Simulation of an Homogeneous Relaxation Model for a three-phase mixture

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Introduction

- Homogeneous relaxation model (HRM) for a three-phase flow with two miscible phases
  - ⇝ Introducing the model
  - ⇝ Numerical study of the convective part
  - ⇝ Beginning of a numerical study of two source terms

Motivations : modeling of a water-vapor-gas flow which can appear during pressurized water reactor accident

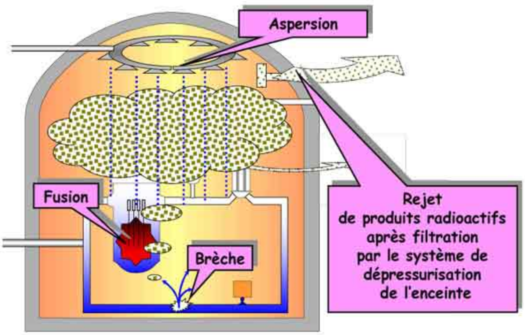


FIGURE – Loss of coolant accidents with primarly failures in pressurized water reactor (IRSN)

Plan

1. Homogeneous relaxation model
2. Numerical study of the convective part
   - Schemes
   - Results
3. A study of two source terms
   - A first comparison
   - Γ_2 study for a two-phase flow model

Thermodynamical description

- Three phases who share the same velocity u : liquid water (l), vapor (v) and inert gas (g)

⇝ Vapor and gas are totally miscible. Introducing mass fractions y_k, volume fractions α_k and energy fractions z_k, the intensive constraints are :

Intensive constraints

- Mass conservation : $1 = y_l + y_g + y_v$
- Energy conservation : $1 = z_l + z_g + z_v$
- Miscibility constraints : $\begin{cases} 1 = \alpha_l + \alpha_g \\ \alpha_v = \alpha_g \end{cases}$

- Intensive description of a state : specific volume τ, internal energy e, gaseous mass fraction y_g and $Y = (y_L, \alpha_l, z_l, z_g)$ other fractions submitted to thermodynamics
- y_g is a constant since the gas is inert
- For a given state (τ, e, Y, y_g), there must exist an unique $Y_{\textsf{eq}}$ corresponding to the thermodynamic equilibrium, which only depends of (τ, e, y_g) and that maximises the entropy $\sigma = \sum_{k=l,g,v} y_k s_k$

Homogeneous relaxation model and its properties [O. Hurisse, L. Quibel, 2019] [H. Mathis, 2019]

- HRM = Euler equations + advection on fractions, thermodynamics effects modeled by source terms Γ :

$$\begin{cases} \partial_t Y + u\partial_x Y = \Gamma \\ \partial_t y_g + u\partial_x y_g = 0 \\ \partial_t \rho + \partial_x \rho u = 0 \\ \partial_t \rho u + \partial_x(\rho u^2 + P) = 0 \\ \partial_t \rho E + \partial_x(\rho E + P)u = 0 \end{cases}$$

- $-\rho\sigma$ is a Lax entropy
- Hyperbolic system as long as the three phases are present

⇝ System closed by given pressure laws and intensive constraints

⇝ Source terms must satisfy the entropy growth according to the second law of thermodynamics

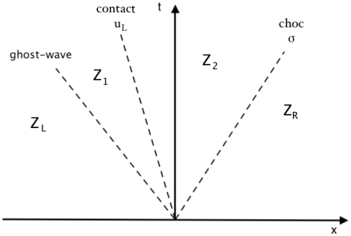
- Rankine-Hugoniot relations to build solutions of Riemann problems :
  - Pressure and velocity conserved through contacts, not fractions
  - Relations through shocks :

$$\begin{cases} [Y] = 0 \\ J = -\frac{[P]}{[u]} \\ J^2 = -\frac{[P]}{[\tau]} \\ [e] + [\tau]\frac{P_L + P_R}{2} = 0 \end{cases}$$

