Simulations of water-vapor two-phase flows with non-condensable gas using a Noble-Able-Chemkin equation of state

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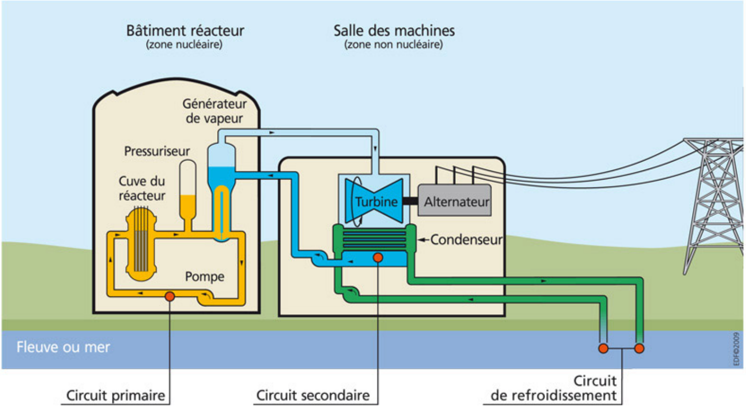
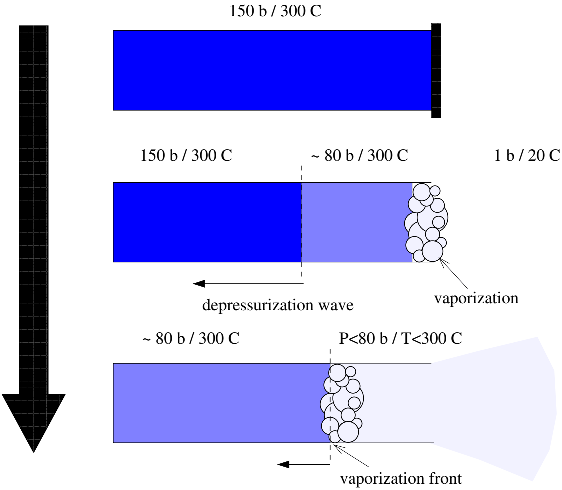
Outline

Pressurized Water Reactors (PWR)



Pressurized Water Reactors (from IRSN website)

Loss of Coolant Accident (LOCA) scenario : breach in the primary circuit

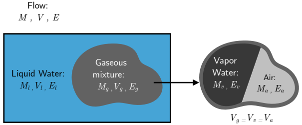


SUPERCANON experiment, representative of a LOCA scenario

Flows of interest

Possible fields :

- Liquid Water (**l**)
- Vapor Water (**v**)
- Non-condensable gas (**a**) : **air**, hydrogen...



Diffuse interface models : the exact interfaces and flow geometry (bubbles...) are NOT known.

Minimal required mathematical properties

In order to achieve code **Verification** :

- **Hyperbolicity of the model** : time stability of numerical solutions.
- **Existence of an entropy inequality** : in order to comply with the second principle of thermodynamics and to define admissible shock waves.
- **Unicity of jump relations** : to correctly define the shock waves.

Other requirements :

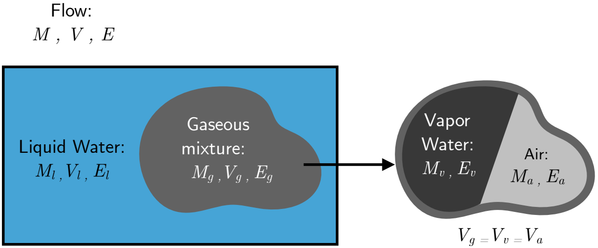
- Ability to handle monophasic flows.
- Preservation of the thermodynamical admissible domain.
- ...

Outline

Chosen homogeneous model

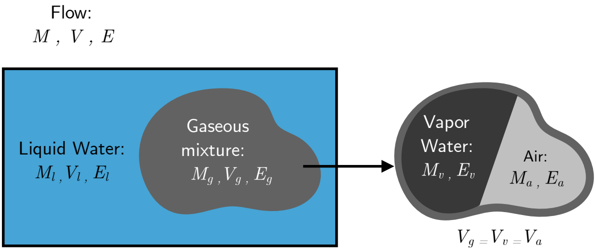
Direct extension of an homogeneous model proposed by T. Barberon and P. Helluy [1], already studied by H. Mathis [2].

Only one equilibrium assumption : kinematic equilibrium between fields.



1. T. Barberon, P. Helluy, Finite volume simulation of cavitating flows, Computers and Fluids 34 (7) (2005) 832–858.
2. H. Mathis, A thermodynamically consistent model of a liquid-vapor fluid with a gas, ESAIM : Mathematical Modelling and Numerical Analysis 53 (1) (2019) 63–84.

