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**Structure and Dynamics
of
Combustion Waves in Premixed Gases**

Paul Clavin
Aix-Marseille Université
ECM & CNRS (IRPHE)

**Lecture II
Governing equations**

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Gaseous mixtures in normal conditions \approx continuum medium
in local equilibrium

mean free path \ll macroscopic length

many microscopic particles \in a fluid "particle"

relaxation time towards equilibrium
of fluid particles \ll macroscopic time scale



internal structure of shock waves

Lecture 2: **Governing equations**

(simplified form, see de Groot et Mazur (1962) or Williams (1985) for more details)

2-1. Conserved extensive quantities

2-2. Continuity

2-3. Fick's law. Diffusion equation

2-4. Conservation of momentum

2-5. Conservation of total energy

Thermal equation

Inviscid flows in reactive gases

Conservative forms

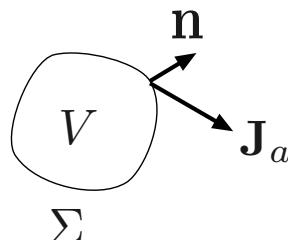
One-dimensional inviscid and compressible flow

2.6. Entropy production

II – 1) Conserved extensive quantities

$$\text{extensive quantities} \quad A_V = \iiint_V \rho a \, d^3\mathbf{r} \quad \begin{array}{l} \text{mass weighted distribution } a(\mathbf{r}, t) \\ \text{mass density } \rho(\mathbf{r}, t) \end{array}$$

conservation equation V fixed $\frac{dA}{dt} = \int_V \int \int [\partial(\rho a)/\partial t] d^3 r = (dA/dt)_1 + (dA/dt)_2$



$$(\mathrm{d}A/\mathrm{d}t)_1 = - \iint_{\Sigma} \mathbf{n} \cdot \mathbf{J}_a \mathrm{d}^2\sigma \quad (\mathrm{d}A/\mathrm{d}t)_2 = \iiint_V \dot{\omega}_a(\mathbf{r}, t) \mathrm{d}^3\mathbf{r}$$

$$(\mathrm{d}A/\mathrm{d}t)_1 = - \iiint_V \nabla \cdot \mathbf{J}_a \, \mathrm{d}^3\mathbf{r}$$

vector field $\mathbf{J}_a(\mathbf{r}, t)$

$$\partial(\rho a)/\partial t = -\nabla \cdot \mathbf{J}_a + \dot{\omega}_a$$

conserved quantities : no production terms $\dot{\omega}_a = 0$
 (mass, momentum and energy)

conserved scalar $a(\mathbf{r}, t)$

$$\partial(\rho a)/\partial t = -\nabla \cdot \mathbf{J}_a$$

conserved vector $\mathbf{a}(\mathbf{r}, t)$
 tensor field $\underline{\mathbf{J}}_a(\mathbf{r}, t)$

$$\partial(\rho \mathbf{a})/\partial t = -\nabla \cdot \underline{\mathbf{J}}_a$$

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II – 2) Conservation of mass: continuity equation

mass is a conserved scalar (classical mechanics)

$$\partial\rho/\partial t = -\nabla \cdot \mathbf{J} \quad \mathbf{J} \equiv \rho \mathbf{u} \quad \partial\rho/\partial t = -\nabla \cdot (\rho \mathbf{u})$$

material (convective) derivative $\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla$

