Computational Modelling of Gas-Liquid Flow in Stirred Tanks

A Thesis Submitted for the Degree of
Doctor of Philosophy

by

Graeme Leslie Lane

BE (Chem, Hons)

The University of Newcastle

Submitted November 2005

Revised submission August 2006

I hereby certify that the work embodied in this thesis is the result of original research and has not been submitted for a higher degree to any other University or Institution.

(Signed) ______________________________________

ACKNOWLEDGEMENTS

I would like to express my gratitude to my supervisor, Professor Geoffrey Evans, for his guidance and advice during the course of this project. I would also like to thank Dr Phillip Schwarz (CSIRO), Dr Peter Witt (CSIRO) and Dr Greg Rigby (formerly at the University of Newcastle) for their valuable assistance with various aspects of the project. I would also like to thank my employer, CSIRO Minerals, whose sponsorship has made this thesis possible.

ABSTRACT

This thesis describes a study in which the aim was to develop an improved method for computational fluid dynamics (CFD) modelling of gas-liquid flow in mechanically-stirred tanks. Stirred tanks are commonly used in the process industries for carrying out a wide range of mixing operations and chemical reactions, yet considerable uncertainties remain in design and scale-up procedures. Computational modelling is of interest since it may assist in investigating the detailed flow characteristics of stirred tanks. However, as shown by a review of the literature, a range of limitations have been evident in previously published modelling methods.

In the development of the modelling method, single-phase liquid flow was firstly considered, as a basis for extension to multiphase flow. A finite volume method was used to solve the equations for conservation of mass and momentum, in conjunction with the k-ε turbulence model. Simulation results were compared with experimental measurements for tanks stirred by a Rushton turbine and by a Lightnin A315 impeller. Comparison was made between different methods which account for impeller motion. Accuracy was assessed in terms of the prediction of velocities, power and flow numbers, the presence of trailing vortices, pressures around the impeller, and the turbulent kinetic energy and dissipation rate. The effect of grid density was investigated.

For gas dispersion in a liquid, the modelling method employed the Eulerian-Eulerian two-fluid equations, again in conjunction with the k-ε turbulence model. The correct specification of the equations was firstly reviewed. Different forms of the turbulent dispersion force were compared. For the drag force, it was found that existing correlations did not properly account for the effect of turbulence in increasing the bubble drag coefficient. By analysing literature data, a new equation was proposed to account for this increase in drag. For the prediction of bubble size, a bubble number density equation was introduced, which takes into account the effects of break-up and coalescence. The modelling method also allows for gas cavity formation behind impeller blades.

Simulations of gas-liquid flow were again carried out for tanks stirred by a Rushton turbine and by a Lightnin A315 impeller. Again, the impeller geometry was included explicitly. A series of simulations were carried out to test the individual effects of various alternative modelling options. With the final method, based on developments in this study, simulation results show reasonable overall agreement in comparison with experimental data for bubble size, gas volume fraction, overall gas holdup and gassed power draw. In comparison to results based on previously published modelling methods, a significant improvement has been demonstrated. However, a number of limitations have been identified in the modelling method, which can be attributed either to the practical limitations on computer resources, or to a lack of understanding of the underlying physics. Recommendations have been made regarding investigations which could assist with further improvement of the CFD modelling method.

TABLE OF CONTENTS