Plan

Study framework

- Fractional step method :
  - ⇝ Convective part solved with Finite Volume method :
    VFRoe-ncv [T. Buffard, T. Gallouët, J.-M. Hérard, 2000]
    Relaxation scheme [C.Chalons, J.-F. Coulombel, 2008]
  - ⇝ ODE on source terms to take thermodynamics into account : $\dot{Y} = \Gamma(Y)$
- Equations of state :
  - ⇝ 3 stiffened gas mixture (3 SG)
  - ⇝ 2 SG + 1 NASG-CK law for liquid water (2 SG + 1 NASG-CK) [L. Quibel, 2020]
- Riemann problems structure : contact + shock

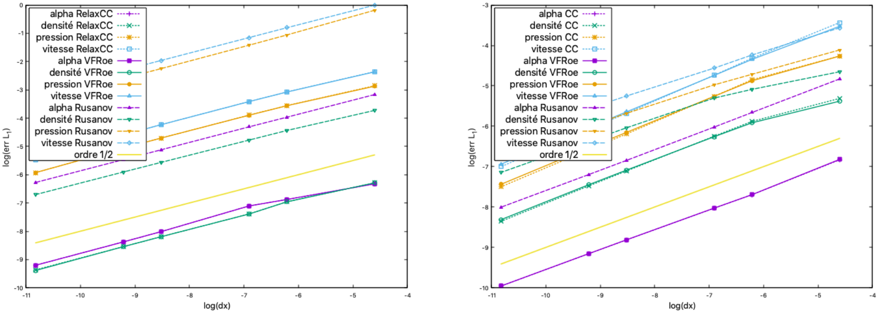


Objectives

Comparing VFRoe-ncv and relaxation schemes on atmospheric and high pressure Riemann problems.

Plan

Convergence results

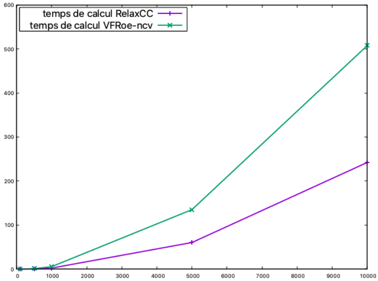


(a) Atm. pressure Riemann problem (b) High pressure Riemann problem

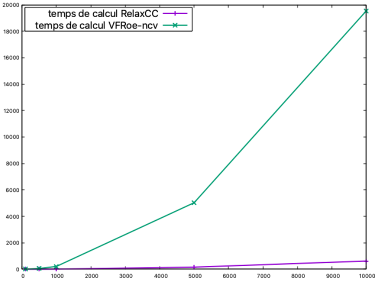
FIGURE – Finite volume schemes convergence curves for a 3 stiffened gas mixture.

- ⇝ Convergence rate of $\frac{1}{2}$
- ⇝ Very similar results between VFRoe-ncv and the relaxation scheme
- Same type of results for a 2 SG + 1 NASG-CK mixture, but more implicite equations to solve, due to the implicit change of variables in the NASG-CK EOS.
- ⇝ Need to improve the robustness of some algorithms for VFRoe-ncv

VFRoe-ncv vs. relaxation scheme



(a) CPU time with respect to number of cells - 3 SG.



(b) CPU time with respect to number of cells - 2 SG + 1 NASG-CK.

FIGURE – Comparison of CPU time for each scheme.

⇝ Relaxation scheme is much faster than VFRoe-ncv, since this last one does variable changes, and so implicit resolutions, at each cell. Consequently, the gap is wider for the more complex EOS mixture 2 SG + 1 NASG-CK.

Convective part conclusion

VFRoe-ncv and the relaxation scheme have similar errors, but the last one is faster and VFRoe-ncv has some lack of robustness.

