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Citation for published version (APA):
Benoij, D. A., de Jong, E. C. J. N., Fey, F. H. A. G., Mullen, van der, J. J. A. M., & Schram, D. C. (1992). On the modelling of flowing thermal plasmas, applied to an inductively coupled plasma. *Journal of High Temperature Chemical Processes*, *1*(3, supplement), 367-372.

Document status and date:
Published: 01/01/1992

Document Version:
Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
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JOURNAL OF HIGH TEMPERATURE CHEMICAL PROCESSES
Colloque, supplément au n°3, Vol 1, Septembre 1992

On the modelling of flowing thermal plasmas, applied to an inductively coupled plasma

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ABSTRACT

The influence of radiative energy losses on the flow and temperature fields in thermal plasmas is reported in this study. The total radiative energy loss in pure argon is calculated with a numerical collisional radiative (CR) model. The flow and temperature fields are calculated numerically for an inductively coupled plama (ICP) which is driven by a 100 MHz *RF* field.

RÉSUMÉ

L'influence des pertes d'énergie radiative dans l'écoulement et dans la distribution en température des plasmas thermiques a ici suscité notre attention. L'énergie radiative totale perdue dans l'argon pur a été calculeé numériquement dans le cadre d'un modèle collisionnel radiatif. L'écoulement et la distribution en température sont calculés numériquement pour un plasma couplé par induction gouverné par un champ *RF* de 100 MHz.

1. INTRODUCTION

The use of thermal argon plasmas can be found in various number of applications. The inductively coupled plasma (ICP) and the expanding cascaded arc are well-known in the field of spectrochemical analysis and deposition of carbon or silicon based films, respectively. In the theoretical study of these plasmas the processes which causes deviations from local thermal equilibrium (LTE) and especially their influence on the flow and temperature fields are investigated. Much attention has been paid to modelling with respect to the understanding of the physical processes and the optimalization of the operation conditions in the various applications. In the characterisation of (thermal) plasmas the knowledge of both the electron and heavy particle temperature is required with respect to elementary balances and transport phenomena, respectively /1/.

To calculate the flow, particle density and temperature distributions a mathematical laminar model is used in which the plasma is considered to be stationary, 2-dimensional axi-symmetric, quasi neutral and is represented by a continuous fluid. Further a 2-temperature model is used to take into account the deviations from LTE. Due to the relatively high frequency of the *RF* field the skindepth is smaller than the radius of the plasma so that a 2-dimensional self consistent electromagnetic field model must be used to calculate the energy incoupling /2,3/. A numerical approach is used to solve the macroscopic mass, momentum and energy balance equations. The model is applied to an ICP. In Fig.1 a schematic view of the ICP is given.

In a recent paper of Proulx et al /4/ it is

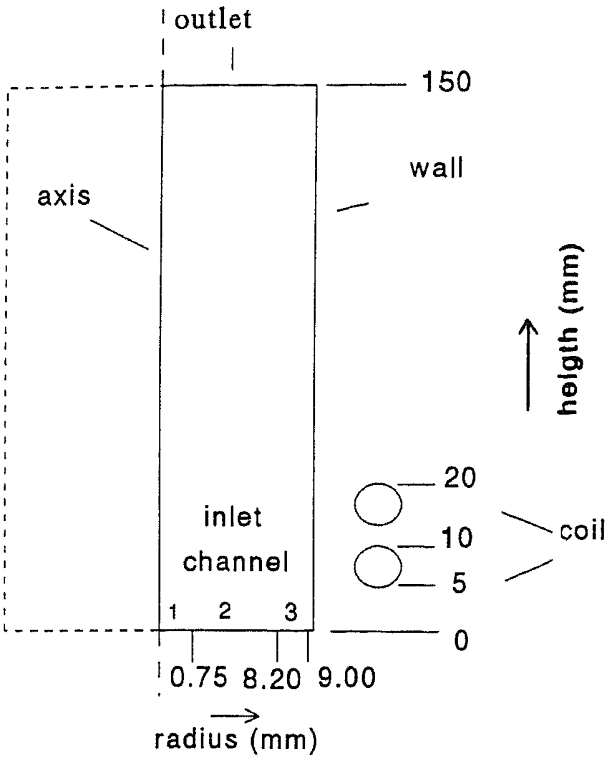

Figure 1. *ICP setup*

shown that the total radiative losses have considerable effect on the energy balance and on the electron number density when the plasma pressure is relatively high such as in thermal plasmas. The total radiative energy loss for wavelenghts from 100 nm to 100 μm is calculated using a collisional radiative model /9,10/. In this way non-equilibrium features on the microscopic level of the atomic state distribution function in the ionizing as well as the recombining part of the plasma are well described.

