# PhD in Energy and Mineral Engineering at PSU

## Nicolás's Research - Reports

Nicolás Bueno[1]    Advisor: Dr. Ayala[1]

[1]Department of Energy and Mineral Engineering
Penn State University

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### Considerations

Test the pseudopotential approach for multicomponent partially miscible mixtures, under the action of a second force, as gravity.

The partition scheme can be proven to work for different Reynolds and Bond (Eotvos) numbers, depicting particular bubble shapes as found by Flit R, Grace JR, Weber M. Bubbles, drops, and particles. New York: Academic Press; 1978.

$$R_e = \frac{\rho_l u_b d_0}{\mu_l} = \frac{u_b d_0}{\nu_l}$$

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

If we fix thermodynamic conditions, $\rho, \Delta\rho, \sigma$ will be fixed. Redifining $R_e$:

$$Re = \frac{\sqrt{g d_0} d_0}{\nu_l} = \frac{\sqrt{g d_0^3}}{\nu_l}$$

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

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

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

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

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

# Initial setup

Domain: 300x300 mesh (2D)
Fluid: Water at 485.33 K ($T_r = 0.75$), and $P_r = 0.092$. $\rho_l^0 = 7.679$, $\rho_v^0 = 0.109$.
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:
$\Delta\rho = 7.59285$, $d_s = 29.45$,
$\Delta P = 0.00378$ ($P_l < 0$).
$\sigma = 0.1112$.

# Spherical regime

First case (150 x 300)

- $g = |\mathbf{g}| =$ -1e-6. $B_o = 0.0592$. $\tau_l = 2.0$, $\nu = 0.5$. $u_b = 0.0121$.
- $R_e^{\mathrm{org}} = 0.713$. $R_e^{\mathrm{mod}} = 0.320$.
- 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. $B_o = 0.592$. $\tau_l = 0.51$, $\nu = 0.0033$. $u_b \approx = 0.35$.
- $R_e^{\text{org}} = 3092$. $R_e^{\text{mod}} = 151.61$
- 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. $B_o = 0.592$. $\tau_l = 0.51$, $\nu = 0.0033$. $u_b \approx = 0.35$.
- $R_e^{\text{org}} = 3092$. $R_e^{\text{mod}} = 151.61$
- 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

# Discussion

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Main discussion points:

- Topic 1
- Topic 2

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And finally everything will be there

# Sample frame title

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## Remark

Sample text

## Important theorem

Sample text in red box

## Examples

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# Two-column slide

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$$E = mc^2$$

- First item
- Second item

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