Simulation of the gas-liquid CO₂ absorption in alkaline aqueous solutions from partially contaminated spherical bubbles and ellipsoidal clean bubbles

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FRAMEWORK: bubble liquid mass transfer coupled with chemical reactions
- Main step of NaHCO₃ production process: dispersion, under the form of bubbles, of an air-CO₂ mixture in an NaHCO₃ - Na₂CO₃ aqueous solution
- Dispersion realized in large scale bubble columns, called the BIR columns (see picture), where a gas-liquid mass transfer of CO₂ occurs
- In the liquid phase, CO₂ is involved in several chemical reactions resulting in precipitation of solid NaHCO₃:
  \[
  \text{CO}_2 + \text{OH}^- \rightarrow \text{HCO}_3^- \quad \text{(1)}
  \]
  \[
  \text{HCO}_3^- + \text{OH}^- \rightarrow \text{CO}_3^{2-} + \text{H}_2\text{O} \quad \text{(2)}
  \]
- In BIR columns, CO₂ is assumed to be transferred across the interface of small bubbles (\(d_b\approx10^{-3}\) m). They seem to have an ellipsoidal shape and a partially contaminated interface \(\Rightarrow\) estimation of the interface characteristic influences on the chemically enhanced bubble-liquid CO₂ transfer rate.

2D-AXISYMMETRICAL MODELING
Notations:
- \(u\): dimensionless velocity vector
- \(p\): dimensionless pressure
- \(a\): dimensionless CO₂ concentration
- \(b\): dimensionless OH⁻ concentration
- \(c\): dimensionless HCO₃⁻ concentration
- \(d\): dimensionless CO₃²⁻ concentration
- \(Re\): particle Reynolds number
- \(Pe\): Péclet number of CO₂
- \(Ha_1\): reaction (1) Hatta number
- \(Ha_2\): reaction (2) Hatta number

Mass balances:
\[
\nabla \cdot \left( \frac{1}{\rho} \frac{\partial \rho}{\partial t} + \rho u \right) = 0
\]
\[
\rho \frac{\partial u}{\partial t} = -\nabla p + \frac{1}{Re} \left( \nabla^2 u + (\nabla u)^T \right)
\]
\[
\rho \frac{\partial a}{\partial t} = - (a \cdot \nabla) u
\]
\[
\rho \frac{\partial b}{\partial t} = - (b \cdot \nabla) u
\]
\[
\rho \frac{\partial c}{\partial t} = - (c \cdot \nabla) u
\]
\[
\rho \frac{\partial d}{\partial t} = - (d \cdot \nabla) u
\]

Chemical reactions:
\[
\n\frac{1}{\rho} \frac{\partial \rho}{\partial t} = \nabla \cdot (\rho u)
\]
\[
\rho \frac{\partial u}{\partial t} = -\nabla p + \frac{1}{Re} \left( \nabla^2 u + (\nabla u)^T \right)
\]
\[
\rho \frac{\partial a}{\partial t} = - (a \cdot \nabla) u
\]
\[
\rho \frac{\partial b}{\partial t} = - (b \cdot \nabla) u
\]
\[
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\]
\[
\rho \frac{\partial d}{\partial t} = - (d \cdot \nabla) u
\]

Numerical resolution
- with COMSOL Multiphysics 3.4 software
- UMFPACK stationary solver is used

Validation
- Comparison with literature correlations for clean and fully contaminated spherical bubbles without reactions: excellent agreement
  [Colloids and Surfaces A 365 (2008), pp. 28-35]

Parameter values
- \(\alpha = 0.003\)
- \(\beta = 4.1\)
- \(\chi = 0.9\)
- \(\chi = 0.7\)
- \(\chi = 0.3\)
- \(\chi = 0.025\)
- \(Ha_1 = 64\)
- \(Ha_2 = 902\)
- \(db = 1\) mm
- \(Re = 200\)
- \(Pe = 10^5\)

SIMULATION RESULTS and DISCUSSION
The CO₂ concentration field in the liquid around the bubble is simulated and the bubble-liquid CO₂ transfer rate is estimated via the computation of the Sherwood number. By comparison with the Sherwood number without reaction, the chemical enhancement factor is estimated.

Study of the ellipsoidal shape bubble with clean interface
- Slip boundary condition at the bubble-liquid interface
- Simulations are realized for the same equivalent diameter \(d_b = 1\) mm.
- The major axis/minor axis W ratio of the ellipsoid goes from 1 (spherical shape) to 2
- For the simulation result presented right here, \(W = 1.72\)

Study of the spherical bubble with partially contaminated interface
- Slip boundary condition at the clean zone of the interface
- No-slip boundary condition at the contaminated zone of the interface
- The contamination angle goes \(\phi_{cap}\) from 0° (clean interface) to 180° (fully contaminated interface)
- For the simulation result presented right here, \(\phi_{cap} = 30°\)

CONCLUSION and FUTURE PLANS
The shape of the bubble and the contamination state of the bubble-liquid interface have a strong influence on the Sherwood number (CO₂ transfer rate) but the variations are barely compensated by the chemical enhancement.

If the shape and the contamination state of the bubbles in a BIR columns are known, a good prediction can be realized with this model by combining these two characteristics.

This model is valid only for the smallest bubbles (not more than 1 mm) \(\Rightarrow\) now the model has to be adapted for the larger ellipsoidal bubbles that have a helical movement.

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