PhD in Energy and Mineral Engineering at PSU

Nicolás's Research - Reports

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Considerations

Goal: Test the pseudopotential approach for partially misc. mixtures, under the action of a second force.

Idea: test different flow regimes based on Reynolds and Bond (Eotvos) numbers, and capture particular bubble shapes, as found by Flit R, Grace JR, Weber M. *Bubbles, drops, and particles*. New York: Academic Press; 1978.

$$R_e = \frac{\rho_l u_b d_b}{\mu_l} = \frac{u_b d_b}{\nu_l}$$

$$B_o = \frac{g \Delta\rho d_b^2}{\sigma}$$

A thermodynamic state fixes $\rho, \Delta\rho, \sigma$. Redifining R_e:

$$Re = \frac{d_b\sqrt{g d_b}}{\nu_l} = \frac{\sqrt{g d_b^3}}{\nu_l}$$

We can sweep the spectrum by fixing g (fixes B_o), and moving ν_l (fixes R_e), as:

$$\nu_l = c_s^2(\tau_l - \frac{\Delta t}{2})$$

$$g = \frac{B_o \sigma}{\Delta\rho d_b^2}$$

$$\nu_l = \frac{\sqrt{g d_b^3}}{R_e}$$

$$\tau_l = \frac{\nu_l}{c_s^2} + \frac{\Delta t}{2}$$

Initial setup

Domain: (!) 300x300 mesh (2D)
Fluid: Water at 485.33 K ($T_r = 0.75$), and $P_r = 0.092$.
$\rho_l^0 = 7.679$ (), $\rho_v^0 = 0.109$. $\rho_r = 70.45$.
Initial condition: Spherical droplet with $d_o = 30$, and $w_o = 8$.

Boundary conditions: The top and bottom boundaries are PERIODIC. On the left and right boundaries a no-slip condition is imposed. At the corners, where there is a PDF that may belong to two boundaries, the enumeration and assignation of conditions is as follows:

- Corner 1 (SW): No-slip (Left)
- Corner 2 (NW): No-slip (Left)
- Corner 3 (SE): No-slip (Right)
- Corner 4 (NE): No-slip (Right)

Parameters: Shan-Chen G=-1.0.
Beta = 0.2076
Time = 100000

Single static simulation:
$\Delta\rho = 7.59285$, $d_s = 29.45$,
$\Delta P = 0.00378$ ($P_l < 0$).
$\sigma = 0.1112$.

Initial setup 2 (Amaya)

Domain: (!) 160x400 mesh (2D)
Fluid: Water at 485.33 K ($T_r = 0.75$), and $P_r = 0.092$.
$\rho_l^0 = 7.679$ (), $\rho_v^0 = 0.109$. $\rho_L/\rho_g = 70$.
$\tau_l = 210.5$. $\tau_g = 0.8$. μ_l/μ_g =10.
Initial condition: Spherical droplet with $d_o = 40$, and $w_o = 8$.

Boundary conditions: Periodic on all boundaries (for static), walls on all boundaries (for dynamic). At the corners, where there is a PDF that may belong to two boundaries, the enumeration and assignation of conditions is as follows:

- Corner 1 (SW): No-slip (Left)
- Corner 2 (NW): No-slip (Left)
- Corner 3 (SE): No-slip (Right)
- Corner 4 (NE): No-slip (Right)

Parameters: Shan-Chen G=-1.0.
Beta = 0.2076
Time = 100000

Single static simulation:
$\Delta\rho = 7.2$ (7.7-0.5), $d_s = 40.0$,
ΔP = 8.5e-3 - 5.87e-3 = 2.623e-3
$\sigma = \Delta P \cdot r = 0.05254$. B_o =10. Then, $g = \frac{\sigma B_o}{\Delta\rho d^2}$ = 4.5e-5. $\mu_l = 0.85$, $\nu_l = 0.1105$. $\tau_l = 0.83$.

Spherical regime

First case (150 x 300)

- $g = |\mathbf{g}| =$ -1e-6. $B_o = 0.0592$. $\tau_l = 2.0$, $\nu = 0.5$. $u_b = 0.0121$.
- $R_e^{\text{org}} = 0.713$. $R_e^{\text{mod}} = 0.320$.
- This is spherical regime, and far away from the other regimes according to the Grace's plot.

Ellipsoidal case

Ellipsoid case (150 x 300)

- $g = |\mathbf{g}| =$ -1e-5. $B_o = 0.592$. $\tau_l = 0.51$, $\nu = 0.0033$. $u_b \approx = 0.35$.
- $R_e^{\mathrm{org}} = 3092$. $R_e^{\mathrm{mod}} = 151.61$
- This simulation is approaching to the Mach velocity limit and a perturbation is moving the bubble from the axis. I decided to open the channel more to avoid the interaction with the wall. I have reasons to believe that the movement beyond the axis is due to whom the corner was assigned to (number of boundary).

