Non-Fickean Diffusion Processes

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Contents

The mixture as a single fluid

"each position $\boldsymbol{x}$ may be occupied simultaneously by several different particles $\boldsymbol{X}_a$, one for each constituent a"

Individual fields

$$\left\| \begin{array}{ll} \rho_a, & \text{individual mass density,} \\ \boldsymbol{v}_a, & \text{individual velocity}, a = 1, ..., n. \\ T, & \text{unique temperature} \end{array} \right.$$

Mass balance and momentum balance for each constituent

$$\begin{aligned} \partial_t \rho_a + \partial_i \rho_a v_a^i &= \widetilde{m}_a, \\ \partial_t \rho_a v_a^j + \partial_i (\rho_a v_a^i v_a^j - t_a^{ji}) &= \widetilde{h}_a^j, \end{aligned}$$

$$\left\| \begin{array}{ll} \widetilde{m}_a, & \text{internal mass production due to chemical reactions,} \\ \widetilde{h}_a, & \text{production of partial momentum due to collisions} \\ & \text{between different constituents,} \\ \boldsymbol{t}_a, & \text{partial stress tensor.} \end{array} \right.$$

Global fields

$$\left\| \begin{array}{ll} \rho = \sum \rho_a, & \text{mass density,} \\ \boldsymbol{v} = \sum \dfrac{\rho_a}{\rho} \boldsymbol{v}_a, & \text{velocity,} \\ T, & \text{temperature.} \end{array} \right.$$

Global balance laws

$$\begin{aligned} \partial_t \rho + \partial_i \rho v^i &= 0, \\ \partial_t \rho v^j + \partial_i (\rho v^i v^j - t^{ij}) &= 0, \\ \partial_t \rho (\varepsilon + 1/2 v^2) + \partial_i (\rho (\varepsilon + 1/2 v^2) v^i - t^{ij} v_j + q^i) &= 0. \end{aligned}$$

$$\left\| \begin{array}{ll} \varepsilon, & \text{internal energy,} \\ \boldsymbol{t}, & \text{stress tensor,} \\ \boldsymbol{q}, & \text{thermal flux} \end{array} \right.$$

Binary mixture

$\boldsymbol{u} = \boldsymbol{v}_1 - \boldsymbol{v}$,	diffusion velocity,
$\boldsymbol{J} = \rho_1 \boldsymbol{u}$,	diffusion flux,
$c = \dfrac{\rho_1}{\rho}$,	mass concentration

Non-Fickean diffusion models

State variables

$$c(\boldsymbol{x}, t), \boldsymbol{J}(\boldsymbol{x}, t), \rho(\boldsymbol{x}, t), \boldsymbol{v}(\boldsymbol{x}, t), T(\boldsymbol{x}, t)$$

Algebraic identity

$$\rho_1 v_1^i v_1^j = J^i v^j + J^j v^i + c\rho v^i v^j + \rho_1 u^i u^j.$$

Hypothesis

$$\rho_1 \boldsymbol{u} \otimes \boldsymbol{u} \approx 0$$

Dynamic law for $\boldsymbol{J}$

$$\partial_t \left(J^k + c\rho v^k \right) + \partial_i \left(J^i v^k + v^i J^k + c\rho v^k v^i - t_1^{ik} \right) = \widetilde{h}^k.$$

Extended thermodynamical model

$$\begin{aligned}
\partial_t\rho + \partial_i\rho v^i &= 0,\\
\partial_t\rho v^j + \partial_i(\rho v^i v^j - t^{ij}) &= 0,\\
\partial_t\rho(\varepsilon + 1/2v^2) + \partial_i(\rho(\varepsilon + 1/2v^2)v^i - t^{ij}v_j + q^i) &= 0,\\
\partial_t\rho c + \partial_i(\rho c v^i + J^i) &= \widetilde{m},\\
\partial_t\left(J^k + c\rho v^k\right) + \partial_i\left(J^i v^k + v^i J^k + c\rho v^k v^i - t_1^{ik}\right) &= \widetilde{h}^k.
\end{aligned}$$

Constitutive relations

Inviscide Mixture

$$t_1^{ij} = -p_1\delta^{ij}, \quad t^{ij} = -p\delta^{ij},$$
$$p_1 = cp.$$

Production of the partial momentum

$$\widetilde{\boldsymbol{h}} = \boldsymbol{v}_1\widetilde{m} + M^{11}\frac{\rho}{\rho_1\rho_2}\boldsymbol{J}, M^{11} = \mathcal{M}^{11}(c,\rho,T)$$

