Numerical study of gas bubbles collective dynamics in the melt influenced with magnetic field

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Abstract
The paper presents numerical study of methane (CH_4) bubbles flow through molten tin (Sn) in electromagnetic (EM) field for cylindrical bubble reactor, which produces hydrogen (H_2) without carbonic acid (CO_2) emission.
Eulerian-Eulerian approach, realized in commercial packages ANSYS CFX and ANSYS Fluent, as well as Boltzmann approach, realized as own code, are used for multiphase flow – liquid metal (continuous phase) and gas bubbles (dispersed phase). Magnetic field is uniform.
Transient distributions of methane flowing in liquid tin, influenced with magnetic field, are discussed.

Key words: bubbles reactor, Euler-Euler approach, Boltzmann approach, multiphase flow, magnetic field, LES

Introduction
The production of hydrogen H_2 without generation of carbonic acid CO_2 may be performed with decomposition of methane $CH_4 \rightarrow C + 2H_2$. The reasonable rate of this endothermic reaction ($\Delta h_0 =$ 74.85 kJ/mol) is reached at temperature values above 600ºC [1]. The main problem of such process is the decreasing of reactor life. The cause is deposition of carbon particles on the reactor walls and catalyst surface; as the consequence is the pressure drop and increase of thermal resistance.

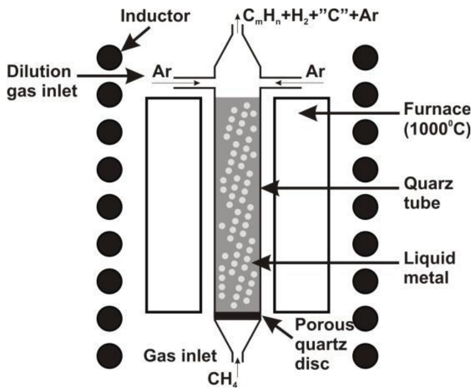

Fig. 1: Liquid metal bubble column for H_2 production without CO_2 emission.

Table 1: Parameters of gas and liquid

Parameter	Unit	Gas	Liquid
Materials	–	methane (CH_4)	tin (Sn)
State	–	ideal gas	molten metal
Operation temperature	*°C*	600	600
Molar mass	*kg/kmol*	16.04	118.71
Density	*kg/m³*	0.224–0.353	6720
Thermal expansivity	K^{-1}	–	$2.24\cdot10^{-5}$
Dynamic viscosity	*kg/(m·s)*	$1.42\cdot10^{-5}$	$1.6\cdot10^{-3}$
Gas–liquid surface tension coefficient	N/m^{-1}	0.518	

A possible way to increase efficiency of production and to control the process is the utilization of magnetic field, produced by direct (DC) or alternating (AC) current source, on electrically conductive liquid, when methane bubbles are flowing through it. The mentioned above process is realized with methane-tin cylindrical bubble reactor (CBR) [2], the scheme of installation is shown in Fig. 1 [3]. Main parameters of methane and tin [4] are gathered in Tab. 1.
Previous consideration of single bubble dynamics [5], which covered both models implementation and experimental verification, are continued in current paper with numerical study of bubbles collective dynamics.

Multiphase Euler-Euler approach for methane bubbles flow through liquid tin
The systems of hydrodynamic equations for two-phase system of gas and liquid (denoted "*g*" and "*l*") consist of continuity, volume conservation and momentum equations according to Euler-Euler approach, which is realized in commercial packages – ANSYS CFX [6] and ANSYS Fluent [7].
The closure of equation system is performed with constrain on the pressure, namely two phases share the same pressure field. Static pressure in liquid depends on height z from the CBR bottom [8] is $p = p_{op} + g_0\rho_l(H_{CBR} - z)$ with

operating pressure p_{op}, gravitational acceleration g_0 and height H_{CBR} of CBR.

The gas density ρ_g is derived from ideal gas law $\rho_g = pM_g/(R_0T)$ with the molar mass of gas phase M_g and universal gas constant $R_0 = 8.314 \cdot 10^3\, kJ/(kmol \cdot K)$.

The flow is assumed isothermal at the operation temperature $T = T_{op}$. The liquid density is uniform constant.

In momentum equations the following interfacial forces, acting on one phase due to the presence of other phase [6,7], are taken into account: ***buoyancy*** force; ***drag*** force; ***lift*** force; ***virtual mass*** force; ***wall lubrication*** force.
The computations for tuning of numerical model show that only ***buoyancy*** and ***drag*** forces may be taken into account because changes of distribution of methane volume fraction due to other forces' contribution does not exceeded 5%.
The ***interphase turbulent dispersion*** force is not applicable for Large Eddy Simulation (LES) model of turbulence. This force may be used along with models of isotropic turbulence such as *k-ω* Shear Stress Transport (SST) model.

