博士論文（要約）

Numerical simulation of bubbly flows with biochemical reactions for water purification systems
（水質浄化システムに関する生化学反応を伴う気泡流の数値シミュレーション）

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論 文 の 内 容 の 要 旨

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A full 3D three-phase numerical model for wastewater purification by the bacterial floc using the microbubbles is developed. The water purification using micro-bubbles has become an important topic due to its enhanced mass transfer effect. Microbubbles are injected into the reactor, and the oxygen obtained from dissolution of micro-bubbles is used up by the bacterial floc floating in the bioreactor for consumption of substrates. The performance of this consumption depends on bubble size and type of injection. By using uniform injection of microbubbles, best dissolution efficiency of microbubbles is observed near the lower region of the bioreactor. Thus, the height of the bioreactor could be significantly reduced without the reduction in the performance. Here, the micro bioreactor model is provided by the mixed Eulerian-Lagrangian formulation for fluid flow, and the tracking of bubble and flow motion in the system. Biochemical reactions based on various literature's including ASM is included in this model for water purification along with gas dissolution and mass transfer of oxygen using the Sherwood number approach. This study is the extension of the works of Murai and Matsumoto (1998) and Gong et al. (2009).

Firstly, the bacterial species modeled with the assumption of continuum nature of it and thus was coupled with Eulerian formulation. The bacterial reactions were modeled using the Monod kinetics and a total of 14 different bacterial types and 56 different species have been included in the model [Grady et al., 2011, Henze et al., 2002]. A complete model of the decay mechanism of the bacteria by Dold et al. (1980) is included in the model where bacteria is seen as undergoing death and lysis continuously. The governing equations include mixed continuity and momentum equations, species conservation equations, bubble motion equations based on force balance on individual bubbles, bubble dissolution equation using Sherwood number approach [Takemura and Yabe, 1999] and mass transfer equation. The biochemical reaction rates for individual species obtained from the reactions is updated into the source term of species conservation equations. Forces considered for translational bubble motion comprises of drag force, buoyancy force, added mass force and the inertial force due to acceleration of fluid around the bubble.

Validation of the biochemical reactions is carried out using the experimental study of Mohan, S. Venkata, et al. (2005). The temporal reaction rates obtained from numerical model and the experimental study were very similar. The sensitivity analysis showed that the results displayed good sensitivity with the biochemical coefficients like yield coefficient, specific growth rate and even the half-saturation constant. Multiple time stepping technique is applied to check for numerically-induced oscillation due to reaction source term and we obtained that the small time step size considered to avoid any instabilities in the bubble plume flow also aids in avoiding numerically-induced oscillation. The simulations have been carried out for heterotrophic organic bacteria with carbohydrates as the source of COD for the current analysis. The height of the tank is varied from 0.4 m to 0.1m (length of base $-$ 0.1m). The injected bubble sizes were studied by varying it from 200 μm to 1000 μm. Different injection systems have also been studied and compared.

The COD reduction curves for 200 μm microbubbles with different injection types are investigated for bioreactor heights of 0.4m, 0.2m and 0.1m (Figure 1). In the case of 0.4m height bioreactors, all injection types gives similar COD reduction rates. But, the on the other hand, shorter reactors gives better COD reduction performance with uniform injection system than central injection systems. And this difference in the performance is inversely proportional to the height.
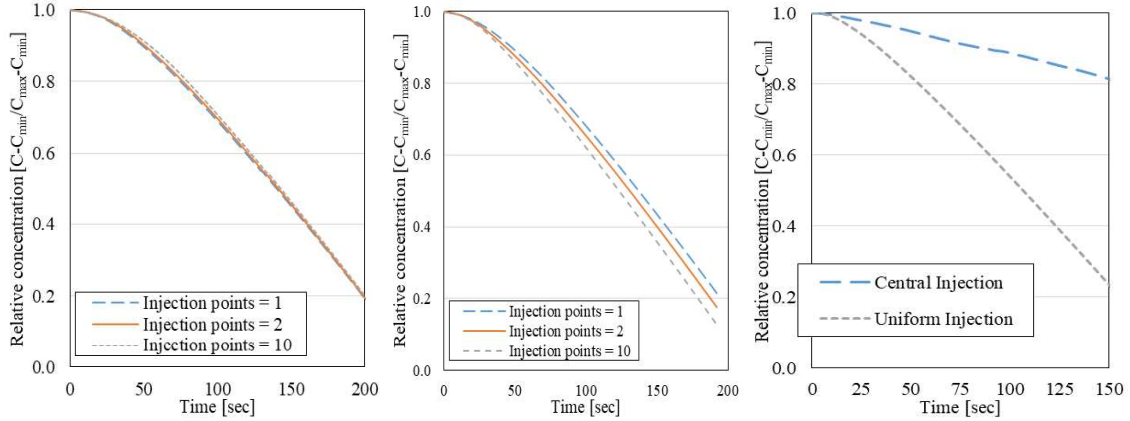