Production of the partial mass

$$\widetilde{m} = \widetilde{m}(c,\rho,T).$$

State equations

$$\varepsilon = \epsilon(c,\rho,T), p = p(\rho,T).$$

Non-reactive mixture. Linear model

Assumptions

Thermal equilibrium

$$T = T_0, \rho = \rho_0, \boldsymbol{v} = 0$$

Partial momentum production

$$M^{11}\frac{\rho_0}{\rho_1\rho_2} = -\frac{p_0}{\rho_0 D}.$$

State variables

$$c(t,x), J(t,x), t > 0, x \in \mathbb{R}$$

Governing equation. Cattaneo equations

$$\begin{aligned} \rho_0\partial_t c + \partial_x J &= 0, \\ \frac{\rho_0 D}{p_0}\partial_t J + \rho_0 D\partial_x c &= -J. \end{aligned} \tag{1}$$

Dimensionless form

$$\partial_t c + \partial_x J = 0,$$
$$\varepsilon \partial_t J + \partial_x c = -J, \qquad \varepsilon = \frac{D^2}{L^2}\frac{\rho_0}{p_0}.$$

Telegraph equation as mathematical model for non-Fickean diffusion

$$\varepsilon \partial_t^2 c + \partial_t c = \partial_x^2 c.$$

Notations

$$\boldsymbol{u} = \begin{pmatrix} c \\ J \end{pmatrix}, \quad \boldsymbol{A}_\varepsilon = \begin{pmatrix} 0 & -\partial_x \\ -\varepsilon^{-1}\partial_x & -\varepsilon^{-1} \end{pmatrix}.$$

Cauchy problem for the non-Fickean diffusion problem (NFDP)

$$\begin{cases} \dfrac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \boldsymbol{A}_\varepsilon \boldsymbol{u} \\ \boldsymbol{u}\big|_{t=0} = \boldsymbol{u}_0 \end{cases}.$$

Cauchy problem for Fickean diffusion (FDP)

$$\begin{cases} \dfrac{\mathrm{d}w}{\mathrm{d}t} = \partial_x^2 w \\ w\big|_{t=0} = c_0 \end{cases}.$$

Theorem. **Assume that the initial datum $\boldsymbol{u}_0$ is a bounded continuous function and $\boldsymbol{u}_0, \partial_x \boldsymbol{u}_0, \partial_x^2 \boldsymbol{u}_0$ belong to $\mathbb{L}^2(\mathbb{R})$. Let**
$\boldsymbol{u}_\varepsilon(t,x)$ be the the solution of the (NFDP),
$w(t,x)$ be the solution of the (FDP).
Then we have the following properties:
(1) Finite speed of propagation. **If the initial datum c_0 has compact support, then the solution $c_\varepsilon(t,x)$ has also compact support for any finite time t**
(2) Fickean diffusion as singular asymptotic limit of non-Fickean diffusion**. The following relations hold**

$$\lim_{\varepsilon\to 0} c_\varepsilon(t,x) = w(t,x),$$

$$\lim_{\varepsilon\to 0} \left(J_\varepsilon(t,x) + \partial_x c_\varepsilon(t,x)\right) = 0.$$

(3) Fickean diffusion as asymptotic limit of non-Fickean diffusion for $t \to \infty$

$$c_\varepsilon(t,x) = w(t,x) + O\big(t^{-1/2}\big) + O\big(\exp(-t/2\varepsilon)\big),\ t \to \infty$$