2. MATHEMATICAL MODEL

Symbols

$\vec{\mathbf{B}}$	magnetic induction
D_A	ambipolar diffusion coefficient
$\vec{\mathbf{J}}$	electric current density
k	Boltzmann constant
n_a	neutral particle numberdensity
n_e	electron number density
n_+	ion number density
p	pressure
S	energy source term
S_{CR}	volumetric ionization coefficient
T_e	electron temperature
T_a	heavy particle temperature
$\vec{v}$	plasma velocity

Greek symbols

α_{CR}	volumetric recombination coefficient
κ_e	electron therm. cond. coef.
κ_a	heavy particle therm. cond. coef.
ρ	density
σ	viscosity tensor

2.1. *Equations*

The five governing transport equations which describes the plasma flow are /5/
mass balance :

$$\vec{\nabla}\cdot(\rho\vec{\mathbf{v}}) = \mathbf{0} \tag{1}$$

$$\vec{\nabla}\cdot(n_e\vec{\mathbf{v}}) - \vec{\nabla}\cdot(\mathbf{D_A}\vec{\nabla}\mathbf{n_e}) = n_e n_a S_{CR} - n_e n_+ \alpha_{CR} \tag{2}$$

momentum equation :

$$\vec{\nabla}\cdot(\rho\vec{\mathbf{v}}\vec{\mathbf{v}}) = -\vec{\nabla}\mathbf{p} + \vec{\nabla}\cdot\sigma + \vec{\mathbf{J}}\times\vec{\mathbf{B}} \tag{3}$$

energy equations :

$$\vec{\nabla}\cdot(\frac{3}{2}\mathrm{n_s k T_s}\vec{\mathrm{v}}) - \vec{\nabla}\cdot(\kappa_\mathrm{s}\vec{\nabla}\mathrm{T_s}) = \mathrm{S(T_s)} \tag{4}$$

where the subscript s stands for electrons or heavy particles. The coefficients S_{CR} and α_{CR} which are in general functions of T_e, T_a, n_e and n_a can be obtained from a collisional-radiative model /6/ and reflect the coupling between the microscopic and macroscopic balance equations. In addition the Maxwell equations for the 2-dimensional EM-field have to be solved simultaneously with Eqn's (1)-(4). Frost's mixture rules are used to calculate the electron transport coefficients and the heavy particle transport coefficients are calculated by Devoto /7/. The source term in the electron energy balance contains the ohmic heating term, elastic energy transfer to the heavy particles, whereas the inelastic contribution and the viscous effects are neglected. For the heavy particles th energy source term contains viscous dissipation and the elastic energy transfer from the electrons. A significant contribution of the inelastic term in the active ionizing zone of the ICP where the temperature is of the order of 8000 K is the radiative energy loss term /8/. For the temperature of interest in the ICP the argon radiation data shows considerable scatter. In the model of Ref.9 in which continuum emission and line radiation are included the plasma is assumed to be in partial LTE which means that the higher excited levels of the neutral system are in Saha equilibrium with the ion ground state. The plasma is optically thin except for the resonance transitions for which the plasma is optically thick. They obtained a simple expression for the total radiative loss valid down to 3000 K. It is not difficult to extend their model to more general plasma conditions valid for ionizing and recombining systems by using a CR-model in which the lower levels of the atomic system are calculated numerically while the upper levels of the atomic system obey an analytical relation /10/.

2.2. Boundary Conditions

The torch has three inlet channels. The argon flow rate at the central channel is $0.2\ell/min$, at the intermediate channel $0.6\ell/min$ and the outer channel $12\ell/min$. At the inlet the heavy particle temperature is 350 K, the axial derivatives of electron density and temperature are zero. On the axis of symmetry the radial velocity component and the gradient of all other variables are zero. At the wall position the velocity is zero, no electron heat flux, the heavy particle heat flux is determined by the wall heat conductivity and a given ionization degree of 10^{-5} is used to determine n_e. At the exit of the torch the axial derivatives are set to zero. The total power input in the ICP is taken to be 500 Watt.

