Including Detailed Chemical Properties in the Modeling of Emerging Turbulent Combustion Systems

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Abstract

Hydrocarbon combustion, involved in more than 90% of the worldwide primary energy consumption, produces most anthropogenic CO2 emissions [1]. Electrification will not entirely replace combustion in the short term for two main reasons: first, batteries exhibit an energy density about 50-100 lower than hydrocarbon fuels. Combustion will, therefore, still be required to power long-distance transport vehicles, such as boats, trucks, or aircraft. Second, many industrial sectors, such as steel, cement, glass, and aluminum, require high temperature (more than 500°C) heat sources that can hardly be delivered without a combustion process.

Developing and optimizing new energy systems that integrate carbon-neutral fuels such as biofuels, efuel, hydrogen or ammonia constitutes a relevant energy scenario to limit global warming. However, sustainable fuels still produce pollutants, in particular NOx. To reduce pollutant emissions, the strategy of combustion engineers is to decrease the temperature of flames by increasing the air-to-fuel ratio. The problem with lean flames is that they are prone to instabilities and extinction, thus causing essential safety issues and mechanical damage [2]. The challenge is to ensure flame stability and minimize pollutant formation by possibly implementing new adapted devices. Combustion engineers need reliable numerical tools for designing future combustion chambers. Advanced modeling of combustion phenomena is required for optimizing the injection system, the combustion chamber geometry, the wall heat transfers but also the pollutant formation. Simulations are also needed to challenge solutions to stabilize low-temperature flames.

The scientific challenges are to model the complex interactions between combustion chemistry and the turbulence of the flow at an affordable computational cost, compatible with industrial constraints [3]. The first difficulty is that the kinetics of combustion involves hundreds of chemical species that react through thousands of elementary reactions. To save computing time, the detailed mechanisms that describe this complex chemistry are reduced before being used in CFD codes. The second issue is related to the modeling of the turbulence / chemistry coupling which is not fully resolved in simulations.

This presentation aims to establish a brief state-of-the-art of both kinetic reduction methods and turbulent combustion models suitable for simulating emerging combustion technologies. The discussion focuses on large eddy simulation (LES) formalism, especially relevant to capture unsteady interactions between chemistry and turbulence. As an illustrative example, the presentation will end by showing

recent simulations of plasma-assisted combustion, an emerging solution to enhance low-temperature flames. The importance of complex chemistry effects on flame stabilization mechanisms are highlighted.

References

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