Sketch of proof. Using the Fourier transform one obtains:
The Fourier transform of the solution

$$\widetilde{\boldsymbol{u}}_\epsilon(t,\xi) = \widetilde{\boldsymbol{\mathcal{E}}}(t,\xi;\varepsilon)\widetilde{\boldsymbol{u}}_0(\xi),$$

and solution

$$\boldsymbol{u}_\epsilon(t,x) = \boldsymbol{\mathcal{E}}(t;\varepsilon) * \boldsymbol{u}_0(x).$$

$$\widetilde{\boldsymbol{\mathcal{E}}}(t,\xi;\varepsilon) = \mathrm{e}^{-\dfrac{t}{2\varepsilon}} \begin{pmatrix} \omega_\varepsilon(t,\xi) + 2\varepsilon\partial_t\omega_\varepsilon(t,\xi) & -2\varepsilon \mathrm{i}\xi\omega_\varepsilon(t,\xi) \\ -2\mathrm{i}\xi\omega_\varepsilon(t,\xi) & -\omega_\varepsilon(t,\xi) + 2\varepsilon\partial_t\omega_\varepsilon(t,\xi) \end{pmatrix},$$

$$\delta = \sqrt{1 - 4\varepsilon\xi^2}, \quad \omega_\varepsilon(t,\xi) = \frac{\mathrm{e}^{\dfrac{t\delta}{2\varepsilon}} - \mathrm{e}^{-\dfrac{t\delta}{2\varepsilon}}}{2\delta}.$$

(1) Finite speed of propagation

Explicit formula for the solution of (NFDP)

$$I(z) = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} \mathrm{e}^{z \sin \phi} \mathrm{d}\phi.$$

$$\begin{aligned} \mathrm{e}^{t/2\varepsilon} c_\varepsilon(t,x) = \ & \frac{c_0(x + t/\sqrt{\varepsilon}) + c_0(x - t/\sqrt{\varepsilon})}{2} + \\ & \frac{t}{4\varepsilon} \int_{-1}^{1} \left[I\left(t \frac{\sqrt{1-y^2}}{2\varepsilon} \right) + \frac{1}{\sqrt{1-y^2}} I'\left(t \frac{\sqrt{1-y^2}}{2\varepsilon} \right) \right] c_0(x + \frac{yt}{\sqrt{\varepsilon}}) \mathrm{d}y \\ & -\sqrt{\varepsilon} \frac{j_0(x + t/\sqrt{\varepsilon}) - j_0(x - t/\sqrt{\varepsilon})}{2} - \\ & \frac{t}{4\varepsilon} \int_{-1}^{1} \frac{y}{\sqrt{1-y^2}} I'\left(t \frac{\sqrt{1-y^2}}{2\varepsilon} \right) j_0(x + \frac{yt}{\sqrt{\varepsilon}}) \mathrm{d}y \end{aligned}$$

(2) Fickean diffusion as singular asymptotic limit of non-Fickean diffusion.

$$\lim_{\varepsilon \to 0} \widetilde{\boldsymbol{\mathcal{E}}}(t,\xi;\varepsilon) = \begin{pmatrix} \mathrm{e}^{-\xi^2 t} & 0 \\ -\mathrm{i}\xi \mathrm{e}^{-\xi^2 t} & 0 \end{pmatrix}.$$

and observe that the function

$$\widetilde{w}(t,\xi) = \mathrm{e}^{-\xi^2 t} \widetilde{c}_0(\xi)$$

solves the (FDP).

Reactive mixture. Structure of the strong detonation waves

Classical Chapman-Jouget theory of the combustion process assets that

"The whole reaction process take place in an infinite thin layer. The reactant being in equilibrium state before shock suddenly reaches after shock another equilibrium state as a product of reaction".

State variables

$$\boldsymbol{U} = (\rho, u, p, c, J).$$

Euler extended equations

$$\frac{\partial \Phi^i(\boldsymbol{U})}{\partial t} + \frac{\partial F^i(\boldsymbol{U})}{\partial x} = P^i(\boldsymbol{U})$$

$$\boldsymbol{\Phi} = \begin{pmatrix} \rho \\ \rho u \\ \rho(u^2/2 + cq) + p/(\gamma - 1) \\ \rho c \\ J + \rho c u \end{pmatrix}$$

$$\boldsymbol{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho(u^2/2 + cq)u + \gamma u p/(\gamma - 1) + qJ \\ \rho c u + J \\ Ju + (\rho c u + J)u + pc \end{pmatrix}, \boldsymbol{P} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \widetilde{m} \\ \widetilde{h} \end{pmatrix}$$

$$p = \rho R T; \varepsilon - \varepsilon_0 = C_V(T - T_0) + cq; \quad q \text{ heat release}$$

Remark. The structure analyzed here take into account the chemical reaction rate and the diffusion phenomena in the reactive zone.