Figure 1: Plot of COD reduction with time for different injection types with 200 μm microbubbles for h=0.4m, h=0.2m and h=0.1m respectively
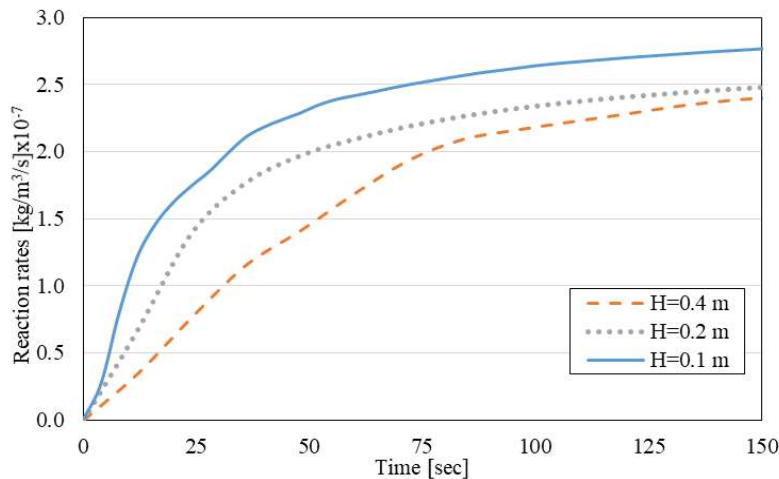

The curves for reaction rates for different heights of the bioreactor with uniform injection system and microbubbles of 200 μm is shown in the Figure 2. The results clearly suggest that it is better to go for shorter bioreactors and the bioreactor height could to be reduced without reduction in the performance of COD removal for microbubbles in uniform injection.

Figure 2: Plots of reaction rates vs time for uniform injection and 200 μm microbubbles

Additionally, we can conclude that for the shorter bioreactor heights, the uniform injection system with microbubbles gives best performance. The microbubbles have very low rising velocity when injected uniformly due to absence of induced flow effects, provides large residence time for microbubbles contrary to the central injection where induced flow effects are large. The uniform injection also ensures uniform distribution of microbubbles across the bioreactor.

For larger bubble sizes (500 μm ~ 1000 μm), uniform injection system performs better than central injection across all the sizes of the bioreactors. The large size of the bubbles provides large rising velocity which signifies the uniformity of the bubbles being the driving factor. Furthermore, the performance of a centrally concentrated injection system in longer bioreactor columns (4:1 to base) is affected both by dissolution rates and bubble retention times (better mixing due to enhanced circulation of fluid by induced flow effects). This is the reason for not obtaining inversely proportionality of performance of the bioreactor to bubble size.

Next, the bacterial concentration is regarded as a floc, thus effectively, the model would be 3D three phase system with Eulerian in liquid phase and Lagrangian in solid and gas phases. The bacterial floc modeling comprises of both the bacterial reactions and motion of the floc. The bacterial floc in our case is considered

to be comprising of approximately 20% of biomass by volume. We've included 14 different bacterial types and 56 different chemical species in our model. Motion of bacterial floc is done through Lagrange tracking and is defined as the force balance of an individual floc. The bubble-particle and particle-particle collisions are modeled using hard sphere model approach with the universal expression coefficient of restitution dependent on stokes number defined by Legendre et al. (2006).

