The use of the Chapman–Jouguet theory for solving the Riemann–problem with vaporization

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Overview

1. Thermodynamic of phase transition
2. The Riemann Problem with equilibrium E.O.S
3. The Riemann Problem out of equilibrium
4. Numerical scheme
5. Numerical results
Thermodynamic model (1/3)

- No Van Der Waals (Euler system is not hyperbolic, difficulty to make a difference between metastable and equilibrium state)

- Two equations of state $\varepsilon_l(P, T)$ and $\varepsilon_g(P, T)$

- Adimensionned coefficients

  $\gamma = -\frac{\tau}{P} \left( \frac{\partial P}{\partial \tau} \right)_s$

  $\Gamma = -\frac{\tau}{T} \left( \frac{\partial T}{\partial \tau} \right)_s$

  $g = \frac{P\tau}{T^2} \left( \frac{\partial T}{\partial s} \right)_\tau$

- Thermodynamic stability requires that

  $\gamma, g \geq 0 \quad \gamma g - \Gamma^2 > 0$
Thermodynamic model (2/3)

- Mixture zone
  - Suppose that fluids are locally non miscible
    \[ V_l + V_g = V_{\text{tot}} \]
  - Optimization of mixture entropy

\[ \implies \text{When the mixture is stable} \]

\[ P_l = P_g \quad T_l = T_g \quad \mu_l = \mu_g \]
Thermodynamic model (2/3)

- Mixture zone

\[ P_l = P_g \quad T_l = T_g \quad \mu_l = \mu_g \]

\[ \mu_l(P, T) = \mu_g(P, T) \implies P = P_{\text{sat}}(T) \]

\[ \tau_l(T) = \tau_l(P_{\text{sat}}(T), T) \quad s_l(T) = s_l(P_{\text{sat}}(T), T) \]
Thermodynamic model (2/3)

- Mixture zone

- 3 E.O.S.

\[
\frac{\gamma - \gamma_m}{\gamma_m} = (\gamma g - \Gamma^2) \left( \frac{T}{\tau} \frac{ds_b}{dP} \right)^2 > 0
\]
Provided \( \frac{dP_{\text{sat}}}{dT} = \frac{s_g(T) - s_l(T)}{\tau_g(T) - \tau_l(T)} > 0 \)

\( \Phi : \begin{pmatrix} y \\ T \end{pmatrix} \mapsto \begin{pmatrix} y \tau_g(T) + (1 - y) \tau_l(T) \\ y s_g(T) + (1 - y) s_l(T) \end{pmatrix} = \begin{pmatrix} \tau \\ s \end{pmatrix} \) is a local diffeomorphism

The mixture equation of state is convex
Thermodynamic model (3/3)

Provided

\[
\frac{dP_{\text{sat}}}{dT} = \frac{s_g(T) - s_l(T)}{\tau_g(T) - \tau_l(T)} > 0 \implies \text{O.K.}
\]

Dodecane, two stiffened gas, coefficients calculated by Lemétayer et al., Int. J. of Thermal Sciences.
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Equilibrium EOS (1/3)

Look for undercompressive waves for the Euler system

\[
\begin{align*}
\partial_t \rho + \partial_x (\rho u) &= 0 \\
\partial_t (\rho u) + \partial_x (\rho u^2 + P) &= 0 \\
\partial_t (\rho E) + \partial_x ((\rho E + P)u) &= 0
\end{align*}
\]

with

\[
E = \varepsilon + \frac{1}{2} u^2
\]

\(\varepsilon, P, \rho\) are linked with an E.O.S.
Equilibrium EOS (1/3)

- Look for undercompressive waves for the Euler system
- Variables are function of $\xi = x/t$

\[ \pm \rho c = \rho (u - \xi) \]
\[ \pm \rho du + dP = 0 \]
\[ d\varepsilon + P d\tau = 0 \implies S = \text{cste} \]

- We take $P$ as a parameter, all the thermodynamic is known thanks for $P$ and $S$. $u$ is obtained by integrating

\[ \pm \rho du + dP = 0 \]

Is that integration affected by phase transition?
Equilibrium EOS (2/3)

Consequences for characteristic curves
Equilibrium EOS (2/3)

- Consequences for characteristic curves
- Characteristic curves in point $A$

![Diagram showing characteristic curves in a liquid mixture at point $A$.](image-url)
Equilibrium EOS (2/3)

- Consequences for characteristic curves
- Characteristic curves in point $A$  \implies OK
- Characteristic curves in point $B$
Equilibrium EOS (2/3)

- Consequences for characteristic curves
- Characteristic curves in point $A$ $\implies$ OK
- Characteristic curves in point $B$ $\implies$ non regular wave ???

But do $A$ and $B$ really exist?
Existence of $A$ and $B$ depends on the behaviour of isentrope near the saturation curves.

Regular fluid:
Existance of $A$ and $B$ depends on the behaviour of isentrope near the saturation curves.

- Regular fluid: Isentropes cross the saturation curve from the pure phase to the mixture
- Retrograde fluid:

\[ T \]

\[ S \]
Existence of $A$ and $B$ depends on the behaviour of isentrope near the saturation curves.

