

Lecture 5

Conditions at a discontinuity Dimensionless parameters

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Conservation conditions at an interface

The time rate of a change of a quantity $\varphi(\mathbf{x}, t)$ over a given volume \mathbb{V} , moving with velocity \mathbf{V}_I is¹

$$\frac{d}{dt} \int_{\mathbb{V}} \varphi dV = \int_{\mathbb{V}} \frac{\partial \varphi}{\partial t} dV + \int_{\mathbb{S}} \varphi (\mathbf{V}_I \cdot \mathbf{n}) dS$$

Applied to mass conservation ($\varphi = \rho$) we

$$\frac{d}{dt} \int_{\mathbb{V}} \rho dV = \int_{\mathbb{V}} \frac{\partial \rho}{\partial t} dV + \int_{\mathbb{S}} \rho (\mathbf{V}_I \cdot \mathbf{n}) dS$$

Using the continuity equation

$$\int_{\mathbb{V}} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} \right) dV = 0 \quad \text{or} \quad \int_{\mathbb{V}} \frac{\partial \rho}{\partial t} dV + \int_{\mathbb{S}} \rho (\mathbf{v} \cdot \mathbf{n}) dS = 0$$

$$\frac{d}{dt} \int_{\mathbb{V}} \rho dV = - \int_{\mathbb{S}} \rho (\mathbf{v} - \mathbf{V}_I) \cdot \mathbf{n} dS$$

¹ This is the multidimensional analogue of Leibnitz's theorem from calculus; it is a kinematic relation, not a law of fluid mechanics.

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When the control volume shrinks to the surface \mathbb{S}_I

$$\lim_{\mathbb{V} \rightarrow 0} \underbrace{\left\{ \frac{d}{dt} \int_{\mathbb{V}} \rho dV \right\}}_{=0} = - \int_{\mathbb{S}_I} \left[\rho^+ (\mathbf{v}^+ - \mathbf{V}_I) \cdot \mathbf{n}^+ + \rho^- (\mathbf{v}^- - \mathbf{V}_I) \cdot \mathbf{n}^- \right] dS$$

no mass accumulation or source/sink of mass at the interface.

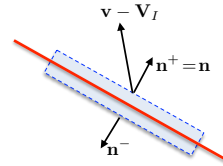
$$\rho^+ (\mathbf{v}^+ \cdot \mathbf{n} - V_I) - \rho^- (\mathbf{v}^- \cdot \mathbf{n} - V_I)$$

$$[\rho (\mathbf{v} \cdot \mathbf{n} - V_I)] = 0$$

$$[p \mathbf{n} + \rho (\mathbf{v} \cdot \mathbf{n} - V_I) \mathbf{v} - \boldsymbol{\Sigma} \cdot \mathbf{n}] = 0$$

results from the momentum equation,. Similarly we can derive jump relations for energy and species concentrations.

In fluid mechanics, discontinuities are allowed within the continuum framework, provided the variables across the surface of discontinuity are such as to satisfy the fundamental conservation laws, or the appropriate *jump conditions*.



“pillbox” control volume
 \mathbf{V}_I is the velocity of the interface (control surface)

$$V_I = \mathbf{V}_I \cdot \mathbf{n}$$

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If viscosity is negligible

$$[\rho (\mathbf{v} \cdot \mathbf{n} - V_I)] = 0$$

$$[p \mathbf{n} + \rho \mathbf{v} (\mathbf{v} \cdot \mathbf{n} - V_I)] = 0$$

$$[\rho (h + \frac{1}{2} v^2) (\mathbf{v} \cdot \mathbf{n} - V_I) + \mathbf{q} \cdot \mathbf{n}] = 0$$

$$[\rho Y_i ((\mathbf{v} + \mathbf{V}_i) \cdot \mathbf{n} - V_I)] = 0$$

The momentum jump can be decomposed into normal and tangential components, to give

$$[\rho (\mathbf{v} \cdot \mathbf{n} - V_I)] = 0$$

$$[p + \rho (\mathbf{v} \cdot \mathbf{n} - V_I) (\mathbf{v} \cdot \mathbf{n})] = 0$$

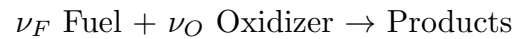
$$[\mathbf{n} \times (\mathbf{v} \times \mathbf{n})] = 0$$

Rankine-Hugoniot relations

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Non-dimensional Equations

In the following the chemistry will be represented by a global one-step (irreversible) reaction



describing the combustion of a single fuel.