Validation of the biochemical reactions is again carried out using the experimental study of Mohan, S. Venkata, et al. (2005) and the temporal reaction rates obtained from numerical model and the experimental study are found to be very close to each other. The validation of bacterial floc motion and collision is carried out through the experimental study of Zhang et al. (1999). The trajectories of particles from experiment and numerical simulation are observed to be very similar as shown in the Figure 3. The sensitivity analysis of the validation study of floc motion showed high sensitivity with density and size of the particles.
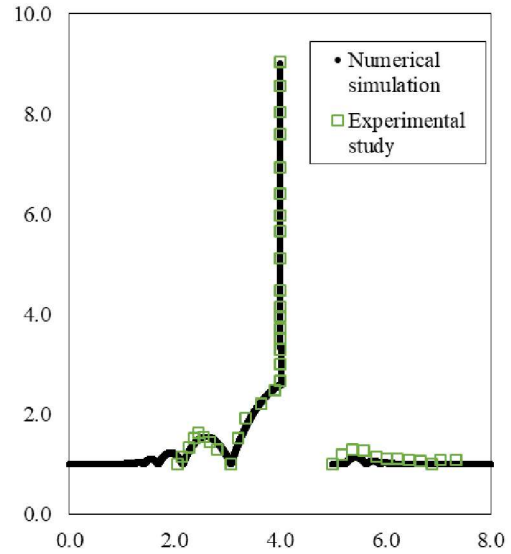

Figure 3: Validation of floc motion and collision

Both the models; biochemical reactions model and bacterial floc model give consistent results for uniform injection system. But, the results are different for central injection system. Primary reason being the consideration of concentration as floc, which ensures easy motion of flocs away from the presence of bubbles due to being heavier than liquid and buoyancy of bubbles. The dissolution efficiencies for different cases of mass flow rates is compared at t=60s. Also, comparison with Gong et al. (2009) is shown. The Figure 4 shows the better dissolution efficiencies of uniform injection over central injection.
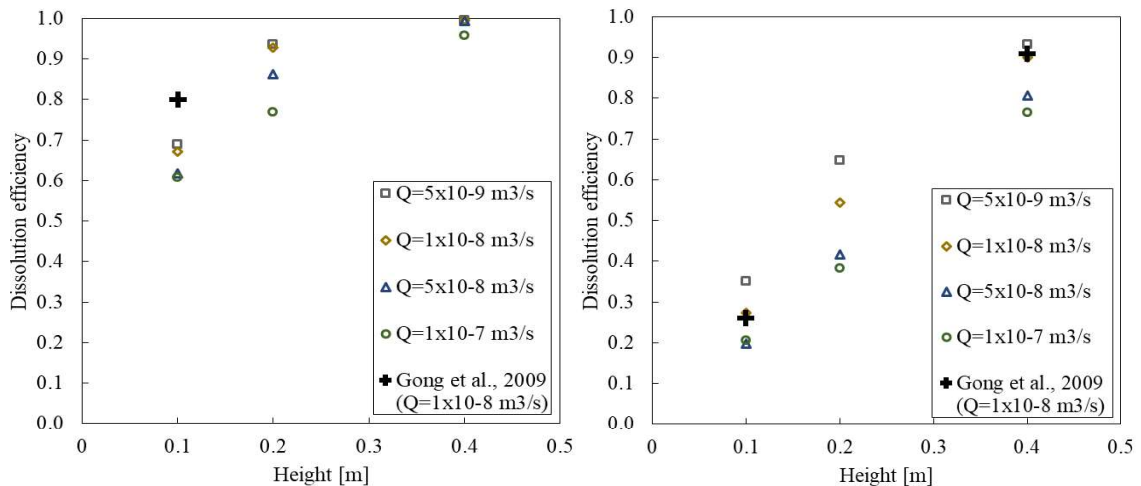

Figure 4: Bubble dissolution efficiency for different mass with UI and CI at t=60s (d$_b$=200 µm, h=0.1m)

