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CFD Simulations of Absorption Reaction in Carbon Solidification Processes

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Abstract

Carbon capture and storage (CCS) is a promising task solution for reduction of CO_2 emission from ships. To meet the IMO proposed target of 20% CO_2 reduction from shipping by 2020, proposal of solidifying CO_2 separated from engine exhaust had been made and tested by the authors. Laboratory experiment [1] on CO_2 absorption has illustrated the feasibility of solidifying carbon onboard ships. To further verify the accuracy of results from CO_2 absorption experiment, simulation with computational fluid dynamics (CFD) of the CO_2 absorption and solidification processes is carried out, including system modelling and meshing, reactions simulating and post-CFD treatments. Eulerian multiphase model and species transport model are applied for the simulation. These models will present the interaction between gas phase (CO_2) and chemical solution in both physical phase interactions and chemical reactions between the species. The mass fractions of Na_2CO_3 in solution are monitored during the absorption process. Conclusions has been reached that the simulation results have a good agreement with the experiment results.

KEY WORDS: *CFD simulation, chemical absorption, environment protection.*

1. Introduction

Maritime environment protection has drawn a huge attention of current maritime societies. Now inspired by onshore CCS applications, the idea of maritime CCS for ships is under researching. The objective of applying CCS on board is to reduce the emission of CO_2 from marine transportations by capture the carbon in fuel oil and temporarily storage on ship board. However, mechanically introducing will bring many undesired impacts, such as huge power requirements for CO_2 phase conversion, large space occupation of liquefied CO_2 and severe demands of storage tank materials. Our project discards the liquefaction procedure and instead, carbon solidification with chemical reactions is proposed. After experiment conducted by authors, simulation is necessary to give a theoretical view of absorption process. ANSYS Fluent is one powerful CFD software which could simulate multi-phase flow and species reaction. Furthermore, the simulation will be introduced during the design stage of real ship installation in order to arrange pipes and locale tanks.

2. Principles of reactions and experiment rigs

Carbon solidification with chemical reactions is based on two chemical processes including CO_2 absorption and CO^{3-} ions precipitation. The following chemical equations are presenting the reaction principles:

$$CO_2\,(g) + 2NaOH\,(l) = Na_2CO_3\,(l) + H_2O\,(l) \quad -\Delta H_1 \tag{1}$$

$$Na_2CO_3\,(l) + CaO(s) + H_2O = CaCO_3\downarrow\,(s) + 2NaOH\,(l) \quad -\Delta H_2 \tag{2}$$

Exhaust gases from marine engines will first be bypassed into a membrane system by a gas blower to provide a concentrated CO_2 gas. Then the concentrated gas will be fed into a reaction tank which contains NaOH solution. According to reaction 1, CO_2 will react with NaOH and generated Na_2CO_3 and water. After the CO_2 absorption process, the solution in tank will be treated by adding CaO and CO^{3-} will be precipitated as $CaCO_3$ based on reaction 2. NaOH is generated during the precipitation and the solution will be recycled. Based on these reactions, CO_2 from the exhaust gases are eventually captured and stored in a solid form.

Based on the principles of the solidification processes introduced above, two steps of experiment are designed: chemical absorption and precipitation, and physical filtration. Figure 1 is the experiment rig used for absorption processes. Pure gas from CO_2 is fed into the measuring cylinder which contains prepared NaOH solution. The gas goes through a gas regulator and a flow meter to adjust pressure and flow rate. Fitting with a pipe, a gas diffuser is applied to generate gas bubbles in order to increase the contact area between gas and solution. The weight changes in CO_2 tank and measuring cylinder are measured with two scales.

