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A simplification of pyrolytic reaction model of hydrocarbon fuel and its application in simulation of heated channel flow

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ABSTRACT

The pyrolytic reaction model plays an important role in studying heat and mass transfer of heated channel flow with pyrolysis because of the influence of pyrolysis on mass and energy balance. So, focusing on the application of pyrolysis reaction model of hydrocarbon fuel in simulation, an approach to simplify the pyrolytic reaction model of hydrocarbon fuel was proposed to reduce the computational workload of simulation. The basic idea of simplification lies in the fact that species with similar critical properties have similar thermophysical properties, and they could be represented as single specie based on corresponding states principle (CSP), so the number of specie equations in the numerical model was significantly reduced according to combining species in products. Numerical tests indicate that the relative difference, caused by simplification, is within 1%. In addition, the species equations are decreased from 18 to 10 and the computational efficiency is doubled. Therefore, this simplification could serve as an effective way for pyrolytic reaction model of hydrocarbon fuel in terms of model accuracy and efficiency.

1. Introduction

The regenerative cooling technology by using endothermic hydrocarbon fuel on board has been considered to be an effective solution for thermal protection of scramjet [1–4]. The endothermic hydrocarbon fuels flows through parallel channel (hydraulic diameter 1–2 mm) of cooling panels designed outside of combustor and is used for cooling before combustion [5–9]. The hydrocarbon fuel begins to pyrolyze with the temperature of fuel increasing up to temperature, typically > 500 °C [2], so, a much higher heat absorption rate is obtained through a series of endothermic reactions. However, the heat and mass transfer in cooling channel is different from that in the convective heat transfer without chemical reaction because of the influence of pyrolysis on mass and energy balance [10–13]. So, in order to guide the design of cooling panel, the heat and mass transfer in heated flow with pyrolysis attract significant research interests [14–17].

In order to predict transformations of mass and energy in reaction, it is of great significance to establish an appropriate pyrolytic reaction model. Since the pyrolysis is complicated, generally, reaction model is simplified according to eliminate the redundant species and reactions based on the chemical reaction kinetics. For example, Sheu et al. [18] developed a three-step global model to predict the pyrolysis of Norpar-13. Jiang et al. [19] investigated experimentally the flow and heat-transfer behavior of thermal cracking n-decane and proposed a global pyrolysis model with 18-species for conversion less than 13%. Ward et al. [20] proposed proportional product distribution chemical model (PPD) and developed a one-step global model, containing 18 species in products. Meng et al. [21] proposed a PPD model with 12-species based

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Nomenclature

A	pre-exponential factors, s^{-1}
C	mole concentration of species, mol m^{-3}
D	diameter, m
$\boldsymbol{F,G}$	vector of convective flux
L	length of channel, m
N	mole fraction
$\boldsymbol{Q}$	primitive variables, $\mathbf{Q} = [P \ u \ \upsilon \ T \ Y_1 \ \cdots \ Y_{n-1}]$
S	source term $\mathbf{S} = [0 \ 0 \ 0 \ 0 \ M_1\dot{\omega}_1 \ \cdots \ M_{n-1}\dot{\omega}_{n-1}]$
T	time, s
$\boldsymbol{U}$	velocity vector, m s^{-1}
Y	mass fraction of species
x,y	two coordinate directions of Cartesian coordinate system
a,b	coefficients of EoS
C_p	Constant pressure specific heat, J kg^{-1} K^{-1}
E	activation energy, kJ mol^{-1}
k_f	rate constant, s^{-1}
M	molecular weight, kg/mol
P	pressure, Pa
R_o	universal gas constant, 8.3145 J mol^{-1} K^{-1}
$\boldsymbol{s}$	surface normal vector, m^2
T	temperature, K
V	molar volume, m^3 mol^{-1}
u, υ	x-component and y-component of velocity, m s^{-1}
r	radius, m

