Simulation of CF_4 Abatement via a Direct-Current Non-transferred Nitrogen Torch

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ABSTRACT

This paper proposes a numerical modeling to predict the abatement process of green-house gas in a reaction chamber via a non-transferred, direct-current torch, where the magneto-hydrodynamic equations, i.e., the continuity, momentum, energy and current continuity equations together with turbulence transport equations are solved with a parallelized finite volume approach. The thermal plasma is assumed in local thermal equilibrium, and a kinetics model is adopted to consider the transport phenomena as well as the chemical reactions of various species arising in the decomposition process. The proposed numerical model is capable of delivering a quantitative prediction of the destruction and removal rate at various operation conditions.

1. Introduction

In the proposed approach, a direct-current thermal plasma flow subjected to an applied electric and a self-induced magnetic field is described by a steady magnetohydrodynamic model, where the continuity, momentum and energy equations incorporated with a turbulence model are solved to predict the flow characteristics of the plasma jet. The plasma flow is under the assumption of being electrically neutral, optically thin and in local thermal equilibrium (LTE) [1]. The operation focus on the average performance of the plasma torch leads to the expropriation of a time-averaged approach. Here, only the azimuthal magnetic field contributed by the electric arc present inside the torch is considered.

2. Method

The steady form of the continuity equation for the thermal plasma flow is expressed as

$$\nabla \cdot (\rho \mathbf{U}) = 0, \tag{1}$$

where ρ denotes the density and $\mathbf{U}$ the velocity vector. The steady form of the momentum equation for the thermal plasma flow is given as

$$\mathbf{U} \cdot (\nabla \rho \mathbf{U}) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{U}) + \rho \mathbf{f} + \mathbf{j} \times \mathbf{B}, \tag{2}$$

where p represents the pressure, μ the apparent viscosity ($=\mu_m+\mu_t$), μ_m the fluid viscosity, μ_t the turbulent viscosity, f the gravitational force, $\mathbf{j}$ the current density and $\mathbf{B}$ the induced magnetic field. The steady form of the energy conservation for the thermal plasma flow is shown as

$$\mathbf{U} \cdot \nabla(\rho c_p T) = \nabla \cdot (\kappa \nabla T) + \mathbf{U} \cdot \nabla p + \mathbf{j} \cdot \mathbf{E} + \frac{5k_B}{2e}(\mathbf{j} \cdot \nabla T) - E_R + \mu|\dot{\boldsymbol{\gamma}}|^2, \tag{3}$$

where c_p is the specific heat, T the gas temperature, κ the apparent thermal conductivity ($=\kappa_m+\kappa_t$), κ_m the thermal conductivity, κ_t the turbulent thermal conductivity, $\mathbf{E}$ the electric field, k_B the Boltzmann constant, e the charge carried by an electron, E_R the radiation loss and the magnitude of shear rate $|\dot{\boldsymbol{\gamma}}|$. The steady form of the current conservation for the thermal plasma flow is described as

$$\nabla \cdot (\sigma \nabla \phi) = 0, \tag{4}$$

where σ stands for the electric conductivity and ϕ the electric potential. The electric field $\mathbf{E}$ is further determined from $-\nabla\phi$, the current density j is defined by $\sigma\mathbf{E}$ and the induced magnetic field B is defined by $\nabla\times\mathbf{A}$, where the vector $\mathbf{A}$ is solved from the Poisson equation $\nabla^2\mathbf{A} = \mu_0\mathbf{j}$ and μ_0 is the magnetic permeability. The steady form of the $k-\varepsilon$ turbulence model to calculate the turbulent kinetic energy k and its dissipation rate ε is denoted as

$$\nabla \cdot (\rho \mathbf{U} k) = G - \rho\varepsilon + \nabla \cdot \left[\left(\mu_m + \frac{\mu_t}{c_k}\right)\nabla k\right], \tag{5}$$

$$\nabla \cdot (\rho \mathbf{U} \varepsilon) = \frac{\varepsilon}{k}(c_1 G - c_2 \rho\varepsilon) + \nabla \cdot \left[\left(\mu_m + \frac{\mu_t}{c_\varepsilon}\right)\nabla \varepsilon\right], \tag{6}$$

where G is the production of turbulent kinetic energy based on a revised model [2], ($c_\mu, c_k, c_\varepsilon, c_1, c_2, c_t$) the constants of the standard $k-\varepsilon$ turbulence model, μ_t the turbulent viscosity and k_t the turbulent thermal conductivity. The steady form of the transport equations of electron and ions are employed to describe the transport of charged particles with a drift-diffusion approximation.

$$\nabla \cdot (n_e \mathbf{U}) + \nabla \cdot \boldsymbol{\Gamma}_e = R_{e,p} - R_{e,c}, \tag{7}$$

$$\nabla \cdot (n_i \mathbf{U}) + \nabla \cdot \boldsymbol{\Gamma}_i = R_{i,p} - R_{i,c}, \tag{8}$$

where n_e states the electron density, n_i the ion density, R_e the source term of electron and R_i the source term of ions. The production and consumption of charged species are distinguished by the subscripts p and c appearing in their source term. The electron flux $\boldsymbol{\Gamma}_e$, as well as the ion flux $\boldsymbol{\Gamma}_i$, is defined as

$$\boldsymbol{\Gamma}_e = -D_e \nabla n_e - \mu_e n_e \mathbf{E}, \tag{9}$$

$$\boldsymbol{\Gamma}_i = -D_i \nabla n_i + \mu_i n_i \mathbf{E}, \tag{10}$$

where D_e denotes the diffusion coefficient of electron, D_i the diffusion coefficient of ions, μ_e the electron mobility and μ_i the ion mobility. The steady form of the transport equation for neutral species is shown as

$$\nabla \cdot (n_i \mathbf{U}) + \nabla \cdot \boldsymbol{\Gamma}_i = R_{i,p} - R_{i,c}, \tag{11}$$

where n_i and R_i denote the density and source term of the neutral species i, respectively. The flux $\boldsymbol{\Gamma}_i$ of the neutral species i is stated as

$$\boldsymbol{\Gamma}_i = -D_i \nabla n_i, \tag{12}$$

where D_i denotes the diffusion coefficient of the neutral species i.

