Modelling of Bubble Breakage and Coalescence in Stirred and Sparged Bioreactors Using the Euler-Lagrange Approach with VOF

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Abstract

Gas-liquid systems are commonly used in industry to carry out biochemical reactions. Such process must be carried out to ensure sufficient mass transfer while there is no damage to the living cells/microorganisms. The overall performance is influenced mainly by the bubble size distribution (BSD) and process parameters such as the impeller speed and gas sparging rate. The correct prediction of BSD is important to choose optimal process parameters and thus meet the requirements of a given cell culture. This work is aiming to utilize computational fluid dynamics (CFD) for prediction of bubble breakage and coalescence at the level of the individual bubbles. Such approach then allows us to predict the whole BSDs under broad range of process parameters. In return, this can help us to determine suitable process parameters necessary to achieve the required conditions inside the vessel. The gas-liquid system of the stirred and sparged bioreactor was modelled utilizing the Euler-Lagrange (EL) approach together with volume of fluid (VOF) method for modelling of the liquid level. The continuous phases were modelled using a 3D time-dependent problem using the Reynolds-averaged Navier-Stokes (RANS) method with a realizable k-ε model for the description of turbulence. The motion of discrete Lagrangian bubbles was tracked by Newton's equation of motion with inclusion of the breakage and coalescence of individual bubbles. For bubble coalescence, the model developed by Prince and Blanch and further modified by Sommerfeld and Sungkorn for use in the Lagrangian approach to bubbles was used. For breakup, a model developed by Martínez-Bazán was used. There, the effect of daughter distribution function (DDF) on the resulting gas dispersion was studied. Two differently sized vessels with very similar geometry (one Rushton turbine impeller, three baffles, rounded bottom, etc.) were modelled. First one was the Minifors vessel with a working volume of 3.5L and as second reactor we used larger vessel with a total volume of 30L. For smaller Minifors vessel the impeller speeds ranged from 200 to 500 rpm, while the gas feed rate was constant and reached a value of 0.33 vvm. On the other hand, for larger 30L reactor impeller speeds in range of 360 to 470 rpm and gas feed rate of 0.01 vvm was used. To validate the whole CFD model, we compared the BSDs obtained from the simulations against experimentally measured BSDs. Subsequently, a general characterization of the studied system was performed in terms of the volumetric mass transfer coefficient (k_La) and the maximum hydrodynamic stress (τ_{VS}) to which the cell could be exposed.

Keywords: CFD, gas-liquid, Euler-Lagrange, VOF, scale-up, break-up, coalescence, stirred/sparged vessel