Alma Mater Studiorum – Università di Bologna

DOTTORATO DI RICERCA IN

Ingegneria Civile, Chimica, Ambientale e dei Materiali, Ciclo XXXII

Extended Abstract of the PhD Thesis entitled

# Computational Fluid Dynamics Analysis of Two-Phase Chemical and Biochemical Reactors

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**Summary and problem addressed**

In this work, the numerical analysis of turbulent two-phase processes in stirred tanks and bioreactors is performed with a computational fluid dynamics (CFD) approach.

Different modelling strategies are studied, tested and developed to improve the prediction of mixing phenomena, interphase interactions and bio-chemical reactions in chemical and process equipment. The systems studied in this work are a dilute immiscible liquid-liquid dispersion and dense solid-liquid suspensions, both in stirred tanks of standard geometry, a gas-liquid system consisting of a dual impeller vortex ingesting fermenter for the production of biohydrogen, analyzed in two configurations of the supports for the attached growth of biomass, two bioreactors, of different scale and configuration, subject to substrate concentration segregation.

Purposely collected experimental data and data from the literature were extensively used to validate the numerical results and either confirmed the goodness of the models and the modelling techniques, helped the definition of the limits and the uncertainties of the model formulations or guided the development of new models.

In all cases, particular attention was devoted to the precision of the numerical solution and to the validation with experimental data to quantify the appropriateness of the models and the accuracy of the CFD predictions.

In particular, CFD is exploited to investigate different turbulent two-phase processes in mechanically stirred tanks and bioreactors. The turbulent phenomena are described in the context of the Reynolds Averaged Navier-Stokes (RANS) equations, while the two-phase fluid mechanics is modelled with an Euler-Euler approach, with the so-called Two-Fluid Model (TFM).

The objective of this research was to study the two-phase fluid dynamics in chemical and process equipment and to develop modelling strategies to describe the relevant physics in the system. Different interphase closure models were studied and tested to improve the prediction of mixing phenomena, interphase interactions and bio-chemical reactions. Particular attention was devoted to determining the ordered discretization error (Grid Convergence study) to assess the *precision* of the solution, and to the validation with experimental data to quantify the *accuracy* of the CFD predictions.

In particular, in this work the following aspects are addressed:

– a dilute immiscible liquid-liquid mixture in a stirred tank of standard geometry was studied and the droplet dispersion was described by means of a Population Balance Model solved with the Quadrature Method of Moments. The effect of the turbulence dissipation rate and its correct prediction on the droplet breakup kernel is assessed. This work has been published in Maluta et al. (2021);

- dense solid-liquid suspensions in a flat-bottomed fully-baffled tank stirred with a mixed-flow impeller were analyzed. The effects of the turbulence modelling, the interphase momentum transfer terms and the coupling between the phases on dense solid-liquid suspensions were assessed and the impact of the different terms on the solid distribution and suspension was quantified. The work has been published in Maluta et al., (2019a);
- the production of hydrogen in an attached growth bioreactor in which two impellers entrained gas from the head space and distributed it to strip the product from the liquid phase was modelled. The turbulent gas-liquid fluid dynamics, the interphase mass transfer mechanism and the product removal from the gas current were implemented in a comprehensive modelling strategy, comparing two geometrical configurations. This work has been published in Maluta et al. (2019b);
- a lab scale and an industrial scale fermentation processes were investigated and glucose concentration fluctuations on the metabolic maintenance cost of a population of *Escherichia coli* were modelled with an Eulerian model. The segregations were described simplifying the fluid dynamics by means of a probabilistic approach based on the Interaction by Exchange with the Mean (IEM) mixing model. This study has been published in Maluta et al. *Biochemical Engineering Journal* (2020).

**Background**

The goal of the research presented was to investigate different turbulent two-phase processes in mechanically stirred tanks and bioreactors by means of numerical simulations. Different phenomena were studied in the context of the RANS-TFM approach, in which the segregation of the phases required specific modelling of the different closure terms to describe the fluid dynamics behavior, the interphase interactions and the effects within each single phase, such as the biomass metabolism or the evolution of the drop diameters.

The investigation concerned different laboratory scale equipment involving dispersed particle/droplets/bubbles in a continuous liquid phase, with the purpose in mind to identify a modelling method for industrial-scale equipment for each specific system. As a result, the direct resolution at all turbulent length and time scales, the entire particle-fluid interface, the particle-fluid interaction forces, the particle-particle collision and particle-wall collision events is not possible.

