Modelling dc glow discharges in a wide range of currents with Comsol Multiphysics. New results, fortes and weaknesses

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Modelling of a DC glow discharge in a wide current range is performed by means of a steady-state solver of commercial software Comsol Multiphysics. Two discharge models are treated: the basic model of glow discharges and a detailed model which takes into account atomic and molecular ions, atomic excited states, excimers, and non-locality of electron energy. Complex behaviour of the discharge was found in two different situations: in the framework of the detailed model in a parallel-plane discharge and in the framework of the basic model in a cathode boundary layer discharge. This behaviour is manifested through a retrograde section limited by two turning points. Being very interesting by themselves, the results illustrate suitability of Comsol Multiphysics for modelling DC glow discharges in a wide current range, but also reveal unfortunate limitations of this powerful tool.

1. Introduction

Recently, multiple solutions existing in the framework of the theory of DC glow discharges have been computed for the first time [1, 2]. Some of these solutions describe modes associated with normal spots, while others describe patterns with more than one spot similar to those observed in the experiments, e.g. [3].

The multiple solutions [1, 2] have been computed by means of commercial software Comsol Multiphysics. One of very strong points of Comsol Multiphysics is the possibility of practical and reasonably straightforward modelling of complex systems, which gas discharges definitely are. Another forte is the possibility of using powerful steady-state solvers, which are indispensable for a systematic study of multiple modes; see discussion in [1]. Another forte is the possibility to specify the discharge current as a control parameter without the need to introduce an external circuit, and to switch seamlessly between discharge current and voltage, a feature which is indispensable for calculation of the most of multiple modes since they possess turning points and their CVCs possess extrema.

The fact that Comsol Multiphysics has allowed finding a new and important class of solutions [1, 2, 4] in the classical model by itself attests to its power. Furthermore, when Comsol Multiphysics is applied to more complex models, then new and surprising results can be obtained even setting aside the multiple solutions: the glow discharge can manifest complex behaviour in apparently simple situations. This complex behaviour does not seem to have been detected in previous works. On the other hand, weaknesses of Comsol Multiphysics become visible, which in some cases severely hinder calculations and are difficult to overcome since, as opposed to home-made codes and despite the flexibility of the software, there is not much room for adjustment of routines included in Comsol Multiphysics. In this work, examples of complex behaviour of glow discharge will be shown and weaknesses of Comsol Multiphysics discussed.

2. The model

The modelling was performed in the framework of the basic model of glow discharges and also in the framework of a more detailed model. The basic model comprises equations of conservation of a single ion species (molecular ions) and the electrons, transport equations for the ions and the electrons written in the local approximation, and the Poisson equation. The detailed model takes into account atomic and molecular ions, atomic excited states, excimers, and non-locality of electron transport and kinetic coefficients. Data on transport and kinetic coefficients employed in the basic and detailed models can be found in [1] and [5], respectively.

Two discharge configurations have been considered. One is the simple parallel-plane configuration: a cylindrical discharge tube with the bases serving as electrodes and the lateral surface (wall) being insulating. The other is a cathode boundary layer (CBL) discharge configuration comprising a cathode-dielectric-anode system with perforated anode and dielectric (a configuration similar to the one used in experiments, see figure 1 of [6]). The interectrode gap in the parallel-plane configuration is 0.5mm. The radius of the opening and the thickness of dielectric in the CBL configuration are 0.5mm as well. Results reported in this work refer to the plasma-producing gas being xenon under the pressure of 30Torr. The steady-state solver of Comsol Multiphysics, version 4.1 was used.

3. Results and discussion

The first example of complex behaviour was found in the parallel-plane configuration in the framework of the detailed discharge model. The solid line in figure 1 depicts the current density voltage characteristic (CDVC) calculated in 1D, i.e., with account of variation of discharge parameters only along the axis of the discharge. The CDVC is qualitatively similar to that described by the classic von Engel and Steenbeck solution, except for the *S*-shaped section in the range 200 $\mathrm{Am}^{-2} < j < 300\ \mathrm{Am}^{-2}$. The existence of the *S*-shape in the CDVC of the 1D discharge has apparently not been reported previously and is a surprising result. Also shown in figure 1 is the CDVC of the 1D discharge calculated without account of stepwise ionization (dashed line). It can be seen that the *S*-shape disappears when stepwise ionization is neglected.

Figure 1 is a clear illustration of the above mentioned fortes of Comsol Multiphysics. The whole CDVC was found, including the whole of the *S*-shape. If a nonstationary solver were used, it would be hardly possible to calculate at least some sections of the *S*-shape even in the 1D geometry being considered: one needs to specify the discharge voltage as a control parameter in order to pass through a turning point, however this may render the discharge unstable against 1D perturbations [4].

