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论文

碳氢燃料点火燃烧的简化化学反应动力学模型

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摘要 基于``准稳态''方法建立了一套复杂化学反应动力学模型简化方法和相应的软件SPARCK. 并以3种典型的碳氢燃料------甲烷、乙烯和庚烷为研究对象，从甲烷点火燃烧的GRI2.11详细基元反应动力学模型出发简化得出了包含14个组分10步总包反应形式的简化化学反应动力学模型，从乙烯燃烧的51组分365详细基元反应模型出发简化得出了包含20个组分16 步总包反应形式的简化化学反应动力学模型，从庚烷点火燃烧的160组分1540详细基元反应模型出发简化得出了包含26个组分22步总包反应形式的简化化学反应动力学模型. 通过对典型激波管试验的结果对比可以看出：得到的简化反应动力学模型能较为有效地再现详细基元反应模型的反应机理，具有较高的计算精度. 在工程计算中有较好的应用前景.

关键词 简化化学反应动力学模型 `准稳态"假设方法 碳氢燃料 点火延时 甲烷 乙烯 庚烷

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Development of reduced chemical reaction kinetic model for hydro-carbon fuel combustion

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Abstract

A method based on quasi-steady state approximation (QSSA) is used to construct a reduced chemical kinetic model for the ignition and combustion of Hydro-carbon fuel, and a software package named SPARCK (Software Package for Reduction of Chemical Kinetics) is developed. Firstly, this method and software is applied to reduce the detailed elementary chemical kinetic model GRI2.11 for the combustion of methane, and a reduced global reaction kinetic model containing 14 species and 10 global reactions is obtained. Secondly, when this method and software is applied to the detailed elementary chemical kinetic model of ethylene combustion which containing 51 species and 365 elementary reactions, a reduced global reaction kinetic model involving 20 species and 16 global reactions can be obtained. Finally, for the combustion of heptane, a reduced global reaction kinetic model involving 26 species and 22 global reactions is obtained from a detailed mechanism having 160 species and 1540 elementary reactions by this method. After using these reduced kinetic models to numerically simulate the typical fuel ignition process in the shock tube, it can be seen that these reduced models can represent the ignition mechanism of the detailed kinetic models quite well and with good accuracies.

Key words reduced chemical kinetic model quasi-steady state approximation hydro-carbon fuel ignition delay methane ethylene heptane

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