


Dynamics of bubble population undergoing mass transfer and coalescence in a glass forming liquid

Franck Pigeonneau¹, Annabelle Laplace², **Luiz Pereira**³

¹Mines-Paristech PSL Univ. - Centre of Material Forming, Sophia Antipolis, France

²CEA, DES, ISEC, DE2D, University of Montpellier, Marcoule, France

³University of Munich (LMU), Department of Earth and Environmental Sciences, Theresienstraße 41, 80333 Munich, Germany



1. Problem statement

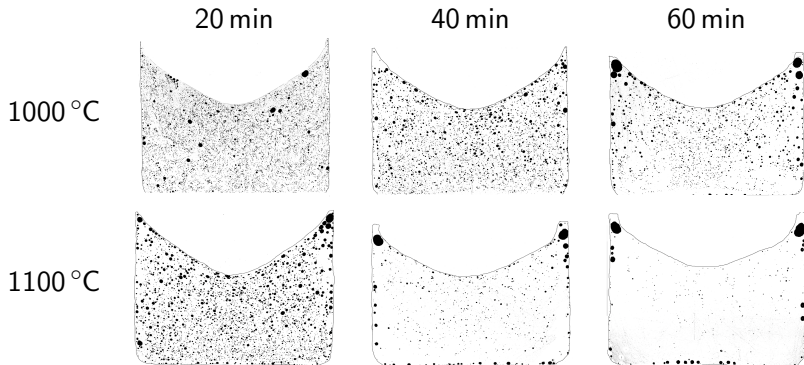


Figure 1: Binarized optical microscope images¹.

¹L. Pereira et al.: Experimental study of bubble formation in a glass-forming liquid doped with cerium oxide, in: *J. Am. Ceram. Soc.* 103 (2020), pp. 2453–2462.

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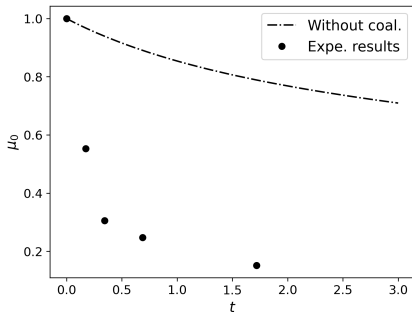


Figure 2: Bubble density vs. t obtained experimentally at $T=1100$ °C.

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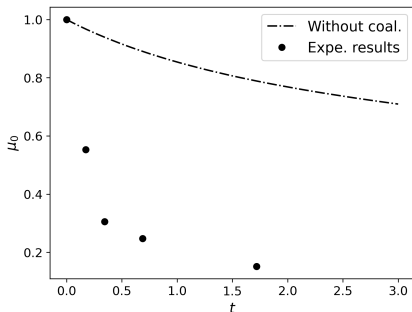


Figure 2: Bubble density vs. t obtained experimentally at $T=1100^\circ\text{C}$.

According to Cable²:

Coalescence is obviously an important phenomenon during the early stages of melting but the conditions favourable to the coalescence of bubbles have been little investigated.

²M. Cable: A study of refining. Part 2: Mechanisms of refining, in: *Glass Technol.* 2 (1961), pp. 60–70.

1. Problem statement
2. Population balance equation
3. Direct quadrature method of moments
4. Numerical results
5. Synthesis & perspectives

2. Population balance equation

- The conservation of the PDF is given by the Liouville equation³:

$$\frac{\partial f}{\partial t} + \nabla \cdot (\mathbf{v}f) + \frac{\partial(\dot{a}f)}{\partial a} + \sum_{i=1}^{N_g-1} \frac{\partial(\dot{x}_{g,i}f)}{\partial x_{g,i}} = h(\mathbf{x}, t; a, \mathbf{x}_g), \quad (1)$$

³D. Ramkrishna: Population balances. Theory and application to particulate systems in engineering, [San Diego 2000](#).

⁴F. Pigeonneau: Mechanism of mass transfer between a bubble initially composed of oxygen and molten glass, in: [Int. J. Heat Mass Transfer 54 \(2011\)](#), pp. 1448–1455.

