行政院國家科學委員會補助專題研究計畫簡易報告

噴射式大氣電漿源之模擬研究-2D 與-3D 平行化流體模型(一年)

Development and Applications of Parallellized 2D and 3D Fluid Modeling Codes for Atmospheric Pressure Plasma Jet (1 Years)

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中文摘要

　　噴射式大氣電漿源的特色為電漿可以從電極噴出，電漿面極小，能量集中，處理效率高，沒有 arcing 問題，應用效果是大氣電漿中最好的，在工業的應用包括局部清潔及處理用途。因此，對噴射式大氣電漿源(APPJ)有基礎的認識，在發展設備上是很重要的。在本研究計畫中我門計劃使用流體模式模擬噴射式大氣電漿，我門使用適於處理複雜幾何與計算平行化的有限元素法(FEM)離散求解 APPJ 的物理方程式。

　　在提出的三年計畫中，在第一階段中我們首先使用 Stabilized FEM 在 Fluid Modeling 的架構下發展一套程式用以模擬二維/軸對稱座標系統，Fluid Modeling 考慮帶電粒子的漂移-擴散傳輸，使用 Stabilized FEM 處理如鞘層區電漿參數變化較劇烈的地方。程式中重要假設包含利用 drift-diffusion approximation 求解帶電粒子的動量通量。所有的模擬程式將被平行化在 PETSc 的 AO 資料結構下。此後，程式可以再任何平行化的機器上執行例如 PC clusters。

關鍵字: 二維，噴射式大氣電漿(APPJ)，Stabilized FEM，流體模型。

Abstract

Atmospheric Pressure Plasma Jet (APPJ) represents one of the future important low-temperature plasmas used in modern materials processing. Its importance stems from its wide applications, such as surface cleaning, dry etching, sputtering and photoresistor stripping, in addition to its low cost as compared to low-pressure plasmas. Thus, fundamental understanding of the plasma physics within APPJ is important in developing this kind of processing equipment. In this proposed research project, we intend to apply the fluid modeling technique to simulate the atmospheric pressure plasma jet (APPJ), in which the INER is currently interested. We shall employ the finite element method (FEM) for all the PDEs involved in describing the APPJ since it is more flexible both in treating complicated geometry and parallel implementation. Stabilized FEM shall be used to discretize the continuity equation for all charged species considering the large drift term in the sheath, Considering the flat or round APPJ, in which INER is interested, we will first develop a simulation code for 2D/axisymmetric coordinate system in the first phase and then extend it into a 3D version in later phases to deal with more realistic operating conditions. All simulation codes will be parallelized under the AO (Application Ordering) framework of PETSc.

In this proposed one-year project, we have developed and verified a parallelized 1D and 2D/axisymmetric fluid modeling code using stabilized FEM. Note stabilized FEM is used to treat plasma properties with large gradient, such as in the sheath. Important assumptions include drift-diffusion approximation for the momentum fluxes of charges species and cross sections for evaluating transport coefficients.

Keywords: two-dimenisional, Atmospheric Pressure Plasma Jet, Stabilized FEM, Fluid Modeling.

I. INTRODUCTION

For the past two decades, studies in low-temperature (non-thermal) atmospheric-pressure (AP) non-equilibrium plasmas have attracted tremendous attention due to their numerous emerging applications, including electrostatic precipitation, ozone production, electromagnetic reflection, absorption, and phase shifts, plasma mitigation of the shock waves in supersonic/hypersonic flows,

surface treatment, thin-film deposition, chemical decontamination, biological decontamination and medical applications, to name a few[Becker *et al.*, 2004]. These excited applications would not have been possible were it not based on the extensive basic research on the generation and sustainment of relative large volumes of non-thermal ("cold") plasmas at atmospheric pressure and relatively small input power. Thus, fundamental understanding of the AP plasmas using various kinds of gases mixtures under different types of power sources becomes very important in optimizing the generation of cold plasma at lower cost.

Several distinct features have made the non-thermal AP plasmas very appealing in practical applications. First, being thermally non-equilibrium in these plasmas, second, the use of atmospheric pressure increases the opportunity of generating chemically active species (radicals) due to three-body processes, such as excited dimmers and trimers. Third, the use of atmospheric pressure greatly reduces the operational cost without the need of using sealed chamber, vacuum pumps, which is very expensive in procurement and maintenance. However, generating plasma at atmospheric pressure often requires very large applied voltage which is very power-consuming. Thus, how to effectively reduce the level of power input becomes a critical issue.

