APPROXIMATE METHOD OF CALCULATION OF CHEMICALLY REACTING GAS MIXTURES OF DETONATION PRODUCTS

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Abstract: Based on the assumption of the existence of the partial chemical equilibrium in the detonation products, an approximate method for calculating composition of the detonation products is developed. The method uses the assumption of the existence of extremum of Helmholtz free energy for a given density, temperature, and molecular weight of the detonation products mixture. Without significant loss of accuracy to the solution of stiff differential equations, a detailed kinetic mechanism can be replaced by one differential equation and a system of algebraic equations. This method is always consistent with the detailed mechanism and can be used separately or in conjunction with the solution of a stiff system, replacing it when bimolecular reactions are near equilibrium.

Keywords: chemical kinetics; chemical equilibrium; products of explosion; numerical modeling of gas-dynamic problems in chemically reacting flow; stiff system

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