



Analysis of operator splitting errors for near-limit flame simulations



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ABSTRACT

High-fidelity simulations of ignition, extinction and oscillatory combustion processes are of practical interest in a broad range of combustion applications. Splitting schemes, widely employed in reactive flow simulations, could fail for stiff reaction–diffusion systems exhibiting near-limit flame phenomena. The present work first employs a model perfectly stirred reactor (PSR) problem with an Arrhenius reaction term and a linear mixing term to study the effects of splitting errors on the near-limit combustion phenomena. Analysis shows that the errors induced by decoupling of the fractional steps may result in unphysical extinction or ignition. The analysis is then extended to the prediction of ignition, extinction and oscillatory combustion in unsteady PSRs of various fuel/air mixtures with a 9-species detailed mechanism for hydrogen oxidation and an 88-species skeletal mechanism for *n*-heptane oxidation, together with a Jacobian-based analysis for the time scales. The tested schemes include the Strang splitting, the balanced splitting, and a newly developed semi-implicit midpoint method. Results show that the semi-implicit midpoint method can accurately reproduce the dynamics of the near-limit flame phenomena and it is second-order accurate over a wide range of time step size. For the extinction and ignition processes, both the balanced splitting and midpoint method can yield accurate predictions, whereas the Strang splitting can lead to significant shifts on the ignition/extinction processes or even unphysical results. With an enriched H radical source in the inflow stream, a delay of the ignition process and the deviation on the equilibrium temperature are observed for the Strang splitting. On the contrary, the midpoint method that solves reaction and diffusion together matches the fully implicit accurate solution. The balanced splitting predicts the temperature rise correctly but with an over-predicted peak. For the sustainable and decaying oscillatory combustion from cool flames, both the Strang splitting and the midpoint method can successfully capture the dynamic behavior, whereas the balanced splitting scheme results in significant errors.

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1. Introduction

Near-limit phenomena such as ignition and extinction are of practical interest in a broad range of combustion applications. High-fidelity simulations with detailed chemical kinetics are essential for the reliable prediction of such phenomena, although the large number of species and reactions, as well as chemical stiffness, pose significant computational challenges. Furthermore, while the size of reaction models can be systematically reduced through skeletal reduction and timescale analysis [1], chemical stiffness typically remains in reduced chemistry models, such that low-cost explicit solvers are in general not applicable for the partial differential equations (PDEs) governing reactive flows. The incorporation of stiff detailed chemical kinetics in combustion simulations is challenging. A variety of numerical methods have been developed [2–20], among which operator splitting schemes have been widely applied to reactive flow simulations. For example, a multi-implicit spectral deferred corrections (MISDC) strategy, second-order accurate in time, has been developed for the low Mach number reacting system to reduce the inherent splitting error [14–17]. It couples advection, diffusion, and reaction by including effects of other processes in fractional discretization. In contrast, to reduce the cost associated with stiff chemistry integration, another class of splitting schemes separate chemical reactions from other physical processes into fractional chemical sub-steps, such that implicit solvers can be applied only for the local chemistry integration [2–10]. In addition, significant progresses have been made recently in the development of fast reaction mapping approximation such as *in situ* adaptive tabulation and dynamic adaptive chemistry [20–23].

Among the most frequently used splitting schemes is the Strang splitting approach [2,3], which is second-order accurate for sufficiently small time step size, and has been routinely employed, for example, in the probability density function (PDF) simulations of turbulent reactive flows for composition evolution [7]. The weak second-order accuracy of time stepping in the PDF component of a large eddy simulation (LES)/PDF simulation is achieved by performing integration of transport and mixing terms twice with half time step, and a full time step for reaction in between [24]. Recently, the Strang splitting scheme has been further combined with tabulation for efficient reactive flow simulations with detailed chemical kinetics [5]. For steady-state reaction–diffusion systems, the Strang-splitting error may introduce displacement from the original systems, for which Speth et al. [9] proposed the balanced splitting to further improve the prediction of steady state solutions.

The accuracy of splitting schemes is well understood in the limit of sufficiently small integration time step size, which is typically substantially smaller than those adopted in most practical simulations [10,25]. For instance, a time step in the order of micro-second was applied for the LES/PDF simulation of a jet flame with a reduced mechanism consisting of 20 species [24], which is substantially larger than the fast chemical timescales that are less than a nano-second. For stiff reaction–diffusion systems, Sportisse [25] argued that the Strang splitting could maintain second-order accuracy even with a time step size larger than the fast chemical time scales, provided there is an attractive manifold and the chemical parts are integrated at the first and last fractional steps. Second-order convergence of the Strang splitting has been reported in a large number of studies, e.g. in an unsteady freely-propagating premixed methane/air laminar flame [10].

More recently, the Strang splitting scheme was found to fail for a stiff reaction–diffusion system when significant radical source is present in the non-chemical source terms [18]. The chemical source term may respond drastically differently due to the missing transport term during the integration of the chemistry sub-steps and therefore incur $O(1)$ integration errors unless the splitting time step size is comparable to or smaller than that required for explicit integration. As an example of practical significance, it was found that the Strang splitting may also fail in predicting the near-limit extinction phenomena in unsteady perfectly stirred reactors (PSRs) [19], while the exact cause of the large error is not clear. The impact of operator-splitting on the accuracy of the simulations of turbulent flames exhibiting local extinction/re-ignition instance is unclear, which merits a systematic analysis of the effects of operator splitting errors on near-limit combustion phenomena, including extinction, ignition and oscillatory combustion.

In this study, theoretical analysis on a reaction–diffusion model is first performed showing that errors induced by the decoupling of fractional steps may lead to significant errors on the predictions of extinction and ignition. Then the analysis is extended to the prediction of ignition, extinction and oscillatory combustion in unsteady PSRs of various fuel/air mixtures. A 9-species detailed mechanism of hydrogen oxidization [26] and an 88-species skeletal mechanism for *n*-heptane [27] are employed in the numerical tests, together with a Jacobian-based analysis for timescales. The tested schemes include the Strang splitting [2,3], the balanced splitting [9], and a new midpoint method. As an outline of this paper, the reaction–diffusion model systems are formulated in Section 2, with the characteristic times being analyzed based on Jacobian matrices. The different splitting methods are presented in Section 3. Then the theoretical analyses of the splitting errors for near-limit phenomena are detailed in Section 4, followed by numerical tests in Section 5. Conclusions are in Section 6.

2. Reaction–diffusion model systems

The spatially discretized governing equations of a reactive flow can be expressed as:

$$\frac{d\phi}{dt} = \mathbf{S}(\phi) + \mathbf{M}(\phi, \mathbf{x}, t), \quad (1)$$

where $\phi = \{\mathbf{Y}, h^s\}$ is the composition, \mathbf{Y} and h^s are the mass fractions of the n_s chemical species and the sensible enthalpy of the mixture, respectively; and \mathbf{S} and \mathbf{M} are the rate-of-change of the composition due to chemical reactions and mixing

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