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Mathematical modeling of gas-liquid flows in bioreactors

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Motivation and Aim: The actual challenge for the researchers is to obtain a relevant model describing liquid and gas turbulent flows [1–4] to develop new bioreactor solutions [5] which tend to maximize gas mass transfer by creating a large gas surface area per unit volume and maintaining this high surface area on the large areas of the total volume of the bioreactor. The methanotrophic microorganisms consume methane as a substrate and breathe dissolved oxygen: ensuring the uniformity of its distribution in volume makes a decisive contribution to the key performance indicators of the system [6]. In order to solve this problem, it is necessary to calculate the predicted values of the gas mass transfer coefficient at various points of a closed contour.
Methods and Algorithms: Two models were developed.
Large scale two-phase continuum model, which includes Navier-Stokes equation for liquid and ideal gas, VOF (volume of fluid) model to describe the interfacial interaction and the model of turbulence which is the modification of k-ε model. This model can be used in both low- and high-Reynolds calculations. In first case, the laminar sublayer is resolved by the grid (no wall functions are used), in the second case, the laminar sublayer is not resolved (wall functions are used). The second case, the laminar sublayer is not resolved (wall functions are used). This model satisfactorily predicts the position of the laminar-turbulent transition on the solid surface. The model makes it possible to evaluate the flow intensity modes in different parts of the bioreactor, to identify areas of stagnation, recirculation vortices and zones of high turbulence.
Low scale model of dispersed bubbles transport in liquid continuum, including also Navier-Stokes equation for the continuous liquid phase, convection-diffusion model of dispersed bubble phase transport, convection-diffusion model of mass transfer for the dispersed bubble phase to account for bubble dissolution/growth. Among the main features accounting for gravity, lift and drag forces, bubbles sticking together, their repulsion from the wall should be mentioned. Worth noting that the model has been successfully verified for bubble flows in laminar flows [1].
Results: Two models were constructed to describe the process of displacement of the gas and liquid phase in the bioreactor. The large-scale model allows to localize the areas of bubble flows, zones of high turbulence, stagnation/unequal mixing. The low-scale model allows to simulate dispersed bubble flows, the distribution of bubble concentration over the volume, and the contact area of the phases.
Both models allow optimizing the bioreactor design for the target operating modes and evaluating the mass transfer properties.

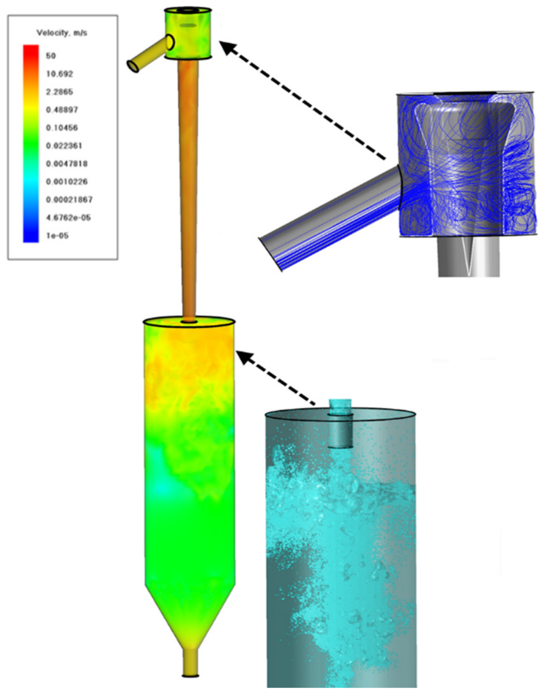

Fig. 1. Liquid velocity (color) and streamlines (blue lines) into bioreactor

Conclusion: The highest priority of the simulations was to determine the mass exchange ratio $K_L = \frac{dC/dt}{a(Cp-C)}$ of the gas fraction, i.e. the intensity of gas dissolution in the liquid. Here $C(t)$- dissolved gas concentration, Cp – equilibrium concentration of dissolved gas, a-phases contact area. Mass exchange is known to reach its local maximal intense in the areas with bubble flow. Thus, the simulations might be reduced to defining the bubble flow regions (ejector, tank) with model (1) and simulating these regions more detailly with taking into account model (2) to determine phases contact area a as well as K_L prediction.

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