Compressible Euler equations for two phase flows with phase transition

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Outline

Introduction

- Models of Baer-Nunziato type
  - full Euler system to each phase
  - Zein, Hantke, Warnecke. *Modeling phase transition for compressible two-phase flows applied to metastable liquids*, J. Comput. Phys., 229 (2010), pp. 2964-2998.
- Models using one set of Euler equations
  - Dumbser, Iben, Munz. *Efficient implementation of high order unstructured WENO schemes for cavitating flows*, Computers & Fluids, 86 (2013), pp. 141-168.
  - Hantke, Dreyer, Warnecke. *Exact solutions to the Riemann problem for compressible isothermal Euler equations for two phase flows with and without phase transition*, Quarterly of Applied Mathematics, vol. LXXI 3 (2013), pp. 509-540.

Model desription - isothermal case

Isothermal Euler equations

$$\begin{aligned} \rho_t + (\rho v)_x &= 0 \\ (\rho v)_t + (\rho v^2 + p)_x &= 0 \end{aligned}$$

Jump conditions across discontinuities

$$\begin{aligned} [\![\rho(v - W)]\!] &= 0 \\ \rho(v - W)[\![v]\!] + [\![p]\!] &= 0 \end{aligned}$$

Mass flux across discontinuities

$$Z = -\rho(v - W) \qquad \text{with} \qquad Z, W = \begin{cases} Q, S & \text{shock wave} \\ z, w & \text{phase boundary} \end{cases}$$

Kinetic relation

$$z = 0 \quad \text{or} \qquad z = \frac{p_V}{\sqrt{2\pi}} \left(\frac{m}{kT_0} \right)^{3/2} [\![g + e_{kin}]\!]$$

Initial data

Riemann initial data

Equations of state

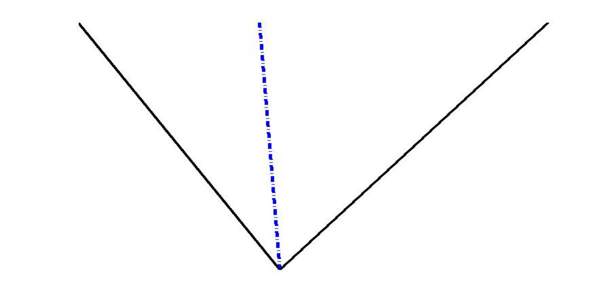
- ideal gas law, Tait equation
- stiffened gas law, generalized stiffened gas law, IAPWS

Results

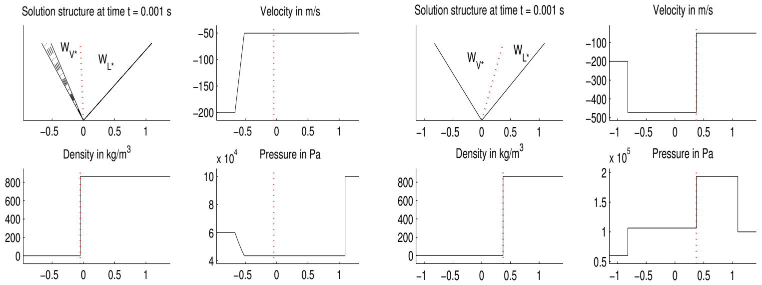
- structure of the solution
- characterization of phase boundaries
- existence results
- uniqueness results
- relashionship between solutions with / without phase transition
- creation of new phases

Isothermal case - structure of the solution

- selfsimilar solution
- two classical waves, one phase boundary
- phase boundary: contact discontinuity or nonclassical discontinuity



Example


Solution structure at time t = 0.001 s
W_{V*}
W_{L*}
Velocity in m/s
Density in kg/m³
Pressure in Pa
x 10⁴
Solution structure at time t = 0.001 s
W_{V*}
W_{L*}
Velocity in m/s
Density in kg/m³
Pressure in Pa
x 10⁵