Reactive shock wave solutions

$$\boldsymbol{U}(x,t) = \begin{cases} \boldsymbol{U}_- \,, x < st, \\ \boldsymbol{U}_+ \,, x > st. \end{cases}$$

Production is concentrated on the line $x - st = 0$

$$P = P(U_-, U_+)\delta(x - st).$$

Rankine-Hugoniot equations

$$-s\left(\boldsymbol{\Phi}(\boldsymbol{U}_+) - \boldsymbol{\Phi}(\boldsymbol{U}_-)\right) + \boldsymbol{F}(\boldsymbol{U}_+) - \boldsymbol{F}(\boldsymbol{U}_-) = \boldsymbol{P}(\boldsymbol{U}_-, \boldsymbol{U}_+)$$

Simple wave solutions

$$\boldsymbol{U}(x,t) = \boldsymbol{U}(x - st)$$

.

$$\frac{\mathrm{d}}{\mathrm{d}y}\big(- s\boldsymbol{\Phi}(\boldsymbol{U}) + \boldsymbol{F}(\boldsymbol{U})\big) = \boldsymbol{P}(\boldsymbol{U})$$

$$\begin{pmatrix} \tau_- \\ T_- \\ c_- \\ J_- \end{pmatrix} \longrightarrow \begin{pmatrix} \tau^{inert} \\ T^{inert} \\ c_- \\ J_- \end{pmatrix} \longrightarrow \begin{pmatrix} \tau^{SD} \\ T^{SD} \\ c_+ \\ J_+ \end{pmatrix}$$

Strong detonation wave

Chemical state variables

$$\begin{pmatrix} c \\ J \end{pmatrix}_- = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \begin{pmatrix} c \\ J \end{pmatrix}_+ = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Thermodynamical state variables

$$\frac{\tau^{SD}}{\tau_-} = \frac{\sigma}{\gamma+1}(1-\beta); \ \frac{T^{SD}}{T_-} = \frac{M_-^2\sigma^2}{(\gamma+1)^2}(1-\beta)(1+\gamma\beta)$$

$$m = \rho(u-s), \ \tau = 1/\rho; a = \sqrt{\gamma p \tau}; M^2 = \frac{m^2}{\gamma p \rho};$$

$$\alpha^2 = h^2/(\omega^2 M_-^2); h^2 = 2(\gamma^2-1)\frac{q}{a_-^2}; \sigma = \gamma + 1/M_-^2;$$

$$\omega = 1 - 1/M_-^2; \beta = \frac{\omega}{\sigma}\sqrt{1-\alpha^2}$$

$$M_-^2 \geq M_{CJ}^2 \equiv 1 + h^2/2 + h\sqrt{1+h^2/4}$$

Simple waves

$$\begin{aligned}
\rho(u-s) &= m \\
\frac{d}{dy}(m^2\tau + p) &= 0 \\
\frac{d}{dy}\left(\frac{\gamma}{\gamma-1}p\tau + m^2\tau^2/2 + q(c+J/m)\right) &= 0 \\
\frac{d}{dy}(c+J/m) &= \frac{\widetilde{m}}{m} \\
\tau m\frac{d}{dy}J + 2Jm\frac{d}{dy}\tau + p\frac{d}{dy}c &= \widetilde{h} - u\widetilde{m}
\end{aligned}$$

Mass production

$$\widetilde{m} = -K\rho\Phi(T)c$$

Partial momentum production

$$\widetilde{h} - u\widetilde{m} = -K\Phi(T)J$$

Hypothesis on the function Φ

$$\Phi(T) > 0, \text{ for } T > T_i, \Phi(T) = 0, \text{ for } T < T_i, \text{and Lipschitz}$$

New chemical variables

$$\begin{aligned}\vartheta &= c + J/m \\ c &= c\end{aligned}$$

Profile of the structure

Dynamical system for chemical variable

$$\begin{cases}\dfrac{\mathrm{d}c}{\mathrm{d}y} &= \dfrac{\gamma M^2}{\gamma M^2 - 1}\Omega\Phi(T)f(\vartheta, c) \\ \dfrac{\mathrm{d}\vartheta}{\mathrm{d}y} &= -\Omega c\Phi(T) \\ \begin{pmatrix}\vartheta \\ c\end{pmatrix}_{y=0} &= \begin{pmatrix}1 \\ 1\end{pmatrix} \\ \begin{pmatrix}\vartheta \\ c\end{pmatrix}_{y\to\infty} &= \begin{pmatrix}0 \\ 0\end{pmatrix}\end{cases}$$

