



**Weierstrass Institute for
Applied Analysis and Stochastics**



Compressible Phase Change Flows and the Existence of Transition Profiles

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1 General Model

2 Compressible / Incompressible Model

1 General Model

- Mass and Momentum Conservation
- Evolution of the Phase Parameter
- Thermodynamical Correctness, Entropy Principle

2 Compressible / Incompressible Model

Two mass densities $\rho_\delta^1, \rho_\delta^2$,

$$\partial_t \rho_\delta^1 + \operatorname{div}(\rho_\delta^1 v) = +\tau_\delta$$
$$\partial_t \rho_\delta^2 + \operatorname{div}(\rho_\delta^2 v) = -\tau_\delta$$
$$\partial_t(\rho v) + \operatorname{div}(\rho v \otimes v + T_\delta) = 0,$$

where the total mass $\rho := \rho_\delta^1 + \rho_\delta^2$

Reaction rate τ_δ :

$$\rho_\delta^1 \xrightarrow{+\tau_\delta} \rho_\delta^2 \quad \rho_\delta^1 \xleftarrow{-\tau_\delta} \rho_\delta^2$$

Tension tensor T_δ consists of pressure tensor P_δ and stress tensor S

$T_\delta = P_\delta - S$, P_δ from the entropy principle,

$$S \equiv S(\rho, \varphi) = \nu_1(\rho, \varphi) \operatorname{div} v \mathbb{I} + \nu_2(\rho, \varphi) \left(\frac{1}{2} (\nabla v + (\nabla v)^T) - \frac{1}{n} \operatorname{div} v \mathbb{I} \right).$$

$\varphi := \rho_\delta^2 / \rho$ phase parameter - represents mass fraction

$$-\tau_\delta = \partial_t \rho_\delta^2 + \operatorname{div}(\rho_\delta^2 v) = \partial_t(\varphi \rho) + \operatorname{div}(\varphi \rho v) = \rho(\partial_t \varphi + v \cdot \nabla \varphi)$$

$$\begin{aligned} \implies \quad & \partial_t \rho + \operatorname{div}(\rho v) = 0 \\ & \rho(\partial_t \varphi + v \cdot \nabla \varphi) = -\tau_\delta \\ & \partial_t(\rho v) + \operatorname{div}(\rho v \otimes v + T_\delta) = 0 \end{aligned}$$

Aim

Derive a Diffuse Interface Model which approximates a Sharp Interface Model consisting of Compressible / Incompressible Flow

Free Energy Density $\varepsilon > 0, \delta > 0$, later ε as function of δ

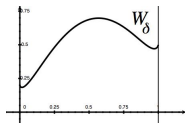
$$f_\delta(\varrho, \varphi, \nabla\varphi) := \frac{1}{\varepsilon} W^\varepsilon(\varrho, \varphi) + \frac{1}{\delta} W^\delta(\varrho, \varphi) + \delta h(\varrho) \frac{|\nabla\varphi|^2}{2} + U(\varrho, \varphi),$$

where W^δ double-well potential, local minima $m_1 = 0$ and $m_2 = 1$ and $h(\varrho) > 0$ is an arbitrary function,

$$W^\varepsilon := (\varrho - \varrho^*)^2 \varphi^2$$

$\varrho^* = \text{constant} > 0$ (Incompressible density)

U Free energy of the bulk phases



$\varphi := \varrho_\delta^2 / \varrho$ mass fraction, $\tau_\delta := \eta_\delta(\varrho, \varphi) \mu$, $\eta_\delta(\varrho, \varphi) > 0$, μ chemical potential
 $\implies \varrho(\partial_t \varphi + v \cdot \nabla \varphi) = -\eta_\delta(\varrho, \varphi) \mu$

For example $\mu := \frac{\delta f_\delta}{\delta \varphi}$ or $\mu := -\Delta \frac{\delta f_\delta}{\delta \varphi}$