Model description - nonisothermal case

- Euler equations
- Equations of state
- Jump conditions across discontinuities [1]

$$
\begin{aligned}
0 &= \frac{\partial \rho_I}{\partial t} - [\![z]\!] \\
0 &= \frac{\partial (\rho_I w)}{\partial t} - [\![zv]\!] + [\![p]\!] \\
0 &= \frac{\partial e_I}{\partial t} + [\![-z(e + \frac{p}{\rho} + \frac{1}{2}(v-w)^2) + q]\!]
\end{aligned}
$$

- Kinetic relation

$$z = 0 \qquad \text{or} \qquad z = \quad ?$$

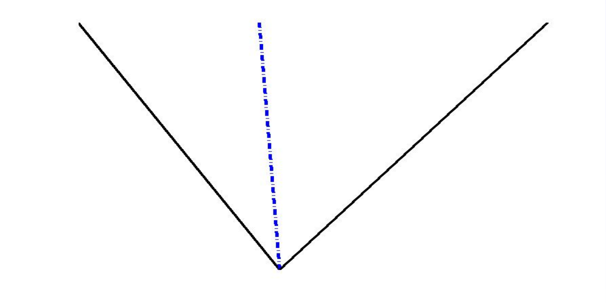
- Entropy condition

$$0 \leq \zeta = \frac{\partial s_I}{\partial t} + [\![-zs + \frac{q}{T}]\!]$$

[1] Dreyer, On Jump Conditions at Phase Boundaries for Ordered and Disordered Phases, WIAS Preprint, 869, 2003

Case I: $z = 0$ - no phase transition

- Balances across the phase boundary simplify
- $$v_L = v_V = w \qquad p_L = p_V$$
- Phase boundary is a contact wave



The exact solution is selfsimilar and can be constructed easily.

Case II: $z \neq 0$ - phase transition may occur

- Simplifying assumptions: $\rho_I = 0, e_I = 0 \quad \Rightarrow \quad \frac{\partial s_I}{\partial t} = 0$
- Balances across the interface

$$
\begin{aligned}
0 &= [\![z]\!] \qquad \Leftrightarrow \qquad 0 = [\![\rho(v-w)]\!] \\
0 &= -z[\![v]\!] + [\![p]\!] \\
0 &= z[\![(e + \frac{p}{\rho} + \frac{1}{2}(v-w)^2)]\!]
\end{aligned}
$$

- Entropy condition

$$0 \leq \zeta = -z[\![s]\!]$$

- Kinetic relation

$$z \sim -[\![s]\!]$$

Case IIa: $z \neq 0$

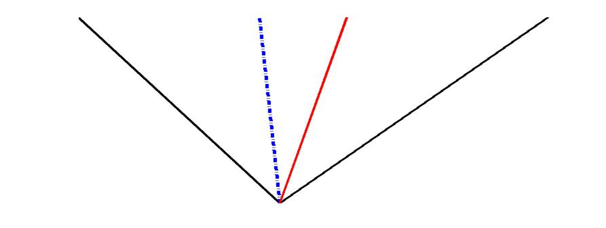
- Entropy condition

$$0 \leq \zeta = -z[\![s]\!]$$

- Kinetic relation

$$z \sim -[\![s]\!]$$

- The exact solution is selfsimilar and can be constructed easily.
- Two classical shock or rarefaction waves, contact wave, phase boundary



- Problem: Thermal equilibrium cannot occur. Only evaporation processes are possible.

Case IIb: $z \neq 0$

We need more general assumptions!