The reaction will be assumed of order n_F, n_O , with respect to the fuel/oxidizer, and an overall order $n = n_F + n_O$. The reaction rate will be assumed to obey an Arrhenius law

$$\omega = \mathcal{B} \left(\frac{\rho Y_F}{W_F} \right)^{n_F} \left(\frac{\rho Y_O}{W_O} \right)^{n_O} e^{-E/\mathcal{R}T}$$

with an overall activation energy E and a pre-exponential factor \mathcal{B} (treated as constant).

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For simplicity, we will treat $\mu, \lambda, \rho D_i$ constants (although most of the theoretical development could accommodate a temperature-dependent λ) so that

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

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \mu \left[\nabla^2 \mathbf{v} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{v}) \right] + \rho \mathbf{g}$$

$$\rho \frac{DY_i}{Dt} - \rho D_i \nabla^2 Y_i = -\nu_i W_i \omega, \quad i = F, O$$

$$\rho c_p \frac{DT}{Dt} - \lambda \nabla^2 T = \frac{Dp}{Dt} + \Phi + Q \omega$$

$$p = \rho \mathcal{R}T/W$$

$$\omega = \mathcal{B} \left(\frac{\rho Y_F}{W_F} \right)^{n_F} \left(\frac{\rho Y_O}{W_O} \right)^{n_O} e^{-E/\mathcal{R}T}$$

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Characteristic values:

the fresh unburned state p_0, ρ_0, T_0 (satisfying $p_0 = \rho_0 \mathcal{R} T_0 / W$) for p, ρ, T .

a characteristic speed v_0 to be specified

the diffusion length $l_D \equiv \lambda / \rho c_p v_0$ for distances

the diffusion time l_D / v_0 for t

This choice is clearly not unique and there may be other length, time, and velocity scales that, for a given problem, could be more relevant.

We will use the same variables for the dimensionless quantities; i.e. after substituting $v^* = v / v_0$ say, we remove the * superscript.

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

$$\rho \frac{D\mathbf{v}}{Dt} = -\frac{1}{\gamma M^2} \nabla p + \text{Pr} \left[\nabla^2 \mathbf{v} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{v}) \right] + \text{Fr}^{-1} \rho \mathbf{e}_g$$

$$\rho \frac{DY_F}{Dt} - L e_F^{-1} \nabla^2 Y_F = -\omega$$

$$\rho \frac{DY_O}{Dt} - L e_O^{-1} \nabla^2 Y_O = -\nu \omega$$

$$\rho \frac{DT}{Dt} - \nabla^2 T = \frac{\gamma - 1}{\gamma} \left(\frac{Dp}{Dt} + \gamma \text{Pr} M^2 \Phi \right) + q \omega$$

$$p = \rho T$$

$$\omega = D \rho^n Y_F^{n_F} Y_O^{n_O} e^{-\beta_0 / T}$$

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Dimensionless Parameters

$$M = \frac{v_0}{\sqrt{\gamma p_0 / \rho_0}} \quad \text{Mach number}$$

$$\text{Fr} = \frac{v_0^2 / l_D}{g} \quad \text{Froude number}$$

$$\text{Pr} = \frac{\mu c_p}{\lambda} \quad \text{Prandtl number}$$

$$\text{Le}_i = \frac{\lambda / \rho c_p}{\mathcal{D}_i} \quad \text{Lewis number of species } i$$

Note that $\text{Pr}^{-1} = \rho_0 v_0 l_D / \mu = Re$ where Re is the Reynolds number based on the diffusion length. The Reynolds number based on a hydrodynamic length L will be large because typically $L \gg l_D$.

$$\beta_0 = E / \mathcal{R} T_0 \quad \text{Activation energy}$$

$$q = \frac{Q / \nu_F W_F}{c_p T_0} \quad \text{heat release}$$

$$\nu = \frac{\nu_O W_O}{\nu_F W_F} \quad \text{mass weighted stoichiometric coeff.}$$

numerator is the heat release per unit mass of fuel

$$D = \frac{(l_D / v_0)}{[(\rho_0 / W_F)^{n_F - 1} (\rho_0 / W_O)^{n_O} \mathcal{B}]^{-1}}$$

$$\text{Damköhler number} \\ = \frac{\text{flow time}}{\text{reaction time}}$$

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Low Mach Number Approximation

The propagation speed of ordinary deflagration waves is in the range 1-100 cm/s, namely much smaller than the speed of sound (in air $a_0 = 34,000$ cm/s).

$$M \ll 1$$

$$\text{momentum equation} \Rightarrow \nabla p = 0$$

$$p = P(t) + \gamma M^2 \hat{p}(\mathbf{x}, t) + \dots$$

will all other variables expressed as $\mathbf{v} + \gamma M^2 \hat{\mathbf{v}} + \dots$

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla \hat{p} + \text{Pr} [\nabla^2 \mathbf{v} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{v})] + \text{Fr}^{-1} \rho \mathbf{e}_g$$

$$\rho \frac{DT}{Dt} - \nabla^2 T = \frac{\gamma - 1}{\gamma} \frac{dP}{dt} + q \omega$$

$$\rho T = P(t)$$

acoustic disturbances travel infinitely fast, and are filtered out.