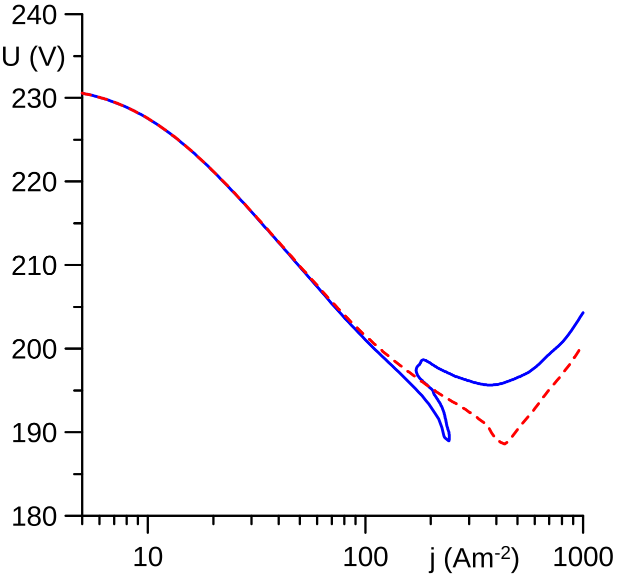


Figure 1: CDVC of the 1D glow discharge. Solid: detailed model. Dashed: stepwise ionization neglected.

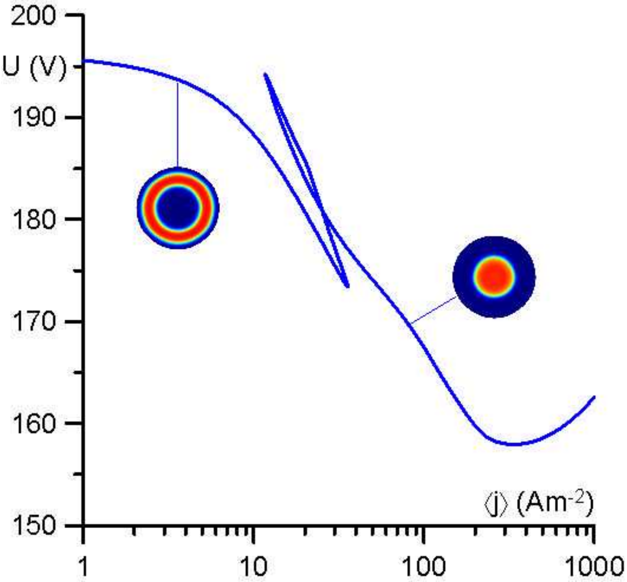
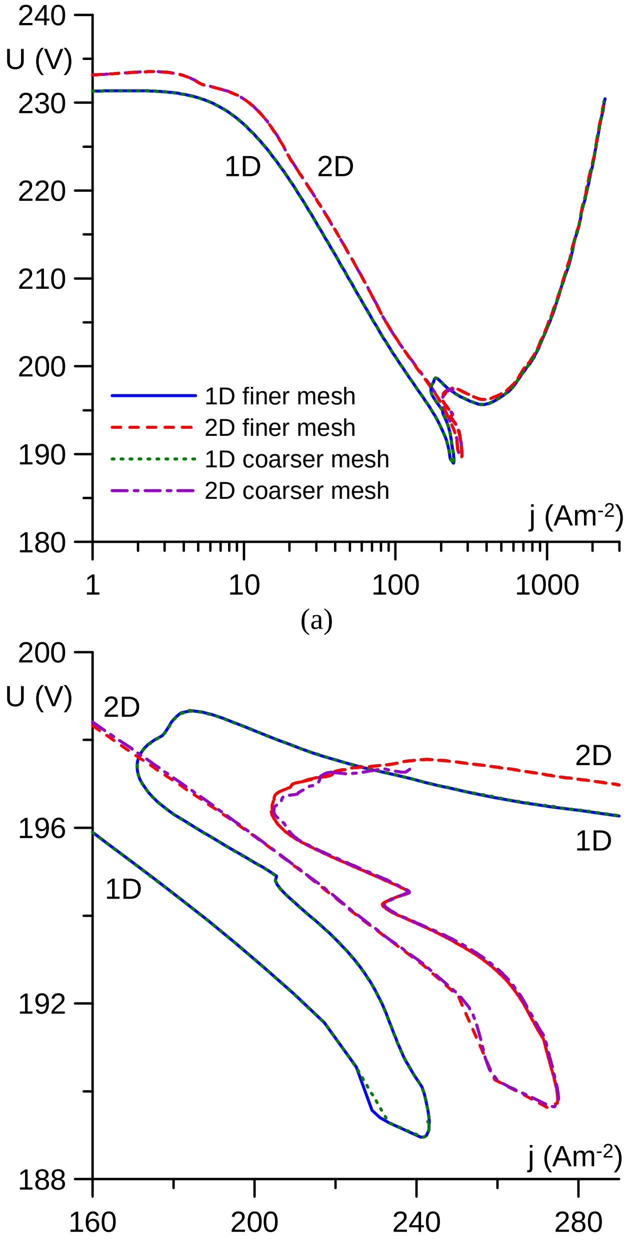