In this realm, the major strength of the TFM model is the viability of application at trial scale with a realistic representation of the equipment geometry, that is the target of any design and geometrical optimization method. Strengths and limitations of the TFM model for the investigate two-phase flows are different depending on the main physical characteristics of the specific turbulent multiphase equipment under investigation, namely: the dispersed phase mean volume fraction, the dispersed phase volume fraction distribution in the equipment volume, the dispersed phase size distribution, the operating mode for the dispersed phase (batch as in the case of droplets and particles, continuous for bubbles). In addition, possible inter-phase mass transfer, chemical or biochemical reactions, if present, must be considered.

For those processes that are critically affected by the turbulent flow field of the continuous phase (e.g. bubble/droplet breakage and coalescence) the same limitations of single-phase RANS-based simulations and the same attention to numerical verification that are already well known from previous investigations have to be kept in mind. The dispersed phase mean and local volume fraction determines the level of interactions.

- In case of one-way coupling, as in the investigated liquid-liquid stirred tank, fluid-particle interaction models for TFM models are generally well established, provided that a realistic size of the dispersed phase is either know a-priori (as is the case of inert solid particles or narrow size distribution of bubbles or droplets) or determined by population balance models in case of wide size distribution. In this latter case, limitations are mainly concerned with the breakage and coalescence models and with the RANS based prediction of the liquid phase turbulent flow field, due to the dependency of breakage and coalescence mechanisms on the turbulent field.
- In case of two-way coupling the effect of the dispersed phase on the turbulent field may have a significant impact, either enhancing or dumping turbulent fluctuations. In the incomplete suspension of dense solid-liquid mixtures, for instance, the lack of an established turbulence dumping model due to the settled layer of particles leads to an overprediction of an interphase, resulting in incorrect suspension of the solids from the bottom of the tank.
- In case of four-way coupling the interactions between particles, such as collisions, are generally modelled as ensemble averaged phenomena. Collisions of particles in dense solid-liquid suspensions in fully turbulent stirred tanks was either proved to have a negligible or a relevant contribution in predicting the volume fraction distribution of the dispersed phase above the just suspended impeller speed, $N_{JS}$. On the other hand, a related

phenomenon as the particle packing is essential in correctly predict the suspension, but its modelling so far relies on a numerical approach.

– For very large dispersed phase concentration, the dominant flow regime may change due to phase inversion, inter-particle collisions, enhanced aggregation phenomena, etc. In these conditions, the Euler-Euler model limits are pushed, and a reliable prediction of the flow fields needs additional models to take the changed physics into account. This is the case of unsuspended solids on the tanks bottom, where inter-particle collision is the main momentum exchange mechanism and the effect of interstitial fluid becomes less important, thus becoming a granular flow regime.

**Main results**

The validation of the numerical results with experimental data has been systematically performed and either confirmed the goodness of the models and the modelling techniques (such as in the case of liquid-liquid turbulent field, in the solid volume fraction profiles in complete suspension conditions, in the bioreactor fluid dynamics and in the chemical species evolution in time as predicted by the metabolic model) or it was instrumental in understanding the limits and the uncertainties of the model formulations (as, for instance, in the prediction of the DSD of diesel fuel in water and in the solid volume fraction profiles in incomplete suspension conditions) helping in some cases the development of new models (for example in the implementation of a TFM interfacial model for the mass transfer of gas in water and in the formulation of the maintenance rate dependence on the substrate fluctuations).

The main specific results achieved in the thesis are summarized in the following.

Liquid-Liquid dispersions in stirred tanks:

- experimental data confirmed that, in the investigated system and operating conditions, the diluted dispersed phase has a negligible impact on the mean and fluctuating variables of the continuous phase;
- RANS-TFM predictions of the turbulent field satisfactorily agree with single-phase results from the literature;
- the simulations underpredict the DSD, suggesting that specific tuning of the breakup kernel parameters is needed;
- grid effects are relevant and need to be properly addressed beforehand;
- a novel scalar correction for the breakup kernel derived from local quantities is proposed.

