NUMERICAL MODELING OF GAS BUBBLE DYNAMICS IN LIQUID METAL IN APPLIED DC MAGNETIC FIELD

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Abstract. Apart from common steam reforming process the thermal decomposition of methane is regarded as an alternate route to producing hydrogen and elemental carbon with out of CO_2 emissions. Chemical reaction of decarburation can be ensured by means of methane bubbly flow through a molten metal bath and additionally controlled by external electromagnetic field. On this stage of research model for single bubble rise in presence of external DC magnetic field, based on VOF approach is developed. Model is verified, in absence of applied field, for different liquid types (water solution, GaInSn) at different flow conditions, obtained bubble terminal shapes and velocities reveal a fine correlation with existing experimental and model results. Bubble rise dynamics is studied in GaInSn in longitudinal/transversal DC magnetic field, appropriate rise characteristics and their dependencies on field strength are in agreement with existing (experimental/model) predictions.

1. Introduction

One of the possibilities to produce H_2 without forming CO_2 is decomposition of CH_4 [1]:

$$CH_4 \rightarrow C + 2H_2, \ (\Delta h_0 = 74.85 \text{ kJ/mol}).$$

Due to fact that reaction of decarburation is endothermic the temperature must be above 600 ˚C for the reaction to proceed at a reasonable rate. The main problem for this process is the deposition of the nanocarbon particles on the reactor walls (or catalyst surface), which causes the pressure to drop and creates thermal resistance, thereby decreasing reactor life. Alternative way is realization of reaction ensuring a methane bubbly flow through a molten metal bath and for process control and increase of efficiency use applied DC/AC magnetic field.

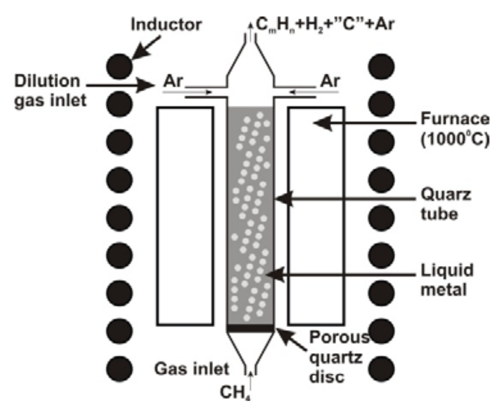


Figure 1: Liquid metal bubbly column for H_2 production without CO_2 emission.

Knowledge of single bubble rise properties (characteristic force coefficients: drag, lift, acceleration) can be used for implementation in bubble cloud behavior model like Euler-Euler, Euler-Lagrange which, in turn, can be used for description of methane thermal cracking reactor (Figure 1). In appropriate context great challenge is attributed to the tracking of sharp interface between the gas bubble and the surrounding liquid, classical difficulty causes: discontinuity of the physical properties across the fluid interface, geometric complexity caused by bubble deformation, numerical smearing of interface between the gas bubble and the surrounding liquid, effects of surfactants on the interface. Mentioned factors are dependent on the mesh quality and in majority of cases significantly increase calculation time. In the present work for appropriate problem class there was examined applicability of VOF method implemented in *ANSYS Fluent*, obtained results for different liquids (water solution, GaInSn) are compared with existing experimental approaches [2].

2. Rising bubble model

Bubble rise dynamics in electrically conductive liquid in external DC EM field can be characterized by the following set of equations:

$$\frac{\nabla^2 \boldsymbol{B}}{\mu_{mag}\sigma_{el}} + (\boldsymbol{B}\cdot\nabla)\boldsymbol{U} - (\boldsymbol{U}\cdot\nabla)\boldsymbol{B} = 0, \tag{1}$$

$$\boldsymbol{j} = \sigma_{el}(-\nabla\varphi + [\boldsymbol{U}\times\boldsymbol{B}]), \tag{2}$$

