Detonation Cell Sizes from Detailed Chemical Kinetic Calculations

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Abstract

A correlation between calculated from detailed chemical kinetic models characteristic reaction zone widths and experimentally measured or numerically simulated detonation cell sizes is analyzed. An approach is proposed to generalize such a correlation, taking into account multidimensional structure of real detonations. It is based on the characteristic reaction zone width δ calculated at initial conditions representative for a multidimensional detonation wave. The ratio A of the detonation cell size λ to characteristic reaction zone width δ is considered to be a function of two stability parameters (reduced effective activation energy and heat release). The generalization of the λ/δ-correlation is evaluated against experimental data and results of multidimensional calculations. An analytical expression is suggested to describe the dependence of A-constant on the stability parameters.

Introduction

The detonation cell size is commonly used to measure detonation sensitivity or detonability. For this reason, the subject of many studies was assessment of the cell sizes of different mixtures using both measurements and theoretical models. Attempts have been made to relate δ to λ using detailed chemical reaction mechanisms. Detailed ZND analyses were made by Westbrook, Urtiew, Moen et al., Shepherd, Kumar, Tieszen, et al, Stamps, et al., and Ciccarelli, et al. [1-6]. Calculations were for H_2 and C_nH_n fuels mixed with O_2 and diluted with N_2, H_2O, Ar, He, and CO_2. The results have shown that the ZND model captures qualitatively the effects of mixture composition, temperature, and pressure on cell size provided that a suitable choice is made for the constant A which relates the calculated reaction zone width to the measured cell size. However, it appears to depend on the mixture composition and initial conditions, and varies in the range of about 10^2.

In the present work, a correlation between calculated from detailed chemical kinetic models characteristic reaction zone widths and experimentally measured or numerically simulated detonation cell sizes is further analyzed. The objective is to develop a model for estimation of the detonation cell size on the basis of detailed chemical kinetic calculations.

Generalization of λ/δ - correlation

The main limitation of the ZND models was found to be due to the difference in reaction conditions in 1D and multi-D detonations. It was suggested, also, that parameters which influence that influence stability of the wave and regularity of the cellular structure and can be of much importance for the cell size estimation. Reduced activation energy and heat release represented by E_a/RT_{ps} and T_{vn}/T_0 were chosen as main stability parameters. A simple model was proposed to generalize λ/δ - correlation. It is based on δ calculated for representative range of reaction conditions in multi-D detonations. Reduced activation energy E_a/RT_{ps} was defined as an average parameter describing sensitivity of the reaction time to the shock strength. Calculations of characteristic reaction zone times were made using CHEMKIN-II code [8] with chemical model of Shepherd [1].

A simplified approach may be suggested to take into account reaction conditions in multidimensional detonations. The effective initial conditions for chemical reaction can be characterized approximately by the state behind the shock with velocity ranging from $1.0D_{cj}$ to $1.6D_{cj}$. This is rather wide range that should cover most of the possible reaction conditions in multidimensional detonations. Different parts of reactants proceed through different sequences of states in a multidimensional detonation wave. This means that it should be a range of characteristic chemical times and corresponding chemical length scales. The problem is to define effective average values which correlate with the detonation cell size. The comparison was made using average values of δ and E_a calculated over different ranges of shock speeds ($D_1 \div D_2$). The best correlation between the experimental cell

sizes and calculated reaction zone widths was found for the following set of parameters (D_1/D_{cj}=1.0 and D_2/D_{cj}=1.6) which represents the widest range of conditions (compare Fig. 1 and Fig. 2).

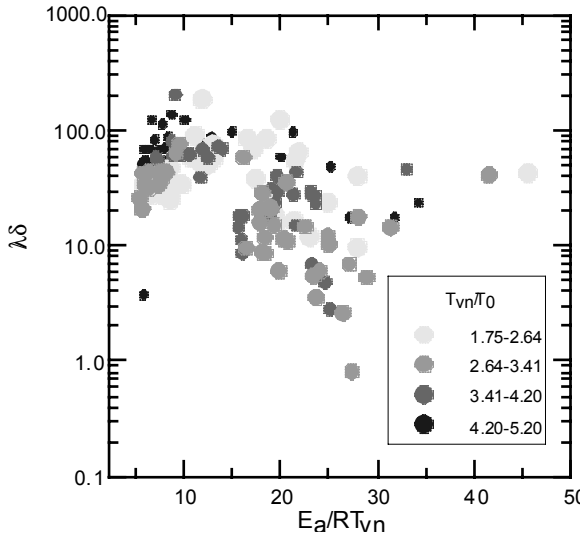

Figure 1. Ratio of λ/δ (von Neumann state initial conditions) as a function of E_a/RT_{vn} and T_{vn}/T_0 for hydrogen-air-steam mixtures at different initial temperatures and pressures.