Figure 2: CVC of the 2D glow discharge. CBL discharge configuration.

Complex behaviour similar to that depicted in figure 1 may be present not only in situations where detailed kinetics is included in the model. In figure 2, the CVC is shown of the 2D (axially symmetric) discharge in the CBL configuration calculated in the framework of the basic model.

Surprisingly, the CVC of the discharge exhibits a loop. (In fact, there is no major difference between this loop and the *S*-shape seen in figure 1: what matters is that in both cases the discharge possesses a retrograde section limited by two turning points.) The discharge is associated with a pattern comprising a ring spot at the cathode in the range of discharge currents below the loop and a spot at the center of the cathode in the range of currents above the loop. Note that neither spot is normal, i.e., the effect of normal current density is absent. The loop is associated with a transition from the pattern with a ring spot into the pattern with a central spot. This transition is smooth and occurs as follows: the inner radius of the ring spot decreases and then turns zero (i.e., the ring spot becomes a circle) and the outer radius is somewhat reduced. Note that although methods of numerical simulations of microdischarges are generally well developed, e.g. [7 - 11], no retrograde sections have apparently been reported. A possible reason is that the complex behaviour exhibited in figure 2 can hardly be noticed if a time-dependent solver is employed. On the other hand, it is relatively easy to calculate it with Comsol Multiphysics due to the possibility of a seamless switching between discharge current and discharge voltage as the control parameter.



(a)

(b)

Figure 3: CDVCs of the 1D mode calculated on different meshes. (a) General view. (b) Detail of the *S*-shape.

Let us give a few examples of limitations revealed by Comsol Multiphysics when applied to the detailed model contemplating multiple ion species, multiple ionization channels, diffusion of excited states, and non-locality of the kinetic and transport coefficients of electrons, even in the simplest parallel-plane geometry. In figure 3, CDVCs are shown of the 1D mode calculated in different ways in the framework of this model: in the 1D geometry with the use of the same mesh as in figure 1 (solid line); in the 1D geometry with the use of a numerical mesh with half as many elements (every other node was removed; dotted line); in the 2D geometry with reflecting lateral wall of the discharge tube and the tube radius of 0.5mm (dashed line); in the same 2D geometry with the use of a numerical mesh with half as many elements in each direction (every other node in each direction removed; dashed-dotted line). The parts of the CDVCs manifesting the *S*-shape are shown in figure 3b.

The effect of the mesh on 1D calculations is hardly visible. For 2D calculations the effect of the mesh cannot be seen in figure 3a but can be seen in figure 3b: the calculation of the 1D discharge in the 2D geometry with the coarser mesh was not possible at higher currents. There is a visible difference between the CDVCs calculated in the 1D and 2D geometries. The difference decreases as the discharge current increases, but it does not decrease with a refinement of the numerical mesh.

It should be stressed that the trend exhibited by CDVCs calculated in 1D and 2D is the same, even in the range where the *S*-shape occurs, and the numerical difference is not large. Therefore, this difference can hardly discredit the above results. On the other hand, the fact that the difference between the 1D and 2D calculations of the 1D discharge does not decrease with a refinement of the numerical mesh is not immediately clear and therefore worrying.

Figures 1 and 3 refer to the case of reflecting lateral wall. An attempt to introduce an account of neutralization of charged particles at the lateral wall in the framework of the detailed model was undertaken. Several variants of boundary conditions for the electron number and energy at the insulating wall have been tested, including those indicated in the user manual of the Plasma Module of Comsol Multiphysics. (This is a recently released simulation tool specifically designed for modelling of gas discharges. It allows users to build glow discharge models with complex kinetic schemes and an equation of conservation of electron energy.) However, the iterations failed to converge in the case where neutralization of charged species at the wall was fully taken into account.