In general there are several types of AP plasma sources. They include DC and low-frequency plasmas, and high-frequency AP plasmas using radio frequency, microwave or respectively pulsed power sources [Becker *et al.*, 2004]. Optimal use of various kinds of AP plasmas requires the fundamental understanding of fluid mechanics, heat transfer, plasma chemistry, plasma kinetics and interaction between charged particles and electromagnetic field. Due to its intrinsic complexity, most researches are still based on exeperimental observations, expect Kushners's group, which is necessary in efficiently optimizing the performance in practical applications. In Kushner's group, both finite difference and finite element methods have been used to solve fluid modeling equations [http://uigelz.ece.iastate.edu/GroupMembers/KushnerMJ.html]. However, there are three important numerical issues that remain unsolved in plasma fluid modeling technique. First, the model can be solved by Newton-Krylov-Schwarz type scheme using the inexact Newton iterative scheme [Hwang, 2005]. Second, no three-dimensional version of plasma fluid modeling code is available. Third, there is no scalable parallelized version of plasma fluid modeling code. Based on the above observations, there is a need to develop a plasma fluid modeling code which includes the following features: parallel processing, fully coupled axisymmetric/three-dimensional equation solver and flexibility in treating complex geometry of objects.

II. BASIC GOVERNING EQUATIONS

In this section, we will describe the governing equations, preliminary FEM discretization, Newton-Krylov-Swartz (NKS) scheme in turn. In addition, PETSc library which is the backbone of the proposed numerical solver will also be introduced briefly for completeness.

Governing Equations

We consider an atmospheric plasma system consisting of electron and ions. In the following, variables with subscript *e, p* represent properties for electron and ion respectively. Note these coefficients for charged species are all functions of E/P alone, which is the well known local-field approximation (LFA). In addition, all momentum fluxes in the continuity equations of charged species are modeled based on drift-diffusion approximation. We assume that thermal state of the electrons can be described by a single electron temperature T_e, while the heavy particles, including ions are in thermal equilibrium with a single temperature T. In what follows, we will describe all conservation equations for charged and neutral species along with the filed equation (Poisson's equation) describing the variation of electric field.

Continuity equations

Continuity equation for *ion species p*, either positive or negative charge, can be written as,

$$\frac{\partial n_p}{\partial t} + \vec{\nabla} \cdot \vec{\Gamma}_p = S_p \qquad (1)$$

where

$$\vec{\Gamma}_p = -\mu_p n_p \vec{E} - D_p \vec{\nabla} n_p \qquad (1a)$$

$$S_p = S_p(n_e, n_i, \alpha_{iz}) \qquad (1b)$$

Note the form of source term as shown in eq. (1b) can be modified or added according to the modeled reactions describing how ion species p is generated or destroyed. Boundary conditions at walls are applied considering thermal diffusion flux and drift diffusion flux.

Continuity equation for electron species e can be written as,

$$\frac{\partial n_e}{\partial t} + \vec{\nabla} \cdot \vec{\Gamma}_e = S_e \qquad (2)$$

where

$$\vec{\Gamma}_e = -\mu_e n_e \vec{E} - D_e \vec{\nabla} n_e \qquad (2a)$$

$$S_e = S_e(n_e, n_i, \alpha_{iz}) \qquad (2b)$$

Similar to S_p, the form of S_e can also be modified or added according to the modeled reactions which generate or destroy the electron. Boundary conditions at walls are applied considering thermal diffusion flux and drift diffusion flux.

Electron energy density equation

In this proposed research electron energy density equation is solved. Electron kinetic energy, defined as $\varepsilon_e = \frac{3}{2} K_B T_e$, can be written as

$$\frac{\partial}{\partial t}(\frac{3}{2} K_B n_e T_e) + \vec{\nabla} \cdot (\frac{5}{2} K_B T_e - \frac{5}{2} K_B n_e D_e \vec{\nabla} T_e) = -e \vec{E} \cdot \vec{\Gamma}_e - S_e I_{iz}$$

$$(3)$$

Note I_{iz} is the ionization energy of the neutral species. On the right-hand side of the energy equation, the terms in turn represent the Ohmic heating, the loss of electron energy due to ionization and energy transfer to heavy particles due to elastic collisions,

respectively. Of course, energy loss due to excitation can be modeled by adding a source term to the right-hand side of energy equation. However, it can be absorbed into the first term of the right-hand side of energy equation for simplicity as demonstrated in Liau *et al.*, [2003] for argon AP plasma. Boundary conditions for electron energy at walls are applied considering drift and thermal induced energy transport.