An axisymmetric flow assumption with nontrivial

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azimuthal component is adopted in this approach. The aforementioned governing equations are then written in the form of a cylindrical coordinate system (z,r,θ), where the axial velocity u in the z direction, the radial velocity v in the r direction and the azimuthal velocity w in the θ direction represent the three components of the velocity **U**. The binary mixing theory [3] and Langevin approach [4] is employed to estimate the diffusion coefficient of the neutral species and charged particles, respectively.

The aforementioned governing equations through a finite volume discretization are transformed into an integral form for the control volumes in space. The linearized system of equations is solved by a SIP solver to determine field variables. The decomposition modeling is divided into two modeling steps. The plasma flow is first predicted to deliver the required flow characteristics before solving the following kinetic model of chemical reactions. Cartesian grids due to its computational efficiency and stability are adopted to discretize the computational domain. The aforementioned numerical scheme is implemented in an in-house code PTCAX, which utilizes a linear domain decomposition scheme to parallelize the flow computation on a Cartesian grid via the MPI library [2].

3. Results and Discussion

The nitrogen plasma torch is designed with a length (L_T) of 140 mm and an inner radius (r_i) of 12 mm, whereas 6 mm is employed for the diameter of both electrode spots. The reaction chamber connected to the plasma torch is measured with a length of 619 mm together with an inner diameter 50 mm. The inlet sizes of the of working gas and the processing gas are measured 12.5 mm and 7.8 mm, respectively. The carbon tetrafluoride is presumed well premixed with nitrogen and water vaper before the processing gas is injected into the hollow troch. The center of the cathode spot is located at the torch axis. A flowrate of 400 L/min nitrogen is employed to operate the gas abatement system. One fourth of the working gas is used in the plasma torch to sustain the non-transferred, DC arc, whereas the rest is adopted to carry the green-house gas, CF_4 into the reaction chamber to interact with the high-temperature thermal plasma ejecting from the upstream plasma torch. The average voltage drops between two electrodes is measured 225 V with a working current of 80 A in a corresponding experiment.

The plasma temperature can be elevated over 1000 K within the tubular torch, except the locations close to the vicinity of the gas inlet. A small region near the cathode spot predicted with high temperature up to 11 kK is depicted close to the centerline. A minor temperature gradient without thermal concentration is found around the anode spot (z=133 mm, r=12 mm). Figure 1 depicts the temperature characteristics inside a direct-current, non-transferred, rod-type plasma torch with nitrogen as the plasma gas as well as the flow field feature inside its reaction chamber. The thermal plasma principally shows apparent temperature gradients in the radial direction from a high-temperature region mainly contributed by the Joule heating. In the reaction chamber, the cold processing gas vertically meets the hot plasma jet in the upstream region of the reaction chamber. An effective mixing of two gas streams leads to relatively uniform temperature distribution between 1000 K and 1300 K from z=300 mm. Fig. 2 compares the species densities at the outlet of the reaction chamber with CF_4 at 11800 PPM.

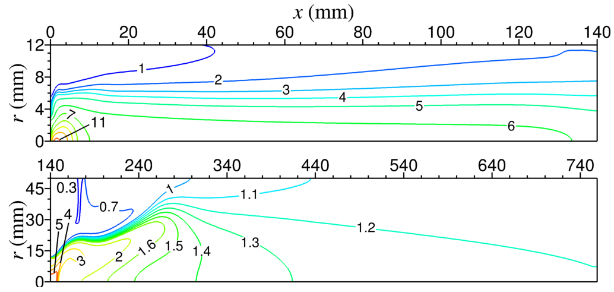

Fig. 1 Temperature distribution inside the plasma torch (upper) and the reaction chamber (lower), where the contour is expressed in kK.

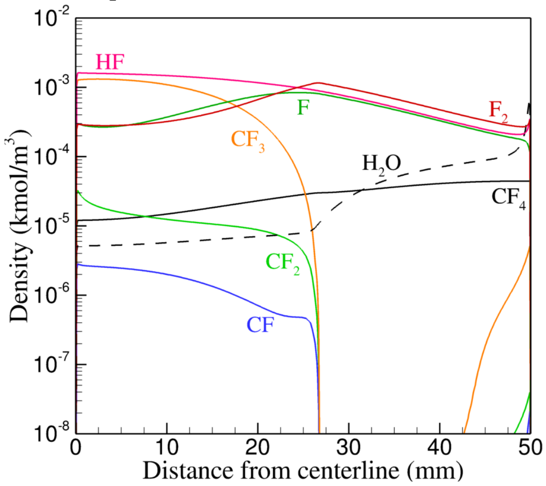

Fig. 2 Comparison of species densities at the outlet of the reaction chamber with CF_4 at 11800 PPM.

4. Concluding Remarks

This study proposes a steady and axisymmetric MHD model to predict the carbon tetrafluoride decomposition inside a reaction chamber, where a direct-current plasma torch operating with nitrogen is employed as its heat source. A finite volume approach is employed to discretize the governing equations of the proposed MHD flow model with the related kinetics model. The proposed model gives a favorable agreement with the corresponding experiment.

References

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