$$\frac{1}{\rho} \frac{D\rho}{Dt} = -\nabla \cdot \mathbf{u}$$

continuity equation

$$\frac{1}{v} \frac{Dv}{Dt} = \nabla \cdot \mathbf{u} \quad v \equiv 1/\rho$$

Lagrangian form of conservation equations

$$\partial(\rho a)/\partial t = -\nabla \cdot \mathbf{J}_a + \dot{\omega}_a$$

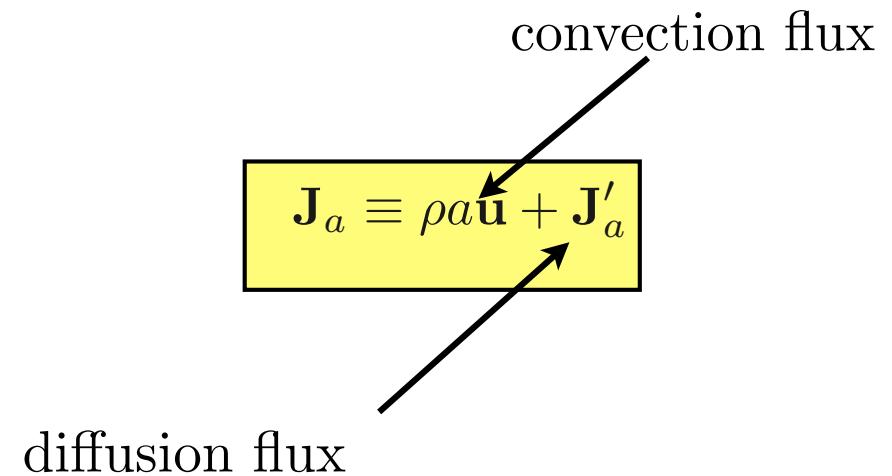
$$\rho D a / D t = -\nabla \cdot \mathbf{J}'_a + \dot{\omega}_a$$

conserved scalar:

$$\partial(\rho a)/\partial t = -\nabla \cdot \mathbf{J}_a$$

$$\rho D a / D t = -\nabla \cdot \mathbf{J}'_a$$

$$\mathbf{J}_a \equiv \rho a \hat{\mathbf{u}} + \mathbf{J}'_a$$



II – 3) Fick's law. Diffusion equation

mass fraction $Y_i = \rho_i / \rho$ $\sum_i Y_i = 1$

inert mixture mass fraction of species is a conserved scalar

$$\rho D Y_i / D t = -\nabla \cdot \mathbf{J}'_i \quad \sum_i \mathbf{J}'_i = 0$$

Kinetic theory of gas (binary diffusion in an abundant species)

Fick's law :

$$\mathbf{J}'_i = -\rho D_i \nabla Y_i$$

$$D_i > 0$$

$$\rho D Y_i / D t = \nabla \cdot [\rho D_i \nabla Y_i]$$

diffusion equation

$$\rho D_i \approx \text{cst.}$$

$$\mathbf{u} = 0$$

$$\partial Y_i / \partial t = D_i \Delta Y_i$$

archetype of irreversible phenomenon

(random walk)

Diffusive damping. Dissipative phenomenon

$$\partial Y / \partial t = D \Delta Y \quad D > 0 \quad [D] = (\text{length})^2 / \text{time}$$

Fourier analysis

$$Y(\mathbf{r}, t) = \sum_{\mathbf{k}} \tilde{Y}_{\mathbf{k}}(t) e^{i\mathbf{k} \cdot \mathbf{r}} \quad k = |\mathbf{k}|$$

$$d\tilde{Y}_{\mathbf{k}}(t)/dt = -(Dk^2)\tilde{Y}_{\mathbf{k}}(t) \quad \tilde{Y}_{\mathbf{k}}(t) = \tilde{Y}_{\mathbf{k}}(0)e^{-Dk^2 t}$$



Green function Self-similar solution

Fourier 1824

$$\partial G / \partial t = D \Delta G$$

$$t = 0 : G(\mathbf{r}, 0) = \delta(\mathbf{r}) \quad G(\mathbf{r}, t) = \frac{1}{(4\pi Dt)^{3/2}} e^{-r^2/4Dt} \quad r = |\mathbf{r}| \quad \iiint G(\mathbf{r}, t) d^3 \mathbf{r} = 1$$

probability distribution of the test particle

number density

$$\partial n / \partial t = D \Delta n$$

$$n(\mathbf{r}, t) = N G(\mathbf{r}, t) \quad n(\mathbf{r}, t) = \iiint n(\mathbf{r}', 0) G(\mathbf{r} - \mathbf{r}', t) d^3 \mathbf{r}'$$

