# Combination of Multi-Component Equilibria with CFD in Modeling Fast Reactive Processes

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The chemical change in a transport system is controlled either by the rate of chemical reactions or by heat and mass transfer effects. In CFD applications, the chemical reactions are usually modeled using finite rate kinetics. However, when some or all reactions are fast, the chemical state in a volume element is determined by the transfer conditions. In such a case, the local equilibrium assumption is valid.

The thermodynamic multi-component program ChemApp [1] was ported to the CFD software Fluent [2] via user defined functions to facilitate solving of equilibrium chemistry simultaneously with CFD modeling of species mixing. In this approach, Fluent is used to solve the species transport without chemical reactions and the chemical equilibrium in each control volume is solved using ChemApp. Two methods to use the output of the ChemApp solver, i.e. the equilibrium concentrations of the chemical species, were considered.

In the first method, each computational cell in the CFD mesh was assumed to be ideally mixed, and the species concentrations were forced to the thermodynamic equilibrium values. However, the chemical reactions are molecular-level processes and the reaction rate for infinitely fast reactions is limited by the mixing rate, which is controlled by turbulence. The second method assumes that the equilibrium state is reached only in the turbulent fine structures responsible for micromixing. The eddy dissipation concept (EDC) was then used to calculate the species mass transfer between the fine structures and the surrounding fluid.

A neutralization process, where sodium hydroxide solution was neutralized in a stirred reactor by adding dissolved carbon dioxide in the mixture, was used as a test case for the modeling approach. The methods to couple ChemApp to Fluent were compared by monitoring the pH distribution in the reactor as a function of time.

[1] Eriksson, G., Hack, K., and Petersen, S.: *ChemApp - a programmable thermodynamic calculation interface.* In Hirsch, J. ed.: Werkstoffswoche '96, Symposium 8: Simulation, Modellierung, Informationssysteme, page 47. DGM Informationsgesellschaft mbH, D-60486 Frankfurt, Germany 1997, ISBN 3-88355-236-4
[2] *Fluent Users' guide - Release 6.2*, Fluent Inc., 2005.