Miscibility and immiscibility constraints



$$\alpha_k = \frac{V_k}{V} \text{ (volume fraction) ; } y_k = \frac{M_k}{M} \text{ (mass fraction) ; } z_k = \frac{E_k}{E} \text{ (energy fraction).}$$

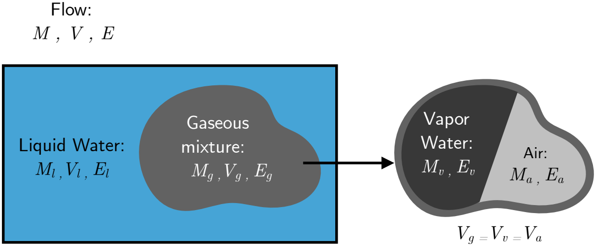
Immiscibility constraints :

$$V_l + V_g = V;$$
$$M_l + M_g = M;$$
$$E_l + E_g = E.$$

Miscibility constraints :

$$V_v = V_a = V_g;$$
$$M_v + M_a = M_g;$$
$$E_v + E_a = E_g.$$

Miscibility and immiscibility constraints



$$\alpha_k = \frac{V_k}{V} \text{ (volume fraction) } ; y_k = \frac{M_k}{M} \text{ (mass fraction) } ; z_k = \frac{E_k}{E} \text{ (energy fraction).}$$

$$\alpha_l + \alpha_v = 1; \quad \alpha_v = \alpha_a;$$

$$y_l + y_v + y_a = 1;$$

$$z_l + z_v + z_a = 1.$$

System of equations and closures

$$
\begin{cases}
\dfrac{\partial}{\partial t}(\rho) + \dfrac{\partial}{\partial x}(\rho U) = 0 \\
\dfrac{\partial}{\partial t}(\rho U) + \dfrac{\partial}{\partial x}\left(\rho U^2 + P\right) = 0 \\
\dfrac{\partial}{\partial t}(\rho E) + \dfrac{\partial}{\partial x}(\rho U E + U P) = 0 \\
\dfrac{\partial}{\partial t}(\rho \alpha_v) + \dfrac{\partial}{\partial x}(\rho U \alpha_v) = \rho \dfrac{\alpha_v^{\mathrm{eq}} - \alpha_v}{\lambda} \\
\dfrac{\partial}{\partial t}(\rho y_v) + \dfrac{\partial}{\partial x}(\rho U y_v) = \rho \dfrac{y_v^{\mathrm{eq}} - y_v}{\lambda} \\
\dfrac{\partial}{\partial t}(\rho z_v) + \dfrac{\partial}{\partial x}(\rho U z_v) = \rho \dfrac{z_v^{\mathrm{eq}} - z_v}{\lambda} \\
\dfrac{\partial}{\partial t}(\rho y_a) + \dfrac{\partial}{\partial x}(\rho U y_a) = 0 \\
\dfrac{\partial}{\partial t}(\rho z_a) + \dfrac{\partial}{\partial x}(\rho U z_a) = \rho \dfrac{z_a^{\mathrm{eq}} - z_a}{\lambda}
\end{cases}
$$

- ρ : mixture density $(kg.m^{-3})$;
- ρU : mixture momentum $(kg.m^{-3})$;
- ρE : mixture total energy $(J.m^{-3})$.

$$\mathbf{W} = (\rho, \rho U, \rho E, \rho\alpha_v, \rho y_v, \rho z_v, \rho y_a, \rho z_a).$$

Closures for :

- pressure P ?
- relaxation time λ ?

Outline

Thermodynamical planes

Potential	Entry plane	"Gibbs relation"	Conjugate variables
μ	(P, T)	$d\mu = -sdT + \tau dP$	$\tau = \left.\frac{\partial \mu}{\partial P}\right\|_T ; s = -\left.\frac{\partial \mu}{\partial T}\right\|_P$
s	(τ, e)	$ds = \frac{P}{T}d\tau + \frac{1}{T}de$	$\frac{P}{T} = \left.\frac{\partial s}{\partial \tau}\right\|_e ; \frac{1}{T} = \left.\frac{\partial s}{\partial e}\right\|_\tau$

- μ : chemical potential (J) in pressure P (Pa) - temperature T (K) plane ;
- s : specific entropy $(J.K^{-1}.kg^{-1})$ in specific volume τ $(m^3.kg^{-1})$ - internal energy e $(J.kg^{-1})$ plane ;

Thermodynamical closure

P defined with a **complete Equation Of State** (EOS).

1. Given EOS : specific entropies

$$s_l(\tau_l, e_l) \quad ; \quad s_v(\tau_v, e_v) \quad ; \quad s_a(\tau_a, e_a).$$

2. Phasic Gibbs relation : $T_k ds_k = de_k + P_k d\tau_k$.

$$\frac{P_k}{T_k} = \left.\frac{\partial s_k}{\partial \tau_k}\right|_{e_k} \quad ; \quad \frac{1}{T_k} = \left.\frac{\partial s_k}{\partial e_k}\right|_{\tau_k}.$$

3. Mixture entropy given by :
$s = (1 - y_v - y_a)s_l(\tau_l, e_l) + y_v s_v(\tau_v, e_v) + y_a s_a(\tau_a, e_a)$.

4. Mixture Gibbs relation can be deduced :
$Tds = de + Pd\tau + \partial_{\alpha_v} s|_{e,\tau,y_k,z_k} d\alpha_v + \partial_{y_v} s|_{e,\tau,\alpha_v,y_a,z_k} dy_v + \partial_{z_k} s|_{e,\tau,\alpha_v,y_k} dz_k,$

$$P = \frac{(1-\alpha_v)\frac{P_l}{T_l} + \alpha_v(\frac{P_v}{T_v} + \frac{P_a}{T_a})}{\frac{1-z_v-z_a}{T_l} + \frac{z_v}{T_v} + \frac{z_a}{T_a}} \quad ; \quad \frac{1}{T} = \frac{1 - z_v - z_a}{T_l} + \frac{z_v}{T_v} + \frac{z_a}{T_a}.$$

Requirements for an admissible EOS

1. Mathematical sufficient conditions to ensure model hyperbolicity :
   - specific entropy s_k is strictly concave with respect to internal specific energy e_k and specific volume τ_k ;
   - temperature $T_k = \left(\dfrac{\partial s_k}{\partial e_k}\right)\Big|_{\tau_k}^{-1}$ is strictly positive.

