Modified three-step chemical model for the critical height for detonation propagation

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The numerical simulation of detonations is a powerful tool to analyze the flow field in detail. However, to date, these provide mostly qualitative insight and lack predictive capabilities. Previous studies [1, 2] have shown that while simplified one-step and three-step chain-branching schemes fitted using conventional methods fail to reproduce limiting behaviors (i.e., quenching), detailed chemistry showed good agreement with experimentally reported limits [1]. However, their high computational cost make large scale three-dimensional simulations and extensive parametric studies inaccessible. An interesting approach was proposed in [3] in which $D_n - \kappa$ curves were used as a fitting target in order to improve the predictive nature of simplified schemes. Results thus far are encouraging [3] and show a significant improvement over previous work dealing with the prediction of the critical reactive layer height required for sustained detonation propagation under yielding confinement.

In the present work, we are concerned with the modified three-step model first introduced by Taileb et al. [4] that retains the features of the scheme proposed by Dold & Kapila [5], once again, in a effort to develop predictive simplified kinetics schemes. In [4], molecular weight and specific heat ratio changes were taken into account and the reaction rate was modified by calibrating the free parameters of the scheme to match the entire thermicity profile with that obtained using detailed chemistry. In addition to the above modifications, here, the dependency of the local density in the initiation reaction, as well as that of the square of the local pressure in the termination reaction were included. The latter changes to the reaction rates, allowed to reproduce the correct reaction rate dependence on the initial pressure. Next, the modified three-step chain-branching scheme will be tested on the critical reactive layer height problem, and hope to present our results to the community as a work-in-progress poster.

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