Algebraic curve for mechanical variables

$$\begin{cases}\dfrac{\tau}{\tau_-}(\vartheta) &= \dfrac{\sigma}{\gamma+1}(1-\zeta) \\ \dfrac{T}{T_-}(\vartheta) &= \dfrac{M_-^2\sigma^2}{(\gamma+1)^2}(1-\zeta)(1+\gamma\zeta) \\ M^2(\vartheta) &= \dfrac{1-\zeta}{1+\gamma\zeta}, \qquad \zeta = \dfrac{\omega}{\sigma}\sqrt{1-\alpha^2(1-\vartheta)}\end{cases}$$

$\boldsymbol{U}_-$		$\boldsymbol{U}^{inert}$		$\boldsymbol{U}^{SD}$
$\begin{pmatrix}\tau_- \\ T_- \\ 1 \\ 1\end{pmatrix}$	$\longrightarrow$	$\begin{pmatrix}\tau(1) \\ T(1) \\ 1 \\ 1\end{pmatrix}$	$\longrightarrow$	$\begin{pmatrix}\tau(0) \\ T(0) \\ 0 \\ 0\end{pmatrix}$

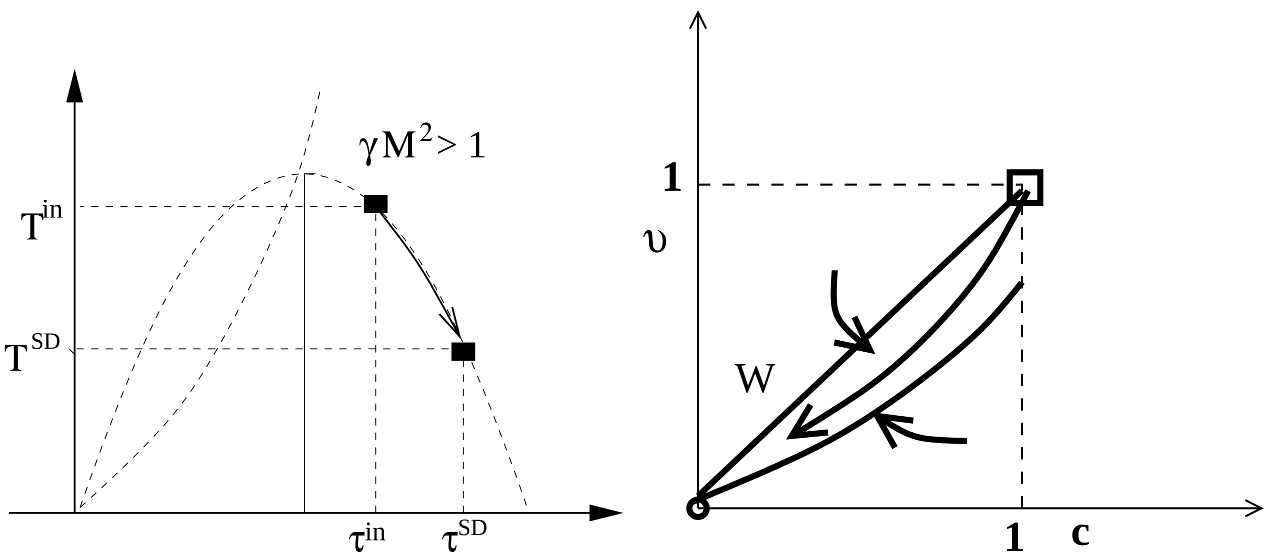

Figure 1: Orbit of the state variabiles in reacting zone.

Theorem. **If the Mach number M_- and heat release q satisfy the following conditions:**

$$M_-^2 \geq M_{CJ}^2, \quad \text{for } \gamma \geq 3$$

$$\begin{cases} \dfrac{3\gamma - 1}{(3-\gamma)\gamma} > M_-^2 > M_{CJ}^2, \\ q \leq \dfrac{\gamma^2 - 1}{2(3-\gamma)(3\gamma-1)}, \end{cases} \quad \text{for } 1 < \gamma \leq 3$$

then there exists a solution of the differential system. The solution remains in the region W for any $y > 0$.

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