Interdisciplinary computational fluid dynamics

Computational Fluid Dynamics (CFD) is the science of predicting fluid velocities and pressure fields via computers, and is a discipline that historically has received enormous attention. CFD model development involves the solution of the partial differential equations describing fluid momentum and continuity balances, and usually requires a fluid dynamicist, physicist, applied mathematician or other computational fluid flow specialist.

Interdisciplinary CFD evolves when the physical problem becomes further complicated by other mechanisms such as energy transport, electrical potential, or chemical reactions to name a few. When such physical phenomena are present, the situation changes dramatically and a host of additional disciplines are required to achieve successful simulations for industrial application. The resulting coupled CFD models are manifested in the interplay between fluid mechanics, computer science, numerical stability, experimentation, and interdisciplinary engineering judgement. On September 23, 1994 Wendell H. Mills from Engineering Computer Corporation (Warrensville Hts., Ohio) has described some interdisciplinary CFD projects he has been working on and, in particular, focused on thermal flow in a burner used in oil refinery reformer units.

2.1 Industrial interdisciplinary CFD

The four major ingredients of interdisciplinary CFD are:

(i) The mathematical model; deriving from scientific or engineering first principles the equations describing the momentum, energy, mass transfer, radiation, chemical relations, turbulence, electric forces, etc.

(ii) Physical properties for the model; this means (a) identifying the boundary conditions and sources, such as heat losses, flow rates, heat or mass sinks, (b) determining the physical coefficients of conductivities, specific heats, densities, activation energies, diffusivities, viscosities, resistivities, etc. from both the literature and experimentation whenever possible.

(iii) The computational model; that is, developing a complete computer software program which computationally solves the model equations.
The easiest way is to use shells, i.e., commercially available interdisciplinary fluid flow codes, as the basic starting point, and to make the necessary modifications depending on the particular physical and geometric conditions in the model under study. The numerical solution involves discretization of the fluid flow region; it must be stable (small changes in the parameters should result in only small changes in the solution).

(iv) Computational process simulation; this means that (a) the computational results must be validated (by experimentation or by the existing literature) after tuning up (or calibrating) the unspecified parameters, (b) the numerical simulation of the process behavior under different operating conditions can be adjusted without significant cost (i.e., in a "capital-free" manner), (c) the numerical simulation is effective tool for process design, scale-up, trouble-shooting, improvement, and control and optimization.

W. Mills mentioned briefly some of the projects he has been working on, such as

(i) Determine retrofit design improvements to eliminate vapor recirculation in oil refinery distillation units;

(ii) Redesign refinery chimney flarestack burner tips to eliminate tip burnout;

(iii) Determine process conditions which achieve specified heat transfer within refinery tubular reactor combustion zones.

Problem (i) involves momentum, continuity and turbulence; problem (ii) involves also chemical reaction and energy, and problem (iii) requires, in addition, surface-to-surface radiation and gas-to-surface radiation.

We shall go into the details of problem (iii).

Figure 2.1 describes schematically a refinery tubular reactor unit. The unit is a cylinder of length 3-4 meters and diameter of the cross-section 10-20 cm. The crude oil flows in the inner tube where chemical processes are taking place to refine the oil. The chemical process requires, ideally, a uniform temperature in the range of 2000-3000°F. The outer pipe surrounding the inner tube serves as burner which is to provide and maintain the desired uniform temperature.

Figure 2.2(a) shows the fuel tube tip (where crude oil enters). Fuel to the burner (the outer pipe) is supplied through the small discs in the annulus. Figure 2.2(b) describes schematically how fuel and air are supplied; here we shall be concerned only with the chemical processes inside the outer tube.

The objective is to develop 3D computer model to simulate temperature, gas flow velocities and fuel combustion within the burner; to run the