Application of the Tabulation of Dynamic Adaptive Chemistry method for CFD simulations including detailed oxidation mechanisms.

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Abstract

Detailed oxidation mechanisms are required for more realistic computational fluid dynamics (CFD) simulations of the combustion phase in internal combustion engines (ICE). They allow to describe the oxidation of complex fuel mixtures over a wide range of operating conditions. Including detailed oxidation mechanisms is, however, computationally expensive since the time integration of the species mass fractions involves to solve a large system of stiff nonlinear ODE, hence restricting their use to very simplified cases.

Different approaches were reported to reduce the computational effort. The most successful techniques are based on mechanism reduction and solution storage and retrieval.

We developed a new method termed tabulation of dynamic adaptive chemistry (TDAC). This method combines a reduction scheme, the dynamic adaptive chemistry (DAC) [1, 2], with a storage/retrieval algorithm, the in situ adaptive tabulation (ISAT) [3, 4]. It has been implemented in the Lib-ICE code which is a set of applications and libraries for ICE simulations developed under the OpenFOAM® technology.

This presentation describes how TDAC takes advantage of the features of ISAT and DAC in ICE simulations to substantially reduce the computational time. It also develops the details about the implementation of the coupling and it introduces the new improvements of the ISAT algorithm that make it more suitable for ICE simulations.

In the context of Homogeneous Charge Compression Ignition (HCCI) engines, we have compared the method with direct integration using several mechanisms (ranging from 44 to 857 species) in simplified geometries. The results obtained with TDAC and with direct integration are in very good agreement. In a more complex geometry, using a 857-species iso-octane mechanism [5], we have also validated the method with the experimental data of Hessel et al. [6]. A speed-up factor of about 300 is achieved compared to the direct integration which is well about what was previously reported for HCCI simulations using only ISAT (up to 10) or DAC (between 15 and 70 in single-cell simulations and depending on the mechanism used).

Accordingly, the TDAC method is a significative improvement to solve the oxidation kinetics in engine simulations as it allows to include detailed mechanisms in complex geometry where the direct integration is not feasible.

Keyword : ISAT, Dynamic Adaptative Chemistry, HCCI, Internal Combustion Engine, CFD

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