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II – 4) Conservation of momentum

Momentum is a conserved vector (isolated system)

$$\rho D\mathbf{u}/Dt = -\nabla \cdot \underline{\underline{\Pi}} - \rho g \mathbf{e}_z,$$

surface force (stress tensor) $\underline{\underline{\Pi}} = p \underline{\underline{I}} + \underline{\underline{\pi}}$

↑
thermodynamic pressure (isotropic)

↑
gravity (body force)

Viscous stress tensor

$$\underline{\underline{\pi}} \equiv -2\eta(\underline{\underline{\nabla u}})^{(s)} - \underline{\underline{I}}(\xi - 2\eta/3)\nabla \cdot \mathbf{u}$$

Navier Stokes equations

$$\rho D\mathbf{u}/Dt = -\nabla(p + \rho gz) + \eta \Delta \mathbf{u} + (\xi + \eta/3)\nabla(\nabla \cdot \mathbf{u})$$

↑
gravity

Viscous shear diffusivity

$$D_{vis} = \eta/\rho$$

Euler equations

$$\rho D\mathbf{u}/Dt = -\nabla p$$

non dissipative equations

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II – 5) Conservation of total energy

internal energy,
 (Additive in a gas when interactions are neglected)

$$e_{int} = e_T + e_{chem}$$

thermal energy, chemical energy (chemical bonds),
 (kinetic + rotational & vibrational energy)

total energy

$$e_{tot} = |\mathbf{u}|^2/2 + e_T + e_{chem} + \dots$$

total energy is a conserved scalar

$$\partial(\rho e_{tot})/\partial t = -\nabla \cdot \mathbf{J}_{e_{tot}} \quad \rho D e_{tot}/Dt = -\nabla \cdot \mathbf{J}'_{e_{tot}} \quad \mathbf{J}'_{e_{tot}} \equiv \mathbf{J}_{e_{tot}} - \rho e_{tot} \mathbf{u}$$

Inviscid and **inert** flows
 (first law of thermodynamics)

Euler equation \Rightarrow $\frac{1}{2}\rho \frac{D}{Dt}|\mathbf{u}|^2 = -\mathbf{u} \cdot \nabla p = -\nabla \cdot (p\mathbf{u}) + p\nabla \cdot \mathbf{u}$

$$\mathbf{J}'_q \equiv \mathbf{J}'_{e_{tot}} - p\mathbf{u}$$

heat flux, ?

$$\rho D(e_T + e_{chem})/Dt = -\nabla \cdot \mathbf{J}'_q - p\nabla \cdot \mathbf{u}$$

heat work done

$$p\nabla \cdot \mathbf{u} = \rho p(D\rho^{-1}/Dt)$$

Fourier law

(simplest form of heat flux)

$$\mathbf{J}'_q = -\lambda \nabla T,$$

thermal conductivity

$$\delta e_T = c_V \delta T \quad \text{thermal diffusivity } \quad |_{13} \quad D_T \equiv \lambda / \rho c_V \quad [D_T] = (\text{length})^2/\text{time}$$

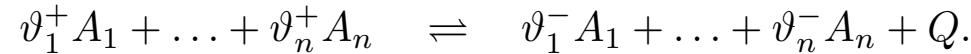
inert material $e_{chem} = \text{cst.}$
 no flow $\mathbf{u} = 0$

