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The combustion and multiphase group

Over recent years, much progress has been made in the development of combustion models for numerical simulations of engineering systems. Although much of the theory is still unclear, the application of these models to real systems seems to be in reach. It is hence not surprising that industrial and commercial interests were well represented in the combustion and multiphase group. However, the main emphasis of most of the projects was in fundamental theory and modeling. The combustion and multiphase group was the largest group of this years' summer program. It had contributions in the general areas of multiphase and combustion science and modeling, but also in fires and radiation, and combustion instabilities and control. This section includes reports on twelve projects: Two related to multiphase flows, five in the area of combustion science and modeling, two related to fires and radiation, and three on combustion instabilities and control.

The projects in multiphase flows are related to liquid gas interfaces and Lagrangian spray models. It is well known that the level set approach to simulate two-phase flows does not guarantee mass conservation of the individual phases. To insure mass conservation, the level set scalar has to be appropriately corrected, for example by a volume of fluid method. The project of Boersma *et al.* explores the effect of such a level set correction method on the higher order interface properties, for instance the curvature. It is found that local correction methods introduce significant errors in the interface curvature. A correction extension method is then proposed addressing this problem and leading to a significant reduction of curvature errors. LES/Lagrangian spray modeling of multiphase flows in critical in simulating practical combustion devices. In a different project, Pozorski *et al.* studied the impact of sub-grid turbulence on particle motion. It was shown from DNS data that filtering affects preferential concentration. A stochastic model was proposed for reconstructing the residual velocity field.

Recent breakthroughs in premixed combustion modeling has increased the computational accessibility of such systems. Bilger recently proposed a new marker field method to track combustion in low Damköhler number premixed configurations. Using a fictional scalar field, the project of Bilger *et al.* analyzed a direct mapping between this field and the reaction progress-variable. DNS of low-Damköhler number premixed combustion is used for an *a priori* testing of the model. A second project related to premixed combustion is that of Huh *et al.*, who recently proposed a premixed turbulent combustion model based on zone-conditional averages. In contrast to Bilger's model, this model has been formulated for the high Damköhler number case. The aim of the present project was to test closure assumptions for the turbulent burning velocity using DNS data. An entirely different approach to combustion modeling in LES is the filtered-density function approach. In such LES-FDF methods, the integration of the chemical source term is computationally expensive. Pope *et al.* studied the use of ISAT to accelerate this computation for LES-FDF. Using several parallel computation paradigms, they identified potential bottlenecks in using ISAT algorithms and demonstrated substantial speed-up compared with the direct integration.

From an industrial perspective, combustion models must be computationally inexpensive. With this constraint in mind, Goldin *et al.* proposed the constructed-PDF model as a possible extension of conventional laminar-flamelet models. By using detailed chemistry and the Linear-Eddy Model to model a simplified flow configuration, a look-up table is created. Using this lookup table, simulations have been performed for a series of turbulent diffusion flame, showing good agreement with experimental data. A real-world application of combustion modeling was the objective of the project of Kim *et al.*. A simulation of a Pratt & Whitney aircraft engine combustor was initiated. One of the obstacles encountered was the modeling of the injection process, which involves a liquid jet impingement on a wall and the formation and development of a liquid wall film. As a result of the project, different film models have been developed and simulations for the combustor have been initiated.

Another highly complex problem of practical interest is the simulation of accidental fires. Tieszen *et al.* studied mixing in such flows by performing LES for a buoyant helium plume. It was found that conventional sub-filter modeling was insufficient and could not reproduce the Rayleigh-Taylor instabilities at the base of the plume. Different models have been proposed and applied in simulations with varying filter width. Also related to accidental fires was the project by Jensen *et al.*. A comparative study of different solution methods of the radiative transfer equation was performed using the temperature fields from simulations of a 2 m pool fire. The applied models include discrete transfer method, different discrete ordinate techniques, and a moment method using the so called M_1 closure.

Another group investigated specific issues related to the design and optimization of combustion devices. In such systems, a major issue is to develop fast optimization processes to be able to adjust, for example, the positions and flow rate distribution of dilution jets in a gas turbine burner in order to reach a predefined outlet temperature profile. This issue was the focus of the work of Debiane *et al.* who applied modern optimization methods to a model flame and showed the potential of their approach to control the flame length, temperature and NO_x emission. Recent experimental experience shows that optimization procedures can also be dangerous: optimizing performances and pollution often leads to instabilities. The development of LPP devices (Lean Premixed Prevaporize) for gas turbines is a good example of experimental design optimization which meets most performance and pollution objectives, but in many cases, leads to high and unacceptable instability levels. Studying and predicting such instabilities using numerical tools was the topic of the other projects. The computation of acoustic resonators (such as combustion chambers) is indeed still a challenge because of the lack of an appropriate formulation of boundary conditions. Prosser and Schlüter proposed and studied a new original boundary condition formulation based on a low-Mach number approximation to improve existing characteristic methods for compressible codes. The objective of the project of Martin *et al.* was to revisit the Rayleigh criterion which is the most commonly used tool to describe instabilities: the recent development of compressible LES for combustion allows now to replace this criterion by a detailed analysis of the budget of acoustic energy. Such a budget was studied in the case of a staged turbulent combustor in which the level of oscillation was controlled by the outlet boundary condition. Finally, as LES will still remain very expensive for a long time, additional tools are needed for design and optimization of thermoacoustic oscillations in industry: the last project (Benoit *et al.*) shows how acoustic analysis can be coupled to LES to predict the growth rates of all acoustic modes in a reacting configuration. Here the objective was to show that LES information can be injected into a Helmholtz acoustic solver to retrieve the unstable modes and eventually control them through different outlet conditions.

Heinz Pitsch and Thierry Poinsot