2. In practical simulations : the EOS needs to be available in several thermodynamical planes :
   - in (e, τ)-plane (internal energy - specific volume) : to get the right shock waves without too numerical difficulties ;
   - in (P, T)-plane (pressure - temperature) : not mandatory, but enables to use a robust algorithm for computing the thermodynamical equilibrium[3].

3. Gloria Faccanoni, Samuel Kokh, and Grégoire Allaire. "Modelling and simulation of liquid-vapor phase transition in compressible flows based on thermodynamical equilibrium." ESAIM : Mathematical Modelling and Numerical Analysis 46.5 (2012) : 1029-1054.

Stiffened gas

$$s_k(e_k, \tau_k) = C_{v_k} \ln((e_k - Q_k - \Pi_k \tau_k)\tau_k^{\gamma_k - 1})) + s_k^0$$

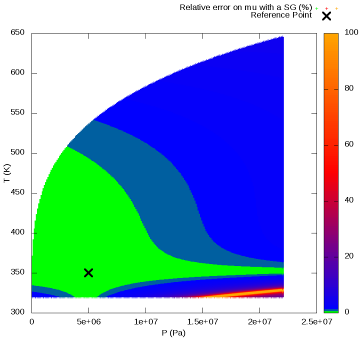
$$\mu_k(P_k, T_k) = \gamma_k C_{v,k} T_k + Q_k - T_k(\gamma_k C_{v,k} \ln(T_k) - (\gamma_k - 1) C_{v,k} \ln(P_k + \Pi_k) + k_k)$$

Pros :

+ Very easy to change of thermodynamical plane (explicit formula).
+ SG EOS is admissible (in terms of convexity) under natural physical conditions.
+ Low CPU-time consuming.

Cons :

- accurate only in a restricted domain, close to a reference point.



Noble-Able Chemkin stiffened gas (NASG-CK) for liquid water

$$\mu_l(P_l, T_l) = \mu_l^0(T_l) + b_l P_l + \mathcal{C}_l(T)\ln(P_l + \Pi_l),$$
$$\mu_l^0(T_l) = RT_l\left(A_l(1-\ln(T_l)) - \frac{B_l}{2}T_l - \frac{C_l}{6}T_l^2 - \frac{D_l}{12}T_l^3 - \frac{E_l}{20}T_l^4 + \frac{F_l}{T_l} - G_l\right),$$
$$\mathcal{C}_l(T_l) = C_{v,l}(\gamma_l - 1)T_l.$$

$$P_l(\tau_l, T_l) = \frac{C_{v,l}(\gamma_l - 1)T_l}{\tau_l - b_l} - \Pi_l$$

$$\boxed{\begin{array}{l} P(\tau, T) = \dfrac{rT}{\tau - b} + \dfrac{a}{\tau^2} \\ \text{cf : Van der Waals EOS} \end{array}}$$

$$C_{p_l}(T_l) = R(A_l + B_l T_l + C_l T_l^2 + D_l T_l^3 + E_l T_l^4).$$

Pros :

+ More accurate.

Cons :

- Inversion towards (e, τ)-plane not explicit.
- NASG-CK EOS is admissible if the following condition holds :

$$C_{p_l}(T_l) - C_{v\,l}(\gamma_l - 1) > 0.$$

NASG-CK inversion towards (e, τ)-plane

1. $P_l = P_l(\tau_l, T_l)$: $P_l = \dfrac{C_{v,l}(\gamma_l - 1)T_l}{\tau_l - b_l} - \Pi_l = P_l(\tau_l, T_l)$;
2. then, $e_l = e_l(\tau_l, T_l)$:

$$e_l = RT_l\left(A_l + \frac{B_l}{2}T_l + \frac{C_l}{3}T_l^2 + \frac{D_l}{4}T_l^3 + \frac{E_l}{5}T_l^4 + \frac{F_l}{T_l}\right) - C_{v,l}(\gamma_l - 1)T_l + \Pi_l(\tau_l - b_l);$$

3. T_l can be deduced from τ_l and e_l by implicitly solving the previous equation, one equation with one unknown (for instance with a secant method algorithm).

Choice of EOS coefficients [6]

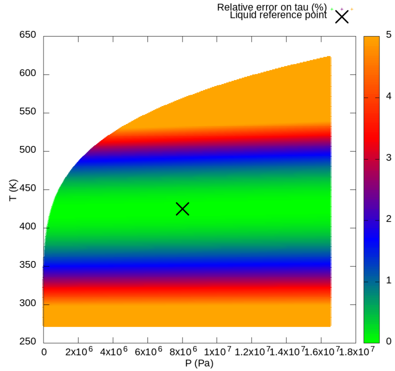
- NASG-CK :
  - A_l, B_l, C_l, D_l, E_l : by fitting μ_l, τ_l, $C_{p,l}$ on IAPWS-IF97 [4] data ;
  - γ_l, $C_{v,l}$, Π_l, b_l : from an extension of an empirical method [5], by imposing some quantities (τ_l, $\alpha_{P,l}$, $C_{v,l}$ and c_l) at a reference point ($P_0 = 80bar, T_0 = 425K$) ;
  - F_l, G_l : by fitting $(\mu_l - \mu_v)(T^{sat}_{IAPWS}(P))$.
- SG : γ_k, $C_{v,k}$, Π_k, Q_k, k_k obtained by fitting μ_l, τ_l, $C_{p,l}$ on IAPWS-IF97 data.