Greek

P	density, kg m^{-3}
$\dot{\omega}$	reaction rate, mol s^{-1} m^{-3}
α,δ_1, δ_2	coefficients of EoS
μ	dynamic viscosity, Pa·s
κ	empirical parameter of binary interaction
Γ	preconditioning matrix
ω	acentric factor
ν	specific volume, m^3 kg^{-1}
λ	thermal conductivity, W $m^{-1}K^{-1}$
Φ	physical quantities

Subscripts

In	inlet
c	critical property
v	viscosity
i,j	species
u, υ	x-component and y-component of physical quantity
R	reactant
M	mixture

on the Ward's work. Since specie equations are employed to describe the mass conservation of components in flow field, it can be seen from above reaction model that many species equations are still included in simulation.

In this paper, focusing on the application of pyrolytic reaction model of hydrocarbon fuel in simulation, a simplification was developed reduce the computational workload of simulation and efficiently implemented to the numerical study of heat and mass transfer in heated channel flow. Unlike the simplification on the base of chemical reaction kinetics, the present simplification is based upon corresponding states principle (CSP) and reduces the number of components in products while the model accuracy is still maintained. As a result, the number of species equations in governing equations is significantly reduced and the computational time for the simulation is decreased.

2. Simplification of pyrolysis reaction model

2.1. Pyrolysis reaction model

The hydrocarbon fuel is actually a complicated mixture with hundreds of hydrocarbon species, so, n-alkanes were selected in previous studies instead of mixture [20,21]. The PPD model of n-decane, proposed by Ward et al., was used as study object and baseline in present analysis [20]. The PPD model is validated to be able to predict the chemical compositions of mild pyrolysis of n-decane at a pressure range, 3.45–11.38 MPa [20]. The overall reaction model could express as follow:

$$\begin{aligned} C_{10}H_{22} \Rightarrow \ & 0.151H_2 + 0.143CH_4 + 0.256C_2H_4 + 0.126C_2H_6 + 0.230C_3H_6 \\ & + 0.180C_3H_8 \\ & + 0.196C_4H_8 + 0.102C_4H_{10} + 0.171C_5H_{10} + 0.124C_5H_{12} \\ & + 0.195C_6H_{12} + \\ & 0.089C_6H_{14} + 0.169C_7H_{14} + 0.072C_7H_{16} + 0.152C_8H_{16} \\ & + 0.012C_8H_{18} + \\ & 0.053C_9H_{18} + 0.003C_9H_{20} \end{aligned} \tag{1}$$

The reaction rate of reactant could be expressed as:

$$\dot{\omega}_R = \frac{dC_R}{dt} = -k_f C_R \tag{2}$$

where

$$k_f = A \exp\left(-\frac{E}{R_0 T}\right)$$

where $A = 1.6 \times 10^{15}$ s^{-1}, $E = 263.7$ kJ/mol.

2.2. Simplification

Based on the law of corresponding states, the equilibrium properties, depending on certain intermolecular forces, are related to the critical properties in a universal way [22]. So, the species with such similar critical properties as critical temperature (T_c), critical pressure (P_c), specific volume (V_c), etc. have the similar thermophysical properties. Therefore, the basic idea of simplification lay in the fact that some species with similar critical properties have similar thermophysical properties, and can be represented as single specie based on CSP.

As shown in Table 1, it can be seen by comparing critical properties of species in PPD model that the two species with same carbon number have the similar critical properties. Therefore, as shown in Fig. 1, the two species with same carbon number were grouped together by mixing rules based on CSP and represented by single species. As a result, a simplified global pyrolysis reaction model with fewer species was built for simulation. The mixing rules for equation of state (EoS) are shown as follow [23]:

$$M_m = \sum_i n_i M_i \tag{3}$$

$$a\alpha = \sum_{i=1} \sum_{j=1} n_i n_j a_{ij} \alpha_{ij} \tag{4}$$

$$a_{ij}\alpha_{ij} = \sqrt{a_i a_j \alpha_i \alpha_j}(1 - \kappa_{ij}) \tag{5}$$

$$b = \sum_{i=1} n_i b_i \tag{6}$$