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Unless $P(t)$ is specified, we are missing an equation, since p has been replaced by two variables P and \hat{p} . An equation in bounded problems can be obtained as follows:

$$\rho \frac{\partial T}{\partial t} + \rho \mathbf{v} \cdot \nabla T - \nabla^2 T = \frac{\gamma-1}{\gamma} \frac{dP}{dt} + q\omega$$

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

$$\frac{\partial(\rho T)}{\partial t} + \nabla \cdot (\rho \mathbf{v} T) - \nabla^2 T = \frac{\gamma-1}{\gamma} \frac{dP}{dt} + q\omega$$

$$\frac{1}{\gamma} \frac{dP}{dt} = -\nabla \cdot (P \mathbf{v} - \nabla T) + q\omega$$

$$\frac{1}{\gamma} \int_{\mathbb{V}} \frac{dP}{dt} dV = - \int_{\mathbb{S}} (P \mathbf{v} - \nabla T) \cdot \mathbf{n} dS + q \int_{\mathbb{V}} \omega dV$$

on the surface \mathbb{S} , $\mathbf{v} \cdot \mathbf{n} = 0$ and for adiabatic conditions $\partial T / \partial n = 0$.

$$\frac{dP}{dt} = \frac{\gamma q}{\mathbb{V}} \int_{\mathbb{V}} \omega dV$$

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The *low Mach number equations* are (with the "hat" in p removed), therefore

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

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \text{Pr} [\nabla^2 \mathbf{v} + \frac{1}{3} \nabla(\nabla \cdot \mathbf{v})] + \text{Fr}^{-1} \rho \mathbf{e}_g$$

$$\rho \frac{DY_F}{Dt} - Le_F^{-1} \nabla^2 Y_F = -\omega$$

$$\rho \frac{DY_O}{Dt} - Le_O^{-1} \nabla^2 Y_O = -\nu \omega$$

$$\rho \frac{DT}{Dt} - \nabla^2 T = \frac{\gamma-1}{\gamma} \frac{dP}{dt} + q\omega$$

$$\rho T = 1$$

and when the underlying pressure does not change in time, $P = 1$.

Unless otherwise indicated, we will be mostly concerned in the following with this set of equations.

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Coupling Functions

For unity Lewis numbers the operator on the left hand side of these three equations is the same.

$$\begin{aligned}\rho \frac{DY_F}{Dt} - Le_F^{-1} \nabla^2 Y_F &= -\omega \\ \rho \frac{DY_O}{Dt} - Le_O^{-1} \nabla^2 Y_O &= -\nu\omega \\ \rho \frac{DT}{Dt} - \nabla^2 T &= q\omega\end{aligned}$$

The combinations $H_F = T + qY_F$ and $H_O = T + qY_O/\nu$ (and hence $Y_F - Y_O/\nu$) satisfy reaction-free equations

$$\rho \frac{DH_i}{Dt} - \nabla^2 H_i = 0$$

leaving only one equation with the highly nonlinear reaction rate term. This is a great simplification, but as we shall see, small variations of the Lewis numbers from one produce instabilities and nontrivial consequences.

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The constant-density approximation

~~$$\rho T = 1$$~~

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} &= 0 \\ \rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) &= -\nabla p + \text{Pr} \left[\nabla^2 \mathbf{v} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{v}) \right] + \text{Fr}^{-1} \rho \mathbf{e}_g\end{aligned}$$

solve to determine \mathbf{v}

$$\begin{aligned}\rho \left(\frac{\partial Y_F}{\partial t} + \mathbf{v} \cdot \nabla Y_F \right) - Le_F^{-1} \nabla^2 Y_F &= -\omega \\ \rho \left(\frac{\partial Y_O}{\partial t} + \mathbf{v} \cdot \nabla Y_O \right) - Le_O^{-1} \nabla^2 Y_O &= -\nu\omega \\ \rho \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) - \nabla^2 T &= q\omega\end{aligned}$$

with the given \mathbf{v} solve for T, Y_F, Y_O .

often referred to as the *diffusive-thermal* model

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