For computations of two-phase gas-liquid system commercial software packages are used, where the following discretization schemes for momentum, continuity and volume conservation equations are used:
• finite element method (FEM) in ANSYS CFX
• volume of fluid (VOF) method in ANSYS Fluent, which is suitable for evaluation of liquid and gas volume fractions.
The test computations for the air-water flow in the rectangle bubble column have been performed. The characteristic ("snake-like") distributions of air volume fraction and velocity vectors field [3,5] are obtained in 2D (mesh ~2 500 elements) and 3D (mesh ~32 500 elements) computations using steady-state or transient SST model of turbulence.
The numerical study of the methane-tin flow in CBR have been performed with LES models of turbulence using the structured 3D mesh (~400 000 elements) with the inflation in vertical direction from the inlet zone to the outlet zone.
To ensure the stability of computations for the transient flow regime the time step is chosen in the range 0.001–0.005 *sec*, which corresponds to the Courant number value less than the unity. When flow changes in time are extremely fast (magnetic field "switching on"), to gain the computations stability the time step is chosen < 0.0001 *sec*.

A lattice Boltzmann model for numerical simulation of dynamics of bubble flow
The lattice Boltzmann method (LBM) is a relatively recent computational approach based on kinetic theory for solving fluid mechanics and other physical problems [9,10]. In brief, the LBM consists of solving the lattice Boltzmann equation for the evolution of a distribution function $f(\vec{x}, \vec{v}, t)$ as they move and collide on a lattice. LBM is originated from the Boltzmann equation: $\frac{\partial f}{\partial t} + \vec{\xi}\nabla_x f + \vec{a}\nabla_\xi f = \Omega(f)$ with velocity $\vec{\xi}$, acceleration $\vec{a}$ and the collision operator $\Omega(f)$. The numerical simulation using the LBM model of the rising process of randomly generated bubbles in rectangular domain with 250×1250 lattice is carried out (Figs. 2, 3), the non-slip boundary conditions are imposed in all directions. The density ratio ρ_l/ρ_g between the fluid and gas is 1000 and viscosity ratio ν_l/ν_g is 100.

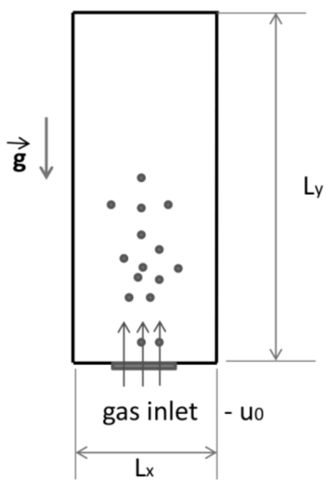

Fig. 2. Rectangular column scheme.

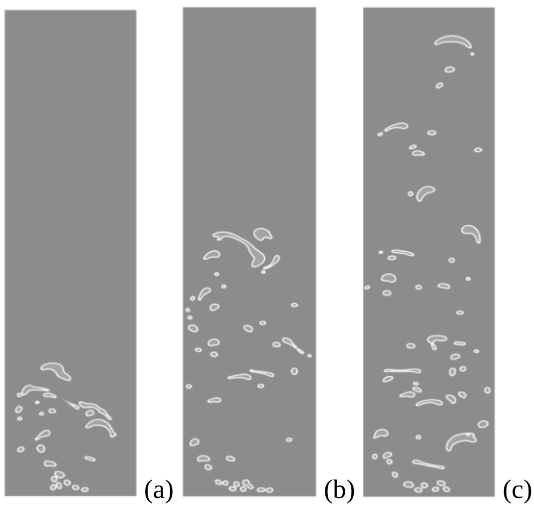

Fig. 3. Randomly generated bubbles in rectangular column $L_x = 0.5$ *m*, $L_y = 2.5$ *m*: ρ_l/ρ_g =1000; ν_l/ν_g =100: (a) t = 21.5 *s*; (b) t = 48.0 *s*; (c) t = 90.0 *s*.

Electromagnetic force

In the case of electrically conductive liquid, which flows with velocity $\vec{\mathrm{v}}_l$ in external magnetic field with induction $\vec{B}$, the dynamics of two-phase system depends on EM force $\vec{f}_l^{EM}$, which is the results of interaction of electrical current, induced by liquid motion, and magnetic field,

$$\vec{f}_l^{EM} = \vec{j}_l \times \vec{B} \qquad \vec{j}_l = \phi_l \sigma_l^{EM} \left(-\nabla \varphi + \vec{\mathrm{v}}_l \times \vec{B} \right) \tag{1}$$

with volume fractions of liquid ϕ_l, electrical conductivity of liquid σ_l^{EM} and electrical potential φ.