$$\nabla\cdot\boldsymbol{U} = 0, \tag{3}$$

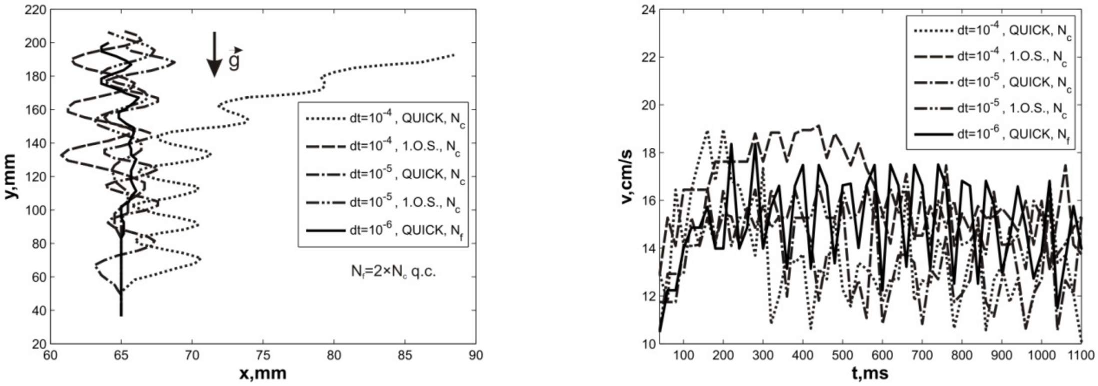
$$\frac{\partial \boldsymbol{U}}{\partial t} + (\boldsymbol{U}\cdot\nabla)\boldsymbol{U} = -\frac{\nabla p}{\rho_l} + \nu_l\nabla^2\boldsymbol{U} + \boldsymbol{f}, \tag{4}$$

where $\boldsymbol{B}$ is magnetic field induction, $\boldsymbol{j}$ – current density, $\boldsymbol{U}$ - velocity, p - pressure, ν_l - kinematic viscosity, $\boldsymbol{f}$ - sum of volume forces, e. g. gravitational: $\boldsymbol{f}_g = \boldsymbol{g}$ and Lorentz force: $\boldsymbol{f}_L = [\boldsymbol{j}\times\boldsymbol{B}]$. First pair of equations describes EM nature of the process: Induction equation (1), where free charges/displacement currents are neglected, for process magnetic Reynolds number: $Rm \ll 1$, in turn equation (2) corresponds Ohm's law. The second pair of equations characterizes hydrodynamic processes of conductive viscous liquid that is considered as incompressible (3). Momentum balance is achieved on account of equation (4).

Because the system contains two phases a dynamics of their boundary should also be described. This can be done by means of coupling magnetohydrodynamics (MHD) module and Volume of Fluid (VOF) technique implemented in *ANSYS Fluent.*

3. Bubble free emersion in simple liquids

3.1. Analysis of numerical effects. In industrial applications density of primary phase $\rho_l \sim 10000$ kg/m^3, numerical effects in case of such systems can play significant role, thus their impact on physical results should be studied very carefully. It is known fact: to obtain accurate results appropriate momentum equation discretization should have high order of precision. However, how these results are dependent on mesh quality and time discretization is rather unclear for appropriate systems under consideration. To study this effects on rather popular for CFD applications QUICK scheme (which is based on a weighted average of second-order-upwind and central interpolations of the velocity) there was considered 2D planar circular air bubble emersion (ρ_{air} = 1.2 kg/m^3, η_{air} = 18 μPa·s, D = 4 mm) in GaInSn eutectic (ρ_{GaInSn} = 6361 kg/m^3, σ_{el} = 3.27 MS/m, σ = 2.2 mPa·s) initialized at the bottom of rectangular fluid domain ($x = 33\cdot D$ and $y = 63\cdot D$) in the beginning of calculation, obtained results for bubble trajectory and velocity are shown on Figure 2a,b. For fixed mesh in case of QUICK scheme there can be seen strong dependence on time step (dotted, dash-dotted and solid line). If time step is too large than there is not observed transition from straight rise trajectory to zig-zagging, bubble rise is initially oscillatory. With decrease of time step there is observed decrease of oscillation amplitude and increase of velocity. Very close results to most precise (QUICK with small enough time step: $dt = 10^{-6}$ s and number of quadratic



(a) (b)

Figure 2: Time step, mesh quality and momentum discretization scheme influence on 2D bubble rise dynamics in liquid metal (a) - trajectory (b) - velocity.

Cells: N_f = 265980, correspondent solid lines) can be obtained with 1 – order scheme (velocity quantities at cell faces are determined by assuming that the cell-center values represent a cell-average value and hold throughout the entire cell) (with $dt = 10^{-5}$ s and N_c = 147364, correspondent dash-dash-dotted lines), due to numerical stability of this approach. It can be concluded that 1 – order scheme have better (with lower computational costs) convergence properties than high order scheme when spatial-time discritization is not high. In general, it can be concluded that for single bubble rise in GaInSn appropriate Courant condition: $Udx/dt < C$ instead of traditional $C = 1$, in case of usage of 1 – order scheme must be $C \approx 0.05$. Recently in [3] there was considered bubble rise in aluminum (ρ_{Al} = 2380 kg/m^3) also in 2D approach, it was stated that for numerical simulations of such system in case of 2 – order scheme: $C < 0.2$.

