Application of the complete flux scheme to radio frequency discharge models

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Abstract. This paper is concerned with the application of transient complete flux scheme to a radio frequency discharge model in a one-dimensional geometry. The transient complete flux scheme and exponential difference scheme are used to discretize plasma fluxes in space. Temporal discretization is performed by using implicit Euler method and the 2-step backward differentiation formula of first and second orders. Numerical experiments are carried out to evaluate the order and level of accuracy. The results obtained by the complete flux scheme prove to have uniformly second-order accuracy for the spatial error and coincide with solutions calculated from the fourth-order deferred correction technique.

1. Introduction
A radio-frequency (RF) discharge generates a bulk plasma containing nearly the same number of positive and negative particles and a sheath containing predominantly positive ions; both of them are periodically modulated by the RF field. Radio frequency discharges are widely used for plasma processing [1] in the microelectronics industry. Plasma processing is a key fabrication step for manufacturing integrated circuits, for example, for etching, deposition and modification of thin films.

Simulations of RF discharges under various operating conditions have been reported in the literature [2-6]. The discretization methods for solving models numerically include first-order upwind [7], central difference [8], exponential difference [9] schemes (EDS), the finite element method [10], and the fourth-order deferred correction technique [11].

The goal of this paper is to show the high performance of the transient complete flux scheme (TCFS) for radio frequency discharge models. In order to make direct comparison with the literature we choose an argon RF discharge model whose results have been reported in [5, 11].

The complete flux scheme (CFS) was developed by Ten Thije Boonkkamp and Anthonissen [12] for advection-diffusion-reaction equations. Ten Thije Boonkkamp et al. [13] extended CFS to advection-diffusion-reaction systems. Later the author and Mihailova et al. applied CFS further to a local field approximation model and a local energy approximation model in a one-dimensional DC configuration and showed that CFS was ten times more accurate [14]. The author and ten Thije Boonkkamp et al. [15] established a rigorous mathematical proof that the CFS is second-order convergent, uniformly in the grid Péclet number, even in the presence of source terms. Ten Thije Boonkkamp et al. [16] extended the CFS to time-dependent conservation laws and the scheme is referred to as the transient complete flux scheme (TCFS). It was shown that for drift-dominated problems, the TCFS is second-order accurate in space, provided the solution is smooth.
In this paper we apply the TCFS to a RF glow discharge model. Although RF discharge model has the same geometry and assumptions as for the DC discharges considered in [14], there are four main differences between the RF discharge model and the DC discharge model. First, the input power for the RF discharge is a radio frequency voltage instead of direct currents. Second, in the source term of the energy balance equation of the RF discharge model the energy loss due to elastic collisions is omitted. Third, the transport and reaction rate coefficients of the RF discharge are assumed to be constants while these coefficients were assumed to be functions of the mean electron energy or the reduced electric field for the DC discharge models. Finally, the boundary conditions of the RF discharge are given by homogeneous Dirichlet boundary condition for electrons and electron energy density and homogeneous Neumann boundary conditions for ions, while these for the DC discharges were given by the more physical flux boundary conditions. The implementation of the TCFS was found to give accurate simulation results that correctly reflect the expected physical behaviour of an argon plasma under the simulated operating conditions. Comparing the results with those generated by the fourth-order deferred-correction technique [11], our results demonstrate excellent agreement, both quantitatively and qualitatively. From the error analysis we see that the TCFS yields uniformly second-order solutions in space. Additionally, we investigated the influence of the time integration. The second-order 2-step backward differentiation formula (BDF2) [17] was compared with the first-order implicit Euler method. The former converges much faster than the latter as the time step decreases. To conclude, the TCFS in combination with the BDF2 is an accurate and efficient numerical scheme for solving the RF discharge model.