[Alt 2009], Objectivity

Isothermal case: entropy principle is equivalent to the free energy inequality;

$$\text{Total free energy density: } f_{\text{tot}} = f_{\delta} + \frac{1}{2} \varrho |v|^2, \quad f_{\delta} = f_{\delta}(\varrho, \varphi, \nabla \varphi)$$

$$\text{Free energy flux: } \psi_{\text{tot}} = f_{\text{tot}} v + T_{\delta}^T v + \psi, \quad \text{where } \psi = -(\partial_t \varphi + v \cdot \nabla \varphi) f_{\delta|_{\nabla \varphi}},$$

the solution (ϱ, v, φ) of the system satisfy the inequality

$$\begin{aligned} \partial_t f_{\text{tot}} + \operatorname{div}(f_{\text{tot}} v + T_{\delta}^T v + \psi) &= \partial_t f_{\delta} + \operatorname{div}(f_{\delta} v + \psi) + Dv \cdot T_{\delta} \\ &= -\frac{1}{\varrho} \eta_{\delta}(\varrho, \varphi) \left(\frac{\delta f_{\delta}}{\delta \varphi} \right)^2 - Dv \cdot S \leq 0. \end{aligned}$$

- as usual, $\nu_1, \nu_2 > 0$, so that $Dv \cdot S \geq 0$; $\eta_{\delta} > 0$;
- and where **Pressure tensor** P_{δ} :

$$\begin{aligned} P_{\delta} &\equiv P_{\delta}(\varrho, \varphi, \nabla \varphi) = (-f_{\delta} + \varrho f_{\delta|\varrho}) \mathbb{I} + \nabla \varphi \otimes f_{\delta|\nabla \varphi} \\ &= \left(\frac{1}{\varepsilon} p_{W^{\varepsilon}}(\varrho, \varphi) + \frac{1}{\delta} p_{W^{\delta}}(\varrho, \varphi) + p_U(\varrho, \varphi) + \delta p_h(\varrho) \frac{|\nabla \varphi|^2}{2} \right) \mathbb{I} + \delta h(\varrho) \nabla \varphi \otimes \nabla \varphi \end{aligned}$$

with $p_U(\varrho, \varphi) := -U(\varrho, \varphi) + \varrho U|_{\varrho}(\varrho, \varphi)$, $p_{W^{\delta}}$, p_h dito

the last two summands (terms with $\nabla \varphi$) stand for the '**surface tension**' between the different phases;

1 General Model

2 Compressible / Incompressible Model

- Diffusive Interface Model
- Sharp Interface Model - Bulk Region
- Sharp Interface Model - Interface
- Interfacial Profile

Assume: $W^\delta(\varrho, \varphi) := \varrho W(\varphi)$, $W(m_1) \neq W(m_2)$
 $\eta_\delta = 1/\delta$, $W^\varepsilon(\varrho, \varphi) := (\varrho - \varrho^*)^2 \varphi^2$

Connection of both parameters

$$\delta \equiv \delta(\varepsilon) = \varepsilon^2$$

The incompressible limes slower than the sharp interface limes

$$\partial_t \varrho + \operatorname{div}(\varrho v) = 0, \quad (1)$$

$$\partial_t(\varrho v) + \operatorname{div}(\varrho v \otimes v) + \nabla \left(\underbrace{\frac{1}{\varepsilon} p_{W^\varepsilon}(\varrho, \varphi)}_{=0} + \frac{1}{\varepsilon^2} p_{\varrho W}(\varrho, \varphi) + p_U(\varrho, \varphi) \right) \quad (2)$$

$$+ \varepsilon^2 \operatorname{div} \left(p_h(\varrho) \frac{|\nabla \varphi|^2}{2} \mathbb{I} + h(\varrho) \nabla \varphi \otimes \nabla \varphi \right) = \operatorname{div}(S),$$

$$\delta \varrho (\partial_t \varphi + v \cdot \nabla \varphi) = -\frac{1}{\varepsilon} W_{|\varphi}^\varepsilon(\varrho, \varphi) - \frac{1}{\varepsilon^2} \varrho W'(\varphi) - U_{|\varphi}(\varrho, \varphi) \quad (3)$$

$$+ \varepsilon^2 \operatorname{div}(h(\varrho) \nabla \varphi),$$

where

$$p_{W^\varepsilon}(\varrho, \varphi) = (\varrho - \varrho^*)(\varrho + \varrho^*) \varphi^2$$

