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Discretization of the Joule heating term for plasma discharge fluid models in unstructured meshes

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ABSTRACT

The fluid (continuum) approach is commonly used for simulation of plasma phenomena in electrical discharges at moderate to high pressures (>10's mTorr). The description comprises governing equations for charged and neutral species transport and energy equations for electrons and the heavy species, coupled to equations for the electromagnetic fields. The coupling of energy from the electrostatic field to the plasma species is modeled by the Joule heating term which appears in the electron and heavy species (ion) energy equations. Proper numerical discretization of this term is necessary for accurate description of discharge energetics; however, discretization of this term poses a special problem in the case of unstructured meshes owing to the arbitrary orientation of the faces enclosing each cell. We propose a method for the numerical discretization of the Joule heating term using a cell-centered finite volume approach on unstructured meshes with closed convex cells. The Joule heating term is computed by evaluating both the electric field and the species flux at the cell center. The dot product of these two vector quantities is computed to obtain the Joule heating source term. We compare two methods to evaluate the species flux at the cell center. One is based on reconstructing the fluxes at the cell centers from the fluxes at the face centers. The other recomputes the flux at the cell center using the common drift-diffusion approximation. The reconstructed flux scheme is the most stable method and yields reasonably accurate results on coarse meshes.

1. Introduction

Fluid (continuum) models have been used since the 1960s to simulate plasma discharge phenomena. Fluid models describe the transport of electrons, ions and neutral species using moments of the species Boltzmann equation coupled to electromagnetic field equations. These models provide spatial and temporal information on averaged properties such as species density and species temperature in discharges and the electromagnetic fields in the discharge. A wide variety of plasmas such as low-pressure glow discharges [1–3], radio-frequency plasma discharges [4–6], dielectric barrier discharges [7], microdischarges [8–11] and streamers [12] have been simulated using the fluid modeling framework.

A typical fluid model solves the following governing equations. The species continuity equation determines the individual species number densities (n_k) in the discharge as follows

$$\frac{\partial n_k}{\partial t} + \vec{\nabla} \cdot \vec{\Gamma}_k = \dot{G}_k, \tag{1}$$

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where, k represents the species index, $\vec{\Gamma}_k$ is the species drift-diffusion flux, and $\dot{G}_k$ is the gas-phase species generation rate through plasma chemical reactions. The self-consistent electric potential is determined using the electrostatic Poisson's equation

$$\nabla^2\phi + \frac{e}{\varepsilon_0}\sum_{k=1}^{K_g} Z_k n_k = 0, \tag{2}$$

where, ϕ is the potential, e is the unit electric charge, ε_0 is the permittivity of free space, K_g is the total number of gas species, and Z_k is the charge number of species k (e.g. -1 for electrons). Electron transport coefficients and the rate coefficients of electron impact reactions are a strong function of the electron energy distribution function which may be parameterized by a local electron temperature (T_e) [8–11]. In case the local fluid approximation is not used, fluid models include an electron energy equation to determine the electron energy density $\left(e_e = \frac{3}{2}k_B T_e n_e\right)$ in the discharge

$$\frac{\partial e_e}{\partial t} + \vec{\nabla}\cdot\left(\frac{5\vec{\Gamma}_e e_e}{3n_e}\right) - \vec{\nabla}\cdot(\eta_e\vec{\nabla}T_e) = -e\vec{E}\cdot\vec{\Gamma}_e - \frac{3}{2}k_B n_e\frac{2m_e}{m_{k_b}}(T_e - T_g)\bar{\nu}_{e,k_b} - e\sum_{j=1}^{I_g}\Delta E_j^e r_j, \tag{3}$$

where, η_e is the thermal conductivity of electrons, k_B is the Boltzmann's constant, m_e and m_{k_b} are the particle mass of electron and dominant background gas species, respectively, $\bar{\nu}_{e,k_b}$ is the electron momentum transfer collision frequency with the background gas, ΔE_j^e is the energy lost per electron (in eV units) in an inelastic collision event represented by a gas-phase reaction j, r_j is the rate of progress of a reaction j (in $\mathrm{m^{-3}\ s^{-1}}$ units), and I_g is the total number of gas-phase reactions. The electrostatic field is determined from the electrostatic potential as $\vec{E} = -\vec{\nabla}\phi$. Finally, the gas temperature (T_g) can be determined through the gas energy equation

$$\frac{\partial}{\partial t}\sum_h n_k h_{k,sens} + \vec{\nabla}\cdot\sum_h \vec{\Gamma}_k h_{k,sens} - \vec{\nabla}\cdot\left(\sum_h \eta_k\vec{\nabla}T_g\right) = -e\sum_h Z_k\vec{\Gamma}_k\vec{E} + \frac{3}{2}k_B n_e\frac{2m_e}{m_{k_b}}(T_e - T_g)\bar{\nu}_{e,k_b} - e\sum_{j=1}^{I_g}\Delta E_j^g r_j, \tag{4}$$

where, $h_{k,sens}$ is the sensible enthalpy of species k, η_k is the thermal conductivity of species k, ΔE_j^g is the energy lost from the thermal pool in an inelastic collision event represented by a gas reaction j, and the index h indicates the summation over all the heavy species. The above gas energy equation uses the constant pressure assumption and neglects fluid mechanical viscous dissipation.

The Joule heating source term, i.e. the first term on the RHS of (3) and (4), constitutes the main source term in the electron energy balance and often times for the gas energy equation. Since reaction rates due to electron impact are exponential functions of the electron temperature, small deviations in the electron energy density can result in significant changes in the predicted discharge characteristics. Most reaction rates also depend on the number density of the background gas, and therefore on the gas temperature. The accuracy of the method used to compute the Joule heating term in the energy balance equations is therefore critical. As shown in [13], the stability of the numerical scheme also depends on the technique used to compute the source term of the electron energy equation owing to temporal stiffness introduced by this term for several types of plasma discharge problems.

Complex two-dimensional or three-dimensional geometries are now commonly encountered in the modeling of plasma discharges. Local mesh refinement is often needed to capture the steep gradients in the number density and in the electric field profiles. To optimize mesh resolution, adaptive mesh techniques can be pursued [12]. For these reasons, the use of unstructured meshes is necessary, as it already is the case for computational fluid dynamics. Robust and accurate numerical methods to simulate gas discharges on unstructured meshes must therefore be developed. Several issues specific to the self-consistent simulations of plasma phenomena using a cell-centered finite-volume approach arise in the context of unstructured meshes, the treatment of the Joule heating term being one. Here we discuss a simple and accurate approach for the numerical treatment of this term in the context of a cell-centered finite-volume discretization of the plasma discharge governing equations on generalized unstructured meshes. The technique can be used on structured meshes as well, where it reduces to a simplified numerical stencil.

2. Numerical method

The governing equations (1)–(4) can be cast in an integral form, by integrating over an arbitrary control volume V as

$$\int_v \frac{\partial\alpha}{\partial t}dV + \int_{\partial V}\vec{\Gamma}_\alpha\cdot dS = \int_V S_\alpha dV, \tag{5}$$

where, α is the dependent variable (the species number densities n_k, the electrostatic potential ϕ, the electron energy densities e_e, or the gas temperature T_g), $\vec{\Gamma}_\alpha$ are the fluxes, and S_α are the source terms. In the cell-centered finite-volume scheme for a fixed non-moving mesh, the following spatial discretization is used to approximate (5)

$$V_{\mathrm{cell}}\frac{\partial\alpha_{cc}}{\partial t} + \sum_f \Gamma_{\alpha,fc}A_f = V_{\mathrm{cell}}S_{\alpha,cc}, \tag{6}$$