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On the Necessary Grid Resolution for Verified Calculation of Premixed Laminar Flames

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Abstract. We consider the grid resolution necessary to resolve combustion in a mixture of calorically imperfect ideal gases described by detailed kinetics and multicomponent transport. Using the steady premixed laminar flame as a paradigm, the required spatial discretization to capture all detailed physics in the reaction zone is found via 1) determination of the finest grid used in a standard software tool which employs adaptive mesh refinement, 2) examination of peak values of intermediate species mass fractions in the flame zone as a function of grid size, 3) a formal grid resolution study, and 4) a robust new eigenvalue analysis developed to estimate the finest length scale. Application to laminar premixed flames in hydrogen-air flames reveals that the finest length scale is on the order of 10^{-4} cm for combustion at atmospheric pressure. Resolution at this scale is shown to be necessary to capture detailed species mass fraction profiles; other features such as steady flame speeds and equilibrium thermochemical properties do not have such a stringent length scale requirement.

AMS subject classifications: 65, 76, 80

Key words: Length scales, premixed flames, detailed kinetics.

1 Introduction

Here we will employ a few basic numerical strategies to develop reliable tools which can give estimates of the grid size necessary for a mathematically verified calculation of reacting flows. The estimates are developed for a simple configuration: a one-dimensional steady laminar flame. Indeed, it may come as a surprise that such straightforward tools as grid convergence studies of laminar flames have not been highlighted in the literature.

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But that is in fact the *status quo*, and the absence of such studies, coupled with the ultimate need for accurate reacting flow calculations for more complex scenarios, justifies the straightforward exercise presented here.

There is some ambiguity in the combustion literature about what constitutes a resolved solution. Many consider a calculation to be resolved if certain global or derived quantities, such as steady flame speed, are insensitive to grid size. Indeed, these are necessary conditions. However, as discussed by Roache [1], convergence of only global quantities is not a sufficient indicator of a fully resolved solution, and taken alone can lead to incorrect conclusions. While a derived quantity may be a function of all dependent variables, it may be insensitive to errors in some of them. Which variables they are insensitive to is problem-dependent, and impossible to determine *a priori*. In the context of a combustion problem, the fact that one may be using a grid which captures the correct flame speed offers no guarantee that species mass fractions have been accurately predicted.

Here, we follow Roache [1] and adopt the more rigorous characterization of a resolved solution as one in which *all dependent variables throughout the domain* are insensitive to changes in discretization size. This more demanding characterization is fully consistent with standard notions found in the broader mathematical and scientific computing literature, cf. [2–6]. The exercise of demonstrating the harmony of the discrete solution with the foundational mathematics is known as verification [7]. Neglecting this issue can give rise to solutions whose macro-behavior depends on the size of the grid and the algorithm that has been used to solve the mathematical model.

For multi-scale problems, verification is difficult due to the range of the scales, which may span many orders of magnitude. Nonlinearity can induce significant coupling across the scales so that errors at small scales can rapidly cascade to the large scales. Moreover, the strength of the coupling across the scales is not known *a priori*. So, all the physical scales of the mathematical model have to be captured in order to have full confidence that predictions are repeatable, grid-independent, and thus verifiable. The main aim of this paper is to estimate the required spatial resolution to capture all physical scales in a standard multi-scale problem: the steady one-dimensional laminar premixed flame propagating freely at atmospheric pressure in a stoichiometric mixture of hydrogen-air described by detailed kinetics and multi-component transport.

In a complementary study, two of the authors [8] gave a robust method to provide an accurate determination of the finest length scale in the reaction zone of a Chapman-Jouguet detonation based on spatial eigenvalue analysis. It was concluded that the required spatial discretization for detonations in hydrogen-air mixtures initially at atmospheric pressure is $\sim 10^{-4}$ cm. Here, the method employed in [8] to calculate the length scales for gas phase detonation is implemented with modification for deflagration. The method is reliable in that it has little dependence on the details of the underlying numerical method used to calculate the laminar flame. It simply requires a local determination of the state of the system. As such, it is able to estimate accurately the length scales using a fundamental mathematical approach. Lastly, the present study extends some of our