

ChemNet™ CFD Post-Processing for Simulation of P. F. Technologies With Detailed Chemistry

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Computational fluid dynamics (CFD) has become established as the most effective and efficient framework for developing integrated designs for furnaces fired with coal and other pulverized fuels (p. f.). Comparable simulation methods are also being developed for dense-phase flow fields. The rudimentary chemistry submodels in such simulations have not necessarily limited the accuracy of the basic design output; for example, CFD furnace simulations are useful because combustion rates are determined by mixing rates between various injected air streams and the fuel streams from individual burners. So the impact of chemical kinetics is secondary, and the limitations of the rudimentary chemical submodels are not immediately apparent.

However, rudimentary process chemistry is unsuitable for advanced power system applications. One essential application presents obvious challenges: Transport gasifiers and other fluidized gasifiers operate at moderate temperatures, where time scales for the chemical kinetics are comparable to, or slower than, mixing rates. Even for the high temperatures imposed in entrained flow gasifiers, accurate chemical kinetics are essential because chemistry in the gas phase determines the concentrations of the primary char gasification agents (CO_2 , H_2O , CO , and H_2). Only part of the steam is injected into the reactor, and all four concentrations change continuously in time while volatiles are reformed by chemistry in the gas phase and the char is gasified. Rudimentary chemical submodels are also too simple to forecast emissions in fuel switching or co-firing scenarios; or to describe emissions that form in gas cleaning systems, like Hg-species, SO_3 , and $\text{PM}_{2.5}$. Clearly, many other problems require detailed reaction mechanisms.

One obvious remedy would be to incorporate more chemistry into the reactor simulations, but the progress in this direction during the past two decades has been imperceptible. Fact is, it is not possible to incorporate elementary reaction mechanisms with even the most rudimentary submodels for turbulent mixing, particle dispersion, and radiation transfer, and this situation is not expected to change in the foreseeable future.

Since the late 1990's, Dr. Ranzi at ENEL in Italy; Prof. Glarborg in Denmark; Dr. Kilpinen in Finland; and Niksa Energy Associates (NEA) in the U. S. have been developing a methodology to quantitatively specify an equivalent network of idealized reactor elements directly from a multiphase reactor simulation, such as an ordinary CFD simulation. In NEA's methodology, this post-processing uses the flow and thermal fields, but ignores the species concentration fields, which reflect the rudimentary chemical submodels. These concentration fields are superseded by simulations of each reactor in the network with full elementary reaction mechanisms for the gas phase and on soot, and the most advanced mechanisms available for the devolatilization, oxidation, and

gasification of the solid fuel. The applications completed to date comprise lab-scale flames of various coals at pressures from 0.1 to 3.0 MPa; 1 MW_{th} flames of three forms of biomass co-fired on four coals; two full-scale, coal-fired furnaces; and a 1D entrained-flow gasifier operated with diverse coal types. In each instance, only 1 or 2 parameters had to be calibrated with baseline performance data because the detailed mechanisms directly connect to fuel properties. Yet the accuracy of the conversion and emissions predictions far surpasses ordinary CFD, and the simulations were usually completed in tens of minutes on ordinary PCs.

Perhaps the most important practical benefit of this methodology is that it weakens and sometimes breaks the connection between the accuracy of the simulation results and the amount of calibration data available for the project. Since detailed chemical reaction mechanisms are directly connected to fuel properties, new rate parameters do not need to be assigned for every fuel in the process simulations, as with rudimentary chemical submodels. Consequently, once the mixing characteristics have been established with calibration data, fuel compositions, stoichiometric ratios, and temperatures can be varied over broad ranges without the need to recalibrate.

The method is currently constrained by its labor requirements. Our demonstration cases were developed with extensive manual operations on the primary CFD flowfield to specify the equivalent reactor networks, which are cost prohibitive. To circumvent this obstacle, organizations with (i) the pertinent chemical reaction mechanisms, such as NEA; (ii) the skills to automate the post-processing of the multiphase flowfield, such as Intelligent Light; and (iii) the software capabilities to manage simulations based on elementary reaction mechanisms, such as Reaction Design should be teamed to develop a fully automated implementation. Given such a software platform, a broad community of specialists working on advanced power generation technologies will be able to utilize realistic process chemistry in their design applications. The benefits will be especially substantial in applications in which chemistry controls, such as, in p. f. furnaces (in-furnace NO_x reduction; O₂ injection; high-temperature air preheat; reburning; CO emissions; soot emissions as portions of PM_{2.5}, LOI; and fuel quality impacts), during multifuel gasification (soot yields; fuel quality impacts on trace species and product quality), polygen processes (diverse feedstocks; reforming at moderate temperatures; oils production) and in gas cleaning systems (Hg emissions; impact of SO₃ on plume opacity; alkali vapor emissions).

For numerous case studies see

S. Niksa and G.-S. Liu, "Advanced CFD Post-Processing for P. F. Flame Structure and Emissions," 28th Int. Technical Conf. on Coal Utilization and Fuel Systems, Coal Technology Assoc., Clearwater, FL, March, 2003.