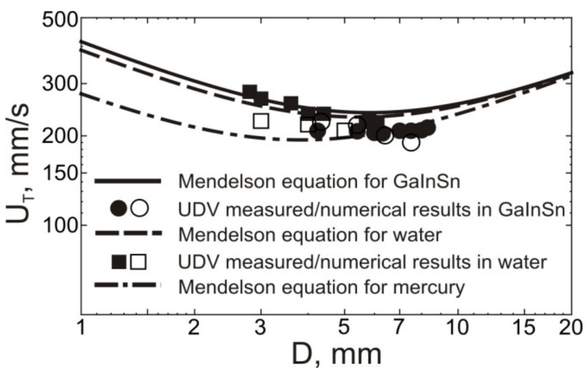


Figure 3: Termianl bubble velocity vs. equivalent bubble diameter in various liquids [2].

To check physical correctness of chosen numerical approach there was considered 3D bubble rise ($N = 2\square10^6$) in GaInSn and also in pure water due to very similar ρ_l/σ ratios (same bubble shape characteristics) of both liquids, appropriate results compared with experiment/theory [2,4] (Figure 3), there can be seen good correlation.

3.2. DC magnetic field influence on a rise dynamics. For demonstration of models ability to describe physical aspects of DC magnetic field influence on bubble rise there was considered 2D system. General mechanism of appropriate influence is shown on Figure 4. With increase of applied field induction there is observed damping of bubble induced vortex structures which is accompanied with increase of bubble rise velocity. However when field strength is enough to suppress all vorticity in bubble wake there is observed decrease in relative velocity as well as damping of oscillations in field transversal directions. Bubble rise (D = 4 mm) trajectories for different field orientations (longitudinal/transversal) and induction values are presented on Figure 5a,b. From simulation results for bubble trajectories there can be observed domination of parallel velocity components to appropriate field direction in moderate induction value range. When field is strong enough surprisingly in both cases observed straightening of appropriate rise trajectories, however similar straightening process is also observed in transversal field for 3D bubble rise in mercury [5].

There was considered 3D bubble rise in applied longitudinal field (B = 0.3 T), obtained result comparison with experiment [2] for relative drag coefficients vs. interaction parameter are shown on Figure 6. In general there is observed tendency that for smaller bubbles drag coefficient increase with increase of field value, similar tendency is also observed in case of liquid metal flow past insulating sphere. In turn, for larger bubbles is observed reverse tendency: decrease of drag coefficient with increase of interaction parameter, this is stimulated by coupling between bubble elongation in fields direction and modification of bubble wake due to applied field. There can be seen qualitative correspondence between experiment and numerical prediction in case of Bo = 2.2, however for Bo = 3.4; 4.9 there is sufficient deviation, this is due to presence of impurities in melt of appropriate experimental setup [2], in turn, occurrence of oxides in melt diminishes the surface tension significantly [6]. Thus in experiment $C_D/C_D(N = 0)$ character change (symmetry brake) is observed at smaller Bond number value comparing to corresponding numerical model result (Bo ~ 6.6), from physical point of view it can be expected, because in last case surface tension decreasing factors are not present, this mean that with increase of diameter Lorentz force influence on bubble shape will be smaller, due to increased surface tension force. Contrary in [7] using immersed boundary method symmetry brake is observed at even smaller Bond number value than in experiment [2]. In case when B = 1 T appropriate model predicts increase of relative drag experienced by bubble with increase of Bond number (Figure 7), in general such tendency could be expected, because in this case Lorentz force impact on bubble shape is balanced by surface tension force, thus impact on rise process is possible only through wake modifications, like in case of small bubbles (Figure 6). In turn, increase of Bond number in field absence indicates increase in rise velocity, in applied field this will lead to larger Lorentz force values, thus larger drag values. Similar tendency in relation between drag and Bond number like in Figure 7 is observed in case of bubble rise in transversally applied DC magnetic field [5]. In general, obtained model results

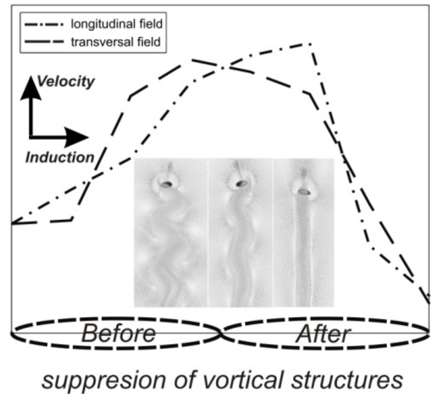
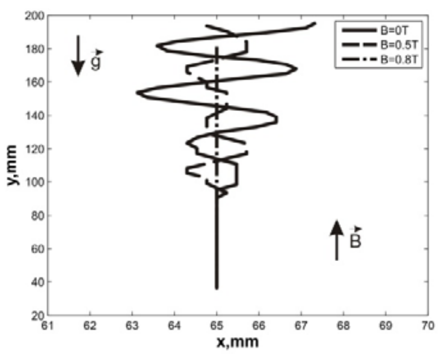
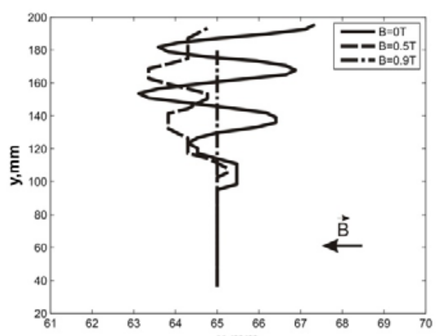