Ellipsoid case (300 x 300)

- $g = |\mathbf{g}| =$ -1e-5. $B_o = 0.592$. $\tau_l = 0.51$, $\nu = 0.0033$. $u_b \approx = 0.35$.
- $R_e^{\mathrm{org}} = 3092$. $R_e^{\mathrm{mod}} = 151.61$
- The ellipse shape of the bubble was better seen in this case, although eventually it moves away from the center. For the most part of the simulation, the ellipsoid maintains, although it is important to understand if the viscosity of the gas phase plays any role in the deformation (”plasticity” of the bubble).
- Apr 15/22. The ellipse is not moving anymore from the center.

Dimples

Dimples case (300 x 300)

- $g = |\mathbf{g}| =$ -2e-3. $B_o = 118$ $\tau_l = 0.72$, $\nu = 0.07348$. $u_b \approx =$.
- $R_e^{\text{org}} =$. $R_e^{\text{mod}} = 100$
- The gravity value is too high and the method is diverging too soon. Not even with G = -0.1 or g = 1e-4.

Dimples case (3000 x 3000)

- $d_o = 300$. $g = |\mathbf{g}| =$ -1e-5. $B_o = 61$. $\tau_l = 0.993$, $\nu = 0.164$ $u_b \approx =$.
- $R_e^{\text{org}} =$. $R_e^{\text{mod}} = 100$
- Did not run

Dimples case (3000 x 3000)

- $d_o = 300$. $g = |\mathbf{g}| =$ -1e-5. $B_o = 61$. $\tau_l = 5.43$, $\nu = 1.64$ $u_b \approx =$.
- $R_e^{\text{org}} =$. $R_e^{\text{mod}} = 10$
- Did not run

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Forcing scheme

Taking advantage of the mutual interactions between components, the pseudopotential is accounting only for attraction between components, while an extra term accounts for the usual repulsion term:

$$F_i^\sigma = -\frac{1}{c_s^2\delta t}\sum_\alpha w_\alpha e_{\alpha,i}[\frac{R_sT}{1-b_m\rho} - c_s^2]\rho_\sigma(\mathbf{x}+\mathbf{e}_\alpha\delta t)$$
$$-\psi^\sigma\sum_{\sigma_2} G_{\sigma,\sigma_2}\sum_\alpha w_\alpha e_{\alpha,i}\psi^{\sigma_2}(\mathbf{x}+\mathbf{e}_\alpha\delta t)$$

Where ψ and G_{σ,σ_2} are defined as:

$$\begin{aligned}\psi^\sigma &= \rho^\sigma\sqrt{\frac{a^\sigma}{f(b\rho)}}\\ G_{\sigma,\sigma_2} &= \frac{2(\Lambda_{\sigma,\sigma_2}-1)}{c_s^2\delta t}\end{aligned} \tag{1}$$

where $f(b\rho)$ is the density-dependent polynomial in the denominator of the attraction term in the cubic equation of state. Here, the terms a, b are given in mass-basis, so proper conversions must be taken care of.

Taylor Expansion

Generic form:

$$F_i = \sum_\alpha T(\mathbf{x} + \mathbf{e}_\alpha \delta t) w_\alpha \mathbf{e}_\alpha$$

Replacing the Taylor expansion of T

$$F_i = T(\mathbf{x}) \sum_\alpha w_\alpha \mathbf{e}_\alpha + \partial_j T \delta t \sum_\alpha w_\alpha \mathbf{e}_\alpha \mathbf{e}_\alpha^j + \frac{\delta t^2}{2} \partial_j \partial_k (T) \sum_\alpha w_\alpha \mathbf{e}_\alpha \mathbf{e}_\alpha^j \mathbf{e}_\alpha^k + \frac{\delta t^3}{6} \partial_j \partial_k \partial_l (T) \sum_\alpha w_\alpha \mathbf{e}_\alpha \mathbf{e}_\alpha^j \mathbf{e}_\alpha^k \mathbf{e}_\alpha^l$$

Continuum approach:

$$F_i = c_s^2 \delta t \partial_i T + \frac{c_s^4 \delta t^3}{2} \partial_i \partial_{kk}(T)$$