Solid-Liquid suspension in stirred tanks:

- in the operating conditions considered, the so-called granular model formulation did not provide any contribution to the TFM in the prediction of the solid distribution in the stirred tank for solid volume fractions up to 0.15, provided that a packing limit was included;
- in complete suspension conditions the coupling between TFM and the proper interphase forces provided reliable radial profiles of solid volume fraction; o in the investigated incomplete suspension conditions the accuracy of the numerical radial concentration profiles was unsatisfactory;
- the turbulent dispersion force significantly contributes to the solid suspension and distribution in the stirred tank; o specific models to account for particle-particle interactions and advances in the modelling of the effects of the solid phase on the liquid turbulent field and of the turbulent dispersion in the incomplete suspension of solids are needed.

Biohydrogen production in stirred fermenters:

- a modelling strategy for the fermentative production and stripping of biohydrogen in the self-ingesting stirred tank reactor was implemented;
- the interphase flux of hydrogen was modelled with a local mass transfer coefficient from the literature, a novel interfacial area formulation for the TFM and the Henry's gas law;
- the kinetics of a simplified biochemical reaction for hydrogen production was described with a substrate inhibition model and implemented in porous supports for attached growth biomass;
- the performances of two reactor configurations were tested with a local and an instantaneous analysis of the reaction rate, the interphase hydrogen fluxes and the two-phase fluid dynamics;
- geometrical changes were proposed based on the local behaviour of the bioreactor;
- the two-impeller configuration allows the circulation of stripping gas to enhance recovery. - *Escherichia coli* fermentation in bioreactors:
- a probabilistic mixing model was derived and implemented in the context of the software ADENON to describe the substrate inhomogeneities in fed-batch systems; o results from the IEM and the compartment model agree, proving that a simplified mixing model could suffice when just substrate segregation is important.
- the adoption of the simplified IEM model does not worsen the agreement with the experiments from the literature; o the simulation with an IEM model of highly segregated heterogeneous bioreactors is faster and computationally cheaper than CFD and CMA;

- a simplified model tying the maintenance rate of a population to the variance of the substrate concentration distribution was developed, implemented, validated against experimental data and discussed both from a Lagrangian and from a Eulerian perspective;
- introducing in the Pirt's law a dependence of the cell maintenance costs on the substrate concentration fluctuations improved the agreement with the experimental data.

**Relevant publications**

1. Maluta, F., Buffo, A., Marchisio, D., Montante, G., Paglianti, A., Vanni, M. Effect of turbulent kinetic energy dissipation rate on the prediction of droplet size distribution in stirred tanks(2021) **International Journal of Multiphase Flow**, 136, art. no. 103547. *DOI: 10.1016/j.ijmultiphaseflow.2020.*103547
2. Maluta, F., Pigou, M., Montante, G., Morchain, J. Modeling the effects of substrate fluctuations on the maintenance rate in bioreactors with a probabilistic approach (2020) **Biochemical Engineering Journal**, 157, art. no. 107536. *DOI: 10.1016/j.bej.2020.107536*
3. Maluta, F., Paglianti, A., Montante, G. RANS-based predictions of dense solid–liquid suspensions in turbulent stirred tanks (2019) **Chemical Engineering Research and Design**, 147, pp. 470-482. *DOI: 10.1016/j.cherd.2019.05.015*
4. Maluta, F., Paglianti, A., Montante, G. Modelling of biohydrogen production in stirred fermenters by Computational Fluid Dynamics (2019) **Process Safety and Environmental Protection**, pp. 342-357. *DOI: 10.1016/j.psep.2018.09.020*

**Conference contributions**

- Maluta F., Paglianti A., Montante G., Predictions of dense solid-liquid stirred tanks by RANS-based two fluid model simulations, 16th *Multiphase Flow Conference and Short Course: Simulation, Experiment and Application*, Dresden, Germany, 13 - 16 Novembre 2018;
- Maluta, F., Carletti, C., Paglianti, A., Montante, G., Numerical simulation of solid distribution and liquid mixing time in dense solid suspensions in a stirred tank, *10th World Congress of Chemical Engineering*, Barcelona, Spain, 1-5 Ottobre, 2017;
- Maluta F., Montante, G., Paglianti, A., Modelling of bio-hydrogen production in stirred fermenters by computational fluid dynamics, 9th International *Conference on Environmental Engineering and Management* – ICEEM09, Bologna, Italy, 6 - 9 Settembre 2017;
- Montante, G., Maluta, F., Paglianti, A., CFD modelling of biohydrogen production in a self-ingesting stirred tank, *ISMIP9 - International Symposium on Mixing in Industrial Processes 9*, Hyatt Regency, Birmingham, 25-28 Giugno 2017;