Formal Matched Asymptotic Expansion in ε

$$\varepsilon \searrow 0$$

'Low Mach Number Limit' as $\varepsilon \searrow 0$, then $\delta = \varepsilon^2 \searrow 0$,

Outer Expansion $\varrho(t, x) = \varrho_0(t, x) + \varepsilon \varrho_1(t, x) + \delta \varrho_2(t, x) + \mathcal{O}(\varepsilon^2)$

$$v(t, x) = v_0(t, x) + \varepsilon v_1(t, x) + \delta v_2(t, x) + \mathcal{O}(\varepsilon^2)$$

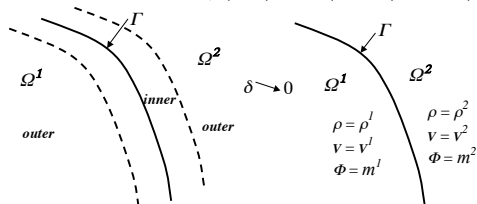
$$\varphi(t, x) = \varphi_0(t, x) + \varepsilon \varphi_1(t, x) + \delta \varphi_2(t, x) + \mathcal{O}(\varepsilon^2)$$

Interfacial Expansion $\varrho(t, y + \delta r \vec{n}_\Gamma(t, y)) = R(t, y, r)$

$$\varrho(t, x) = R(t, y, r) = R_0(t, y, r) + \varepsilon R_1(t, y, r) + \delta R_2(t, y, r) + \mathcal{O}(\varepsilon^2)$$

$$v(t, x) = V(t, y, r) = V_0(t, y, r) + \varepsilon V_1(t, y, r) + \delta V_2(t, y, r) + \mathcal{O}(\varepsilon^2)$$

$$\varphi(t, x) = \Phi(t, y, r) = \Phi_0(t, y, r) + \varepsilon \Phi_1(t, y, r) + \delta \Phi_2(t, y, r) + \mathcal{O}(\varepsilon^2)$$



$\varrho_1, v_1,$ and φ_1

are perturbations in the bulk regions

$R_1, V_1,$ and Φ_1

are perturbations in the interfacial regions

For $t > 0$, there is an unknown free interface Γ_t , $\Omega = \Omega_t^1 \cup \Gamma_t \cup \Omega_t^2$,

Bulk Region: Compressible / Incompressible Navier-Stokes system

$$\partial_t \varrho^1 + \operatorname{div}(\varrho^1 v^1) = 0, \quad \text{in } \Omega_t^1$$

$$\partial_t(\varrho^1 v^1) + \operatorname{div}(\varrho^1 v^1 \otimes v^1 + T^1(\varrho^1, m_1)) = 0,$$

$$\operatorname{div} v^2 = 0, \quad \text{in } \Omega_t^2$$

$$\varrho^* (\partial_t v^2 + \operatorname{div}(v^2 \otimes v^2)) + \operatorname{div} T^2(\varrho^*, m_2) = 0,$$