- Regular fluid: Isentropes cross the saturation curve from the pure phase to the mixture
- Retrograde fluid: Isentropes cross the saturation curve from the mixture to the pure phase

Liquid saturation curve is always regular. Vapor saturation curve exhibits often at least one retrograde part.
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Out of equilibrium Riemann problem (1/4)

- metastable states (Thomson et al., JFM 1986 and 1988; Simoes-Moreira, JFM 1999)

\[ \text{metastable state} \]

\[ \Rightarrow \text{need for a multiphase code} \]
Out of equilibrium Riemann problem (1/4)

- metastable states (Thomson et al., JFM 1986 and 1988; Simoes-Moreira, JFM 1999)
- A phase transition wave is a self–similar discontinuity
  \[ M = \frac{u_2 - u_1}{\tau_2 - \tau_1}, \]
  \[ M^2 = -\frac{p_2 - p_1}{\tau_2 - \tau_1}, \]
  \[ \varepsilon_2 - \varepsilon_1 + \frac{1}{2}(p_2 + p_1)(\tau_2 - \tau_1) = 0 \]

beware! \( \varepsilon_1 \) == E.O.S of the liquid

\( \varepsilon_2 \) == E.O.S of the mixture or the gas

\[ \Rightarrow \] Chapman–Jouguet (CJ) theory
Out of equilibrium Riemann problem (2/4)

- Assumptions for the use of the CJ theory:
  - EOS are convex
  - \( \varepsilon_2(P, \tau) - \varepsilon_1(P, \tau) < 0 \)
  - upstream state \( \notin \) the set of the downstream states
Assumptions for the use of the CJ theory:

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- \( \tau \) increases \( \Longrightarrow \) deflagration
Assumptions for the use of the CJ theory:

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- $\tau$ increases $\implies$ deflagration
- No strong deflagrations $\implies$ subsonic wave
Assumptions for the use of the CJ theory:
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- \( \tau \) increases \( \Rightarrow \) deflagration
- No strong deflagrations \( \Rightarrow \) subsonic wave
Out of equilibrium Riemann problem (3/4)

\[
\delta \varepsilon(y_l) = y_l \varepsilon_l(P, \tau_l(P)) + (1 - y_l) \varepsilon_g(P, \tau_g(P)) \\
- \varepsilon_l(P, y_l \tau_l(P) + (1 - y_l) \tau_g(P)) < 0
\]

\[
\frac{d\delta \varepsilon}{dT}(y_l) = (\tau_g - \tau_l) \frac{T^2}{\tau} \frac{\gamma g - \Gamma^2}{\Gamma} \frac{ds_l}{dT}
\]
Out of equilibrium Riemann problem (3/4)

\[
\delta \varepsilon(y_l) = y_l \varepsilon_l(P, \tau_l(P)) + (1 - y_l) \varepsilon_g(P, \tau_g(P)) < 0
\]

- entropy growth criterion
Out of equilibrium Riemann problem (3/4)

\[
\delta \varepsilon (y_l) = y_l \varepsilon_l (P, \tau_l (P)) + (1 - y_l) \varepsilon_g (P, \tau_g (P))
\]

\[
- \varepsilon_l (P, y_l \tau_l (P) + (1 - y_l) \tau_g (P)) < 0
\]

entropy growth criterion

\[
\frac{ds}{d\tau_0} = \frac{\gamma_m P_0}{T \Gamma_m} \left( \frac{\gamma_l \Gamma_m}{\gamma_m} \left( \frac{\tau_P}{\tau_0} - 1 \right) + \frac{\tau_P}{\tau_0} \left( \frac{\gamma_l}{\gamma_m} - 1 \right) \right)
\]
Out of equilibrium Riemann problem (4/4)

- one indeterminate

![Diagram showing the out of equilibrium Riemann problem with states 0, 0*, vaporization, sonic wave, and contact surface.]
Out of equilibrium Riemann problem (4/4)

- one indeterminate
- A “physical” closure (Lemétayer et al, JCP 2005)
Out of equilibrium Riemann problem (4/4)

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- ... leads to a solution that is not continuous with respect to its initial data!!!
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Numerical method (Continuous model)

- **Multiphase model**

\[
\begin{align*}
\frac{\partial \alpha_k}{\partial t} + u_I \frac{\partial \alpha_k}{\partial x} &= 0 \\
\frac{\partial \alpha_k \rho_k}{\partial t} + \frac{\partial \alpha_k \rho u_k}{\partial x} &= 0 \\
\frac{\partial \alpha_k \rho_k u_k}{\partial t} + \frac{\partial \alpha_k \left( \rho_k u_k^2 + p_k \right)}{\partial x} &= p_I \frac{\partial \alpha_k}{\partial x} \\
\frac{\partial \alpha_k \rho_k E_k}{\partial t} + \frac{\partial \alpha_k u_k \left( \rho_k E_k + p_k \right)}{\partial x} &= u_I p_I \frac{\partial \alpha_k}{\partial x}
\end{align*}
\]

- **problems**
  - How to choose \( u_I, p_I \) ? modelling problem
  - non conservative products
Numerical method (Continuous model)