Plan

A first comparison

All of the following study is done for a 3 SG mixture. For relaxation time scales $\lambda > 0$, we consider :

Type (1) : $\Gamma_1 = \lambda(Y_{\textsf{eq}} - Y)$

- Very used model in homogeneous literature [O. Hurisse, 2014, 2017], [L. Quibel 2019]
- Advantages :

⇝ Exact ODE solved for fixed time scales

⇝ Simple trajectories

- Drawbacks :

⇝ Computation of $Y_{\textsf{eq}}$ that can be very hard depending of the choice of EOS [P. Helluy, L. Quibel 2019]

⇝ Time scales constraints : they must be <u>identical</u>

Type (2) : $\Gamma_2 = \lambda Y(1 - Y)\nabla_Y \sigma$

- Recently introduced in homogeneous models [H. Mathis 2019], comes from full non-equilibrium models literature
- Advantages :

⇝ No need to compute $Y_{\textsf{eq}}$

⇝ Time scales can be <u>different</u> depending on fractions

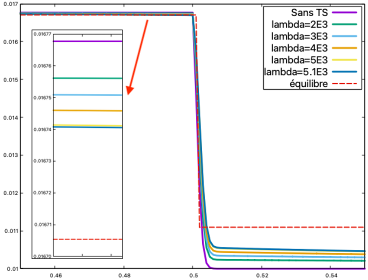
- Drawbacks :

⇝ Need a strong ODE solving method (implicit Euler scheme with Broyden algorithm)

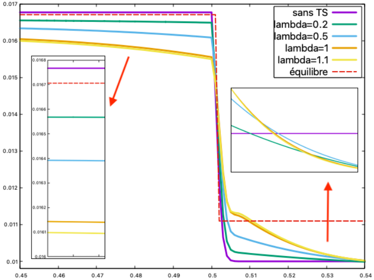
⇝ Far more complex trajectories, no longer monotonous

Coupling with the convective part

- We only consider common time scales according to fractions
- Convective part is solved by the relaxation scheme
- Γ_2's ODE solved by an implicit Euler method



(a) α_l modification by Γ_1.



(b) α_l modification by Γ_2

FIGURE – Atmospheric pressure Riemann problem modification by adding source terms for different time scales. Red dotted lines represents constant states equilibria.

$\rightsquigarrow$ Monotonous evolution towards equilibrium for Γ_1, non monotonous for Γ_2

$\rightsquigarrow$ Limited choice of λ : algorithm fails due to non-admissible states around the contact

Plan

Γ_2 study for a two-phase flow

- In order to simplify the analysis, we study these source terms for a two-phase flow. Thus, the ODE system is reduced to dimension 3 $(Y = (y_l, \alpha_l, z_l))$ that allows us to visualize data in space

⇝ A first numerical study of trajectories brings us to consider $Y(1-Y)\nabla_Y\sigma$ instead of $\nabla_Y\sigma$: solving is easier since $\forall t > 0,\ Y(t) \in]0;1[^3$

⇝ Γ's domain is a convex subset of the open cube, bounded by two planes that come from entropies definitions

- Important features :
  - ⇝ Uniqueness of the inner equilibrium (up to now, lack of a concavity argument)
  - ⇝ An equilibrium on the cube's border is necessary $0_{\mathbb{R}^3}$ or $1_{\mathbb{R}^3}$.

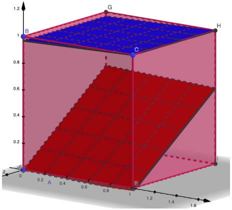


FIGURE – Γ's definition domain for a given $\tau, e)$ in space (y, α, z).

Conclusions

Conclusions

- Two-parts numerical study
  - ⇝ HRM convective part : efficient FV scheme
  - ⇝ Source terms contribution : Γ_1's limits could be avoided thanks to Γ_2

Forecast

⇝ At-equilibrium Riemann problems

⇝ Validation test cases

⇝ Analysis of the two-phase source terms Γ_2

Thank you for your attention !