Reduced kinetic model for the explosive ignition of hydrazine vapor

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The ignition delay time is one of the most important parameter to be considered in detonation ignition, as well as in the deflagration – detonation transition process. Therefore the knowledge of the ignition delays in a hydrazine vapor detonation wave is of crucial importance.

A detailed kinetic model for explosive decomposition of gaseous hydrazine has been built with the most recent kinetic data available, in order to calculate the ignition delays. It consists of 33 reversible reactions and 13 chemical species.

In the Zeldovich, von Neumann, Döring detonation model, the ignition delay represents the lapse of time separating the shock front and the reaction zone. It is defined here, among other definitions leading to the same computational results, in terms of the temperature history of the reactive mixture. Von Neumann parameters are used as the initial conditions in the chemical kinetic model to obtain its value. It is important to note that the ignition delay τ_i is directly related to the induction length Δ_i.

As in most gaseous systems, the detonation cell size λ_i for N_2H_4 vapor is related to the induction length as $\lambda_i = A\ \Delta_i$. Knowing the experimental detonation cell size for pure hydrazine at different initial temperatures and pressures, the average value of the proportionality factor A is found to be 27.5 ± 3.0. However this result does not take into account the influence of pressure-dependant reactions given in the kinetic model nor the N_2H_4 collision efficiency. Considering the last one is of the order of 2 to 3 relative to N_2, a new hydrazine average proportionality factor has been determined to be 80 ± 9. Based on this value and on the computations of Δ_i, it is therefore possible to predict the cell size for any pure N_2H_4 or N_2H_4/ N_2 mixtures.

In a round tube, the detonability limits can be estimated, since a self-sustained detonation cannot propagate in a tube if the cell size λ is larger than πd, where d is the tube diameter. Knowing the detonation cell size for N_2H_4, it is thus possible to predict its detonability limits.

The detailed kinetic model has been reduced for implementation in numerical codes dealing with the simulations of reactive flows. Sensitivity analysis have been performed in order to identify the most important reactions for hydrazine vapor detonation. As a result, the ignition delay and the hydrazine concentration profile are well reproduced with a reduced kinetic model composed of 10 equilibrated reactions (i.e. 20 reactions) and 9 chemical species. However, using this reduced model, the pressure, temperature and concentration of the main products (N_2, H_2, NH_3) at equilibrium are not correctly predicted.

In order to overcome this difficulty, another reduction technique has been used, based on the code KINALC coupled to the Principal Component Analysis of matrix F (PCAF) method. This procedure is a relatively simple and effective tool for finding efficiently the important reactions to be considered in the reduced mechanism. Finally, it leads to a reduced kinetic model of 26 reactions (instead of 66 reactions in the full mechanism) and 11 species. A good agreement is obtained between the full model and this reduced one.