Computational Fluid Dynamics (CFD) for Process Industry

Computational Fluid Dynamics (CFD) is widely applied in process industry, for example in developing the equipment, choosing optimal process parameters or solving wearing problems. Most of the industrial cases involve multiple phases. The rapid development of computer performance and multiphase models has made CFD a powerful technique for obtaining detailed information about the processes, even if the process conditions make the measurements difficult. VTT applies CFD for troubleshooting, for design and scale-up of reactors. VTT has a high level expertise in multiphase CFD of complex processes involving reactions and heat transfer.

Solutions
VTT offers CFD solutions in a wide range of applications in process industry, including:

- Stirred tank reactors: chemical reactors, gas-liquid, solid-liquid and three phase systems, mineral processes, etc.
- Flotation equipment: one, two and three phase models, including particle attachment
- Precipitation: liquid phase chemical equilibrium, nucleation and growth based on supersaturation
- Heat exchangers: conjugate heat transfer, condensation, fouling
- Fluidized bed processes
- Fixed bed reactors: trickle beds, flow models, heat and mass transfer
- Liquid-liquid extraction

We use ANSYS Fluent® and OpenFOAM® to solve the flow equations with user defined submodels. We continuously develop efficient models for solving various multiphase flows. The focus is in methods allowing the simulation of industrial scale process units in acceptable time.

Examples of solution of customer cases
Wearing problem in a client’s mixing mechanism
- Multiphase CFD modelling predicted correctly the location of wearing.
- A number of modifications were modeled in order to find a geometry less susceptible to wear.
- Modelling was an inexpensive way to test several geometry variations.
- In addition, CFD produced valuable information about the general operational performance of the process unit.

CFD results confirmed proper operation of process unit
- Based on tracer measurements, one mixing unit in the process plant was suspected to have a bypassing problem.
- CFD analysis showed unambiguously that the tank was well mixed and no bypassing took place.
- In addition, modelling showed how the measured data was misinterpreted.
- As a result, the expensive repairs were avoided.
Example: Mixing of non-Newtonian fluid
In many industrial processes, the fluid viscosity is shear dependent. VTT is experienced in modeling non-Newtonian flows, taking into account turbulent effects and, in bubbly flows, the bubble induced shear. As an example, a validation simulation of the mixing of nanocellulose pulp in a stirred reactor is shown below. The rheology and velocity profiles were measured at VTT.

Example: Precipitation modeling
Modeling of precipitation processes involves two-phase flow, crystal growth and nucleation kinetics and often complex liquid phase chemistry. Models for precipitation have been implemented at VTT both in CFD and in the multizone model. Benefits of CFD:
- Local reaction zones are found, depending on the reagent feed locations: Measurements usually give information of the process only in a few points
- The effect of rotating speed on precipitation process behavior is easily investigated
- CFD analysis shows the effect of mixing rate on local supersaturation and therefore e.g. on the particle size distribution
- Usable in designing and analyzing the production size reactors

Example: Heat exchangers
CFD is a powerful tool in modeling and optimizing industrial heat exchangers. Conjugate heat transfer simulations can be used for conventional (one phase) heat exchangers. VTT has developed specific models also for condensing heat exchangers. In addition, comprehensive models for particulate fouling in heat exchangers have been developed.

Example: Flotation
CFD has been used in modelling of flotation process equipment to extend the understanding of the process and to find new solutions for saving energy and water. One, two and three phase models are in use (water, solids and air bubbles).

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