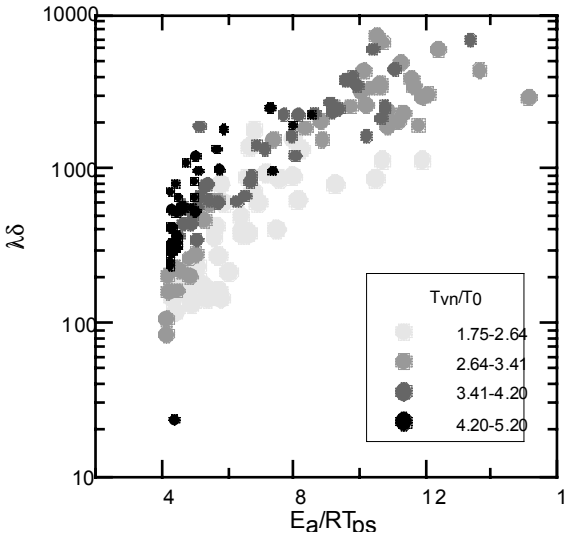

Figure 2. Ratio of λ/δ as a function of E_a/RT_{ps} and T_{vn}/T_0 for hydrogen-air-steam mixtures at different initial temperatures and pressures. Calculations of δ and E_a/RT_{ps} using representative reaction conditions in multidimensional detonations.

The generalization of λ/δ - correlation was evaluated against experimental data. The data were chosen for systems which give the widest possible range of the parameters E_a/RT_{ps}, T_{vn}/T_0. Experimental data were taken for hydrogen hydrogen-air mixtures, hydrogen-air-steam mixtures, H_2/O_2 diluted with Ar and CH_4/O_2 C_2H_4/O_2 C_2H_6/O_2 diluted with Ar and N_2. The range of stability parameters for these systems is shown in Fig. 3.

The ratio of λ/δ was shown to be a function of E_a/RT_{ps} and T_{vn}/T_0 within the accuracy of the experimental data (see Fig. 5). An analytical expression for $\lambda/\delta(E_a/RT_{ps}, T_{vn}/T_0)$ was suggested in the range of $E_a/RT_{ps} = 3 \div 16$, and $T_{vn}/T_0 = 1.5 \div 8$. Mean deviation of the calculated values from experimental data was about 50%. A detailed comparison of the estimated values of cell sizes with experimental data for hydrogen mixtures is presented in Fig. 4. It was found that the model gives reliable estimates of the cell sizes for lean mixtures with and without steam. This was usually a problem for the standard ZND calculations [1, 6]. The effects of elevated temperature and steam dilution are described with good accuracy. The effect of initial pressure is accounted as well.

It was found out that hydrogen and hydrocarbon fuels, systems with different regularity of the cellular structure (Ar and N_2 -dilutants), ordinary and marginal detonations show the same quality of correlation. The estimates for λ, however, should be treated carefully outside the range of variables, where the λ/δ-function was defined. Limitations of CHEMKIN-II code should be also taken into account. It was shown, also, that the function for *A*-constant determined in the frame of the present model works equally good for both computed (from multidimensional simulations) and experimental cell sizes. This may be an argument in favor of the physical assumptions which were chosen in the model.

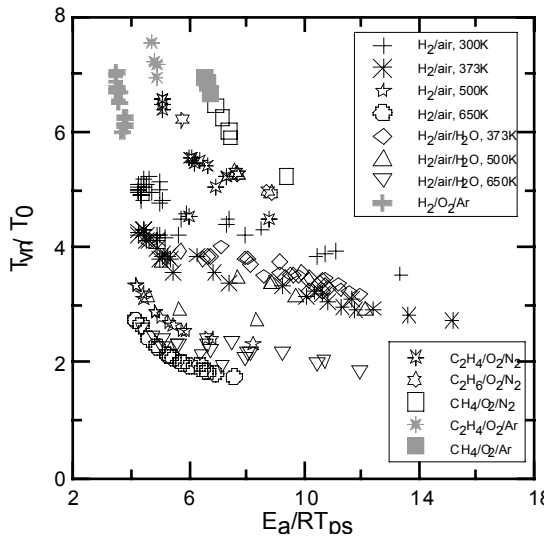

Figure 3. Stability parameters Ea/RTps and Tvn/T0 for different combustible mixtures used in approximation of λ/δ(Ea/RTps, Tvn/T0) function.