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with⁴

$$\mathbf{v} = \mathbf{u} - \frac{\mathbf{g}a^2}{3\nu}, \quad (2)$$

$$\dot{a} = \frac{1}{2a} \sum_{i=1}^{N_g} \text{Sh}(\text{Pe}_i) \mathcal{H}_i \mathcal{D}_i (x_{l,i} - x_{g,i}), \quad \mathcal{H}_i = \mathcal{L}_i RT, \quad x_{l,i} = \frac{C_{l,i}}{\mathcal{L}_i P}, \quad (3)$$

$$\dot{x}_{g,i} = \frac{3}{2a^2} \sum_{j=1}^{N_g} \text{Sh}(\text{Pe}_j) \mathcal{H}_j \mathcal{D}_j (\delta_{ij} - x_{g,i}) (x_{l,j} - x_{g,j}), \quad \forall i = [1; N_g - 1] \quad (4)$$

³Ramkrishna: Population balances. Theory and application to particulate systems in engineering (see n. 3).

⁴Pigeonneau: Mechanism of mass transfer between a bubble initially composed of oxygen and molten glass (see n. 4).

2. Population balance equation

- ▶ To solve the PBE, a size-conditioned density is defined⁵:

$$n(\mathbf{x}, t; a) = \int_{\Omega_{\mathbf{x}_g}} f(\mathbf{x}, t; a, \mathbf{x}_g) d\mathbf{x}_g, \quad (5)$$

- ▶ and a size-conditioned of a quantity G is

$$\langle G|a \rangle = \frac{\int_{\Omega_{\mathbf{x}_g}} Gf(\mathbf{x}, t; a, \mathbf{x}_g) d\mathbf{x}_g}{n(\mathbf{x}, t; a)}. \quad (6)$$

- ▶ After volume average, the PBE becomes

$$\frac{\partial \langle n \rangle}{\partial t} + \frac{\partial (\langle \dot{a} | a \rangle \langle n \rangle)}{\partial a} = \langle S \rangle(t; a) - \frac{\langle n \rangle g a^2}{3\nu}. \quad (7)$$

⁵D. L. Marchisio/R. O. Fox: Computational models for polydisperse particulate and multiphase systems, 2013.

2. Population balance equation

- The coalescence source term, $S(\mathbf{x}, t; a)$, is given by⁶

$$\langle S \rangle(t; a) = \frac{1}{2} \int_0^a \frac{a^2}{(a^3 - a'^3)^{2/3}} K(a', \sqrt[3]{a^3 - a'^3}) \langle n \rangle(t; a') \langle n \rangle(t; \sqrt[3]{a^3 - a'^3}) da' - \langle n \rangle(t; a') \int_0^\infty K(a, a') \langle n \rangle(t; a') da'. \quad (8)$$

- Due to the bubble rising, the coalescence kernel can be written as follows⁷

$$K(a, a') = \frac{g\pi}{3\nu} (a + a')^2 |a^2 - a'^2| E_{\text{col}}(a, a'). \quad (9)$$

⁶Marchisio/Fox: Computational models for polydisperse particulate and multiphase systems (see n. 5).

⁷X. Zhang/R. H. Davis: The rate of collisions due to Brownian or gravitational motion of small drops, in: *J. Fluid Mech.* 230 (1991), pp. 479–504.

2. Population balance equation

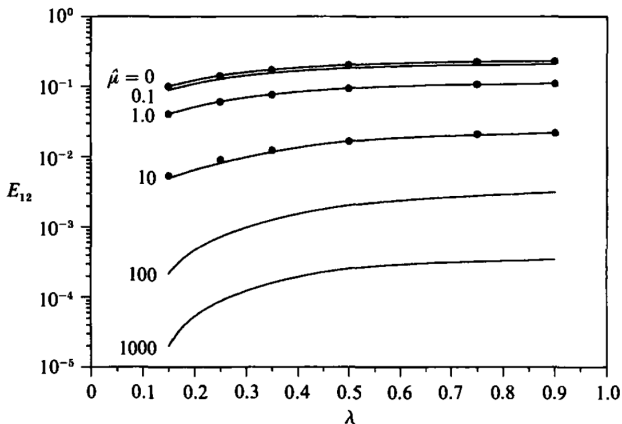


Figure 3: Coalescence efficiency for gravity sedimentation⁸.

⁸Zhang/Davis: The rate of collisions due to Brownian or gravitational motion of small drops (see n. 7).

