On the combination of detailed chemical simulation with CFD-calculations

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Abstract

CFD calculations with high demands on the degree of chemical information, such as are needed for reasons of environmental protection, continue to be no small challenge. A concept is introduced here which achieves two things to a much greater extent than has previously been the case: the degree to which chemical and fluid dynamics modelling can be separated and the extent to which the algorithm can be used by programmers and end users as a black box. This is realised by translating the fluid dynamics model into a system of reaction cells and mixing cells (RCMCS). In this way, a favourable balance is achieved between the amount of labour invested and the degree of chemical information supplied by the simulation. Among other things, the ability to determine unknown parameters of the chemical reaction mechanisms and the functionality of the system with very large reaction mechanisms has been proven.