2. Plasma model

We consider a parallel plate argon RF discharge as shown in Figure 1. The discharge is formed between two parallel infinitely large planar electrodes and the separation between the two electrodes is \(L\). The set of model equations is thus given by

\[
\begin{align*}
\frac{\partial n_{i,e}}{\partial t} + \frac{\partial \Gamma_{i,e}}{\partial x} &= K n_{e} N, \\
\frac{\partial n_{e}}{\partial t} + \frac{\partial \Gamma_{e}}{\partial x} &= -qE n_{e} - K n_{e} H_{i}, \quad \Gamma_{e} = \frac{5}{3} \mu_{e} E n_{e} - \frac{5}{3} D_{e} \frac{\partial n_{e}}{\partial x}, \\
-\frac{d}{dx} \left( \varepsilon_{0} \frac{dV}{dx} \right) &= q(n_{i} - n_{e}), \quad E = -\frac{dV}{dx}
\end{align*}
\]

The values of the transport coefficients and various parameters of the discharge used in the present simulation are the same as in [5], [6] and [11] and listed in Table 1.

The ionization rate coefficient \(K_{ion}\) is based on the experimental data, presented in [18], and reads as follows

\[
K_{ion} = \begin{cases} 
0 & \varepsilon \leq 5.3 \text{ eV}, \\
8.7 \times 10^{-15} (\varepsilon/eV - 5.3) \exp(-4.9/\sqrt{\varepsilon/eV - 5.3}) & \varepsilon > 5.3 \text{ eV}.
\end{cases}
\]
The boundary conditions are listed in Table 2. Electron secondary emission is not taken into account in the boundary conditions of electron density, in contrast to DC discharge studies in the previous chapter. As pointed out in [5] and [6], this simplification is justified because the rate of the electron secondary emission generation is expected to be less than one tenth of the ionization rate.

**Table 1.** Transport coefficients and parameters of the discharge used in the simulation.

| Parameter           | Symbol | Value   | Unit         |
|---------------------|--------|---------|--------------|
| Electron mobility   | $\mu_e$ | 30.0    | m$^2$V$^{-1}$s$^{-1}$ |
| Electron diffusivity| $D_e$   | 120.0   | m$^2$s$^{-1}$  |
| Ion mobility        | $\mu_i$ | 0.14    | m$^2$V$^{-1}$s$^{-1}$ |
| Ion diffusivity     | $D_i$   | 4.0×10$^{-3}$ | m$^2$s$^{-1}$  |
| Ionization energy   | $H_{ion}$ | 15.578  | eV           |
| RF driving frequency| $f$     | 13.56   | MHz          |
| RF driving amplitude| $V_{rf}$ | 40      | V            |
| Electrode separation| $L$     | 0.02    | m            |
| Gas temperature     | $T_g$   | 293     | K            |
| Gas pressure        | $p_g$   | 133.3224 | Pa           |

**Table 2.** Boundary conditions for the simulation.

| Electrode | $n_i$ | $n_e$ | $n_c$ | $V$ |
|-----------|-------|-------|-------|-----|
| $x = 0$   |       | 0     | 0     | 0   |
| $x = L$   |       | 0     | 0     | $V = V_{rf} \sin(2\pi f t)$ |

**3. Numerical methods**

We solve the set of equations in the RF discharge model separately by Gummel iteration. Despite the RF glow discharge model is composed of the same equations as the DC glow discharge [14], we should apply different numerical methods, since the RF discharge is time-dependent. We choose the TCFS to discretize the balance equations of particle densities and electron energy density. The vertex-centered grid used is shown in Figure 2.

**Figure 2.** Uniform vertex-centered grid. Solid circles denote nodal points and squares denote control volumes.

Moving the source term to the right-hand side of the equation and applying the CFS to the quasi-stationary problem we obtain the discretization form for the $j$th control volume as follows:

$$-a_{W,j} n_{j-1} + a_{C,j} n_j - a_{B,j} n_{j+1} = b_{W,j} (s_j - n_{j-1}) + b_{C,j} (s_j - n_j) + b_{B,j} (s_{j+1} - n_{j+1}).$$