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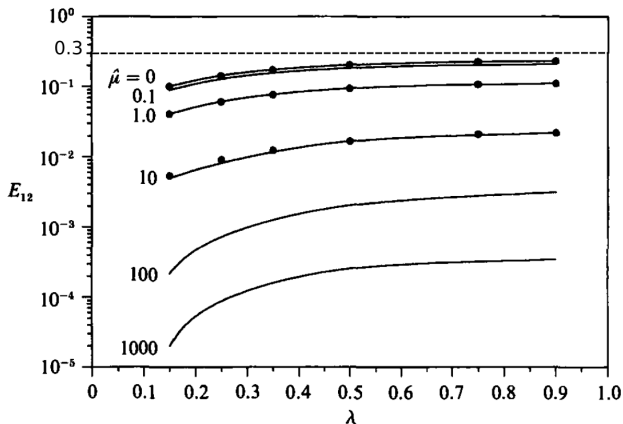


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2. Population balance equation

Table 1: Characteristic quantities for the normalisation.

$$\begin{array}{cccc}
 a & t & \mathbf{v} & \langle n \rangle \\
 a_0 & \frac{3H\nu}{ga_0^2} & \frac{ga_0^2}{3\nu} & \frac{N_0}{a_0} \\
 \varphi_0 = \frac{4\pi a_0^3 N_0}{3}. & & &
 \end{array} \tag{10}$$

$$K(a, a') = K_0 E_{\text{coa}} (a + a')^2 |a^2 - a'^2|, \tag{11}$$

$$K_0 = \pi N_0 a_0^2 H. \tag{12}$$

3. Direct quadrature method of moments

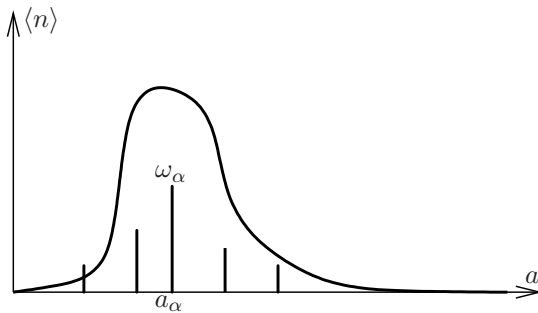


Figure 4: $\langle n \rangle$ vs. a and discrete representation of $\langle n \rangle$.

$$\langle n \rangle(t; a) = \sum_{\alpha=1}^N \omega_\alpha(t) \delta[a - a_\alpha(t)], \quad (13)$$

ω_α : weight, a_α : abscissa.

3. Direct quadrature method of moments

- In direct method, equations are written in ω_α and a_α ⁹:

$$\frac{d\omega_\alpha}{dt} = A_\alpha, \quad \frac{d(\omega_\alpha a_\alpha)}{dt} = B_\alpha, \quad \forall \alpha \in [1, N], \quad (14)$$

$$(1 - k) \sum_{\alpha=1}^N a_\alpha^k A_\alpha + k \sum_{\alpha=1}^N a_\alpha^{k-1} B_\alpha = C_k, \quad \forall k \in [0; 2N - 1], \quad (15)$$

$$C_k = \sum_{\alpha=1}^N \sum_{\beta=1}^N \omega_\alpha \omega_\beta K(a_\alpha, a_\beta) \left[\frac{(a_\alpha^3 + a_\beta^3)^{k/3}}{2} - a_\beta^k \right] + k \sum_{\alpha=1}^N a_\alpha^{k-1} \langle \dot{a} | a_\alpha \rangle \omega_\alpha - \sum_{\alpha=1}^N \omega_\alpha a_\alpha^{k+2}, \quad (16)$$

$$\frac{d\langle x_{g,i} | a_\alpha \rangle}{dt} = \frac{3}{2a_\alpha^2} \sum_{j=1}^{N_g} \text{Sh}(\text{Pe}_{j,\alpha}) \mathcal{H}_j \text{Fo}_j (\delta_{ij} - \langle x_{g,i} | a_\alpha \rangle) (x_{l,j} - \langle x_{g,j} | a_\alpha \rangle), \quad \forall i \in [1, N_g - 1], \quad (17)$$

$$\frac{dx_{l,i}}{dt} = -\frac{3\varphi_0}{2} \sum_{\alpha=1}^N a_\alpha \omega_\alpha \text{Sh}(\text{Pe}_{i,\alpha}) \text{Fo}_i (x_{l,i} - \langle x_{g,i} | a_\alpha \rangle), \quad \forall i \in [1, N_g]. \quad (18)$$

⁹Marchisio/Fox: Computational models for polydisperse particulate and multiphase systems (see n. 5).