- Balances across phase boundaries

$$
\begin{aligned}
0 &= \frac{\partial \rho_I}{\partial t} - [\![z]\!] \\
0 &= \frac{\partial (\rho_I w)}{\partial t} - [\![zv]\!] + [\![p]\!] \\
0 &= \frac{\partial e_I}{\partial t} + [\![-z(e + \frac{p}{\rho} + \frac{1}{2}(v-w)^2) + q]\!]
\end{aligned}
$$

- Entropy condition

$$0 \leq \zeta = \frac{\partial s_I}{\partial t} + [\![-zs + \frac{q}{T}]\!]$$

- Taking into account heat conduction
-

$$\frac{\partial s_I}{\partial t} \neq 0$$

Case IIb: $z \neq 0$

- Simplifying assumptions: $\rho_I = 0$
- Balances across phase boundaries

$$
\begin{aligned}
0 &= [\![z]\!] \qquad \Leftrightarrow \qquad 0 = [\![\rho(v-w)]\!] \\
0 &= -z[\![v]\!] + [\![p]\!] \\
0 &= \frac{\partial e_I}{\partial t} - z[\![(e + \frac{p}{\rho} + \frac{1}{2}(v-w)^2)]\!]
\end{aligned}
$$

- Entropy condition

$$0 \leq \zeta = \frac{\partial s_I}{\partial t} - z[\![s]\!]$$

- $$e_I = e_I(T_I)$$

- Kinetic relation

$$z = \frac{p_V}{\sqrt{2\pi}} \left(\frac{m_0}{kT_I}\right)^{3/2} [\![g + Ts + \frac{1}{2}(v-w)^2 - sT_I]\!]$$

Case IIb: $z \neq 0$ - surfacial tension

$$e_I = -T_I^2 \frac{\partial \frac{\sigma(T_I)}{T_I}}{\partial T_I} \quad \neq const!$$

- $\sigma \equiv const$ cannot be used!
- Eötvös rule? Also a linear relation for σ cannot be used!
- Katayama-Guggenheim rule

$$\sigma = \sigma_0 \left(1 - \frac{T_I}{T_c}\right)^{11/9}$$

may be used.

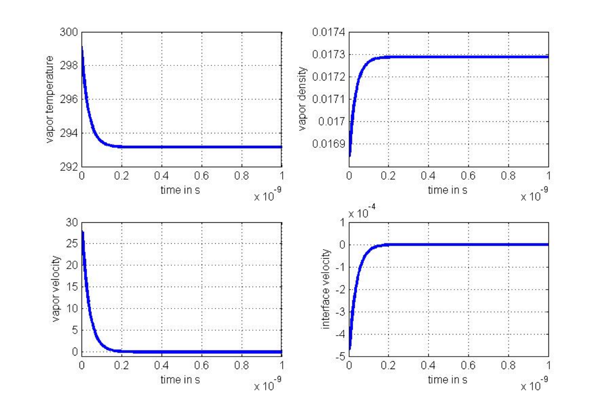
- Problem: Selfsimilarity of the solution is lost!

Examples - behavoir of the phase boundary

- System, that has to be solved
  - balances across the interface
  - kinetic relation
- Initial data: liquid state, initial interface temperature
- Closure conditions
  - ideal gas law for the vapor phase
  - polynomial approximation of the Katayama-Guggenheim rule
- Numerical methods used
  - Newton's method
  - Runge-Kutta method

Example 1

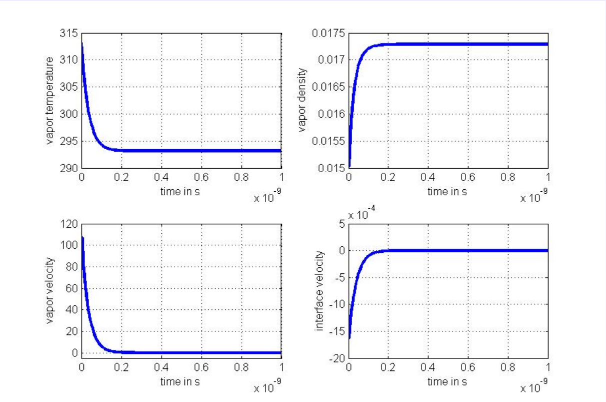
Initial data: $T_L = 293.15K$, $p_L = 2339Pa$, $v_L = 0$, $T_V(0) = 299.15K$



The system runs into a stady state within $t \leq 0.2 \cdot 10^{-9} s$!

