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Improved Stiff ODE Solvers for Combustion CFD A. IMREN, D.C. HAWORTH, Penn State — Increasingly large chemical mechanisms are needed to predict autoignition, heat release and pollutant emissions in computational fluid dynamics (CFD) simulations of in-cylinder processes in compression-ignition engines and other applications. Calculation of chemical source terms usually dominates the computational effort, and several strategies have been proposed to reduce the high computational cost associated with realistic chemistry in CFD. Central to most strategies is a stiff ordinary differential equation (ODE) solver to compute the change in composition due to chemical reactions over a computational time step. Most work to date on stiff ODE solvers for computational combustion has focused on backward differential formula (BDF) methods, and has not explicitly considered the implications of how the stiff ODE solver couples with the CFD algorithm. In this work, a fresh look at stiff ODE solvers is taken that includes how the solver is integrated into a turbulent combustion CFD code, and the advantages of extrapolation-based solvers in this regard are demonstrated. Benefits in CPU time and accuracy are demonstrated for homogeneous systems and compression-ignition engines, for chemical mechanisms that range in size from fewer than 50 to more than 7,000 species.

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