# Multiphase CFD: the use of optimization models and the importance of full scale size in Multiphase Modelling

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**Abstract**

It is well known that Computational Fluid Dynamics (CFD) is a powerful tool for process design and optimization. However, few are the contributions that explore real optimization models to arrive at better equipment design and/or better processes operation. It will be shown the development of an impeller for solid suspension based on a model mixing CFD (the commercial ANSYS CFX software was used for the CFD results) with Optimization (the coomercial software modeFRONTIER was used as the multiobjective design optimization tool) [3]. The combined approach used seven design variables and two nonlinear constraints. The designs were compared in their ability to meet two objectives: to increase the impeller effectiveness, defined as the ratio of pumping number to power number (in other words, the ratio of the pumping capacity to power consumed, normalized to be dimensionless), and to improve the homogeneity of the liquid-solid mixture (by increasing the cloud height). The model arrived at several possible solutions in a Pareto frontier, a set of equally optimal designs, at the end of the procedure. The optimization process was divided into two main steps:

1. A real optimization step, in which the objective functions and constraints were evaluated by the CFD approach.

2. A virtual optimization step, in which well-behaved response surfaces were used to extrapolate the initial results, saving computational time.

A further improvement on the first prototype of the impeller was obtained by imposing a minimun value for the Impeller Power Number ( $N_P$), since very low values for the Power Number restrict the use of the impeller for several industrial applications.

Recent CFD works are showing he importance of using real scale three-dimensional models for process predictions. The particular case of a three-dimensional, three-phase flow model to predict the dynamic behavior of an industrial fluid catalytic cracking (FCC) industrial riser is shown [1], [2]. The CFD model takes into account heat transfer and chemical reactions. A four-lump model was proposed to represent the catalytic cracking reactions in which the heavy oil (gasoil) is converted into gasoline and light hydrocarbon gases. Gas acceleration inside the reactor due to molar expansion and a model to describe undesirable catalyst deactivation by coke deposition on its surface were also considered. The commercial CFD code (Ansys CFX) was used to obtain the numerical data. Appropriate functions were implemented inside the CFX code to model the heterogeneous kinetics and catalyst deactivation.

## References

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[2] G. C. Lopes, L. M. Rosa, M., J. R. Nunhez, and Martignoni. W. P. Numerical study of outlet riser effects on flow patterns and reaction yields in industrial fcc reactors. 2012. *Submitted for publication.*

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