The investigation is conducted for various mass flow rates with three different bubble sizes are shown in the Figure 5. An important observation is the decline in the difference between the curves for uniform injection system with microbubbles of 200 µm in the bioreactor of height 0.1m. The mass flow rate can be significantly reduced by use of microbubbles for shorter bioreactor. The COD reduction studies for microbubbles are carried out for various heights of bioreactors, with constant mass flow rates and bacterial quantity. The curves for reaction rates are plotted in Figure 6 at t=60 s. The analysis shows that the reaction proceeds faster for shorter reactor heights. This is an important conclusion, since apart from enhancing the COD reduction, this will also result in optimization of the space due to reduction in size of bioreactor. The performance of uniform injection system is better than central injection for arguably all the cases studied
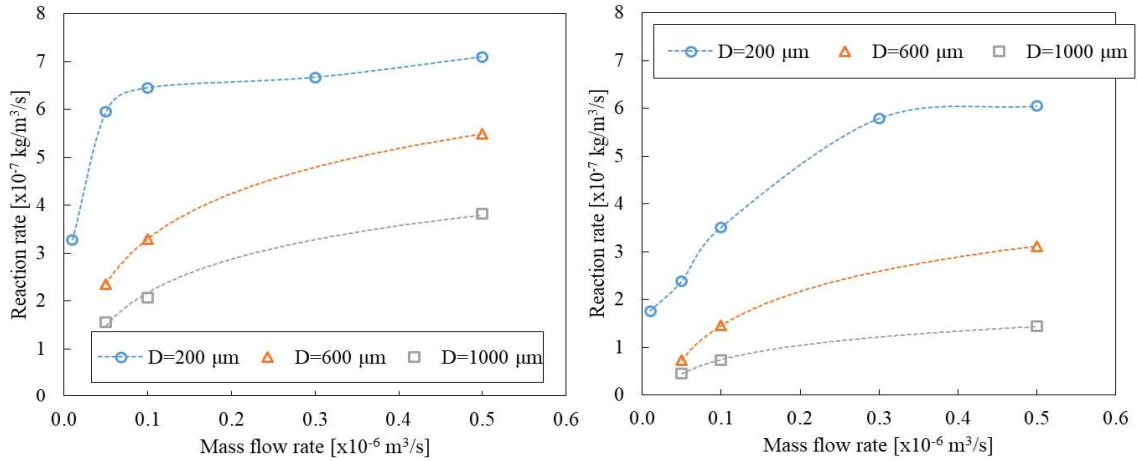
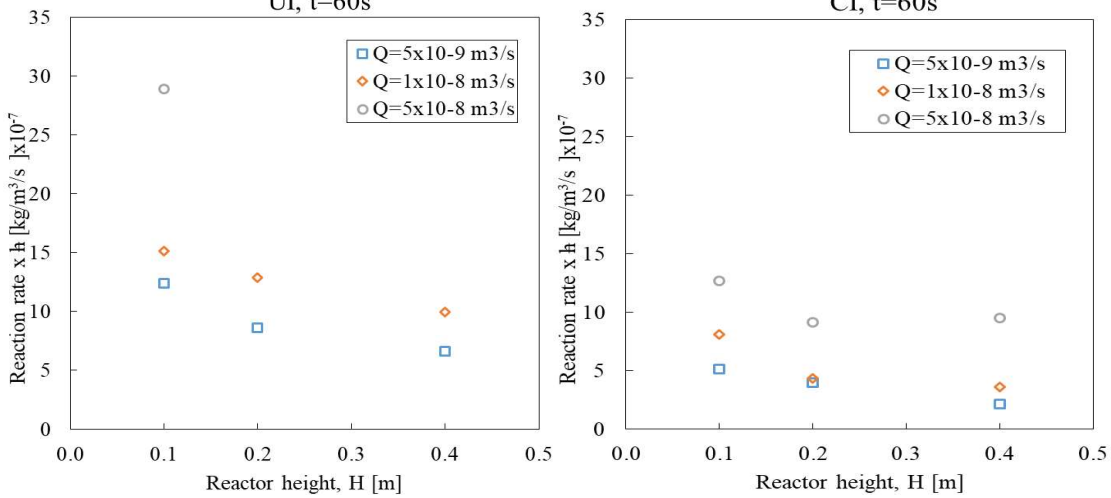**Figure 5: Reaction rate vs mass flow rates for different bubble sizes with UI and CI at t=60s at t=60s (h=0.1m)**

Figure 6: Reaction rate vs reactor heights for different mass flow rates with UI and CI at t=60s (d_b=200 μm)

Parallelization of the system is implemented and is necessary for two reasons; one for expanding it to the industrial scale from lab scale, and to reduce the computation cost. The parallelization includes parallelization of both Eulerian and Lagrangian phases. Eulerian case is a full 3D parallelization. The Lagrangian parallelization calculates the phase parameters of the specific bubbles in the region of their residence for the corresponding node. The weak (Figure 7) and strong scalabilities for varying mass flow rates illustrates attainment of good parallelization.
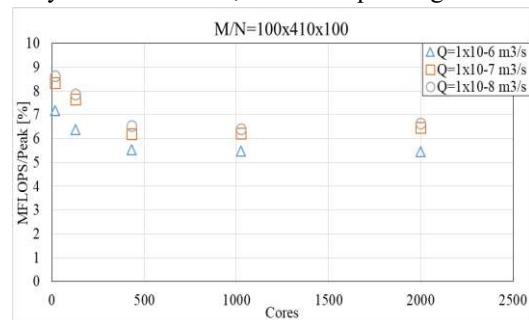

Figure 7: Weak scalability of MPI Parallelization

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