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Structure and Dynamics of Combustion Waves in Premixed Gases

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Lecture 11
Governing equations

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

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

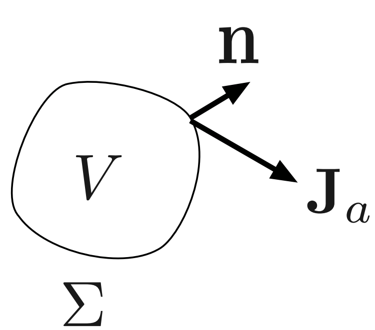
$II-1)$ Conserved extensive quantities

extensive quantities $A_V = \iiint_V \rho a \, \mathrm{d}^3\mathbf{r}$

mass weighted distribution $a(\mathbf{r},t)$

mass density $\rho(\mathbf{r},t)$

conservation equation V fixed $\quad \mathrm{d}A/\mathrm{d}t = \iiint_V [\partial(\rho a)/\partial t] \, \mathrm{d}^3\mathbf{r} = (\mathrm{d}A/\mathrm{d}t)_1 + (\mathrm{d}A/\mathrm{d}t)_2$



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

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

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

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

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

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

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

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

tensor field $\quad \underline{\underline{\mathbf{J}_a}}(\mathbf{r},t)$

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

$II-2)$ Conservation of mass: continuity equation

mass is a conserved scalar (classical mechanics)

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

material (convective) derivative $\dfrac{\mathrm{D}}{\mathrm{D}t} \equiv \dfrac{\partial}{\partial t} + \mathbf{u}.\nabla$

$$\frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\nabla.\mathbf{u}$$

continuity equation

$$\frac{1}{v}\frac{\mathrm{D}v}{\mathrm{D}t} = \nabla.\mathbf{u} \qquad v \equiv 1/\rho$$

Lagrangian form of conservation equations

convection flux

$$\partial(\rho a)/\partial t = -\nabla.\mathbf{J}_a + \dot{\omega}_a \qquad \rho\mathrm{D}a/\mathrm{D}t = -\nabla.\mathbf{J}'_a + \dot{\omega}_a \qquad \mathbf{J}_a \equiv \rho a\mathbf{u} + \mathbf{J}'_a$$

conserved scalar:

diffusion flux

$$\partial(\rho a)/\partial t = -\nabla.\mathbf{J}_a \qquad \rho\mathrm{D}a/\mathrm{D}t = -\nabla.\mathbf{J}'_a$$

!

(definition of the diffusion flux in the equation for energy is slightly different)
see slide 11

$II - 3)$ 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

$$\rho \mathrm{D} Y_i / \mathrm{D} t = -\nabla . \mathbf{J}'_i \qquad \sum_i \mathbf{J}'_i = 0$$

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

Fick's law : $\mathbf{J}'_i = -\rho D_i \nabla Y_i$ $\qquad D_i > 0$

$$\rho \mathrm{D} Y_i / \mathrm{D} t = \nabla . [\rho D_i \nabla Y_i]$$

diffusion equation

$\rho D_i \approx$ cst. $\qquad \mathbf{u} = 0$ $\qquad \partial Y_i / \partial t = D_i \Delta Y_i$

archetype of irreversible phenomenon

(random walk)

Diffusive damping. Dissipative phenomenon

$$\partial Y/\partial t = D\Delta Y \qquad D > 0 \qquad [D] = (length)^2/time$$

Fourier anaysis

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

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

Fourier 1824

Green function   Self-similar solution

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

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

probability distribution of the test particle

number density

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

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

$II-4)$ Conservation of momentum

Momentum is a conserved vector (isolated system)

$$\rho \mathrm{D}\mathbf{u}/\mathrm{D}t = -\nabla . \underline{\underline{\Pi}} \quad -\rho g \mathbf{e}_z,$$

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

thermodynamic pressure (isotropic)

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

Navier Stokes equations (gravity)

$$\rho \mathrm{D}\mathbf{u}/\mathrm{D}t = -\nabla(p + \rho g z) + \eta \Delta \mathbf{u} + (\xi + \eta/3)\nabla(\nabla.\mathbf{u})$$

Viscous shear diffusivity $D_{vis} = \eta/\rho$

Euler equations

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

non dissipative equations

$II-5)$ Conservation of total energy

internal energy, $e_{int} = e_T + e_{chem}$

(Additive in a gas when interactions are neglected)

thermal energy, (kinetic + rotational & vibrational energy)

chemical energy (chemical bonds),

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

total energy is a conserved scalar

$$\partial(\rho e_{tot})/\partial t = -\nabla.\mathbf{J}_{e_{tot}} \qquad \rho\,\mathrm{D}e_{tot}/\mathrm{D}t = -\nabla.\mathbf{J}'_{e_{tot}} \qquad \mathbf{J}'_{e_{tot}} \equiv \mathbf{J}_{e_{tot}} - \rho e_{tot}\mathbf{u}$$