$T^k = p^k \mathbb{I} - s^k$ tension tensor, p^k scalar pressure, s^k stress tensor,

$$\text{in } \Omega_t^1: \quad \varphi = 0$$

$$p^1 \equiv p_V(\varrho^1, m_1),$$

$$s^1 \equiv s(\varrho^1, m_1) = \nu_1(\varrho^1, m_1) \operatorname{div} v^1 \mathbb{I} + \nu_2(\varrho^1, m_1) \left(\frac{1}{2} (\nabla v^1 + (\nabla v^1)^T) - \frac{1}{n} \operatorname{div} v^1 \mathbb{I} \right)$$

$$\text{in } \Omega_t^2: \quad \varphi = 1$$

$$p^2 \text{ unknown,}$$

$$s^2 \equiv s(\varrho^*, m_2) = \tilde{\nu}(\varrho^*, m_2) \Delta v^2$$

Energy-Inequality

$$\int_0^t \int_{\Omega} \frac{1}{\varepsilon} (\varrho - \varrho^*)^2 \varphi^2 dx dt \leq C_{\text{data}} \Rightarrow \varrho = \varrho^* \quad \text{in } \Omega_t^2 \quad \text{for } \varepsilon \searrow 0$$

Then in Ω_t^2 $\varrho(t, x) \approx \varrho_0(t, x) + \varepsilon \varrho_1(t, x)$

Comparison order ε^0

$$\partial_t \varrho_0 + \operatorname{div}(\varrho_0 v_0) = 0,$$

$$\begin{aligned} \partial_t(\varrho_0 v_0) + \operatorname{div}(\varrho_0 v_0 \otimes v_0) + \nabla(p_U(\varrho_0, \varphi_0) + 2\varrho_0 |\varphi_0|^2 \varrho_1 + 2(\varrho_0 - \varrho^*)(\varrho_0 + \varrho^*)\varphi_0 \varphi_1) \\ = \operatorname{div}\left(\nu_1(\varrho_0, \varphi_0) \operatorname{div} v_0 \mathbb{I} + \nu_2(\varrho_0, \varphi_0) \left(\frac{1}{2}(\nabla v_0 + (\nabla v_0)^T) - \frac{1}{n} \operatorname{div} v_0 \mathbb{I}\right)\right). \end{aligned}$$

and $\varrho_0(t, x) = \varrho^*$, $\varphi_0 = 1$ and $\varphi_1 = 0$, then

$$\Rightarrow \varrho^* \operatorname{div}(v_0) = 0, \quad \varrho^* (\partial_t v_0 + \operatorname{div}(v_0 \otimes v_0)) + \nabla(2\varrho^* \varrho_1) = \tilde{\nu} \Delta v_0$$

$$\Rightarrow p(t, x) = 2\varrho^* \varrho_1(t, x), \quad \gamma := \frac{1}{2\varrho^*}$$

that means in Ω_t^2 $\varrho(t, x) \approx \varrho^* + \varepsilon \gamma p(t, x)$

Different Jump conditions on $\Gamma := \{(t, x) : x \in \Gamma_t\}$: $[v]_{\Gamma} \neq 0$ and $[\varrho]_{\Gamma} \neq 0$

Relative interface velocity in normal direction $\lambda := (v_{\Gamma} - v) \cdot \vec{n}_{\Gamma}$

$v_{\Gamma} \cdot \vec{n}_{\Gamma}$ normal interface velocity of Γ , κ curvature

Interface Conditions

$$\left. \begin{aligned} [\varrho\lambda]_{\Gamma} &= 0, & \text{on } \Gamma, \\ -\varrho\lambda[v]_{\Gamma} + [T^k \vec{n}_{\Gamma}]_{\Gamma} &= \operatorname{div}_y^{\Gamma}(\gamma(\mathbb{I} - \vec{n}_{\Gamma} \otimes \vec{n}_{\Gamma})) = \gamma\kappa \cdot \vec{n}_{\Gamma} \vec{n}_{\Gamma} + \nabla^{\Gamma} \gamma, & \text{on } \Gamma, \\ [v]_{\Gamma} &= \omega \vec{n}_{\Gamma}, & \text{on } \Gamma, \\ G(\varrho^1, \varrho^*) &= 0, & \text{on } \Gamma, \end{aligned} \right\}$$