Computations results of methane-tin flow in CBR

Main parameters of installation are gathered in Tab. 2.

Table 2: Geometrical and operational parameters

Geometrical parameters	Unit	Value
Height of column	*m*	1.15
Filing level of the melt	*m*	1.05
Diameter of column	*m*	0.036
Diameter of gas inlet	*m*	0.0072
Diameter of gas bubbles	*m*	0.0001

Operational parameters	Unit	Value
Gas speed at inlet	*m/s*	0.05
Gas volume flow	m^3/s	$2.0 \cdot 10^{-6}$
Gas mass flow	*kg/s*	$7.5 \cdot 10^{-7}$
Induction of magnetic field	*T*	0.5

In the case of ***absence of magnetic field*** the methane jet has the instantaneous “snake-like” shape in the zone near inlet (Fig. 4(a)). Time-averaged (flow time 40 s has been reached) distribution of methane volume fraction is almost axis-symmetrical. Maximum time-averaged speed of methane is $\mathrm{v}_{meth,\max}^{aver}$ ~0.33 *m/s*, which is ~6.5 times greater than speed in inlet opening $\mathrm{v}_{meth}^{inlet}$ = 0.05 *m/s* (Tab. 3). The instantaneous speed of methane may exceed $\mathrm{v}_{meth,\max}^{inst}$ ~1.16 *m/s*. The maximum time-averaged $\mathrm{v}_{tin,max}^{aver}$ and instantaneous $\mathrm{v}_{tin,max}^{inst}$ velocities of tin are of the same range.

The methane jet is essential only near inlet with the maximum height of the jet penetration only 2.5% of the reactor height H_{CBR}. The diameter of jet is comparable with the diameter D_{inlet} of the inlet opening (Tab. 3). Above the inlet zone the distribution of methane is almost uniform.

In the case when the ***constant vertical magnetic field*** is applied, the impact of Lorentz force (the maximum value $f_{\max}^{EM}$ ~$3.3 \cdot 10^5$ N/m^3, the vectors are located in the horizontal plane and are perpendicular to the magnetic field induction) results in thinning-down of the methane jet (Fig. 4 (b)), which the averaged diameter may be estimated as 10% of the diameter D_{inlet} of the inlet opening (Tab. 3).

The penetration of extremely thin methane jet is very fast (archived flow time is approximately 3.5 sec) with time-averaged speed $\mathrm{v}_{meth,\max}^{aver}$ ~2.03 m/s, which is ~40.5 times greater than the methane speed in the inlet opening $\mathrm{v}_{meth}^{inlet}$ = 0.05 m/s (Tab. 3). The height of methane jet penetration is comparable with the reactor height H_{CBR} (Tab. 3).

In the case of the ***constant horizontal magnetic field***, the vectors of Lorentz force (the maximum value $f_{\max}^{EM}$ ~$5.0 \cdot 10^4$ N/m^3) are located in the vertical plane. The prevailing direction of Lorentz force is opposite to the tin flow direction, that is, the magnetic field decelerates the flow of tin and as sequence it decelerates the flow of methane.

The diameter of methane jet is comparable with the inlet opening diameter D_{inlet} (Fig. 4 (c), Tab. 3). This thick and straight methane jet penetrates to approximately 40% of the reactor height H_{CBR} for archived flow time (10 sec) with the time-averaged speed $\mathrm{v}_{meth,\max}^{aver}$ ~0.47 m/s, which is ~9.5 times greater than the methane speed in the inlet opening.

Table 3: Computed characteristic parameters of methane-tin flow

magnetic induction [*T*]	flow time [*s*]	$f_{\max}^{EM}$ [N/m^3]	$\mathrm{v}_{meth,\max}^{inst}$ [*m/s*]	$\mathrm{v}_{meth,\max}^{aver}$ [*m/s*]	methane jet average diameter [*m*]	methane jet maximum height [*m*]
B =0	40	0	1.16	0.33	~$0.35D_{inlet}$	~$0.025\ H_{CBR}$
B_z =0.5	3.5	$3.3 \cdot 10^5$	3.26	2.03	~$0.1D_{inlet}$	~H_{CBR}
B_x =0.5	10	$5.0 \cdot 10^4$	1.18	0.47	~D_{inlet}	~$0.4H_{CBR}$