Resulting pressure;

$$p = c_s^2 \sum_\sigma \rho_\sigma + \frac{c_s^2 \delta t}{2} \sum_\sigma \sum_{\sigma_2} G_{\sigma,\sigma_2} \psi_\sigma \psi_{\sigma_2} + \sum_\sigma (\frac{R_s T}{1 - b_m \rho} - c_s^2) \rho_\sigma$$

$$p = \frac{R_s T}{(1 - b_m \rho)} \rho - \frac{a_m \rho^2}{f(b_m \rho)}$$

Reference

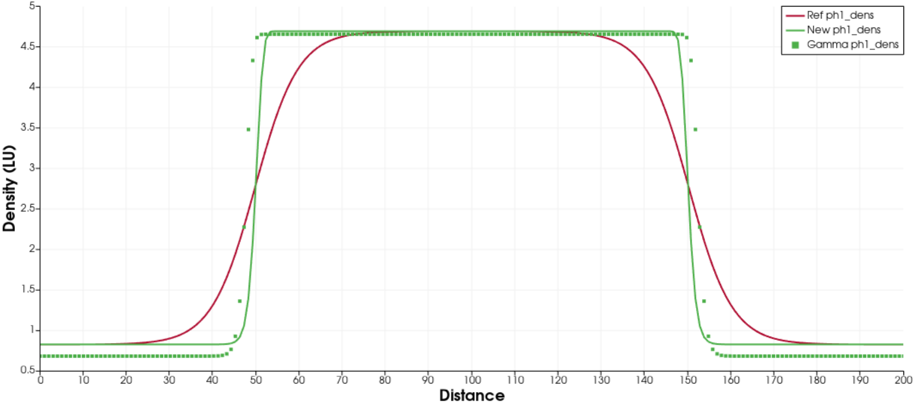
From van der Waals implementation into the phase behavior model (C++):

Name, mw, pc, tc, acen, vc, shift
C3 0.044097 615.8 666.05 0.1522 0.0 0.0
C5 0.044097 488.5 845.80 0.2514 0.0 0.0

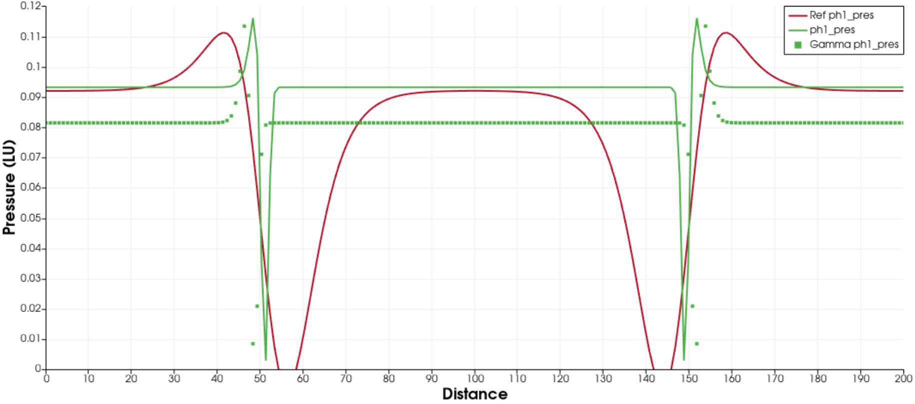
Conditions:
P = 275.36 psi, T = 192.34 F. z = [0.5, 0.5]

Results from flash:
Densities = 13.5852 lb/ft3, 2.3956 lb/ft3
(4.693187 lu, 0.8275917 lu)
Fugacities = 906.34 kPa, 604.423 kPa
(0.043939432 lu, 0.029302344 lu)
Liquid composition = [0.36357, 0.63643]
Gas composition = [0.54527, 0.45473]
Ki = 1.49975, 0.714505. γ = 0.642

Results

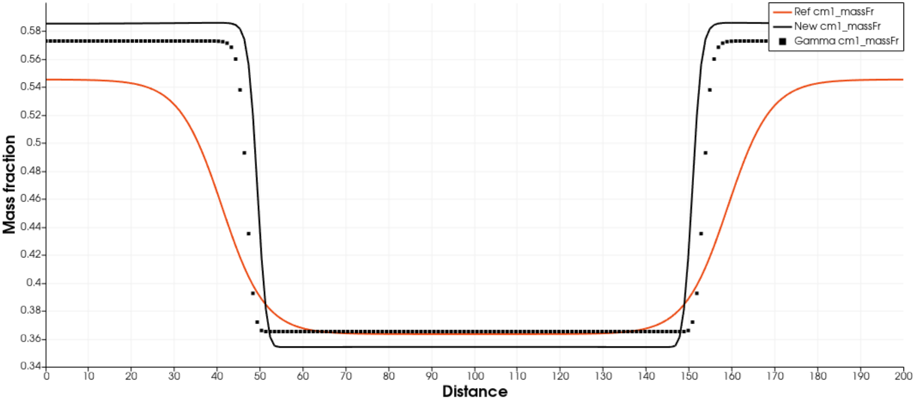

Ref ph1_dens
New ph1_dens
Gamma ph1_dens
Density (LU)
Distance
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200