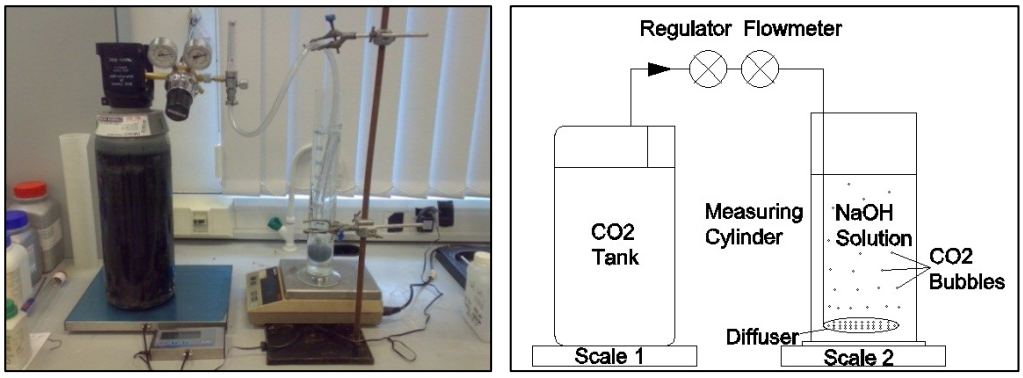

Figure 1 Experiment rigs of absorption processes

3. Methodology

ANSYS Fluent solves conservation equations for chemical species by predicting the local mass fraction of each species, through the solution of a convection-diffusion equation for specified species [2]. The following is the equation of conservation:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \tag{3}$$

where R_i is the net rate of production of species i by chemical reaction and Si is the rate of creation from the dispersed phase and sources. J_i is the mass diffusion flux. $\vec{v}$ is the overall velocity vector (m/s). t presents time and ρ presents density of species.

For Eulerian multiphase model, the concept of phasic volume fractions is introduced and the volume of one phase can is defined as:

$$V = \int_V a dV \tag{4}$$

where a is the volume fraction of phases and the sum of volume fraction of all phases equals to 1.

The continuity equation for phase q is:

$$\frac{1}{\rho_{rq}}\left(\frac{\partial}{\partial t}(a_q \rho_q) + \nabla \cdot (a_q \rho_q \vec{v}_q) = \sum_{p=1}^{n} (\dot{m}_{pq} - \dot{m}_{qp}) + S_q\right) \tag{5}$$

where ρ_{rq} is the phase reference density; $\vec{v}_q$ is the velocity of phase q; $\dot{m}_{pq}$ characterizes the mass transfer from the phase p to q and $\dot{m}_{qp}$ is the mass transfer from q to p; S_q is the source term added.

The equation of energy conservation for each fluid phase is:

$$\frac{\partial}{\partial t}(a_q \rho_q \vec{v}_q) + \nabla \cdot (a_q \rho_q \vec{v}_q \vec{v}_q) = -a_q \nabla p + \nabla \cdot \bar{\tau}_q + a_q \rho_q \vec{g} + \sum_{p=1}^{n} K_{pq}(\vec{v}_p - \vec{v}_q) + \dot{m}_{pq}\vec{v}_{pq} - \dot{m}_{qp}\vec{v}_{qp} + (\vec{F}_e + \vec{F}_{lift,q} + \vec{F}_{vm,q}) \tag{6}$$

where ρ is the density; p is the pressure shared by all phases; g is gravitational acceleration, K is the momentum exchange coefficient between fluid phases and $\vec{F}_e$ are all external forces on phases. $\bar{\bar{\tau}}$ is the stress-strain tensor of q th phase:

$$\bar{\bar{\tau}}_q = a_q \mu_q \left(\nabla \vec{v}_q + \nabla \vec{v}_q^{\,T}\right) + a_q \left(\lambda_q - \frac{2}{3}\mu_q\right) \nabla \cdot \vec{v}_q I \tag{7}$$

where μ_q and λ_q are the shear and bulk viscosity of phase q and I is the unit tensor.

Reaction rate, $k_{f,r}$, between phases is computed using Arrhenius expression:

$$k_{f,r} = A_r T^{\beta_r} e^{-E_r/RT} \tag{8}$$

where A_r is the pre-exponetial factor; β_r is the temperature exponent; E_r is the activation energy for reaction and R is the universal gas constant.

