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CFD Simulation for Bubble Nucleation Rate of Dissolved Gas

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Abstract: The natural gas in Malaysia is high in CO_2 content. The well removal of CO_2 from natural gas can be carried out by using physical absorption method. CO_2 will be absorbed at high pressure and desorbed at low pressure. The objective of this study was to analyze the phenomenon of CO_2 desorption across a venturi nozzle. Dissolved CO_2 gas bubble nucleation in water was studied by using CFD simulation. Models regarding bubble nucleation of dissolved gas and solubility in water at different pressure were written in User Defined Function (UDF) to be incorporated into FLUENT. The main parameters that affect the bubble nucleation are the pressure drop across the nozzle and the number of dissolved gas molecules in solution, which is defined by the solubility at the initial condition. The bubble nucleation rate increased exponentially with pressure drop. The highest bubble nucleation was found to be at the wall of the throat of the nozzle. No bubble nucleation can be detected for area with insufficient pressure drop. The bubble nucleation rate profile was similar as the pressure profile across the nozzle.

Key words: CFD, CO_2 desorption, dissolved gas, bubble nucleation

INTRODUCTION

The natural gas wells available in Malaysia are high in CO_2 content. The removal of CO_2 from the gas stream is important to improve the quality of natural gas. There are many separation technologies available to remove the CO_2 such as chemical absorption, physical absorption and membrane technology. Since the partial pressure of CO_2 in the gas stream is high, physical absorption using physical solvent may be one of the good choice. This technology also known as pressure swing absorption, whereby CO_2 is absorbed at high pressure in the solvent and desorbed from the solvent at low pressure. The solvent can be easily regenerated by bringing down the pressure. The main focus area in current study is the bubble nucleation of dissolved CO_2 from the solvent, which is the solvent regeneration process.

Bubbles can be easily encountered in various places; carbon dioxide gas bubbles forming from carbonated drink, bubbles form when heating up water, cavitations in ship propellers, etc. Gas bubble nucleation generally takes place from supersaturated gas solutions, whereby the gas solution is heated or depressurized. Conceptually, the bubbles will undergo four stages; nucleation, growth, coalesce and collapse.

There are many researchers who studied the fundamental of bubble formation. In the Classical Nucleation Theory (CNT), there is an energy barrier, which is determined by the free energy for bubble nucleation. In general, the nucleation rate, J (cm^{-3} sec^{-1}), also defined as the number of droplets of the new phase appearing per unit time per unit volume, can be calculated using the Eq. 1. The C in Eq. 1 will changed slowly with other parameters in the equation (Lubetkin, 1995):

$$J = C_{\exp} - \frac{\Delta G}{kT} \qquad (1)$$

Later on year 2003, Lubetkin (2003) had concluded that there is an unknown factor that is not included in the nucleation equation. He then identified this unknown factor as the surface activity of the gases which form the bubbles. Besides, some researchers tried to study the bubble nucleation in the Lennard-Jones fluid by using Density Functional Theory (DFT). They claimed that DFT can predict better than CNT for critical bubble that is small, diffused and liquidlike (Shen and Debenedetti, 2001; Dong, 2005). Some researchers also used DFT to predict the bubble nucleation rates in binary fluids. They found out that in some particular cases, bubble nucleation rate may decrease with increase of temperature. Thus, DFT is required to estimate bubble nucleation rate more accurately (Talanquer and Oxtoby, 1995; Talanquer *et al*., 2001). On the other hand, Kwak and Oh (2004) had used a unified approach to find out the gas and vapor bubble nucleation rate. Other than that, gas bubble growth had also been studied by several researchers. They had

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presented several equations that can be used to describe bubble growth dynamics, that take into account of the influence of Laplace pressure on the bubble growth (Kuchma *et al*., 2009; Gor *et al*., 2011). Yamada *et al*. (2008) even studied the bubble formation process up the stage of coalescence.

There are also many numerical studies of cavitation through a venturi nozzle. These studies will simulate the process of bubble formation from water vapor using simplified cavitation model. The model only takes into account the formation of vapor cavity while the dissolved gas bubble effect is assumed negligible. Most of the numerical simulation had successfully presented the cavitation phenomenon through the venturi nozzle, by presenting the volume fraction of the bubble or the void ratio profile (Goncalves *et al*., 2010; Preston *et al*., 2002; Yazici *et al*., 2007; Kozubkova and Rautova, 2009).