Results



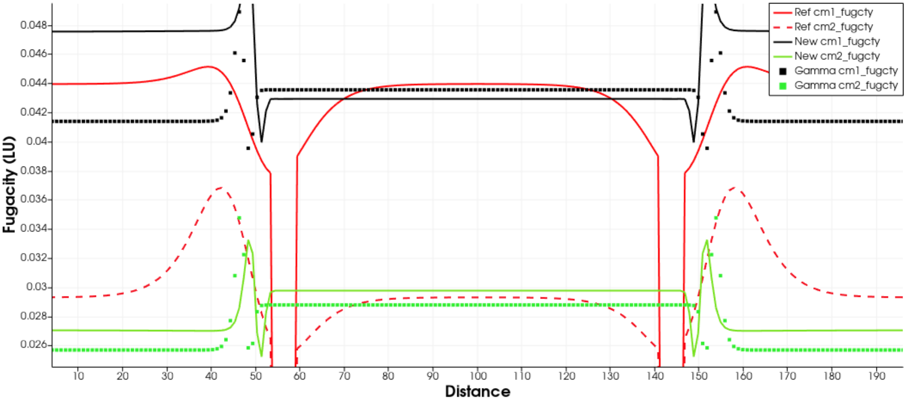
Ref ph1_pres
ph1_pres
Gamma ph1_pres
Pressure (LU)
Distance
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200

Results

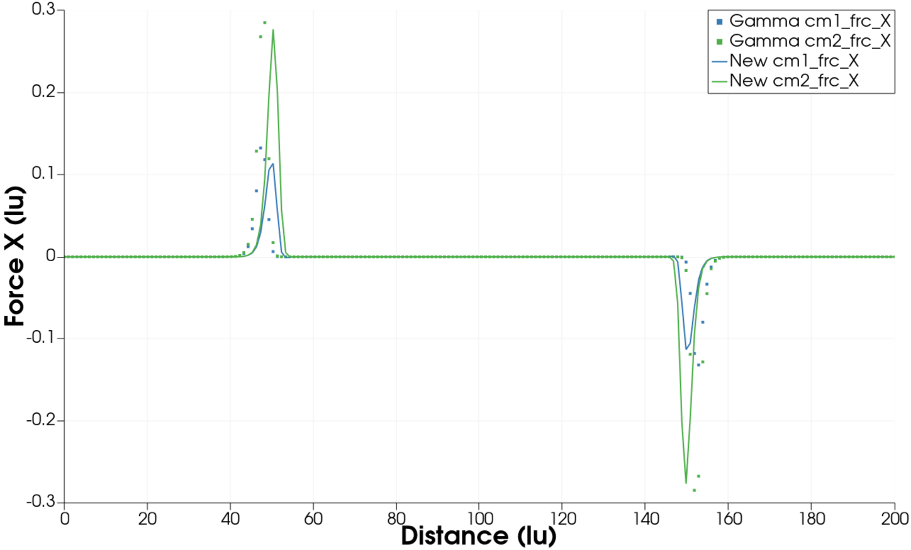


Ref cm1_massFr
New cm1_massFr
Gamma cm1_massFr
Mass fraction
Distance
0.58
0.56
0.54
0.52
0.5
0.48
0.46
0.44
0.42
0.4
0.38
0.36
0.34
0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200

Results


Ref cm1_fugcty
Ref cm2_fugcty
New cm1_fugcty
New cm2_fugcty
Gamma cm1_fugcty
Gamma cm2_fugcty
Fugacity (LU)
Distance
0.048
0.046
0.044
0.042
0.04
0.038
0.036
0.034
0.032
0.03
0.028
0.026
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

Results



Gamma cm1_frc_X
Gamma cm2_frc_X
New cm1_frc_X
New cm2_frc_X
Force X (lu)
Distance (lu)
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
20
40
60
80
100
120
140
160
180
200

Discussion

Report XXX XX - 202X

Main discussion points:

- Topic 1
- Topic 2

Sample frame title

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- Text visible on slide 1

Sample frame title

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- Text visible on slide 1
- Text visible on slide 2

Sample frame title

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- Text visible on slide 1
- Text visible on slide 2
- Text visible on slides 3

Sample frame title

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- Text visible on slide 1
- Text visible on slide 2
- Text visible on slide 4

In this slide

In this slide
the text will be partially visible

In this slide
the text will be partially visible
And finally everything will be there

Sample frame title

In this slide, some important text will be highlighted because it's important. Please, don't abuse it.

Remark

Sample text

Important theorem

Sample text in red box

Examples

Sample text in green box. The title of the block is “Examples”.

Two-column slide

This is a text in first column.

$$E = mc^2$$

- First item
- Second item

This text will be in the second column and on a second tought this is a nice looking layout in some cases.