Inviscid and inert flows

(first law of thermodynamics)

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

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

heat flux,

$$\rho\,\mathrm{D}(e_T + e_{chem})/\mathrm{D}t = -\nabla.\mathbf{J}'_q - p\nabla.\mathbf{u}$$

heat work done

$p\nabla.\mathbf{u} = \rho p(\mathrm{D}\rho^{-1}/\mathrm{D}t)$

Fourier law

(simplest form of heat flux)

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

thermal conductivity

Fourier equation

inert material $e_{chem} = \text{cst.}$

no flow $\mathbf{u} = 0$

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

$\delta e_T = c_V \delta T$ thermal diffusivity , $D_T \equiv \lambda/\rho c_V$ $[D_T] = (length)^2/time$

Reactive flows

elementary reaction

$$\vartheta_1^+ A_1 + \ldots + \vartheta_n^+ A_n \quad \rightleftharpoons \quad \vartheta_1^- A_1 + \ldots + \vartheta_n^- A_n + Q.$$

reaction rate
nb/(volume × time)

$$\dot{W}^{(j)} \equiv (J_+^{(j)} - J_-^{(j)}) \quad \text{and} \quad \vartheta_i^{(j)} \equiv (\vartheta_i^{-(j)} - \vartheta_i^{+(j)}),$$

stoichiometric coefficient

conservation equation for the species

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

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

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

sum over the reactions

equation for the chemical energy

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

heat of the j th reaction

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

sum over the species

enthalpy of formation per unit of mass of species i

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

Thermal balance of inviscid flow of reactive gas

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

heat released by the j^{th} reaction

rate of the j^{th} reaction
(number per unit time and unit volume)

$$\rho\, \mathrm{D}(e_T + e_{chem})/\mathrm{D}t = -\nabla.\mathbf{J}'_q - p\nabla.\mathbf{u}$$

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

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

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

continuity $\Rightarrow \quad -p\nabla.\mathbf{u} = \dfrac{p}{\rho}\dfrac{\mathrm{D}}{\mathrm{D}t}\rho = \dfrac{\mathrm{D}}{\mathrm{D}t}p - \rho\dfrac{\mathrm{D}}{\mathrm{D}t}[(c_p - c_v)T]$

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

thermal equation of an invicid fluid

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

compression conduction chemistry

Governing equations for inviscid flows of reactive gas

$$\frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\nabla.\mathbf{u}, \qquad \rho\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = -\nabla p, \qquad p = (c_p - c_v)\rho T,$$

$$\rho c_p \frac{\mathrm{D}T}{\mathrm{D}t} = \frac{\mathrm{D}p}{\mathrm{D}t} + \nabla.(\lambda\nabla T) + \sum_j Q^{(j)}\dot{W}^{(j)},$$

$$\rho\frac{\mathrm{D}Y_i}{\mathrm{D}t} = \nabla.(\rho D_i \nabla Y_i) + \sum_j \vartheta_i^{(j)}\mathsf{m}_i\dot{W}^{(j)}.$$

stoichiometric coefficient

Conservative form of the energy equation (inviscid approximation)

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

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

convective flux of enthalpy — diffusive flux of total energy

progress variable

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

heat released per unit mass

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

Viscous flow

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

shear viscosity ↘ ↙ bulk viscosity

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

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

one-dimensional compressible flow

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

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

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

(simplest form of heat flux)

$II - 6)$ Entropy production

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

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

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

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

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

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

$$T\frac{\mathrm{D}s}{\mathrm{D}t} = \frac{\mathrm{D}e_T}{\mathrm{D}t} + p\frac{\mathrm{D}(1/\rho)}{\mathrm{D}t} - \sum_i \mu_i \frac{\mathrm{D}Y_i}{\mathrm{D}t}$$

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

inert mixture in one-dimensional geometry

$$J_s = \rho u s - \frac{\lambda}{T}\frac{\partial T}{\partial x},$$

$$\dot{w}_s = \frac{\mu}{T}\left(\frac{\partial u}{\partial x}\right)^2 + \frac{\lambda}{T^2}\left(\frac{\partial T}{\partial x}\right)^2$$

$\mu > 0, \qquad \lambda > 0$

$$\rho\frac{\mathrm{D}s}{\mathrm{D}t} = \frac{\partial}{\partial x}\left(\frac{\lambda}{T}\frac{\partial T}{\partial x}\right) + \dot{w}_s$$

$$\rho T\frac{\mathrm{D}s}{\mathrm{D}t} = \frac{\partial}{\partial x}\left(\lambda\frac{\partial}{\partial x}T\right) + \mu\left(\frac{\partial u}{\partial x}\right)^2$$