Figure 4: General mechanism of field influence on bubble rise.



(a)



(b)

Figure 5: Stationary magnetic field influence on bubble (D = 4 mm) in 2D approach on rise trajectory (a) – longitudinal field (b) – transversal field.

are very promising also due to fact that system is considered on $2x10^6$ element mesh, in turn, appropriate results in [7] are obtained on $83.9x10^6$ element mesh, thus usage of VOF method can lead to considerable decrease of computational costs.

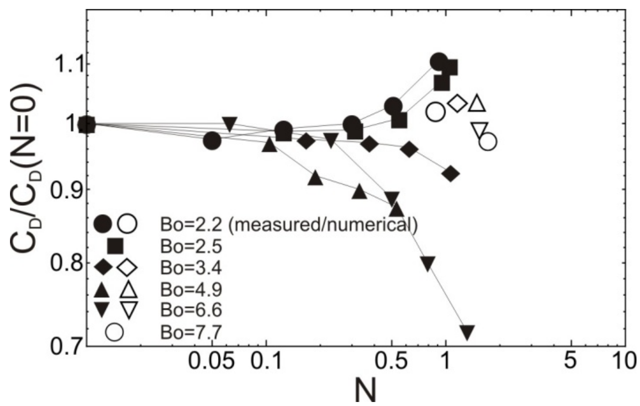


Figure 6: Relative change of drag coefficient vs. magnetic interaction parameter result comparison with experiment [2].

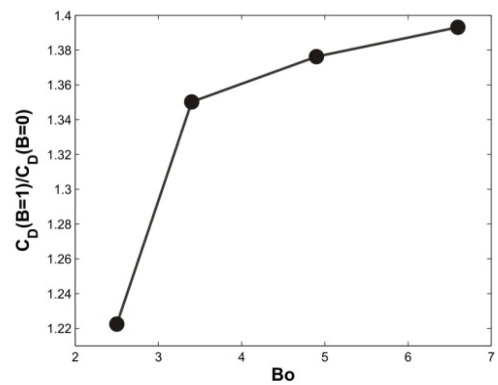


Figure 7: Drag coefficient vs. Bond number in longitudinally applied field (B = 1 T).

4. Conclusions

The obtained model results clearly show ability to describe bubble rise process for different liquid classes. It is shown that for minimization of computational costs for systems with high density ratios 1 - order scheme can be applied for momentum equation and in case of GaInSn appropriate Courant condition: $C < 0.05$ should be taken into account. In case of applied DC magnetic field model give correct physical results, which are in good agreement with experiments [2], for high magnetic field values (B ~ 1 T) model predicts increase of bubble experienced relative drag with increase of Bond number.

5. Acknowledgments.

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6. References

[1] Abanades, A.: Experimental analysis of direct methane cracking, Int. J. Hydrogen Energy 36 (2011) 12877-12886.
[2] Zhang C., Eckert S., Gerbeth G.: Experimental study of single bubble motion in a liquid metal column exposed in a DC magnetic field, Int. J. Multiphase Flow 31 (2005) 824-842.
[3] Liu H., Xie M.Z., Liu H.S., Wang D.Q.: Numerical study on bubble rising behaviour in a reciprocally stirred molten metal flow, Rev. Adv. Mater. Sci. 33 (2013) 195-201.
[4] Mendelson H.D.: The prediction of bubble terminal velocity from wave theory, AlChE J. 13 (1967) 250-253.
[5] Mori Y., Hijikata K., Kuriyama K..: Experimental study of bubble motion in mercury with and without a magnetic field, J. Heat Transfer 99 (1977) 404-410.
[6] Szekely J.: Fluid flow phenomena in metals processing, Academic Press 1979.
[7] Schwarz S., Frohlich J.: DNS of single bubble motion in liquid metal and influence of magnetic field, Proc. Symposium on Turbulent Shear Flow Phenomena, Ottawa, Canada 2011.