4. Wagner, W. and Kretzschmar, H.-J. (2008), "International Steam Tables : Properties of Water and Steam Based on the Industrial Formulation IAPWS-IF97"

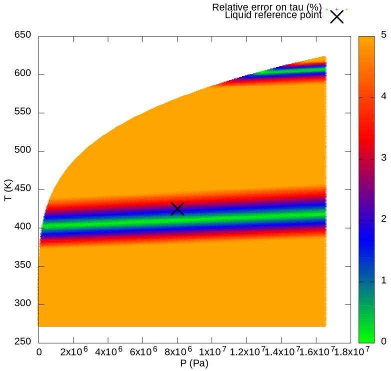
5. F. Daude, P. Galon, Z. Gao, E. Blaud, Numerical experiments using a HLLC-type scheme with ALE formulation for compressible two-phase flows five-equation models with phase transition, Computers and Fluids 94 (2014) 112–138.

6. L. Quibel, Simulation of water-vapor two-phase flows with non-condensable gas, PhD, Université de Strasbourg

NASG-CK VS SG accuracy for liquid water : specific volume τ_l

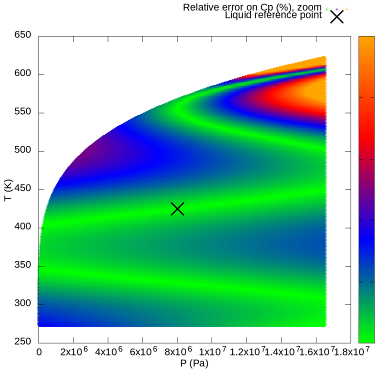


Relative error w.r.t IAPWS : NASG-CK

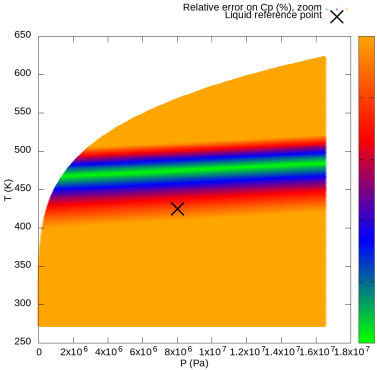


Relative error w.r.t IAPWS : SG

NASG-CK VS SG accuracy for liquid water : heat capacity $C_{p,l}$



Relative error w.r.t IAPWS : NASG-CK



Relative error w.r.t IAPWS : SG

Outline

Chosen EOS

- NASG-CK for liquid :

$$\mu_l(P_l, T_l) = \mu_l^0(T_l) + b_l P_l + \mathcal{C}_l(T)\ln(P_l + \Pi_l),$$
$$\mu_l^0(T_l) = RT_l\left(A_l(1-\ln(T_l)) - \frac{B_l}{2}T_l - \frac{C_l}{6}T_l^2 - \frac{D_l}{12}T_l^3 - \frac{E_l}{20}T_l^4 + \frac{F_l}{T_l} - G_l\right),$$
$$\mathcal{C}_l(T_l) = C_{v,l}(\gamma_l - 1)T_l;$$

- SG for vapor and air ($k = v, a$) :

$$\mu_k(P_k, T_k) = \gamma_k C_{v,k} T_k + Q_k - T_k(\gamma_k C_{v,k}\ln(T_k) - (\gamma_k - 1)C_{v,k}\ln(P_k + \Pi_k) + k_k).$$

General method

The numerical method is based on a fractional step method :

1. **First step** : we account for the convective part of the system.

   First-order explicit and conservative finite volumes schemes are used. By noting : W_i^n the space-average value of W on the mesh cell Ω_i at time t^n, $W_i^{n+1,*}$ at the next time step $t^n + \Delta t^n$ is obtained from :

   $$\Delta x_i(W_i^{n+1,*} - W_i^n) + \Delta t^n \left(F(W_i^n, W_{i+1}^n) - F(W_{i-1}^n, W_i^n)\right) = 0$$

   with F the numerical flux to be defined for each scheme.
   In this work : **Relaxation scheme** [7].

2. **Second step** : the fractions are relaxed in accordance with the source terms, once the thermodynamical equilibrium is computed.

   The thermodynamical equilibrium is the state $(\bar{\alpha}_v, \bar{y}_v, \bar{z}_v, \bar{y}_a, \bar{z}_a)$ which **maximizes the mixture entropy** s for a given specific volume τ and internal energy e.

7. Chalons C., Coulombel J.F., (2008), JMAA, Vol. 348, pp. 872–893

Conditions of thermodynamical equilibrium depending on the present fields

Equilibrium **l** $\oplus$ **(v + a)** :

$$\begin{cases} T_l(\bar{\mathcal{V}}_l, \bar{\mathcal{M}}_l, \bar{\mathcal{E}}_l) = T_v(\bar{\mathcal{V}}_v, \bar{\mathcal{M}}_v, \bar{\mathcal{E}}_v) = T_a(\bar{\mathcal{V}}_a, \bar{\mathcal{M}}_a, \bar{\mathcal{E}}_a) \\ P_l(\bar{\mathcal{V}}_l, \bar{\mathcal{M}}_l, \bar{\mathcal{E}}_l) = P_v(\bar{\mathcal{V}}_v, \bar{\mathcal{M}}_v, \bar{\mathcal{E}}_v) + P_a(\bar{\mathcal{V}}_a, \bar{\mathcal{M}}_a, \bar{\mathcal{E}}_a) \\ \mu_l(\bar{\mathcal{V}}_l, \bar{\mathcal{M}}_l, \bar{\mathcal{E}}_l) = \mu_v(\bar{\mathcal{V}}_v, \bar{\mathcal{M}}_v, \bar{\mathcal{E}}_v). \end{cases}$$