Field equation

There are two field equations that are required the proposed AP plasma fluid modeling code, including Poisson's equation and Maxwell's equation. In the present project, at least the Poisson's equation for electrostatics is solved.

Poisson's equation for electrostatics due to boundary conditions and distribution of charged density can be written as,

$$\vec{\nabla} \cdot (\varepsilon \vec{E}) = -\frac{e}{\varepsilon_0} (\sum_{pos.\ ions} n_p - \sum_{neg.\ ions} n_e) \qquad (4)$$

$$\vec{E} = -\vec{\nabla} \varphi \qquad (5)$$

Note φ is the instantaneous electrostatic potential.

III. NUMBERICAL METHOD

Continuity equations

Since all continuity equations for charged particles are similar in format, only FEM formulation for the electron species is demonstrated here for brevity. In this proposed research, we employ Galerkin-Least Square (or stabilized) FEM [Donea and Huerta, 2003] for discretizing all unsteady convection-diffusion equations. Consider eq. (2) with the mass flux replaced by eq. (2a) as,

$$\frac{\partial n_e}{\partial t} - \mu_e \vec{E} \cdot \vec{\nabla} n_e - D_e \Delta n_e = S_e \qquad (6)$$

We define the residual of the continuity equation as,

$$R \equiv \frac{\partial n_e}{\partial t} - \mu_e \vec{E} \cdot \vec{\nabla} n_e - D_e \Delta n_e - S_e \qquad (7)$$

The form of Galerkin is,

$$\int_{\Omega} \omega_G R = 0 \quad \text{where} \quad \omega_G = \frac{\partial n_e}{\partial u_i} \qquad (8)$$

The form of least-square is,

$$\int_{\Omega} \omega_{Ls} R = 0 \quad \text{where} \quad \omega_{Ls} = \frac{\partial R}{\partial u_i} \qquad (9)$$

Finally, we combine the above two terms by adding them together with a stability parameter τ multiplying least-square eq. as the following form.

$$\int_{\Omega} (\omega_G \frac{\partial n_e}{\partial t} - \vec{\nabla}\omega_G \cdot \mu_e \vec{E} n_e + D_e \vec{\nabla}\omega_G \cdot \vec{\nabla}n_e - \omega_G S_e)$$
$$+ \int_{\Omega} \tau \omega_{Ls}(\frac{\partial n_e}{\partial t} - \mu_e \vec{E} \cdot \vec{\nabla}n_e - D_e \Delta n_e) \qquad (10)$$
$$= \int_{\Omega} \omega_G S_e + \int_{\Omega} \tau \omega_{Ls} S_e - \int_{\Gamma} (-\omega_G \mu_e \vec{E} n_e - \omega_G D_e \vec{\nabla}n_e)$$

Note how the stability parameter τ depends on mobility, diffusity, convective speed and grid size is described in detail in [Franca and Valentin, 2000].

IV. RESULTS AND DISCUSSIONS

Initially, we have conducted a CCP test case [Passchier and Goedheer, 1993] using Galerkin FEM. Unfortunately, We find running a case with 12,500 cells using 32 cpu in INER cluster needs more than 20 days. It is too time-consuming to be practical. So we are currently including stabilized FEM to reduce grid size that will greatly decrease computational time.

We turned back to simulate a quasi-1D RF (P = 0.5 torr, V_{pp} = 200 V, f = 13.56MHz, L = 2 cm) case using Galerkin/least-square FEM and conducted different grid tests to gain the suitable parameter.

The test grids show in Fig. (1) Gap length is 2 cm. It is divided in turn by 40 to 800 grids. Fig. (2) - (4) shows the distribution of electron number density using τ_{Codina}, τ_{Shakib} and τ_{Franca}. Among τ_{Codina} and τ_{Shakib} can be found in [Donea and Huerta, 2003]. From the three figures, we can find τ_{Codina} performs better in coarse grids than τ_{Franca} and τ_{Shakib}.

Completed code was tested on a PC-cluster system with processors up to 32. Results are summarized in Table 1, which shows that parallel efficiency of ~60% can be obtained for 32 processors for the present problem size.