where $\Phi = m_1$ in Ω_t^1 and $\Phi = m_2$ in Ω_t^2 , and

γ surface tension, ω capillarity force,

the two mass densities of the bulk phases are connected by G

$$\omega = \omega[\varrho\lambda] := \int_{m_1}^{m_2} \frac{e_h(R)}{\bar{\mu}(R,s)} \left\{ \frac{1}{2} \frac{1}{h(R)} \sqrt{2 \int_{m_1}^s h(R) R W' d\bar{s}} \right\} ds,$$

$$\gamma = \gamma[\varrho\lambda] := \int_{m_1}^{m_2} \left(1 - \frac{1}{2} \frac{\mu_2(R,s)}{\bar{\mu}(R,s)} \frac{e_h(R)}{h(R)} \right) \sqrt{\int_{m_1}^s 2 h(R) R W' d\bar{s}} ds.$$

Mass flux $M := \lambda^1 \varrho^1 = \lambda^2 \varrho^2$. The function R is the solution of the

Inner Interface Problem

$$\begin{aligned} M^2 \partial_s \left(\left| h(R) g(R, \cdot) \partial_s \left(\frac{1}{R} \right) \right|^2 \right) &= 2 h(R) R \partial_s W \\ \partial_s R(m_1) &= 0, \quad \partial_s R(m_2) = 0. \end{aligned}$$

where $g = \tilde{v}/e_h$, $e_h(z) = [z h(z)]'$ energetic part, and $e_h \geq 0$.

Theorem

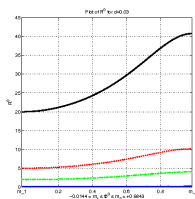
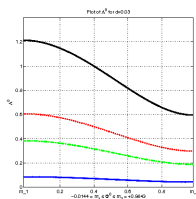
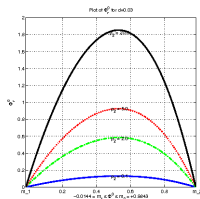
We consider $W(\varphi) := W_0(\varphi) + \varepsilon W_1(\varphi)$.

W_0 and W_1 double-well potentials, twice continuously differentiable functions in φ , local minima on m_1 and m_2 , and local maximum on $s_a = (m_1 + m_2)/2$.

$W_0(m_1) = W_0(m_2)$ and symmetric function on $\varphi = s_a$, $W_1(m_1) \neq W_1(m_2)$, $h \equiv 1$.

\implies

Then, there is a $\varepsilon_0 \in \mathbb{R}_+$ and for each $M \in \mathbb{R} \setminus \{0\}$ has the Inner Interface Problem a solution $R \in C^1([m_1, m_2]) \cap C^2((m_1, m_2))$ as $0 < \varepsilon < \varepsilon_0$.



Let $h \equiv 1$ and $\tilde{\mu} \equiv 1$, then $g(R, \cdot) = 1$. Then

$$M^2 \partial_s \left(\left| \partial_s \left(\frac{1}{R} \right) \right|^2 \right) = 2R \partial_s W \quad \partial_s R(m_1) = 0, \quad \partial_s R(m_2) = 0.$$

Then

$$\partial_s \left(\frac{1}{R} \right) = \frac{1}{|M|} \sqrt{\int_{m_1}^s 2RW' d\bar{s}} \quad \text{and}$$

$$0 = \partial_s \left(\frac{1}{R} \right) (m_2) = \frac{1}{|M|} \sqrt{\int_{m_1}^{m_2} 2RW' d\bar{s}},$$

that is

$$\partial_s \left(\frac{1}{R} \right) = \frac{1}{|M|} \sqrt{\int_{m_1}^s 2RW' d\bar{s}}, \quad \int_{m_1}^{m_2} RW' d\bar{s} = 0$$

