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

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1. Problem statement

Figure 1: Binarized optical microscope images\textsuperscript{1}.

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Figure 2: Bubble density vs. $t$ obtained expérimentally at $T=1100^\circ$C.
1. Problem statement

![Diagram showing bubble density vs. time](image)

**Figure 2**: Bubble density vs. \( t \) obtained expérimentally at \( T=1100^\circ\text{C} \).

According to Cable\(^2\):

*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.*

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 equation:\(^3\):

\[
\frac{\partial f}{\partial t} + \nabla \cdot (vf) + \frac{\partial (\dot{a}f)}{\partial a} + \sum_{i=1}^{N_g-1} \frac{\partial (\dot{x}_{g,i}f)}{\partial x_{g,i}} = h(x, t; a, x_g),
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\]  

(1)

with\(^4\)

\[
v = u - \frac{g a^2}{3 \nu},
\]

(2)

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

(3)

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

(4)

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

\(^4\)Pigeonneau: 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 defined\(^5\):

\[
n(x, t; a) = \int_{\Omega_{x_g}} f(x, t; a, x_g) dx_g,
\]

(5)

- and a size-conditioned of a quantity \( G \) is

\[
\langle G|a \rangle = \frac{\int_{\Omega_{x_g}} Gf(x, t; a, x_g) dx_g}{n(x, t; a)}.
\]

(6)

- After volume average, the PBE becomes

\[
\frac{\partial \langle n \rangle}{\partial t} + \frac{\partial (\langle \dot{a}|a\rangle \langle n \rangle)}{\partial a} = \langle S \rangle(t; a) - \frac{\langle n \rangle ga^2}{3\nu}.
\]

(7)

2. Population balance equation

The coalescence source term, $S(x, t; a)$, is given by

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

$$-\langle n \rangle(t; a') \int_0^\infty K \left( a, a' \right) \langle n \rangle(t; a') da'. \quad (8)$$

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

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

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

2. Population balance equation

Figure 3: Coalescence efficiency for gravity sedimentation\(^8\).

\(^8\)Zhang/Davis: The rate of collisions due to Brownian or gravitational motion of small drops (see n. 7).
2. Population balance equation

![Graph showing coalescence efficiency for gravity sedimentation](image)

**Figure 3**: Coalescence efficiency for gravity sedimentation\(^8\).

\(^8\)Zhang/Davis: The rate of collisions due to Brownian or gravitational motion of small drops (see n. 7).
2. Population balance equation

Table 1: Characteristic quantities for the normalisation.

<table>
<thead>
<tr>
<th></th>
<th>(a)</th>
<th>(t)</th>
<th>(\nu)</th>
<th>(\langle n\rangle)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a_0)</td>
<td>(\frac{3H\nu}{g_0^2})</td>
<td>(\frac{ga_0^2}{3\nu})</td>
<td>(\frac{N_0}{a_0})</td>
<td></td>
</tr>
</tbody>
</table>

\[
\varphi_0 = \frac{4\pi a_0^3 N_0}{3}. \quad (10)
\]

\[
K (a, a') = K_0 E_{coa} (a + a')^2 |a^2 - a'^2|, \quad (11)
\]

\[
K_0 = \pi N_0 a_0^2 H. \quad (12)
\]
3. Direct quadrature method of moments

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

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

\( \omega_\alpha \): weight, \( a_\alpha \): abscissa.
3. Direct quadrature method of moments

In direct method, equations are written in $\omega_\alpha$ and $a_\alpha$:

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

(14)

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

(15)

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

$$
- \sum_{\alpha=1}^{N} \omega_\alpha a^{k+2}_\alpha,
$$

(16)

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

(17)

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

(18)

Marchisio/Fox: Computational models for polydisperse particulate and multiphase systems (see n. 5).
3. Direct quadrature method of moments

1. Initialisation of $2N$ first moments $\mu_k$ 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 algorithm$^{10}$;

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 $\mu_k$.

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4. Compute the $2N$ first $\mu_k$.

In numerical applications: $N = 3$.

\textsuperscript{10}Wheeler: Modified moments and Gaussian quadratures (see n. 10).
4. Numerical results

- Extraction from the 2D images\textsuperscript{11}, the 3D relevant data\textsuperscript{12}.

<table>
<thead>
<tr>
<th>$T$ (°C)</th>
<th>$N_0$ (mm$^{-3}$)</th>
<th>$\varphi_0$</th>
<th>$a_0$ (µm)</th>
<th>$K_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>345</td>
<td>$8.64 \times 10^{-2}$</td>
<td>39.07</td>
<td>33.17</td>
</tr>
<tr>
<td>1050</td>
<td>190</td>
<td>$1.01 \times 10^{-1}$</td>
<td>50.27</td>
<td>30.19</td>
</tr>
<tr>
<td>1100</td>
<td>68.8</td>
<td>$1.11 \times 10^{-1}$</td>
<td>72.91</td>
<td>22.99</td>
</tr>
</tbody>
</table>

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

\textsuperscript{12}A. Baddeley/E. B. Vedel Jensen: Stereology for statisticians, 2005.
4. Numerical results

(a) $T=1000^\circ C$

(b) $T=1050^\circ C$

(c) $T=1100^\circ C$

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

(a) $T=1000\, ^\circ C$

(b) $T=1050\, ^\circ C$

(c) $T=1100\, ^\circ C$

Figure 6: $\mu_0$ vs. $t$. 
4. Numerical results

(a) $T = 1000^\circ C$

(b) $T = 1050^\circ C$

(c) $T = 1100^\circ C$

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

(a) $T = 1000 \, ^\circ C$

(b) $T = 1050 \, ^\circ C$

(c) $T = 1100 \, ^\circ C$

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
  \[ K_0 \sim 1 \rightarrow N_0 > 10^2 \text{ cm}^{-3}. \]  
  \[ (20) \]
- The probability of the coalescence \( \sim 1/\sqrt[3]{N_0} \sim 1 \text{ mm}. \)
- DQMOM is an efficient method to solve PBE.
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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!

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