V. CONCLUSIONS AND FUTURE WORKS

In the current report, we have selected suitable τ for our stabilized FEM. Important conclusions are summarized as follows:
1. The case using Galerkin method for very dense mesh can converge properly, but it takes too much time to be practical.
2. Tests including stabilized term show that the use of τ_{Codina} in stabilized FEM performs the best..
3. Parallel efficiency can reach up to ~60% with 32 processors.

We are now continuing to search a proper stabilized parameter in 2D axisymmetric case to increase computational efficiency.

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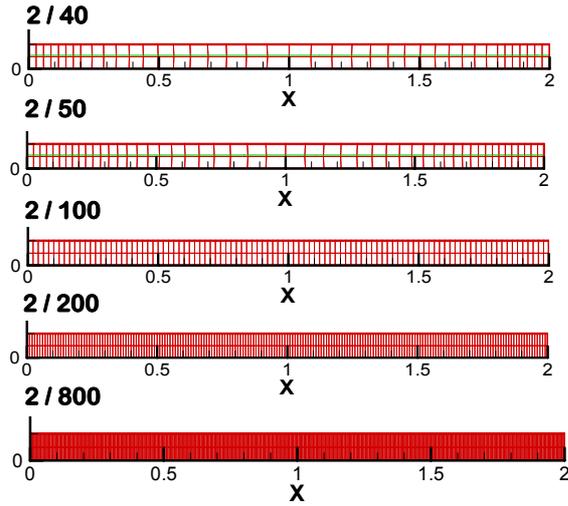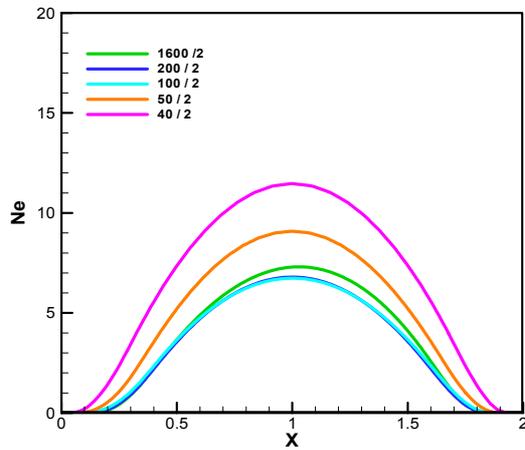
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2 / 100

2 / 200

2 / 800

Fig. 1 Sketch of grid tests.

Fig. 2 Distribution of N_e for τ_{Codina}.
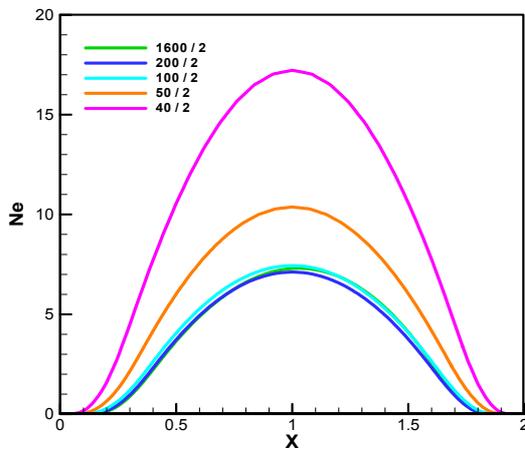
Fig. 3 Distribution of N_e for τ_{Shakib}.
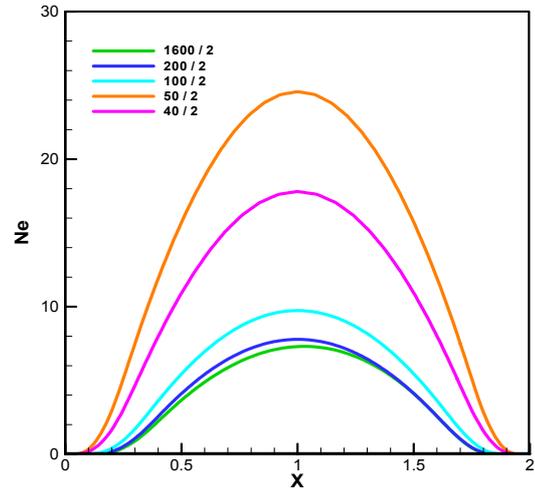
Fig. 4 Distribution of N_e for τ_{Franca}

	1	2	4	16	32
Eff. (ILU(2) / Gmress)	100 %	87.32 %	92.06 %	69.93 %	58.28 %

Table 1. Parallel efficiency of the parallelized FEM code. (Test grid size: 160 x 80 quadrilateral elements)