Equilibrium **l** $\oplus$ **v** :

$$\begin{cases} T_l(\bar{\mathcal{V}}_l, \bar{\mathcal{M}}_l, \bar{\mathcal{E}}_l) = T_v(\bar{\mathcal{V}}_v, \bar{\mathcal{M}}_v, \bar{\mathcal{E}}_v) \\ P_l(\bar{\mathcal{V}}_l, \bar{\mathcal{M}}_l, \bar{\mathcal{E}}_l) = P_v(\bar{\mathcal{V}}_v, \bar{\mathcal{M}}_v, \bar{\mathcal{E}}_v) \\ \mu_l(\bar{\mathcal{V}}_l, \bar{\mathcal{M}}_l, \bar{\mathcal{E}}_l) = \mu_v(\bar{\mathcal{V}}_v, \bar{\mathcal{M}}_v, \bar{\mathcal{E}}_v). \end{cases}$$

Equilibrium **l** $\oplus$ **a** :

$$\begin{cases} T_l(\bar{\mathcal{V}}_l, \bar{\mathcal{M}}_l, \bar{\mathcal{E}}_l) = T_a(\bar{\mathcal{V}}_a, \bar{\mathcal{M}}_a, \bar{\mathcal{E}}_a) \\ P_l(\bar{\mathcal{V}}_l, \bar{\mathcal{M}}_l, \bar{\mathcal{E}}_l) = P_a(\bar{\mathcal{V}}_a, \bar{\mathcal{M}}_a, \bar{\mathcal{E}}_a). \end{cases}$$

Equilibrium **(v + a)** :

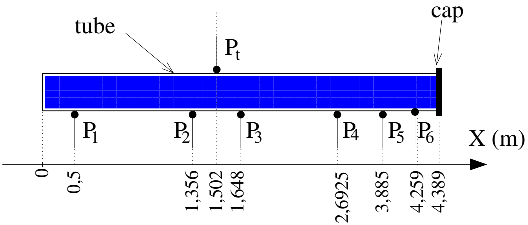
$$T_v(\bar{\mathcal{V}}_v, \bar{\mathcal{M}}_v, \bar{\mathcal{E}}_v) = T_a(\bar{\mathcal{V}}_a, \bar{\mathcal{M}}_a, \bar{\mathcal{E}}_a).$$

+ monophasic cases.

SUPERCANON facility

- LOCA = accidental scenario in which a breach occurs in the primary circuit (**validation** test case).
- SUPERCANON : experimental facility[8], reproducing a LOCA scenario.

A closed tube filled with liquid at 150 *bars* and 300°*C* is suddenly opened in air at 1*bar*.



Experimental dataset : pressure with respect to time at points $P_1, \dots, P_6$ and void fraction at P_t.

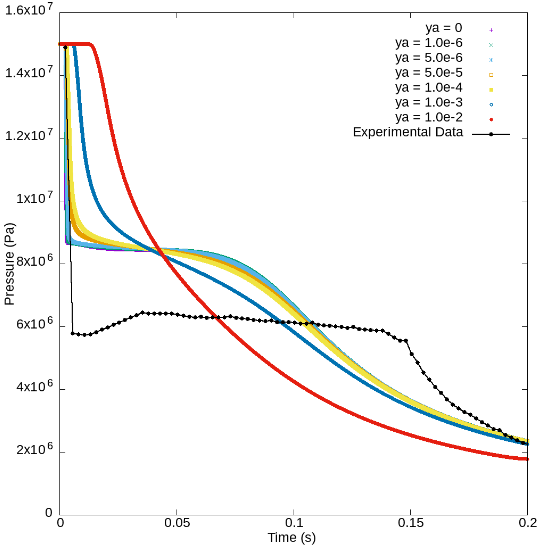
8. B. Riegel, PhD, Contribution à l'étude de la décompression d'une capacité en régime diphasique 1978

At-equilibrium simulations

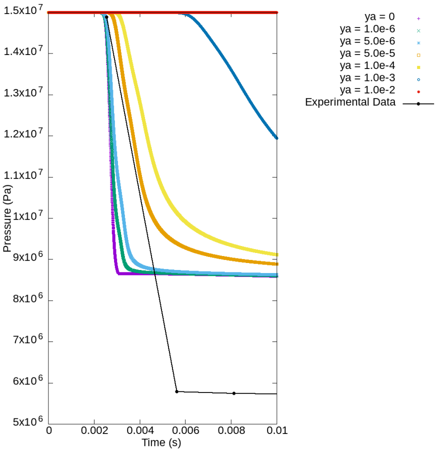
	Left State	**Right State**
Fields in the mixture	Liquid water + Air	Air + Vapor (moist rate=55 %)
y_a ?	various y_a	$y_v = 0.0085162$
Pressure (Pa)	150 bar	1 bar
Temperature (°C)	300 °C	20 °C

Relaxation time $\lambda = 0$.

Results : importance of out-of-equilibrium effects



Results : influence of y_a on the sound speed



Pressure near the tube wall within time.

	Sound speed
Experimental	$\simeq 900 m.s^{-1}$
In pure liquid, NASG-CK (in accordance with IAPWS)	$\simeq 1480 m.s^{-1}$

$\rightarrow$ With a small amount of air ($y_a = 5 \times 10^{-5}$), the depressurization wave travels with a velocity in accordance with the experimental one.