Assumptions

1. Location of bubbles, size, micro-scale details of the flow are unknown
2. Given a set of initial and boundary condition, we consider one experiment as a realisation of this flow.
3. What we expect to observe/compute is an ensemble average of these experiments

1. Equations for each phase
   Euler
   \[ \chi_k \left( \partial_t U_k + \partial_x F_k(U_k) \right) = 0 \]
   + Topological equation for the interface
   \[ \partial_t \chi_k + \sigma \partial_x \chi_k = 0 \]
Numerical method (Continuous model)


1. Equations for each phase
   Euler + Topological equation for the interface

2. Average

\[
\begin{align*}
\partial_t \alpha_k \rho_k + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) &= \mathcal{E} (\rho (\mathbf{u}_k - \sigma) \cdot \nabla \chi_k) \\
\partial_t \alpha_k \rho_k \mathbf{u}_k + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \otimes \mathbf{u}_k + \alpha_k P_k) &= \mathcal{E} ((\rho_k \mathbf{u}_k (\mathbf{u}_k - \sigma) + P_k) \cdot \nabla \chi_k) \\
\partial_t \alpha_k \rho_k E_k + \nabla \cdot (\alpha_k \rho_k E_k \mathbf{u}_k + \alpha_k P_k \mathbf{u}_k) &= \mathcal{E} ((\rho_k E_k (\mathbf{u}_k - \sigma) + P_k \mathbf{u}_k) \cdot \nabla \chi_k) \\
\partial_t \alpha_k + \mathcal{E} (\sigma \cdot \partial_x \chi_k) &= 0
\end{align*}
\]
Numerical method (Continuous model)


1. Equations for each phase
   - Euler + Topological equation for the interface

2. Average

3. Modelling

\[ \mathcal{E} \left( P_k \nabla \chi_k \right) = P_I \nabla \alpha_k \]

\[ \mathcal{E} \left( (P_k \mathbf{u}) \cdot \nabla \chi_k \right) = P_I \mathbf{u}_I \nabla \alpha_k \]

\[ \mathcal{E} \left( \sigma \cdot \nabla \chi_k \right) = \mathbf{u}_I \nabla \alpha_k \]
Numerical method (Continuous model)


1. Equations for each phase
   - Euler + Topological equation for the interface

2. Average
   - Closure Problems

3. Modelling
   - Non conservative Products+ Closure Pbs
Numerical method

a Cell of the mesh. We know \((\alpha, \rho, u, P)\) in each cell
Numerical method

\[ t_{n+1} \]

\[ \sum' \quad \sum \quad \sum \quad \sum \quad \sum \quad \sum'\prime \prime \]

\[ t_n \]

\[ x_{i-1/2} \quad x_{i+1/2} \]

- cut the cell into subcells, taking care of \[ \int_{\Delta x} X = \alpha \]
- do the same for the neighbours cells
Numerical method

Evolution in time
Numerical method

- Averaging procedure
- Probability in the boundary of the cell:

\[
P_{i+1/2}(\Sigma_1, \Sigma_1) = \min(\alpha_i^{(1)}, \alpha_i^{(1)})
\]

\[
P_{i+1/2}(\Sigma_1, \Sigma_2) = \max(0, \alpha_i^{(1)} - \alpha_{i+1}^{(1)})
\]

- see Abgrall/Saurel, JCP, 2003
Numerical method

- extension to reactive flux
- Total vaporization wave

→ replace the contact discontinuity by the vaporization wave
Numerical method

- extension to reactive flux
- Partial vaporization wave

\[ \sigma \]

\[ u^* \]

\[ \text{mixture} \]

\[ \text{gas} \]

\[ \text{liquid} \]
Numerical method

- extension to reactive flux
- Partial vaporization wave

Average of total and partial vaporization wave
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## Vaporisation

### Shock tube

<table>
<thead>
<tr>
<th>Gas</th>
<th>Liquid</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P = 10^5\text{Pa}$</td>
<td>$P = 10^9\text{Pa}$</td>
</tr>
<tr>
<td>$\rho = 0.1\text{kg.m}^{-3}$</td>
<td>$\rho = 3\text{kg.m}^{-3}$</td>
</tr>
<tr>
<td>$u = 0$</td>
<td>$u = 0$</td>
</tr>
</tbody>
</table>
Vaporisation

Density

Vaporisation

Velocity

analytical
computed
Vaporisation

Pressure

Conclusion

- construction of a solution for the Riemann problem with phase transition
  - entropy growth condition
  - continuity of the intermediates states with respect to the initial states
- easy computation thanks for the discrete equation method (right and left states of the Riemann problems are always pure fluids)
Thank you!
Bibliography (1/5)

- Very useful and common books on Hyperbolic problems

- Fitting of EOS with Stiffened gas (in French)
The first paper with the computation of reactive waves with the Discrete equations method

The famous “Liu” solution for liquefaction

THE paper on the Riemann problem with kinks and other dirty tricks in EOS
Some experiments


The solution of Wendroff for the Riemann problem with smooth loss of convexity


On the Discrete Equations Method