In addition to the above-discussed solutions, which exist at all discharge currents, the above models may admit other solutions [1, 2], which are multidimensional, exist in limited current ranges, and describe self-organized spot patterns similar to those observed in the experiment [3]. An attempt to compute these other solutions in the framework of the detailed model in the parallel-plane geometry was only partially successful: it was possible to find 2D modes in some current ranges but not in the whole region of their existence, as opposed to what was done in [1, 2] in the framework of the basic model.

Results not shown here indicate that these difficulties are likely to have originated in the equation of conservation of electron energy. Note that the Plasma Module of Comsol Multiphysics employs the equation of conservation of electron energy written in the same form as the one used in this work, and test calculations performed with the Plasma Module showed that no problems arise from accounting for absorption at the wall, presumably due to a built-in optimization. Unfortunately, the current version (version 4.1) of Plasma Module does not support steady-state solvers. Therefore, this tool cannot be used for a detailed and systematic study of multiple solutions, nor can it be used to describe complex behaviour with *S*-shapes or loops. Nevertheless, the fact that the Plasma Module can deal with the equation of conservation of electron energy suggests that the problem has a solution.

It is interesting to note that a similar difficulty has been encountered in calculations for the CBL configuration in the framework of the basic model with the use of versions 3.5a and older of Comsol Multiphysics: it was impossible to calculate the discharge at all discharge currents. This weakness disappeared with the release of version 4.0.

3. Conclusions

Complex behaviour of the discharge was found using a steady-state solver of Comsol Multiphysics in two different situations. This behaviour is manifested through a retrograde section limited by two turning points. In the case of the 1D discharge calculated in the framework of a detailed model of discharge in xenon between parallel-plane electrodes, this behaviour manifests itself in the plane (j,U) as an S-shaped section of the CDVC and is associated with stepwise ionization. In the case of the axially symmetric discharge in xenon calculated in the framework of a basic model in the cathode boundary layer configuration, this behaviour manifests itself in the plane (I,U) as a loop in the CVC. The effect is a consequence of the geometry of the discharge: the loop is associated with a smooth transition between a pattern with a ring spot at the cathode at low currents and a pattern with a spot at the cathode center at high currents. Both the S-shape and the loop are scientifically very interesting. One could think of further numerical work on these effects and also of experiments.

Complex behaviour has emerged as a consequence of consideration of either a detailed kinetic scheme, or a discharge geometry other than parallel-plane discharge. These results give the impression that complex behaviour in DC glow microdischarges is a rule rather than an exception.

Comsol Multiphysics is a very powerful tool which allows prediction of complex behaviour which may be present even in apparently simple situations; this behaviour can hardly be noticed if time-dependent solvers are used. Like other rapidly developing simulation tools, Comsol Multiphysics has unfortunate drawbacks which manifest themselves under certain conditions. However, past experience shows that new versions of Comsol Multiphysics usually offer significant improvements and add flexibility. One can hope that the weaknesses revealed in this work will be overcome in the near future.

4. Acknowledgments

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5. References

[1] P. G. C. Almeida, M. S. Benilov, and M. J. Faria, Plasma Sources Sci. Technol. 19 (2010) 025019.

[2] P. G. C. Almeida, M. S. Benilov and M. J. Faria, IEEE Trans. Plasma Sci. 39 (2011) to appear.

[3] K. H. Schoenbach, M. Moselhy, and W. Shi, Plasma Sources Sci. Technol. 13 (2004) 177.

[4] P. G. C. Almeida, M. S. Benilov, M D Cunha and M. J. Faria, J. Phys. D: Appl. Phys. 42 (2009) 194010.

[5] P. G. C. Almeida, *Investigation of modes of current transfer in DC glow and arc discharges*, PhD thesis, Universidade da Madeira (2011).

[6] W. Zhu, N. Takano, K. H. Schoenbach, D. Guru, J. McLaren, J. Heberlein, R. May, and J. R. Cooper, J. Phys. D: Appl. Phys. 40 (2007) 3896.

[7] J. P. Boeuf, L. C. Pitchford, and K. H. Schoenbach, Appl. Phys. Lett. 86 (2005) 071501.

[8] E. Muñoz-Serrano, G. Hagelaar, T. Callegari, J. P. Boeuf, and L. C. Pitchford, Plasma Phys. Control. Fusion 48 (2006) B39.

[9] K. Makasheva, E. Muñoz-Serrano, G. Hagelaar, J. P. Boeuf, and L. C. Pitchford, Plasma Phys. Control. Fusion 49 (2007) B233.

[10] T. Deconinck and L. L. Raja, Plasma Processes Polym. 6 (2009) 335.

[11] X. Zhang, X. Wang, F. Liu, and Y. Lu, IEEE Trans. Plasma. Sci. 37 (2009) 2055.