Out-of-equilibrium simulations

	Left State	**Right State**
Fields in the mixture	Liquid water + Air	Air + Vapor (moist rate=55 %)
y_a ?	$y_a = 5 \times 10^{-5}$	$y_v = 0.0085162$
Pressure (Pa)	150 bar	1 bar
Temperature (°C)	300 °C	20 °C

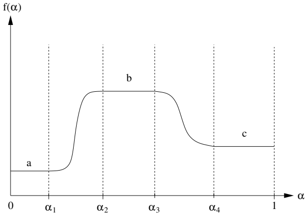
Relaxation time λ :

- defined with a toy law t_{toy} ;
- defined with a simple model, based on nucleation theory t_{nuc}.

Toy law for relaxation time λ

$$\boxed{\lambda = t_{toy} = \lambda_0 f(\alpha_v) \exp\left(- \left(\frac{\alpha_v - \bar{\alpha_v}}{\delta\alpha} \right)^2 \right)}$$

with the following parameters : $\lambda_0 = 10^{-2}$ s et $\delta\alpha = 5.75\ 10^{-4}$, $a = 1$, $b = 0.05$, $c = 0$, $\alpha_1 = 0$, $\alpha_2 = 0.15$, $\alpha_3 = 0.25$, $\alpha_4 = 0.65$.



Definition of the function $\alpha \in [0, 1] \mapsto f(\alpha)$ used for the definition of λ.

Simplified model based on nucleation for relaxation time λ

Hypothesis : out-of-equilibrium effects related to the first bubbles appearance in liquid.

Arrhenius law :

$$\boxed{\lambda = t_{nuc} = \frac{a_0}{\Delta P^3} \exp\left(\frac{\varphi E_a}{k_B T}\right)}$$

$\varphi \in [0, 1]$ such as :

- $\varphi \to 0$: heterogeneous nucleation
- $\varphi = 1$: homogeneous nucleation.

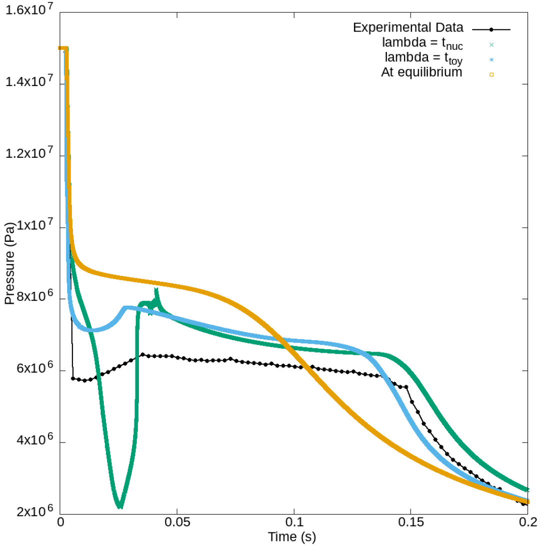
Parameters definition :

- fixed $a_0 = \mathcal{P} \times \mathcal{T}$, $\quad \mathcal{P} = 1 bar; \mathcal{T} = 4.389 m/1481\ m.s^{-1}$,
- variable $\varphi = \begin{cases} 1 & \text{if } y_v + y_a < 10^{-9}, \\ (y_v + y_a)^2 & \text{otherwise.} \end{cases}$

In practical simulations :

- t_{nuc} relevant only while y_v stays small ;
- t_{nuc} is regularized through a cosine function, to avoid too sharp discontinuities : some arbitrary thresholds appear...

First interesting qualitative results



Conclusion and perspectives

Main results :

- NASG-CK EOS is a good compromise between simplicity and accuracy for liquid water.
- Non-condensable gas has an influence on the thermodynamical properties of the mixture, such as the sound speed.
- Out-of-equilibrium effects are important to obtain realistic results on sudden depressurization such as SUPERCANON test case.

Perspectives :

- With three fields, the thermodynamical equilibrium computation may be tricky (numerical threshold on fractions for missing fields).
- Some improvements are needed on relaxation time scale λ modelling.

Some references

- *Preprint* : O. Hurisse, L. Quibel, Simulations of a two-phase flow homogeneous model with a gaseous phase as a miscible mixture of vapor and non-condensable gas.
- T. Barberon, P. Helluy, Finite volume simulation of cavitating flows, Computers and Fluids 34 (7) (2005) 832–858.
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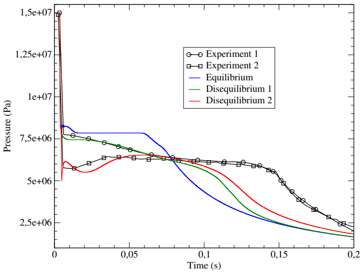
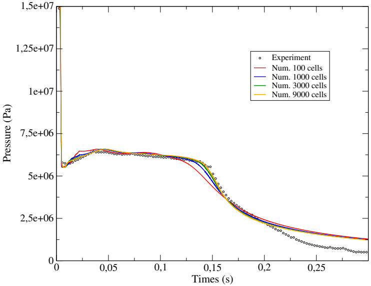
- Gloria Faccanoni, Samuel Kokh, and Grégoire Allaire. "Modelling and simulation of liquid-vapor phase transition in compressible flows based on thermodynamical equilibrium." ESAIM : Mathematical Modelling and Numerical Analysis 46.5 (2012) : 1029-1054.
- P. Boivin, M. Cannac, O. Le Metayer, A thermodynamic closure for the simulation of multiphase reactive flows, International Journal of Thermal Sciences 137 (2019) 640–649.