(5)

where the coefficients $a_{W,j}$, $b_{W,j}$, etc. are defined by
To compare the impact of time integration we use the implicit Euler method and BDF2. Both of them are A-stable [17, Page 145], however, the former is first-order and the latter is second-order. The source term is treated explicitly in each step to keep it from affecting the diagonal dominance of the coefficient matrix in the discrete system. Then, using the Euler method, equation (5) can be discretized as

\[ (b_{W,j} - a_{W,j} \Delta t)n_{j+1}^{k+1} + (b_{C,j} + a_{C,j} \Delta t)n_{j+1}^{k+1} + (b_{E,j} - a_{E,j} \Delta t)n_{j+1}^{k+1} \]

\[ = b_{W,j}n_{j-1}^{k} + b_{C,j}n_{j}^{k} + b_{E,j}n_{j+1}^{k} + \Delta t(b_{W,j}s_{j-1}^{k} + b_{C,j}s_{j}^{k} + b_{E,j}s_{j+1}^{k}). \]  

Using BDF2 for equation (5) we can derive

\[ \left( \frac{3}{2}b_{W,j} - a_{W,j} \Delta t \right)n_{j+1}^{k+1} + \left( \frac{3}{2}b_{C,j} + a_{C,j} \Delta t \right)n_{j+1}^{k+1} + \left( \frac{3}{2}b_{E,j} - a_{E,j} \Delta t \right)n_{j+1}^{k+1} \]

\[ = 2(b_{W,j}n_{j-1}^{k} + b_{C,j}n_{j}^{k} + b_{E,j}n_{j+1}^{k}) - \frac{3}{2}(b_{W,j}n_{j-1}^{k-1} + b_{C,j}n_{j}^{k-1} + b_{E,j}n_{j+1}^{k-1}) \]

\[ + \Delta t(b_{W,j}s_{j-1}^{k} + b_{C,j}s_{j}^{k} + b_{E,j}s_{j+1}^{k}). \]  

The Neumann boundary conditions are approximated by the one-sided second-order difference scheme. At left boundary it is given by

\[ \frac{\partial n}{\partial x}(0) \approx \frac{-3n_0 + 4n_1 - n_2}{2\Delta x}, \]

and at the right boundary by

\[ \frac{\partial n}{\partial x}(L) \approx \frac{3n_{N,w} - 4n_{N,w-1} + n_{N,w-2}}{2\Delta x}. \]  

Discretizing on each control volume and writing the discretized equation in vector form we obtain for the Euler method

\[ (B + \Delta tA)n^{k+1} = Bn^{k} + \Delta tBs^{k}, \]

and for BDF2

\[ \left( \frac{3}{2}B + \Delta tA \right)n^{k+1} = 2Bn^{k} - \frac{3}{2}Bn^{k-1} + \Delta tBs^{k}. \]  

Poisson’s equation is discretized by the central difference scheme. To avoid the time step restriction, the semi-implicit treatment (see [19]) is adopted.

4. Results and discussion

We carry out the simulations in software Matlab. The periodic quasi-steady-state solutions for a period T are presented in Figure 3. In Figure 4 two snapshots of the periodic quasi-steady-state solution for various variables are presented. These solutions are obtained by using a grid consisting of 5120 control volumes and by integrating over 2000 RF cycles. Each cycle is integrated by \( N_{ts} = 640 \) time steps. After 2000 cycles the solutions is regarded as the periodic quasi-steady-state, since the relative differences in \( n_e, n_i \) and \( n_\epsilon \) at the ends of two consecutive periods are less than \( 10^{-6} \). The initial values of the particle densities and the mean electron energy are uniform, \( n_e = n_i = 5 \times 10^{15} \text{ m}^{-3} \) and \( \epsilon = 1 \text{ eV} \).

