Revision of the Detonation Cell Sizes from Detailed Chemical Kinetic Calculations Prediction Model

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The detonation cell size (λ) 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 reaction zone width (δ) to λ using detailed chemical reaction mechanisms. A correlation between calculated from detailed chemical kinetic models characteristic reaction zone widths and experimentally measured or numerically simulated detonation cell sizes was analyzed in a previous work of authors. An approach was proposed to generalize such a correlation, taking into account multidimensional structure of real detonations. It was based on the characteristic reaction zone width 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 was considered to be a function of two stability parameters (dimensionless effective activation energy and parameter describing the relation between chemical energy and initial thermal energy of the combustible mixture). The generalization of the λ/δ correlation was evaluated against experimental data and results of multidimensional calculations. An analytical expression was suggested to describe the dependence of A-constant on the stability parameters. This gives a basis for prediction of the detonation cell sizes from the detailed chemical kinetic calculations in a wide range of mixture compositions and initial conditions. During past years a number of new detailed chemical kinetic schemes are available. Revision of a model was done using new kinetic schemes and range of experimental data used for correlation was widely extended, especially for hydrocarbon containing mixtures. Detailed comparison of the modeled detonation cell size λ and experimentally measured cell size for different types of fuels in a wide range of initial conditions is presented in a work. Analyses and selection of the most suitable detailed chemical kinetic schemes for the presented model is done.