Out-of-equilibrium SUPERCANON simulations, with several EOS



With SG EOS for liquid. [9]



With IAPWS look-up table for liquid. [10]

9. Hurisse O., (2017), Computers and Fluids, Vol. 152.
10. Hurisse O., Quibel L., (2020), ATH2020 proceedings.

Algorithm to compute the thermodynamical equilibrium

- **If** $y_a = 1$: monophasic **a** equilibrium, END.

- **Else if** $y_a = 0$: try to compute a **l** $\oplus$ **v** equilibrium :
  - **If admissible :** **l** $\oplus$ **v** equilibrium, END.
  - **Else** :
    - **If** $s_l(\tau, e) > s_v(\tau, e)$: monophasic **l** equilibrium, END.
    - **Else** : monophasic **v** equilibrium, END.

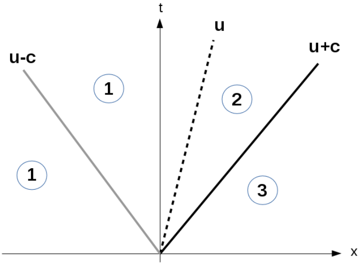
- **Else** : try to compute a **l** $\oplus$ **(v + a)** equilibrium :
  - **If admissible :** **l** $\oplus$ **(v + a)** equilibrium, END.
  - **Else** :
    - **If** $s_{la}(y_a, \tau, e) > s_{va}(y_a, \tau, e)$: **l** $\oplus$ **a** equilibrium, END.
    - **Else** : **(v + a)** equilibrium, END.

Empirical method to fit NASG-CK EOS coefficient

A point $(P_0 = 80bar, T_0 = 425K)$ is chosen :

1. $\tau_0(P_0, T_0)$, $\alpha_{P,0}(P_0, T_0)$, $C_{v,0}(P_0, T_0)$ and $c_0(P_0, T_0)$ are obtained with the IAPWS-97 formulation.
2. ${C_p}^{NASG-CK} = {C_p}^{NASG-CK}(T_0)$.
3. $\mathcal{A}_l = (\gamma^{NASG-CK} - 1) \times {C_v}^{NASG-CK}$ is deduced from c_0 and $\alpha_{P,0}$:
$$\mathcal{A}_l = (\gamma^{NASG-CK} - 1) \times {C_v}^{NASG-CK} = \left(\frac{1}{c_0^2 {\alpha_{P,0}}^2 T_0} + \frac{1}{{C_p}^{NASG-CK}} \right)^{-1}.$$
4. ${C_v}^{NASG-CK} = C_{v,0}(P_0, T_0)$, so that $\gamma^{NASG-CK} = \dfrac{\mathcal{A}_l}{C_{v,0}(P_0, T_0)} + 1.$
5. $\mathcal{B}_l = b_l \times (P_0 + \Pi_l) = (\dfrac{1}{\alpha_{P,0}} - T_0) \times (\gamma^{NASG-CK} - 1) \times {C_v}^{NASG-CK}.$
6. Π_l and b_l are deduced from τ_0 and $\mathcal{B}_l$:
$\Pi_l = \dfrac{\mathcal{B}_l + T_0 \times \mathcal{A}_l}{\tau_0} - P_0$ and $b_l = \dfrac{\mathcal{B}_l}{(P_0 + \Pi_l)}.$

Building of analytical solutions



Riemann problem with one intermediate state ; $U - c$: "ghost wave" ; U : contact wave ; $U + c$: shock wave ; c is the sound speed.

Analytical solution :

- in the domain 1 : initial left state $(\alpha_L, y_L, z_L, U_L, \tau_L, e_L)$;
- in the domain 2 : intermediate state $(\alpha_*, y_*, z_*, U_*, \tau_*, e_*)$;
- in the domain 3 : initial right state $(\alpha_R, y_R, z_R, U_R, \tau_R, e_R)$.

A more accurate EOS : IAPWS-IF97 [11]

In each region, a different EOS is provided with a polynomial obtained by interpolation of experimental data.

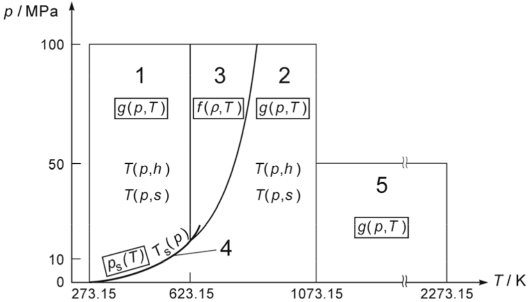


Fig. 1. Regions and equations of IAPWS-IF97.

Pros :

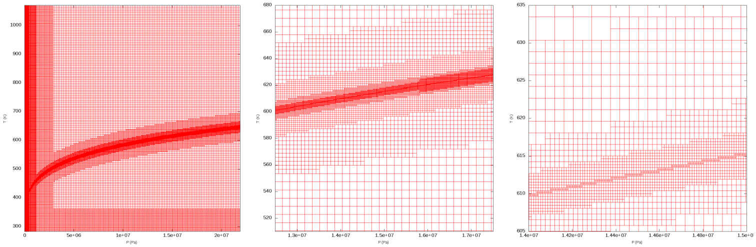
+ Accurate.

Cons :

- High CPU-time consuming : impossible to use it directly in industrial simulations !