Example 2

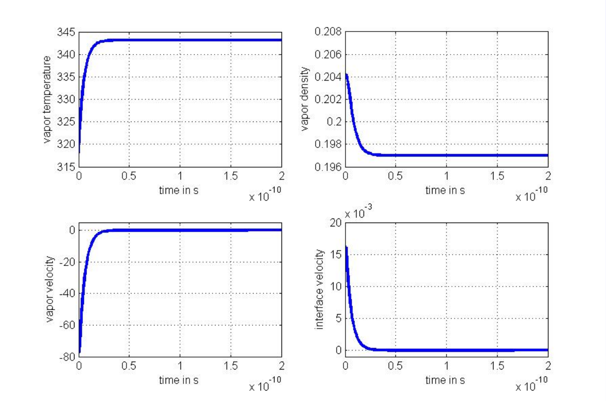
Initial data: $T_L = 293.15K$, $p_L = 2339Pa$, $v_L = 0$, $T_V(0) = 313.15K$



The system runs into a stady state within $t \leq 0.2 \cdot 10^{-9}s$!

Example 3

Initial data: $T_L = 343.15K$, $p_L = 31200Pa$, $v_L = 0$, $T_V(0) = 318.15K$



The system runs into a stady state within $t \leq 0.5 \cdot 10^{-10}s$!

Summary phase boundaries

- similar results for other sets of initial data
- for higher temperatures the process is faster
- analytical proof?
- maybe helpful for numerical solutions?

- Simplifying assumptions have big influence on the solution and its structure.
- $$p_L \geq p_V$$

Creation of new phases

From now on the fluid under consideration is water.

- Situation 1: pure water vapor is compressed
- Situation 2: pure liquid water is expanded

Isothermal case

- For sufficiently high compression of water vapor liquid water is created.
- By sufficiently strong expansion of liquid water water vapor can be created.

Nonisothermal case?

Creation of liquid water

Theorem 1: Nonexistence result (MH, Ferdinand Thein, 2014) [2]

Using the real equations of state for water or any good approximation of the real equation of state condensation by compression cannot occur.

This result holds for

- compressible Euler equations, phase transitions modeled by a kinetic relation
- compressible Euler equations, phase transition modeled using an equilibrium assumption
- models of Baer Nunziato type, phase transition modeled using relaxation terms

[2] Hantke, Thein, Why condensation by compression in pure water vapor cannot occur in an approach based on Euler equations, accepted for publication in Quarterly of Applied Mathematics

Creation of liquid water

Proof.

- uses wave curves
- no intersection point with the saturation line
- no mechanism for phase transition

Consequence.

- no analogous results as in the isothermal case
- minimum requirement for an EOS

Corollary.

- adiabatic processes don't allow creation of liquid water
- if in any process liquid water is created Euler equations cannot be used

Open questions.

- Analogous results for other fluids?
- Analogous results for all fluids?

Creation of water vapor

Theorem 2: Nonexistence result (MH, Ferdinand Thein, 2014)

Using the real equation of state for water or any good approximation of the real equation pure water vapor cannot be created in an approach based on Euler equations and an equilibrium assumption.

This result holds for

- compressible Euler equations, phase transition modeled using an equilibrium assumption
- models of Baer Nunziato type, phase transition modeled using relaxation terms

- The creation of a mixture of water vapor and liquid water (wet steam) is possible.
- The mass fraction of water vapor is bounded

$$\mu \leq 0.5.$$

- Reason: models don't allow entropy production

Choice of the EOS

- classical EOS give very bad descriptions of real fluids
- analysis for IAPWS almost impossible
- using IAPWS is complicated
- using tabled EOS is problematical from mathematical point of view
- generalized Tait equation for water