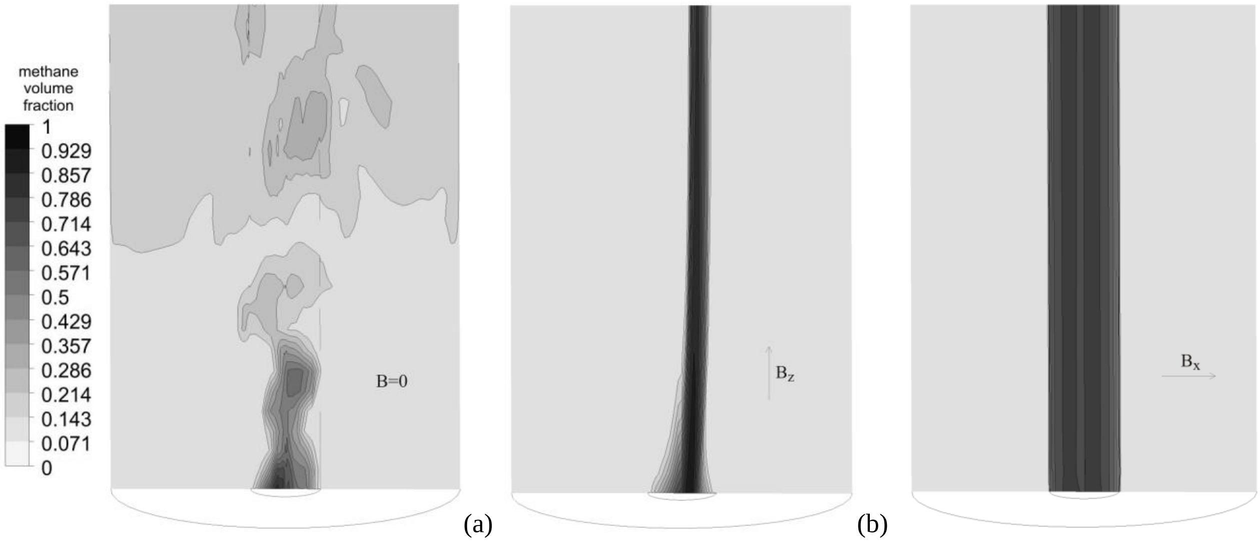

Fig. 4: Methane volume fraction instantaneous distributions in vertical cross-section of CBR inlet zone: (a) t = 40 s, B=0; (b) t = 13.5 s, B_z = 0.5 T ("switched on" for t = 10–13.5 s; (c) t = 20 s, B_x = 0.5 T ("switched on" for t =10–20 s).

Conclusions

√ Two different numerical approaches are developed for studying of methane bubbles collective dynamics interfacing with the liquid tin flow in the cylindrical bubble reactor:

• based on Euler-Euler multi-phase tools of commercial packages ANSYS CFX and ANSYS Fluent with application of *k-ω* Shear Stress Transport and/or Large Eddy Simulation models of turbulence;

• based on lattice Boltzmann method (LBM).

√ Computational results for the methane and tin volume fractions and the velocity vectors in high temperature reactor without magnetic field are of a good qualitative agreement with the experimental and predicted results for the water-air two phase system in the rectangular bubble reactors. The further tuning of numerical approaches will be available on the base of the experiment data in gas and liquid metal system.

√ The constant magnetic field is taken into account using simplified approach in order to estimate the impact of Lorentz force on the methane jet penetration into the liquid tin. The obtained results for distributions of the methane volume fraction show that the vertical magnetic field is narrowing the methane jet and consequently accelerates it. The horizontal magnetic field decelerates the jet and keeps the size of its diameter. The methane jets influenced with the magnetic field are straight, in contrast to the "snake-like" distributions of volume fractions and velocity vectors in the case without magnetic field.

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References

[1] A. Abánades, E. Ruiz, E.M. Ferruelo et al. (2011), International Journal on Hydrogen Energy 36, 12877-12886
[2] Hydrogen from methane without CO_2 emissions (2013). Karlsruhe Institute of Technology, PR 041 (March 21)
[3] T. Steinberg, E. Baake (2014), Elektrowärme International 2, 59-62
[4] V.V. Buhmirov, D.V. Rakutina, Yu.S. Solnishkova (2009), Reference materials for problems solution for "Heat-and-mass-exchange" course, Ivanovo State Power University (in Russian)
[5] A. Tucs, S. Spitans, A. Jakovics, E. Baake (2014), Proceedings of the 9th PAMIR Int. Conference 2, 266-270
[6] Multiphase flow theory (2011), ANSYS CFX-solver theory guide
[7] Multiphase flows (2012), ANSYS Fluent theory guide
[8] W. Lou, M. Zhu (2013), Metallurgical and Materials Transactions 44B, 2013-1251
[9] X. Shan, H. Chen (1993), Physical Review E 47, 1815-1819
[10] I.O. Kurtoglu, C.-L. Lin (2006), Numerical Heat Transfer 50B, 333-351