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Numerical Modeling and Simulation Analysis of Plasma-Liquid Interaction at Atmospheric Pressure

大気圧下におけるプラズマー液体相互作用の数値モデリングと
シミュレーション解析

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Atmospheric pressure plasma has been widely applied to water cleanup treatment, material synthesis, medicine and so on. However, the discharge dynamics including the interaction with liquid and biological interfaces are extremely complex and not understood well. For further development of the plasma applications, theoretical analyses based on numerical modeling and simulations are essential. In this paper, the analytical schemes using fluid models and molecular dynamics were briefly described. The numerical results with the interaction between atmospheric pressure plasma and liquid-biological interface were reviewed for recent topics of plasma application. Moreover, the future prospects for the numerical simulations in this research field were also discussed.

1. Introduction

Presently, we can easily bring plasma radicals into contact with various substances such as fluids and biomaterials by means of non-equilibrium plasma under atmospheric pressure. This plasma technology has been applied to water purification, material synthesis, and sterilization. In particular, plasma medicine is a recent attractive application [1]. However, the interactions among multi-phase interfaces are extremely complicated, and cannot be well understood with only experimental validation. The theoretical modeling and numerical simulation are essential for further insights of the mechanism.

In this paper, the modeling of multiphase including plasma, gas, liquid and biomaterial under atmospheric pressure, and typical numerical methods are briefly described. Some analytical examples of liquid-biological interface are reviewed in the latest topical applications. The prospects of nearest future simulations in this research field are also discussed.

2. Simulation Models and Techniques

In order to model the multiphase of plasma, gas, liquid and biomaterial numerically, we need to consider various complicated and specific conditions and cheese appropriate numerical schemes. As is shown in Fig. 1, fluid models and molecular dynamics are available for above simulations.

Fluid model for plasma physics is a macroscopic method describing statistical average dynamics

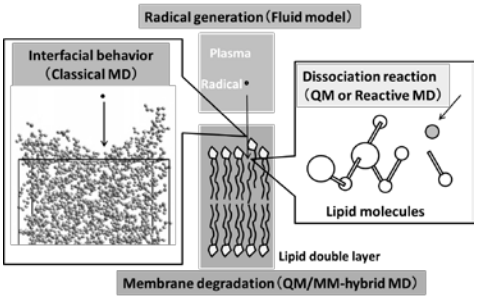

Fig.1. Schematics of an analytical multi-phase model

such as spatio-temporal distributions of particles and fields. This analytical system generally consists of the continuity equations for density of electrons, ions and neutral particles, and Poisson's equation.

Transport parameters and reaction rate coefficients are required in advance. In order to refer electronic swarm parameters, the local field, pseudo-thermal equilibrium or relaxation continuum approximation is adopted.

Fluid model is suitable for faster calculations of high-density plasma behavior under a wide range of electromagnetic field. However, various conditions should be suitably approximated for boundary, energy conservation and interaction.

Molecular dynamics (MD) is a deterministic model of particle behavior in atomic scale. The motion equations of all individual particles are integrated by time step in the order of a femtosecond.

In typical simulations, atoms move by interatomic

force based on quantum atomic potentials. These forces are obtained from classical interatomic potentials referred to as force field or are directly derived from quantum mechanical calculations.

MD can deal with accurate behavior of each particle in fine-grained time and length scale without arbitrary fitting parameters because of the self-consistency in principle. On the other hand, it is difficult to perform long time and large size simulations since the computational load is limited.

3. Examples of Simulations

The streamer propagation through bubble in liquids was simulated using two-dimensional fluid model for treatments of volatile organic compounds by Babaeba and Kushner [2]. Spatial evolution of streamer along the surface of bubble was promoted with an increase of the relative permittivity and conductivity of liquids. The transition of streamer path from axial to surface of bubble strongly depended on the size of bubble, applied voltage and mean free path of photon.

They investigated filament formation in atmospheric pressure dielectric barrier discharges (DBD) and surface charging of human skin tissue with similar numerical technique [3]. The maximum value of intracellular electric field exceeded 100 kV cm^{-1}. This model was upgraded for wound skin filled with blood serum [4].

Shirafuji *et al*. numerically investigated charged particle behavior through gas and liquid phases in DBD with water [5]. Ion accumulation in surface layer of liquid was much larger than that without plasma irradiation. Takeuchi considered mass transfer through gas-liquid interface for radicals [6]. Further detailed framework of multiphase modeling for plasma-biofilm and plasma-tissue interactions was developed by Chen *et al*. [7].

With respect to MD simulations, Minagawa *et al*. investigated the physical behavior of water molecules by the bombardment of positive oxygen ion on plasma-liquid surface [8]. The number of sputtered water molecules, liquid temperature, and penetration depth in liquid were quantified to be a function of various incident energy and electric field strength.

Using reactive force field referred as to ReaxFF, Yusupov *et al*. simulated the interaction of oxygen radicals with water. Their computational results showed that OH, HO_2, and H_2O_2 could diffuse deeply to the liquid layer [9]. They also modeled interaction of radical oxygen species with biological surface such as bacterial cell walls [10] and lipids in skin barrier [11] by similar MD technique. The abstraction of hydrogen played a key role on the degradation of biological surface.

Abolfath *et al*. examined quantum mechanical and molecular mechanical MD (QM/MM-MD) for the reactive interaction of OH radicals with DNA [12]. The selective promotion of hydrogen abstraction from guanine was shown for different spin states of OH – guanine system.

4. Conclusions

For numerical analyses with interactions between plasma and liquid or biological interface under atmospheric pressure, we described the outline of fluid model and molecular dynamics, and overviewed the latest analytical results.

The numerical simulations are available for theoretical and quantitative analyses of further complicated system with respect to boundary shape, interfacial interaction and changes of flow and heat in multiphase.

In the nearest future, the establishment of general models and techniques for multi-physics will be required. We should verify the space division at appropriate time in synthesized multiphase simulations.

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