Figure 3(a) shows that the electrons are subject to oscillations with the variation of the RF voltage. In contrast, the argon ions cannot follow the variation of the voltage and Figure 3(b) illustrates that the ion density is essentially constant with respect to time. This agrees with the fact that the frequency of the electrons (approximately 600 MHz for \( n_e = 5 \times 10^{15} \text{ m}^{-3} \)) is much higher than the radio frequency while that of ions (approximately 2.4 MHz for \( n_i = 5 \times 10^{15} \text{ m}^{-3} \)) is much lower. From Figure 3(c) and 3(d) we can see that the distribution of the potential is flat in the bulk and rapid changes occur in the sheath. Accordingly, the electric field is nearly 0 in the bulk and high fields locate in the sheath. Figure 4(e) shows that electron energy density also varies corresponding to the voltage. From Figure 4(f) we can see that the maximum of the ionization rate coefficient occurs in the momentary cathode sheath, since there the electrons have already been accelerated to possess high energy, see Figure 4(e).
These simulation results qualitatively agree with many of the physical phenomena characteristic of argon plasmas reported in [2, 3, 4, 5, 6].

![Figure 3. Periodic quasi-steady-state results in a cycle. Space-time contours of (a) electron density, (b) ion density, (c) potential, (d) electric field, (e) electron energy density, (f) ionization rate coefficient.](image)

These results generated using the same parameters and conditions are also presented in [5, 11]. We compare the present results with those in [11]; see Figure 4. The present result show excellent agreement both quantitatively and qualitatively with those in [11]. It is worth mentioning that in [11] Davoudabadi et al. used the deferred correction technique. The fluxes due to drift and diffusion are separately approximated and each of them is expressed by a sum of an implicit part and an explicit part. The implicit part is a lower order approximation and the explicit part is the subtraction of a higher order approximation to the lower order approximation [20]. Although more accurate solutions can be obtained using the deferred-correction technique, the procedure of discretization is quite complicated. The discretization procedure of the TCFS is simple and the point is that it yields very similar results with the higher-order scheme. Therefore, the TCFS is preferable from the point of view of accuracy and implementation.

Regarding the solution shown in Figure 3 as the exact solution (h and τ are small enough), we calculate the maximum norm of the spatial discretization errors $e_h$ of the solutions calculated with various grid sizes. Figure 5(a) shows the variation of $e_h$ as a function of $h$ in a double logarithmic plot. The model is also solved by using the EDS. Its maximum norm of the discretization errors are plotted in Figure 5(a) as well. The slopes of the curves from the TCFS are uniformly 2, while these from the EDS gradually changes from 1 to 2 as the grid size $h$ decreases.

To demonstrate the impact of the time integration, we calculate the maximum norm of the discretization error $e_\tau$ in time for various time steps and a fix $h$. We plot $e_\tau$ as a function of $\tau$ in Figure 5(b). The grid used in space has 160 control volumes. We can see that the slopes of the curves from the Euler method are approximately 1 and these from the BDF2 are approximately 2. These results illustrate that the Euler method displays first-order and the BDF2 displays second-order as they should. Additionally, we can see for a given $\tau$ the discretization error of the BDF2 is much smaller than that of the Euler method and to achieve a given accuracy, the time step needed by the BDF2 can be nearly four time larger than that of the Euler method.
Electron densities

Ion densities

Potential

Electric field

Mean electron energy

Ionization rate

Figure 4. Comparison of the quasi-steady-state results of the present work with those presented by Davoudabadi et al. [11]. Two snapshots for $t = 0$ and $t = 0.25T$ in a period are presented.

Figure 5. Double logarithmic plot.

5. Conclusions

A low-cost highly accurate finite volume method is implemented to solve the RF discharge model in a one-dimensional configuration. The performance of the TCFS and the EDS are used to discretize plasma fluxes in space. Temporal discretization is performed by using Euler method and BDF2 of first and second orders. Numerical experiments show that the results obtained by the TCFS have uniformly second-order accuracy for the spatial error and coincide with the solutions calculated from the fourth-order deferred correction technique, while the EDS is second-order accurate only when the grid size is small enough. Moreover, the BDF2 displays second-order accurate for temporal error. To conclude, the TCFS in combination with the BDF2 is an accurate and efficient numerical scheme for solving the RF discharge models.
Present and future work aims at the application of the complete flux scheme to higher-dimensional problems, for example, streamer discharges, for which the improved accuracy of the TCFS has an even greater impact.

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