3. Direct quadrature method of moments

1. Initialisation of $2N$ first moments μ_k from an initial pdf:

$$\mu_k = \int_0^\infty a^k \langle n \rangle(t; a) da = \sum_{\alpha=1}^N a_\alpha^k \omega_\alpha. \quad (19)$$

2. Determine $(a_\alpha, \omega_\alpha)$ from the $2N$ first moments using the Wheeler algorithm¹⁰;
3. Solve the ODE for $\omega_\alpha, \omega_\alpha a_\alpha, \langle x_{g,i} | a_\alpha \rangle$ & $x_{l,i}$ using a RK4.
4. Compute the $2N$ first μ_k .

¹⁰J. C. Wheeler: Modified moments and Gaussian quadratures, in: Rocky Mt. J. Math. 4.2 (1974), pp. 287–296.

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In numerical applications: $N = 3$.

¹⁰Wheeler: Modified moments and Gaussian quadratures (see n. 10).

4. Numerical results

- ▶ Extraction from the 2D images¹¹, the 3D relevant data¹².

Table 2: Initial N_0 , φ_0 , a_0 & K_0 .

T (°C)	N_0 (mm ⁻³)	φ_0	a_0 (μm)	K_0
1000	345	8.64×10^{-2}	39.07	33.17
1050	190	1.01×10^{-1}	50.27	30.19
1100	68.8	1.11×10^{-1}	72.91	22.99

¹¹Pereira et al.: Experimental study of bubble formation in a glass-forming liquid doped with cerium oxide (see n. 1).

¹²A. Baddeley/E. B. Vedel Jensen: Stereology for statisticians, 2005.

4. Numerical results

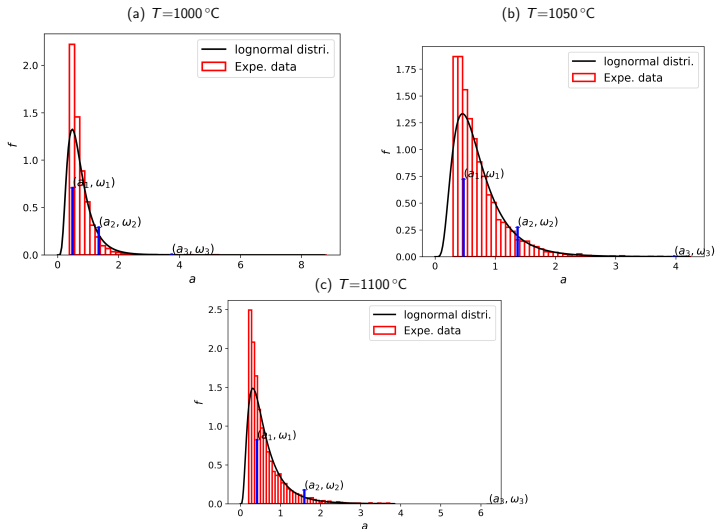


Figure 5: Initial pdf from image analysis at 20 min.

4. Numerical results

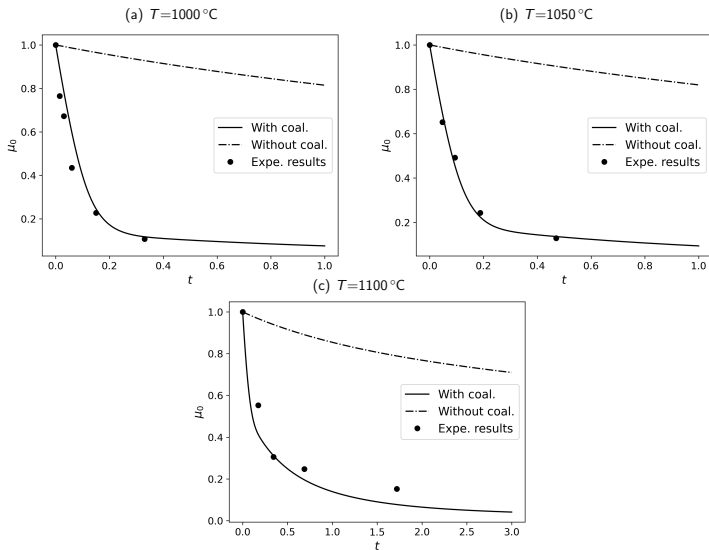


Figure 6: μ_0 vs. t .

