The combustion group

During the CTR 2000 Summer Program, seven projects related to combustion and sprays covered a large variety of topics ranging from the fundamental understanding of spray development and combustion processes to the modeling of real applications. As in previous summer programs, large-eddy simulation (LES) of chemically reacting flows was a main subject. In contrast to previous years, in 2000 the main focus was not only on the development and assessment of combustion models, but also on the evaluation of the merits and feasibility of LES for industrial applications. This trend towards the simulation of practical applications is reflected in the following facts: Three of the seven projects have industrial participation; two of the projects are related to the modeling of spray development, a key issue for modeling real combustion devices, which typically burn liquid fuels; and three projects are related to partially premixed combustion, which is the main combustion mode in many modern gas turbines and piston engines.

An example of the latter is the work by Jiménez, Haworth, Poinsot, Cuenot and Blint. This group extended a project initiated in the 1998 CTR Summer Program where the first direct simulations of premixed flames propagating into a stratified mixture were conducted with full treatment of complex chemistry. In 2000, globally lean mixtures were studied and NO_x formation added. In a parallel project, Haworth studied a new model which combines the capabilities of flamelet and pdf methods. This model has the capacity of handling stratified combustion and pollutant formation.

Legier, Poinsot, and Veynante performed an LES of combustion instabilities in a diffusion burner built at Ecole Centrale Paris for SNECMA. The main issue was to test whether LES could predict the different stabilization processes of this flame.

In an attempt to develop an efficient and robust premixed combustion model for LES of engineering applications, Flohr and Pitsch developed an LES formulation of a turbulent flame speed closure model which was originally proposed for RANS modeling. The model was implemented in a commercial flow solver with LES capability and applied to a generic premixed burner with focus on the combustor response to forced inflow modulations. An important part of this work is the evaluation of the LES capability of the flow solver by comparing DNS results for a turbulent pipe with those obtained using an existing, extensively validated CTR DNS code.

Although reactive flow problems in chemical engineering typically reveal a chemistry considerably different from hydrocarbon chemistry of fossil fuels observed in engine combustion, similar combustion models might be applicable in both cases. During this program, the methyl chloride chlorination process was investigated by Harvey and Pitsch. In order to evaluate the level of modeling complexity required in typical industrial applications, flamelet models were implemented in a RANS and an LES code, and predictions for a model reactor using both codes were compared to simulations neglecting chemical closure. Some important findings are that the temperature is substantially overpredicted if chemical closure is neglected. The LES also exhibited considerably lower scalar dissipation rates and higher maximum temperatures compared to the RANS calculations.

An issue of particular importance to numerical simulations of combustion in technical devices is the modeling of spray dynamics and vaporization. In most gas-turbine combustors and in modern diesel engines, liquid fuels are injected at subcritical temperatures into a supercritical environment. Common spray models fail to predict the transitional behavior which is important in this regime. Oefelein and Aggarwal addressed this problem by developing a unified high-pressure evaporation model which includes the description of transcritical and supercritical processes. The second spray related project by Smith, Cha, Pitsch, and Oefelein performed DNS of evaporating and reacting sprays in isotropic turbulence. Using the analysis of the resulting statistics for the mixture fraction and the scalar dissipation rate, they provided a novel formulation of mixture fraction based combustion models, such as conditional moment closure or unsteady flamelet models, which can be applied to spray combustion.

Heinz Pitsch and Thierry Poinsot