Fourier equation

$$\partial T / \partial t = D_T \Delta T$$

Reactive flows

elementary reaction



reaction rate nb/(volume × time) $\dot{W}^{(j)} \equiv (J_+^{(j)} - J_-^{(j)})$ and $\vartheta_i^{(j)} \equiv (\vartheta_i^{-(j)} - \vartheta_i^{+(j)})$, stoichiometric coefficient

conservation equation for the species

$$\rho D Y_i / D t = -\nabla \cdot \mathbf{J}'_i + \sum_j \vartheta_i^{(j)} \mathbf{m}_i \dot{W}^{(j)},$$

$$\mathbf{J}'_i = -\rho D_i \nabla Y_i$$

$$\rho \frac{D Y_i}{D t} = \nabla \cdot (\rho D_i \nabla Y_i) + \sum_j \vartheta_i^{(j)} \mathbf{m}_i \dot{W}^{(j)} (T, p, \dots Y_k \dots)$$

sum over the reactions

equation for the chemical energy

$$e_{chem} \equiv \sum_i h_i Y_i$$

heat of the j th reaction

$$Q^{(j)} = \sum_{i=1}^n (\vartheta_i^{(j)+} - \vartheta_i^{(j)-}) \mathbf{m}_i h_i (T_o),$$

sum over the species

enthalpy of formation per unit of mass of species i

$$\rho D e_{chem} / D t = - \sum_i \nabla \cdot (h_i \mathbf{J}'_i) - \sum_j Q^{(j)} \dot{W}^{(j)}$$

Thermal balance of inviscid flow of reactive gas

$$e_{chem} \equiv \sum_i h_i Y_i \quad \rho D e_{chem} / Dt = - \sum_i h_i \nabla \cdot \mathbf{J}'_i - \sum_j Q^{(j)} \dot{W}^j$$

heat released by the j^{th} reaction \uparrow rate of the j^{th} reaction
 (number per unit time and unit volume)

$$\rho D(e_T + e_{chem}) / Dt = - \nabla \cdot \mathbf{J}'_q - p \nabla \cdot \mathbf{u}$$

heat flux $\mathbf{J}_q \equiv \mathbf{J}'_q - \sum_i h_i \mathbf{J}'_i \quad \mathbf{J}_q = -\lambda \nabla T$

$$\delta e_T = c_v \delta T \quad c_v \approx \text{cst.} \quad (\text{for simplicity, can be easily removed})$$

$$\rho c_v D T / Dt = \nabla \cdot (\lambda \nabla T) - p \nabla \cdot \mathbf{u} + \sum_j Q^{(j)} \dot{W}^{(j)}$$

continuity $\Rightarrow -p \nabla \cdot \mathbf{u} = \frac{p}{\rho} \frac{D}{Dt} \rho = \frac{D}{Dt} p - \rho \frac{D}{Dt} [(c_p - c_v) T]$

ideal gas law $p = (c_p - c_v) \rho T.$

thermal equation of an invicid fluid

$$\rho c_p D T / Dt = D p / Dt + \nabla \cdot (\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)}$$

compression conduction chemistry

Governing equations for inviscid flows of reactive gas

$$\begin{aligned} \frac{1}{\rho} \frac{D\rho}{Dt} &= -\nabla \cdot \mathbf{u}, & \rho \frac{D\mathbf{u}}{Dt} &= -\nabla p, & p &= (c_p - c_v)\rho T, \\ \rho c_p \frac{DT}{Dt} &= \frac{Dp}{Dt} + \nabla \cdot (\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)}, \\ \rho \frac{DY_i}{Dt} &= \nabla \cdot (\rho D_i \nabla Y_i) + \sum_j \vartheta_i^{(j)} \mathbf{m}_i \dot{W}^{(j)}. \end{aligned}$$

stoichiometric coefficient

Conservative form of the energy equation (inviscid approximation)

$$\partial(\rho e_{tot})/\partial t = -\nabla \cdot \mathbf{J}_{e_{tot}} \quad \mathbf{J}_{e_{tot}} = \mathbf{J}'_{e_{tot}} + \rho e_{tot} \mathbf{u} \quad \mathbf{J}_q + \sum_i h_i \mathbf{J}'_i = \mathbf{J}'_{e_{tot}} - p \mathbf{u}$$

$$\partial(\rho e_{tot})/\partial t = -\nabla \cdot [\rho \mathbf{u} e_{tot} + \mathbf{u} p + \mathbf{J}_q + \sum_i h_i \mathbf{J}'_i] = -\nabla \cdot [\rho \mathbf{u} (e_{tot} + p/\rho) + \mathbf{J}_q + \sum_i h_i \mathbf{J}'_i]$$