4. Numerical results

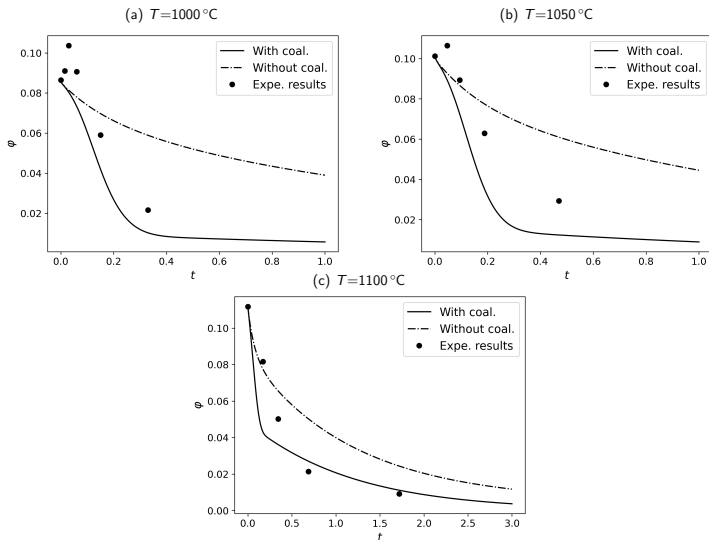


Figure 7: $\varphi = 4\pi\mu_3/3$ vs. t .

4. Numerical results

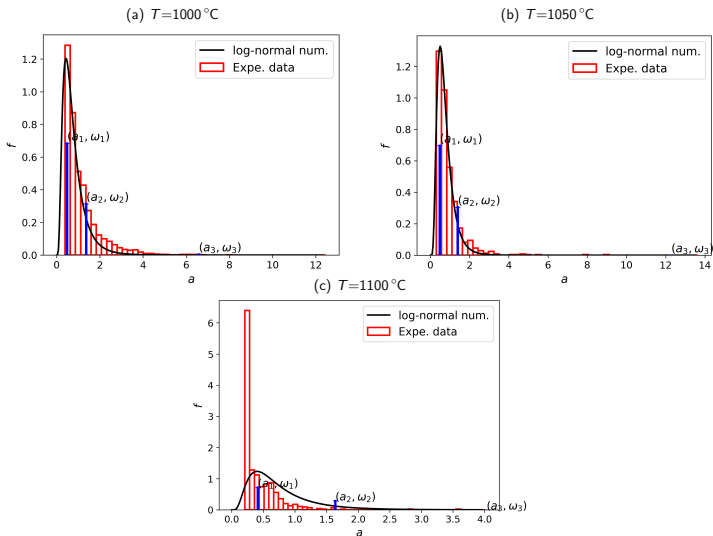


Figure 8: pdf from image analysis at 120 min.

5. Synthesis & perspectives

- ▶ Gravity sedimentation kernel explained the coalescence in a crucible experiment.
- ▶ Coalescence becomes important if

$$K_0 \sim 1 \rightarrow N_0 > 10^2 \text{ cm}^{-3}. \quad (20)$$

- ▶ The probability of the coalescence $\sim 1/\sqrt[3]{N_0} \sim 1 \text{ mm}$.
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- ▶ The probability of the coalescence $\sim 1/\sqrt[3]{N_0} \sim 1 \text{ mm}$.
- ▶ DQMOM is an efficient method to solve PBE.
- ▶ To be used in CFD software (Ansys Fluent).
- ▶ Need a coalescence kernel accounting for fluid motion.
- ▶ Introduce the redox & fining.

5. Synthesis & perspectives

Thank you for your attention!

Contact:

franck.pigeonneau@minesparis.psl.eu