\partial v_i}{\partial x_j} \right)^2 = \sum_{ij} \left( \frac{\partial v_j}{\partial x_i} \right)^2$$

now (I - 3) become :

$$\begin{aligned} \rho \frac{D\mathbf{v}}{Dt} &= \rho \mathbf{g} + \nabla \cdot \tilde{\Sigma} - \nabla \cdot \tilde{I}P \\ \rho \frac{D\mathbf{v}}{Dt} &= \rho \mathbf{g} + \nabla \cdot \tilde{\Sigma} - \nabla P \end{aligned} \quad (\text{I} - 6)$$

and energy equation (I - 5) become;

$$\rho \frac{De}{Dt} = -P \nabla \cdot \mathbf{v} + \Phi - \nabla \cdot \mathbf{q} \quad (\text{I} - 7)$$

Where  $-P \nabla \cdot \mathbf{v}$  is the  $PV$  work and  $\Phi$  is the friction generated heat also  $-\nabla \cdot \mathbf{q}$  is the heat flux.

### Thermal Conduction

Assuming  $\mathbf{q}$  come only from conduction.

From Fourier's law  $\mathbf{q} = -\lambda \nabla T$  ( $\lambda$ ; thermal conductivity).

Then (I - 7) become;

$$\rho \frac{De}{Dt} = -P \nabla \cdot \mathbf{v} + \Phi + \nabla \cdot (\lambda \nabla T) \quad (\text{I} - 8)$$

### Thermodynamics

Properties of state  $P, \rho, T, h, s$

For simple compressible pure substance only two of them are independent.

Assuming ideal gas;

(a)  $P = \rho \bar{R} T$   $\bar{R} = R/w$  is the specific gas constant and  $R$  is the universal gas constant,  $w$  is the molecular mass.

(b) for ideal gas  $e = e(T)$

(c)  $h = e + P/\rho$

(d) mass heat capacity

$$C_p = \left( \frac{\partial h}{\partial T} \right)_p \quad C_v = \left( \frac{\partial e}{\partial T} \right)_v$$

$$\gamma = C_p / C_v \quad \text{thus } \gamma = \gamma(T)$$

$$h = h^0 + \int_{T^0}^T C_p dT$$

$$e = e^0 + \int_{T^0}^T C_v dT$$

where  $h^0$ ,  $e^0$  are the reference enthalpy and internal energy and  $T^0$  is the reference temperature.

$$(e) \quad \frac{P}{\rho} = \bar{R}T \quad \text{thus} \quad \frac{dP/\rho}{dT} = \bar{R}$$

$$h = e + \bar{R}T \quad \text{thus} \quad \frac{dh}{dT} = \frac{de}{dT} + \bar{R}$$

since  $h(P, T)$ ,  $e(1/\rho, T)$

$$\text{thus} \quad \frac{dh}{dT} = \left( \frac{\partial h}{\partial T} \right)_p = C_p \quad \frac{de}{dT} = \left( \frac{\partial e}{\partial T} \right)_v = C_v$$

$$C_p - C_v = \bar{R}$$

$$\gamma - 1 = \bar{R}/C_v \rightarrow C_v = \frac{\bar{R}}{\gamma - 1}; \quad C_p = \bar{R} \frac{\gamma}{\gamma - 1}$$

$$(f) \quad Tds = dh - dP/\rho$$

$$Tds = de + dP/\rho$$

for isentropical flow  $ds = 0 \therefore dh = dP/\rho$

$$dh = C_p dT = \frac{\gamma \bar{R}}{\gamma - 1} dT = \frac{\gamma}{\gamma - 1} d\left(\frac{P}{\rho}\right)$$

$$\frac{dP}{\rho} = \frac{\gamma}{\gamma - 1} d\left(\frac{P}{\rho}\right) \Rightarrow \frac{P}{\rho^\gamma} = \text{constant}$$

(g) Speed of sound

In isentropical condition for general case

ratio of pressure change in relation to density change.

$$\left( \frac{\partial P}{\partial \rho} \right) = a^2$$

for ideal gas in isentropical condition



$$P = C\rho^\gamma$$

$$\frac{\partial P}{\partial \rho} = C\gamma\rho^{\gamma-1} = P \frac{\gamma}{\rho}$$

thus  $a = \sqrt{P\gamma/\rho} = \sqrt{\gamma RT}$  and  $a$  is the sound speed.

(h) Temperature equation

from the left hand side of the energy equation (I - 8)

$$\begin{aligned} \rho \frac{De}{Dt} &= \rho \frac{D}{Dt}(h - P/\rho) = \rho \left[ \frac{Dh}{Dt} - \frac{1}{\rho} \frac{DP}{Dt} + \frac{P}{\rho^2} \frac{D\rho}{Dt} \right] \\ &= \rho \frac{Dh}{Dt} - \frac{DP}{Dt} + \frac{P}{\rho} \frac{D\rho}{Dt} \end{aligned}$$

from continuity equation (I - 2)

$$= \rho \frac{Dh}{Dt} - \frac{DP}{Dt} - P \nabla \cdot \mathbf{v}$$

since  $dh = C_p dT$  assuming  $C_p$  is a constant

$$\frac{Dh}{Dt} = C_p \frac{DT}{Dt}$$

The energy equation become.

$$\begin{aligned} \rho C_p \frac{DT}{Dt} - \frac{DP}{Dt} - P \nabla \cdot \mathbf{v} &= -P \nabla \cdot \mathbf{v} + \Phi + \nabla \cdot (\lambda \nabla T) \\ \rho C_p \frac{DT}{Dt} &= \frac{DP}{Dt} + \Phi + \nabla \cdot (\lambda \nabla T) \end{aligned}$$

Conclusion:

Assumptions: simple compressible pure substances (two free thermodynamic variables)

Newtonian fluid (stress proportional to strain rate) and ideal gas ( $e(T), h(T)$ ) we have  $\rho, \mathbf{v}, P, T \rightarrow 6$  variables

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (\text{I} - 9)$$

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla P + \rho \mathbf{g} + \nabla \cdot \tilde{\mathbf{\Sigma}} \quad (\text{I} - 10)$$

$$\rho C_p \frac{DT}{Dt} = \frac{DP}{Dt} + \Phi + \nabla \cdot (\lambda \nabla T) \quad (\text{I} - 11)$$