In current study, the effect of inlet pressure on dissolved gas bubble nucleation through venturi nozzle will be investigated by using CFD simulation. The simulations were carried out for bubble nucleation of dissolved carbon dioxide gas in water. The gas bubble nucleation model used is based on the model suggested by Kwak and Oh (2004) by using unified approach. The vapor bubble nucleation is assumed to be insignificant.

METHODOLOGY

Model and numerical method: The numerical simulations were carried out by using CFD approach. Gas bubble nucleation model, as suggested by Kwak and Oh (2004), was used in current study. Many factors affecting the gas bubble nucleation are included in the model, such as number of dissolved gas molecules, molecular volume of dissolved gas molecules, enthalpy and temperature of the gas solution. The model was written in user-defined function and hooked into population balance model.

To study the effect of different pressure inlet on the bubble nucleation rate, pressure of 100, 50, 10 and 1 bar were set as the pressure inlet for different cases at 30°C. In addition, the inlet CO_2 mole fraction was also set according to the CO_2 solubility at different pressure as described by Duan and Sun (2003). The number of dissolved gas molecules available in the gas solution, which is one of the important parameters that affect the gas bubble nucleation rate, was determined by the CO_2 solubility. In addition, the well-known k-ε turbulence model was used in the CFD simulation as it has been widely used in various industries to estimate the turbulence flow.

The geometry used in the CFD simulation, by using asymmetric approach, was shown in Fig. 1. The total length of the nozzle was 6 inches and the throat of the venturi nozzle is positioned at x = 1 inch. Hence, bubble nucleation was expected to be the highest at this position.

RESULT AND DISCUSSION

In current study, the effect of different pressure inlet onto the bubble nucleation rate in the venturi nozzle is to be investigated. The main focus of this investigation included the maximum nucleation rate and the bubble nucleation rate profile across the nozzle.

Maximum dissolved gas bubble nucleation rate: The bubble nucleation rate of dissolved CO_2 in water liquid against pressure of the water solution at initial state was shown in Fig. 2. From the figure, there is no CO_2 bubble nucleation for pressure drop of 1 and 5 bars. This phenomenon indicates that the pressure drop is insufficient to form bubble nuclei. In addition, the low number of dissolved gas molecules (due to low CO_2 solubility at low pressure) may also insufficient to form the bubble nucleation. A small bubble nucleation rate can be detected for pressure drop of 10 bars and the bubble nucleation rate greatly increase for pressure drop of 50 and 100 bars. The big jump of bubble nucleation rate was suggesting that the bubble nucleation started to form at the pressure drop of about 10 bars. In addition, the bubble nucleation rate was a few times greater for pressure drop of 100 bars than 50 bars. Hence, generally, the bubble nucleation rate was increased exponentially with pressure drop.

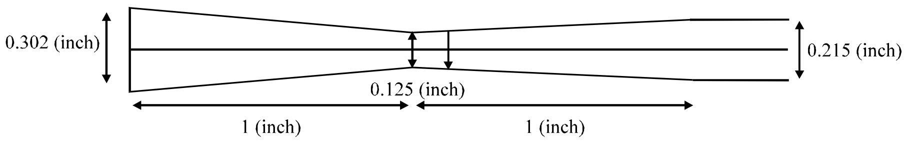
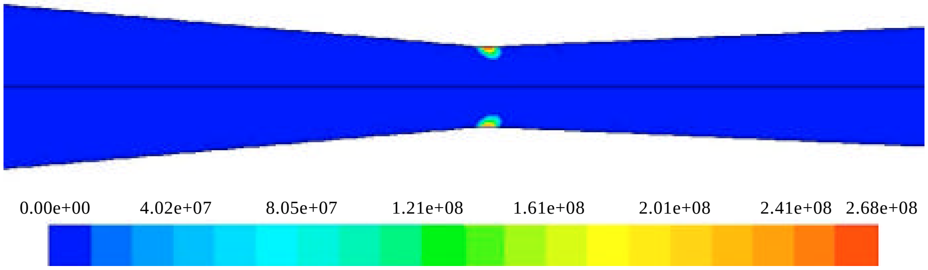
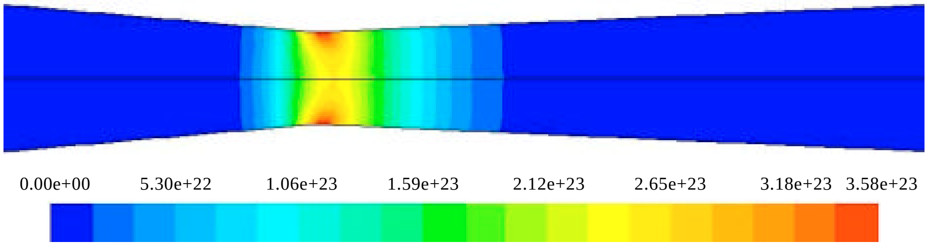
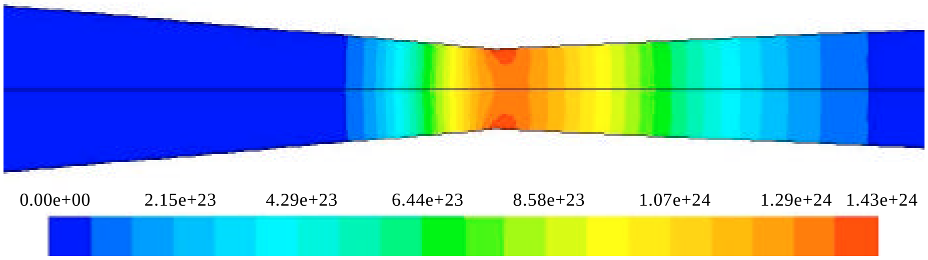