11. Wagner, W. and Kretzschmar, H.-J. (2008), "International Steam Tables : Properties of Water and Steam Based on the Industrial Formulation IAPWS-IF97"

Construction of IAPWS-IF97 look-up table



1. IAPWS EOS is sampled in (P, T)-plane, with local refinement to get a compromise between CPU-time efficiency and accuracy.
2. Gibbs relation has to be fulfilled : $d\mu = -sdT + \tau dP$.
3. μ is $\mathcal{C}^1$; on the widest cells, μ is obtained from IAPWS ; on smaller cells, μ is computed to ensure the continuity of μ, s and τ at the junction between cells of different size.

Comparison of EOS : accuracy/efficiency on a given test case

EOS	SG	NASG-CK	IAPWS look-up table	IAPWS
CPU time ?	1	$\simeq 2$	8	700
Max relative error ?	$\simeq 40\%$	$\simeq 20\%$	10^{-5}	Ref

IAPWS look-up table is much cheaper than the direct IAPWS formulation, for an equivalent accuracy. Its CPU-cost is reasonable with respect to analytical EOS.

Possibility of verification with the look-up table ?

Two Riemann problems have been defined :

1. one using a Stiffened Gas EoS ;
2. one using the look-up table.

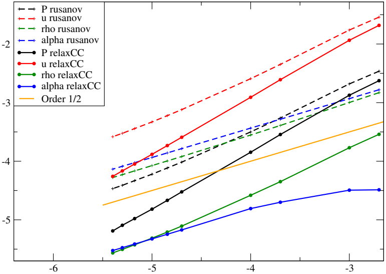
Three convective numerical schemes have been compared on convergence studies :

1. Rusanov scheme [12] ;
2. VFRoe-ncv scheme [13] ;
3. a relaxation scheme proposed by Chalons and Coulombel [14].

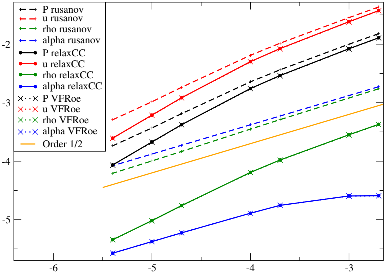
12. Rusanov V., (1961), ZVMMF, Vol. 1, pp. 267–279.
13. Buffard T., Gallouët T., Hérard J.-M., (2000), Computers and Fluids, Vol. 29, pp. 813–847.
14. Chalons C., Coulombel J.F., (2008), Journal of Mathematical Analysis and Applications, Vol. 348, pp. 872–893.

Robustness and accuracy of the relaxation scheme

log(L1-error) VS log(mesh size) (from 100 to 250 000 cells)



Look-up table ;



Stiffened Gas EOS.

- **Verification** is possible with IAPWS look-up table.
- VFRoe-ncv scheme is not robust enough when using the look-up table.
- The relaxation scheme is very robust and far more accurate than Rusanov scheme.

Verification test cases for several configurations with IAPWS look-up table

Waves	Equilibrium	EOS	Initial states Left/Right
Contact	No	LuT	liq. + vap. / liq. + vap.
Shock	No	LuT	liq. + vap. / liq. + vap.
Contact + shock	No	SG	liq. + vap. / liq. + vap.
Contact + shock	No	LuT	liq. + vap. / liq. + vap.
Contact	Yes	LuT	liq. + vap. / liq. + vap.
Shock	Yes	LuT	liq. + vap. / liq. + vap.
Contact + shock	Yes	LuT	liq. + vap. / liq. + vap.
Contact	Yes	LuT	liq. / liq. + vap.
Shock	Yes	LuT	liq. / liq. + vap.

$\rightarrow$ A far more complete study is available in [15].

15. Quibel L., Helluy P., Hurisse, O., (2020), “Assessment of numerical schemes for complex two-phase flows with real equations of state", Computers and Fluids, Vol. 29, pp. 813–847.

Relaxation scheme [16]

One additionnal scalar unknown is introduced $\mathcal{T}$, so that $(\rho\mathcal{T})_i^0 = 1 \ \forall i$.

- New pressure $\Pi = P(\mathcal{T}, s) + a^2(\mathcal{T} - \tau)$;
- Relaxation specific total energy $\Sigma = \dfrac{u^2}{2} + e(\mathcal{T}, s) + \dfrac{\Pi^2 - P^2(\mathcal{T}, s)}{2a^2}$;

where a is a positive constant which should satisfy a stability condition :

$$a^2 > \max(-\partial_\tau p(\tau_r), -\partial_\tau p(\tau_l)) = \max(\frac{|c_l|}{\tau_l}, \frac{|c_r|}{\tau_r}) \tag{1}$$

This enlarged system is solved, with all the characteristic fields linearly degenerate :

$$\left\{ \begin{array}{l} \partial_t \rho + \partial_x(\rho U) = 0 \\ \partial_t(\rho U) + \partial_x(\rho U^2 + \Pi) = 0 \\ \partial_t(\rho\Sigma) + \partial_x(\rho U\Sigma + U\Pi) = 0 \\ \partial_t(\rho Y) + \partial_x(\rho Y U) = 0 \\ \partial_t(\rho\mathcal{T}) + \partial_x(\rho\mathcal{T}U) = \dfrac{1}{\epsilon}\rho(\tau - \mathcal{T}) \end{array} \right. \tag{2}$$

16. Chalons C., Coulombel J.F., (2008), Journal of Mathematical Analysis and Applications, Vol. 348, pp. 872–893.