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NONEQUILIBRIUM OF DISSOCIATION AND RECOMBINATION IN R.F. THERMAL PLASMAS WITH DIATOMIC GAS

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ABSTRACT

RF argon-hydrogen, argon-oxygen and argon-nitrogen thermal plasmas have been formulated to investigate the nonequilibrium of dissociation and recombination of the reactive gases in the plasmas. In an argon-hydrogen and argon-oxygen plasma, the calculated results on a kinetic model is similar to those on an equilibrium model. An argon-nitrogen plasma can not be treated as thermodynamic equilibrium owing to the substantial difference between these results.

1. INTRODUCTION

Thermal plasmas offer a high energy source. RF thermal plasmas are free from electrode contamination. RF plasmas have been used for a number of applications; chemical synthesis, plasma spraying and production of ultrafine powders of various materials.

The temperature, flow and concentration fields in RF plasmas have been calculated numerically to increase the efficiency of chemical reactions. The modeling, however, has not included chemical reactions in the early stage.[1,2] The modeling with chemical reactions has developed on the assumption of local thermodynamic equilibrium.[3] The modeling on a kinetic model for chemical reactions is rather scare.[4]

In the present paper, dissociation and recombination rates of diatomic gases in RF plasmas were taken into account in the calculation model. RF argon-hydrogen, argon-oxygen and argon-nitrogen thermal plasmas under atmospheric pressure have been formulated to investigate the nonequilibrium in the plasmas. These reactive plasmas are very important and elementary. The two-dimensional continuity, momentum, energy and species equations along with the one-dimensional electromagnetic equations were solved simultaneously.

2. NUMERICAL FORMULATION

The flow, temperature and concentration fields in an RF plasma torch were calculated by solving simultaneously the two-dimensional continuity, momentum, energy and species equations with the one-dimensional electromagnetic equations. The RF plasma torch model used in this simulation is shown in **Fig. 1**. Gases issue from circular slits of 2 mm width at the total flow rate of 25 litre/min. Argon issues both from the inner slit (Q1 = 10 litre/min) and from the outer slit (Q2 = 10 litre/min).

Diatomic gas (H_2, O_2 or N_2) issues from the outer slit (Q3 = 5 litre /min). The input power is 8 kW and the frequency is 4 MHz at the torch.

The following assumptions are made for the model: a) laminar flow. b) Local thermodynamic equilibrium only for ionization. The dissociation and recombination rate of hydrogen, oxygen or nitrogen are considered. c) Axially symmetric. d) Optically thin. e) Negligible viscous dissipation. f) Negligible displacement current.

The governing equations are formulated in the cylindrical coordinate as follows;

$$\nabla \cdot (\rho u \Phi) = \nabla \cdot (\Gamma \nabla \Phi) + S \tag{1}$$

where ϕ is called the dependent variable, Γ and S are the diffusion coefficient and the source term, respectively. The governing equations were solved using the SIMPLER[5] algorithm. The calculations were performed for a 12x18 nonuniform grid system in the radial and axial directions, respectively. The convergence criterion was that the mass balance is satisfied to within 0.1%.

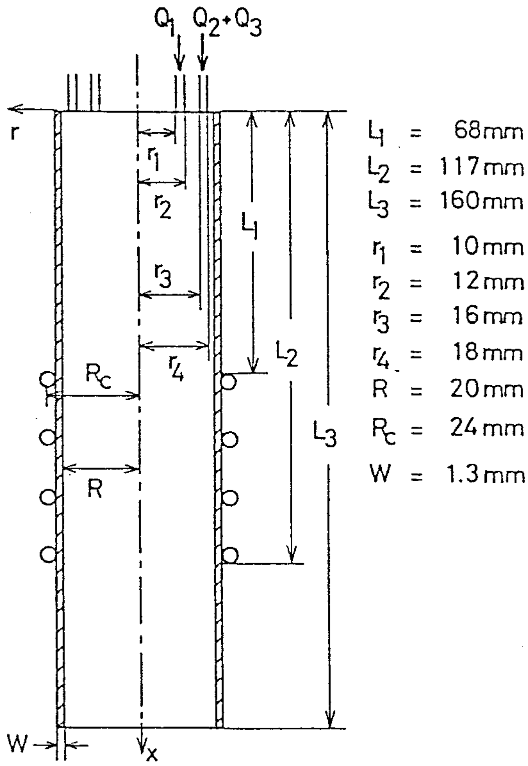

Fig. 1 Calculation model.