4. Assumptions, modelling and simulations

Before the modelling and simulation, a range of assumptions is essential to be applied during these procedures in order to simplify the problem and model geometry:

1. The conditions of surrounding environment are set as following: temperature of 298K, pressure of 101325 Pa and gravity of 9.81m/s^2.
2. As the simulation focusing on reaction in measuring cylinder, the whole rigs are simplified to a 2 dimensional model which is shown in Figure 2.
3. For bubble column simulation, the diffuser is simplified as ten separated inlets at bottom to avoid unstructured grid. For simulation of combining chemical reaction with bubble column, further simplification of inlet is applied for the case of computing intense.
4. The gas fed in is ideal gas. Fluids and gases are both incompressible.
5. The gas bubbles have a minimum diameter of 1e-05 meters.
6. An extension of measuring cylinder is applied to avoid the impacts of backflow on NaOH solution.

The experiment system is modeled with Gambit. The model is a simple column which constituted by solid walls with ten inlets on bottom and one outlet on top. The geometry of the model was using actual scale parameters in experiment. The column height is 0.6 meters and the diameter of column is 0.06 meters. The height of solution in the column is 0.3 meters. The structure grid has a minimum length of 5e-04 m and there are 108000 cells in this model. The flow rate in experiment is 3L/min. Hence, the mass flow rate is 0.001897 kg/s.

The simulation of absorption reaction is based on Fluent and it includes both the reaction and bubble column simulations. Since the simulation involves a chemical reaction and a two-phase flow at the same time, the Eulerian model is selected. It is simply because the only model that compatible with multiphase reaction simulation is Eulerian model. One simulation case of absorption reaction will be presented and it takes 405s to finish the reaction practically. However, with a time step size of 5e-03s, total time steps will be 162000. With support of High Performance Computer from ARCHIE-WeSt, the real time of each iterate is about 2s on 4 cores. Hence, for this case, about 200 CPU-hour are required.

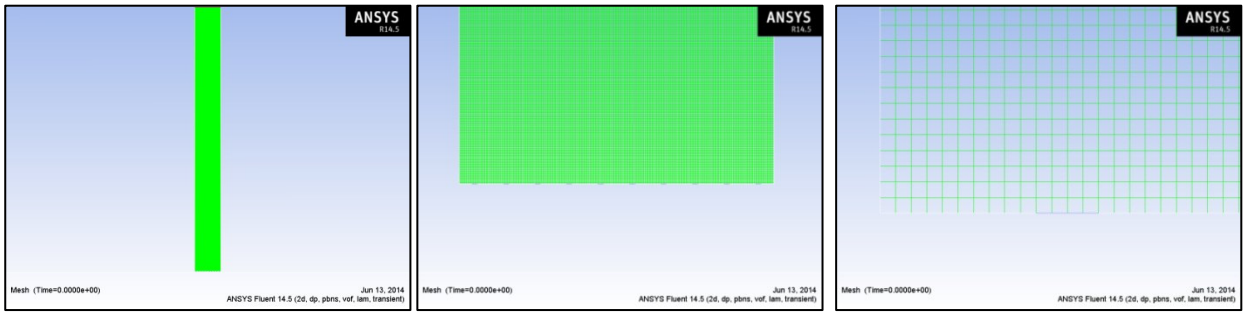

Figure 2 Modeling and meshing of experiment rigs (left: graph of whole model and mesh; middle: the distribution of inlet at the bottom of model; right: the size of meshing)

5. Results from simulations

The bubbles flow in the fluid domain is presented in Figure 3. It indicates the volume fraction contours of solution at t = 0s and t = 3s. It is a 3 second simulation simply because the project is majorly focusing on reaction part and too high computing intensity is another reason.