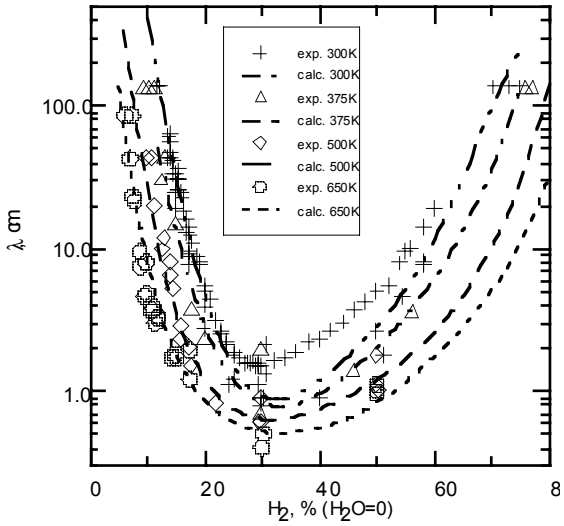

Figure 4. Cell width versus hydrogen concentration at different initial temperatures for hydrogen-air mixtures without steam. Experimental data and calculations.

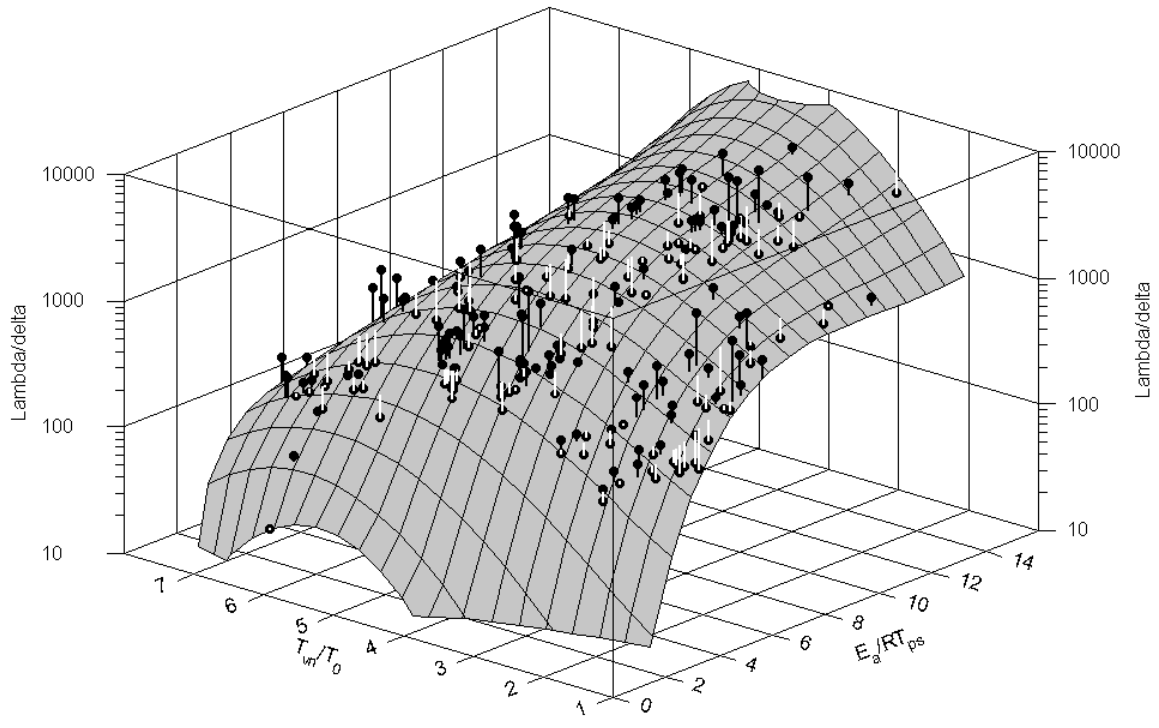

Figure 5. Ratio of λ/δ as a function of Ea/RTps and Tvn/T0. Points are the ratio of experimental cell sizes λ to calculated reaction zone width δ. Surface shows analytical function given by Equation. Black point bars are given for points above the surface, white bars for points below the surface.

An important observation was made concerning the values of effective activation energy. The effective values determined in the frame of the present model appear to be significantly smaller than those calculated using von Neumann initial conditions. This means that the effective temperature sensitivity of reaction time in multidimensional detonations is not as strong as it follows from parameters typical for 1D detonation models. Non-Arrhenius temperature dependence of characteristic reaction time (given by detailed chemistry) is responsible for this difference. Effective activation energy decreases with the increase of initial reaction temperature, at least for the considered types of mixtures. Such a behavior of effective activation energy appeared to be important in the λ/δ correlation. In the model presented here, this behavior was taken into account by choosing representative reaction conditions for multidimensional detonations. Being important for the cellular structure, the changes of effective activation energy over the range of reaction conditions may play a role in dynamic behavior of detonations, as well. Corresponding numerical simulations with simplified reaction models should be more adequate, probably, if such a behavior will be taken into account.

References

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