3. CALCULATED RESULTS

The calculated streamlines, isotherms, degree of dissociation, and concentration contours of H_2 and H in an argon-hydrogen plasma are shown in **Figs. 2 (a)-(e)**, respectively. The dimensionless streamlines are based on the total input flow rate. The temperature field of the argon-hydrogen plasma was varied by the strong recirculating eddy. The strong eddy flattens the temperature gradient in the upstream from the coil region. The concentration contours show that H_2 exists only near the quartz tube wall, while the concentration of H near the wall is negligible. In the high temperature region, the concentration of H_2 can be neglected.

The radial distributions of mass fraction of H_2 and H in the argon-hydrogen plasma on the kinetic model is compared to those on the equilibrium model in **Fig. 3.** The difference between them is little. The results indicates that the dissociation and recombination of hydrogen in an argon-hydrogen plasma can be treated as thermodynamic equilibrium. **Figure 4** shows that an argon-oxygen plasma can be also described as thermodynamic equilibrium. The comparison between the results on the kinetic model and on the equilibrium model in the argon-nitrogen plasma in **Fig.** 5 shows the substantial discrepancy for the distributions of mass fraction of N_2 and N. The discrepancy is due to the relatively high dissociation energy of N_2. This indicates that an argon-nitrogen plasma can not be treated as thermodynamic equilibrium.

4. CONCLUSIONS

Nonequilibrium of dissociation and recombination of reactive gases were investigated with the numerical analysis. An argon-hydrogen and argon-oxygen plasma can be described as thermodynamic equilibrium. An argon-nitrogen plasma, however, can not be treated as thermodynamic equilibrium.