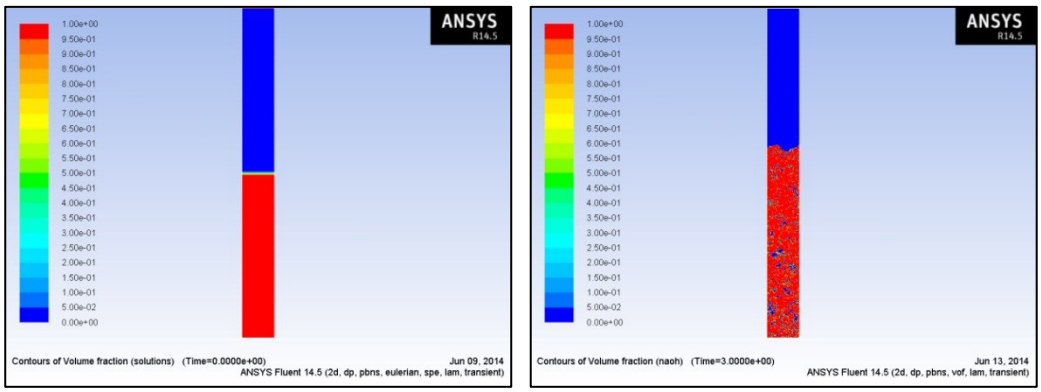

Figure 3 Bubble flow phenomenon under contours of solutions volume fraction (left: contours graph at t = 0s; right: contours graph at t = 3s.)

Table 1 Simulation results: mass fraction of Na_2CO_3 in solution

Flow time(s)	*Mass-Average Mass fraction of Na_2CO_3*
0	0
100	26.02%
200	51.19%
300	75.92%
400	99.87%

For simulation of reaction, mass fraction of Na_2CO_3 in solution phase is monitored. The reaction is completed when the mass fraction of Na_2CO_3 achieved 100%. Hence, in simulation, while it reaches 100%, the simulation is finished. According to equation (8), the reaction rate constant is determined by three factors: pre-exponent factor, activation energy and temperature. Therefore the reaction in CFD simulation is dominated by these factors as well. The simulation will be optimized by controlling these factors in order to achieve reasonable output. Table 1 presents the monitored mass fraction of Na_2CO_3 changing over time and Figure 4 is the comparison of mass fraction change between experiment and simulation. It also presents the volume fraction of solutions at t=400s.

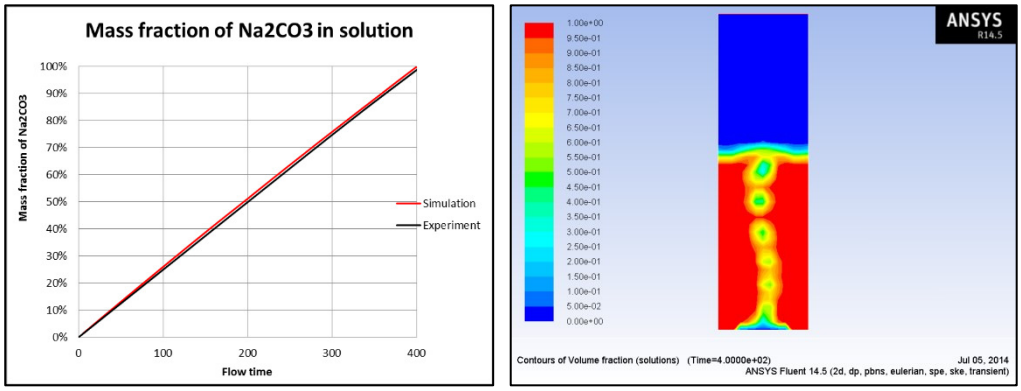

Figure 4 Comparison of Na_2CO_3 mass fractions over time between experiment and simulation results (left); Simulation of absorption reaction at t = 400s (right).

6. Discussions and conclusions

The simulation indicates the varying of bubble sizes and shapes which has a good agreement with the experimental phenomenon. The curve of Na_2CO_3 mass fraction over time also matches well with the experimental result. From the simulation, the CFD simulation of bubble column effect is achieved which illustrates the general movements of bubbles in solution regime. Other than the experiment, the simulation of experiment is another excellent verification to the feasibility of absorption process on capturing CO_2. The result from the simulation is quit consistent with that of experiment. The promising base it provides will be helpful for further verification of all other experiment results and improvement can always be made with higher hardware performance. An experience factor to optimize the simulation is figured out and it will be applied to achieve reasonable results while simulating more complicate models for case ship study.

7. Acknowledgement

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8. Reference

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