convective flux of enthalpy diffusive flux of total energy

progress variable

$$\rho q_m D\psi/Dt \equiv \sum_j Q^{(j)} \dot{W}^{(j)}, \quad \psi \in [0, 1]$$

heat released per unit mass

$$e_{tot} + p/\rho = c_p T + |\mathbf{u}|^2/2 - q_m \psi$$

Viscous flow

$$\underline{\underline{\Pi}} = p \underline{\underline{I}} + \underline{\underline{\pi}}$$

shear viscosity \rightarrow $\underline{\underline{\pi}} \equiv -2\eta(\underline{\underline{\nabla \mathbf{u}}})^{(s)} - \underline{\underline{I}}(\xi - 2\eta/3)\nabla \cdot \mathbf{u}$ bulk viscosity \leftarrow

$$\partial(\rho e_{tot})/\partial t = -\nabla \cdot [\rho \mathbf{u} (c_p T + |\mathbf{u}|^2/2 - q_m \psi) + \mathbf{J}'_q + \mathbf{u} \cdot \underline{\underline{\pi}}]$$

one-dimensional compressible flow

$$\mu \equiv 4\eta/3 + \xi$$

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho u)}{\partial x} \quad \frac{\partial(\rho u)}{\partial t} = -\frac{\partial}{\partial x} \left(p + \rho u^2 - \mu \frac{\partial u}{\partial x} \right)$$

$$\frac{\partial(\rho e_{tot})}{\partial t} = -\frac{\partial}{\partial x} \left[\rho u (c_p T + u^2/2 - q_m \psi) - \lambda \frac{\partial T}{\partial x} - \mu u \frac{\partial u}{\partial x} \right]$$

(simplest form of heat flux)

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II – 6) Entropy production

$$s(\rho, T, \dots Y_i, \dots)$$

entropy is a function of state that is not a conserved quantity

$$\partial(\rho s)/\partial t = -\nabla \cdot \mathbf{J}_s + \dot{w}_s,$$

2nd law of thermodynamics dissipative effects $\Rightarrow \boxed{\dot{w}_s \geq 0}$

$$T\delta s = \delta e_T + p\delta v - \sum_i \mu_i \delta Y_i$$

ideal gas $\frac{(s - s_o)}{c_v} = \ln \left(\frac{p/\rho^\gamma}{p_o/\rho_o^\gamma} \right)$

$$\boxed{T \frac{Ds}{Dt} = \frac{De_T}{Dt} + p \frac{D(1/\rho)}{Dt} - \sum_i \mu_i \frac{DY_i}{Dt}}$$

$$\dot{w}_s = \mathbf{J}'_q \cdot \nabla \left(\frac{1}{T} \right) - \sum_i \mathbf{J}'_i \cdot \nabla \left(\frac{\mu_i}{T} \right) - \frac{1}{T} \underline{\underline{\pi}} : (\underline{\underline{\nabla u}})^{(s)}$$

inert mixture in one-dimensional geometry

$$J_s = \rho u s - \frac{\lambda}{T} \frac{\partial T}{\partial x}, \quad \boxed{\dot{w}_s = \frac{\mu}{T} \left(\frac{\partial u}{\partial x} \right)^2 + \frac{\lambda}{T^2} \left(\frac{\partial T}{\partial x} \right)^2} \quad \mu > 0, \quad \lambda > 0$$

$$\rho \frac{Ds}{Dt} = \frac{\partial}{\partial x} \left(\frac{\lambda}{T} \frac{\partial T}{\partial x} \right) + \dot{w}_s \quad |_{19} \quad \rho T \frac{Ds}{Dt} = \frac{\partial}{\partial x} \left(\lambda \frac{\partial}{\partial x} T \right) + \mu \left(\frac{\partial u}{\partial x} \right)^2$$