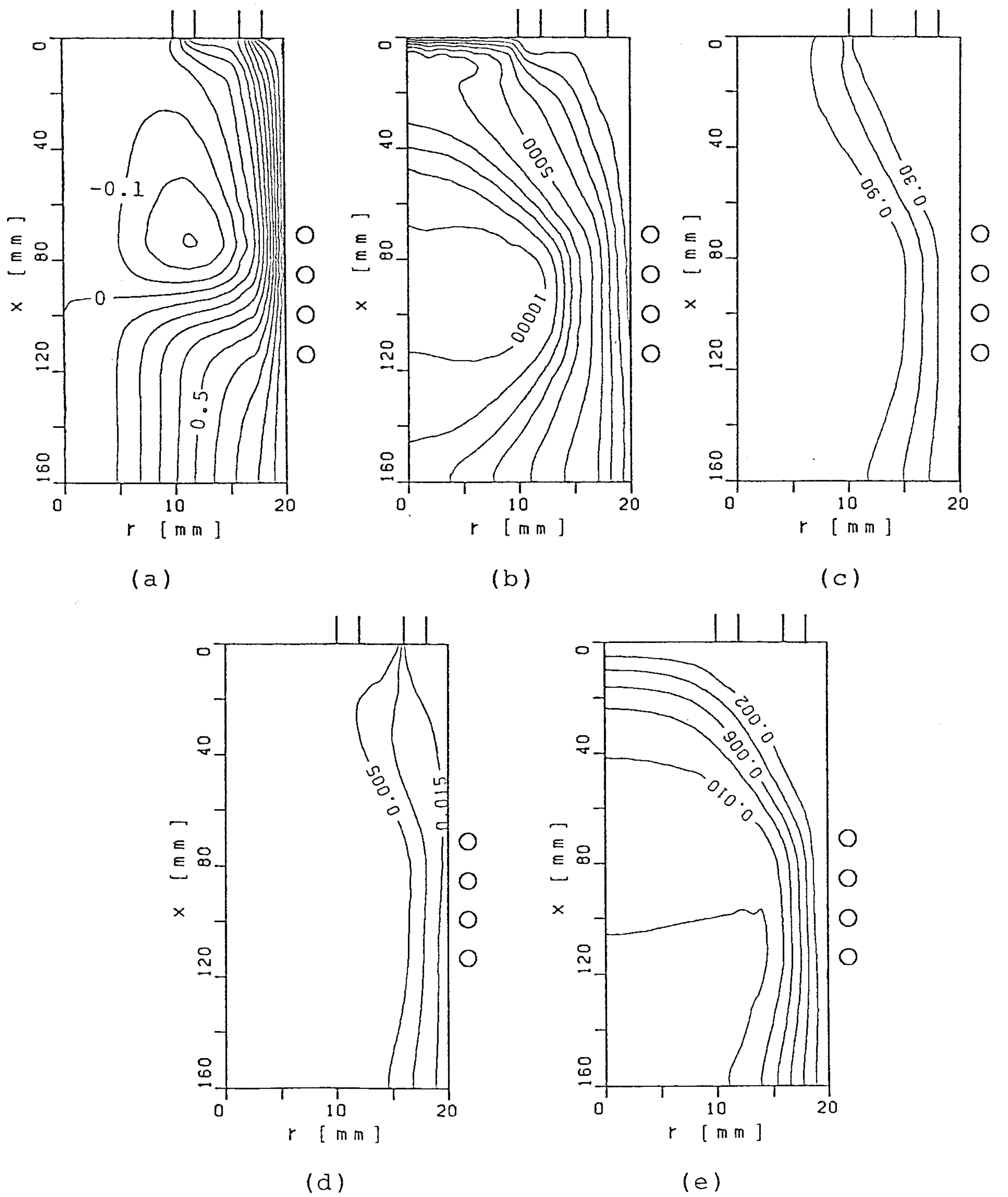

Fig. 2 Streamlines(a), isotherms(b), degree of dissociation(c) and mass fraction of H_2(d) and H(e) (Ar:20 litre/min; H_2:5 litre/min).

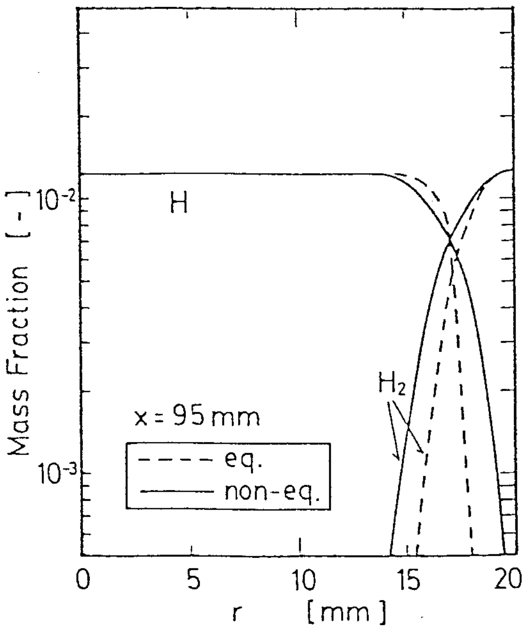

Fig. 3 Mass fraction of H_2 and H for the kinetic and the equilibrium models.

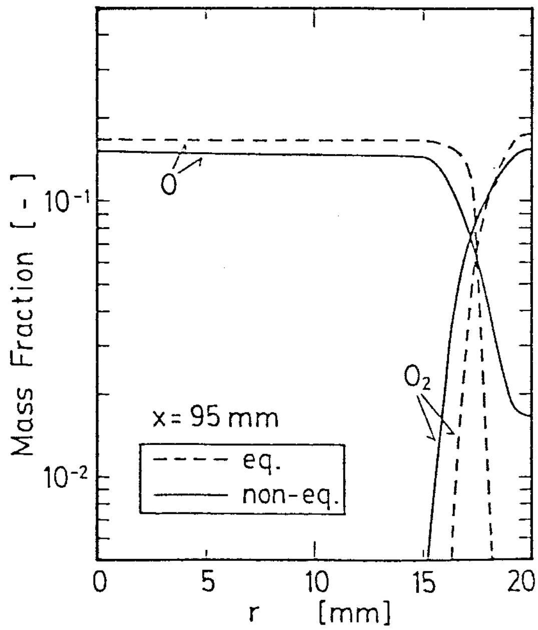

Fig. 4 Mass fraction of O_2 and O for the kinetic and the equilibrium models.

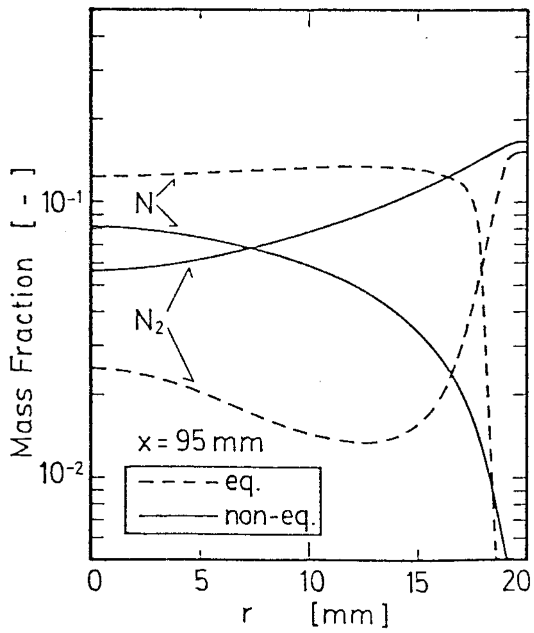

Fig. 5 Mass fraction of N_2 and N for the kinetic and the equilibrium models.

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