Fig. 1: Geometry of nozzle

Table 1: Dissolved gas nucleation rate profile across the nozzle at pressure drop of 10, 50 and 100 bar

Pressure drop (bar)	Nucleation rate profile
10	
50	
100	

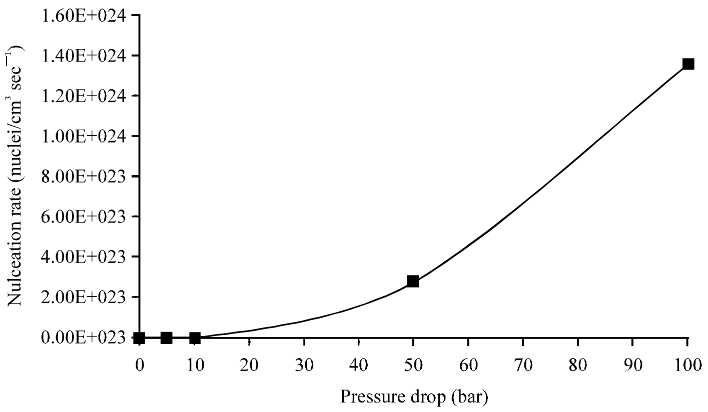


Fig. 2: Maximum bubble nucleation rate vs. pressure drop

Dissolved gas bubble nucleation rate profile: In general, the profile of bubble nucleation rate depends solely on the pressure drop. The number of dissolved gas molecules in water only plays a role to increase the magnitude of nucleation rate but not the profile. A common detailed view of pressure profile across the throat of the venturi nozzle was shown in Fig. 3. All of the five cases shared a common pressure profile at the throat of the nozzle. The pressure was lowest at the throat and recovered at the nozzle diverging section. At the throat of the nozzle, the pressure was even lower near to the wall. Thus, the nucleation rate profile followed the same trend as shown in Table 1. For the 10 bar pressure drop case, sufficient pressure drop to form bubble nuclei was at the region near to the wall. Pressure drop was sufficient for 50 and 100 bar cases and caused bubble nuclei to form

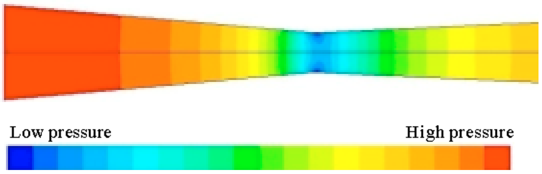


Fig. 3: Common pressure profile across nozzle

even at the middle of the throat. The total area of bubble nucleation was bigger for higher pressure drop across the throat. Technically, there was no nucleation formed before and after the throat.

CONCLUSION

From the results discussed, the pressure drop across the nozzle and the number of dissolved gas molecules in the feed solution played an important role in forming bubble nucleation. The bubble nucleation rate was increased exponentially with the pressure drop and number of dissolved gas molecules. In the other hand, the nucleation rate profile depended only on the pressure profile.

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