Let $B \subset C^0([m_1, m_2])$ closed with

$$B := \left\{ u \in C^0([m_1, m_2]) : 0 < c_k \leq u \leq C_g, \int_{m_1}^{m_2} \frac{W'}{u} ds = 0, u \text{ monotone increasing} \right\}.$$

We introduce the operator

$$F : B \rightarrow C^0([m_1, m_2]), \quad u_1 \in B \mapsto u_3 = F(u_1) \in C^0([m_1, m_2]),$$

where

$$\begin{aligned} u_2(s) &= \frac{1}{|M|} \int_{m_1}^s \sqrt{\int_{m_1}^{\bar{s}} \frac{2W'}{u_1} d\bar{s}} d\bar{s} \\ u_3(s) &= u_2(s) + C(u_2), \quad \text{with} \quad \int_{m_1}^{m_2} \frac{W'}{u_2 + C(u_2)} ds = 0. \end{aligned}$$

1. Existence of $C(u_2)$ - intermediate value theorem
2. F is a non-expanding map - by choosing c_k and C_g
3. F is a contraction - for a weighted norm, Banach fixed point theorem

$$f_\delta(\varrho, \varphi, \nabla\varphi) := \frac{1}{\varepsilon} W^\varepsilon(\varrho, \varphi) + \frac{1}{\delta} W^\delta(\varrho, \varphi) + \delta h(\varrho) \frac{|\nabla\varphi|^2}{2} + U(\varrho, \varphi),$$

Generalization to $h \neq 1$

1. The function h fulfills a special growth condition

$$h(z_2) z_2^{\frac{2-n}{n}} \leq h(z_1) z_1^{\frac{2-n}{n}} \quad \text{for all } z_1 \leq z_2, \quad z_1, z_2 \in \mathbb{R}_+,$$

Then, $e_h(z) \neq 0$ for all $z \in \mathbb{R}$ and surface tension $\gamma > 0$

2. $h > 0$ is an arbitrary continuously differentiable function and bounded from below, that is $h(z) \geq h_s > 0$ for all $z \in \mathbb{R}$

Theorem

Let $W(m_1) \neq W(m_2)$. Then, it exists G with $\mathbf{G}(\varrho^1, \varrho^*) = \mathbf{0}$.

Definition: The function G is defined by solution $R = R[M]$ with $R[M(t, y)](m_1) = \varrho^1(t, y)$, $R[M(t, y)](m_2) = \varrho^*(t, y)$.

- Incompressible limit is a singular limit,

On Ω^1 : compressible

$$\partial_t \varrho'_1 + \operatorname{div}(\varrho'_1 v_1 + \varrho_1 v'_1) = 0,$$

$$\begin{aligned} \partial_t(\varrho'_1 v_1 + \varrho_1 v'_1) + \operatorname{div}(\varrho'_1 v_1 \otimes v_1 + \varrho_1 v'_1 \otimes v_1 + \varrho_1 v_1 \otimes v'_1) + \nabla(p_{U_1|_\varrho}(\varrho_1, m_1)\varrho'_1) \\ = \operatorname{div}(\operatorname{Lin}S) \end{aligned}$$

On Ω^2 : incompressible

$$\partial_t \varrho'_2 + \operatorname{div}(\varrho'_2 v_2 + \varrho^* v'_2) = 0,$$

$$\partial_t(\varrho'_2 v_2 + \varrho^* v'_2) + \operatorname{div}(\varrho'_2 v_2 \otimes v_2) + \varrho^* \operatorname{div}(v'_2 \otimes v_2 + v_2 \otimes v'_2) + \nabla p' = \operatorname{div}(\operatorname{Lin}S)$$

- In compressible flows the sound velocity is finite, there are wave solutions for small perturbations
- In incompressible flows the sound velocity is infinite, but $\varepsilon > 0$ consider $\varrho = \varrho^* + \varepsilon \gamma p$

Thank you for your attention !