2.3. Solution Procedure

Equations (1)-(4) together with the Maxwell equations for the energy incoupling, are solved by the control volume method as described by Patankar /11/. The non-staggered grid approach of Rhie /12/ is incorporated in the SIMPLE algorithme and an orthocurvilinear coordinate system is used. The flexibility of the model can be enlarged by gridgeneration so that an uniform grid can be used always to increase the accuracy.

3. RESULTS AND DISCUSSIONS

For the computational region an uniform grid of 30×20 points is used as a first step, in axial and radial direction, respectively. For the calculations an IBM RISC 6000 system is used. To test our model a calculation is performed in which the ICP configuration of /13/ is implemented. The results were in excellent agreement.

An important difference with our ICP configuration is the operation frequency of the applied field which is 100 MHz whereas it is 3 MHz in /13/. As a result the skindepth in our ICP configuration is of the order of 1 mm while the plasma radius is 9 mm. The energy dissipation is then constricted to a rather small part of the plasma near the wall so that the influence of diffusive transport in that part is considerable and the computational grid might be too coarse. The calculated quantities of main interest from the experimental point of view, are the electron temperature and electron density as a function of the radius. In Fig.2 radial profiles of T_e are shown for 3 different axial positions calculated with the radiative loss according to Miller and Ayen /14/ while in Fig.3 radial n_e profiles are shown for the same axial positions. As can be seen from figures 2 and 3 T_e and n_e have their maximum between 7 and 8 mm for the position 5 mm above load coil (alc). Experimental results show /15/ that T_e and n_e have their maximum for smaller radii, i.e. 6mm so that cooling near the wall or transport to the center is missing in the

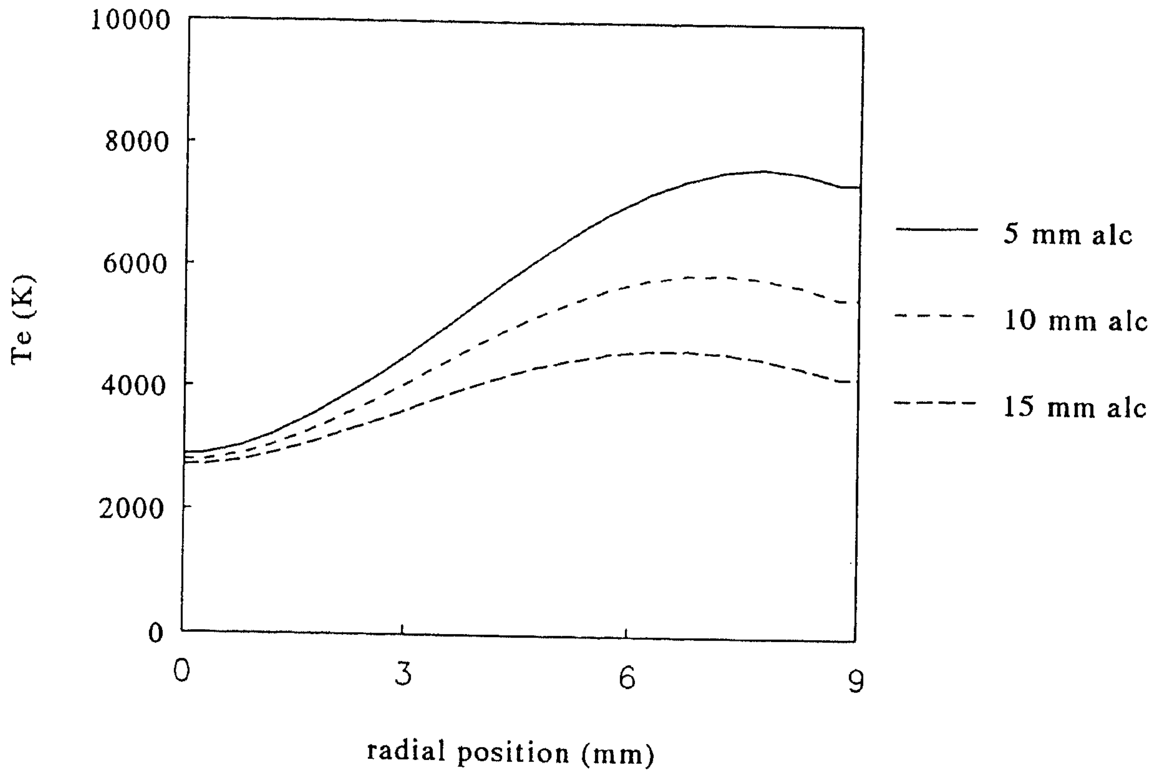

Figure 2. *Radial* T_e *profile*

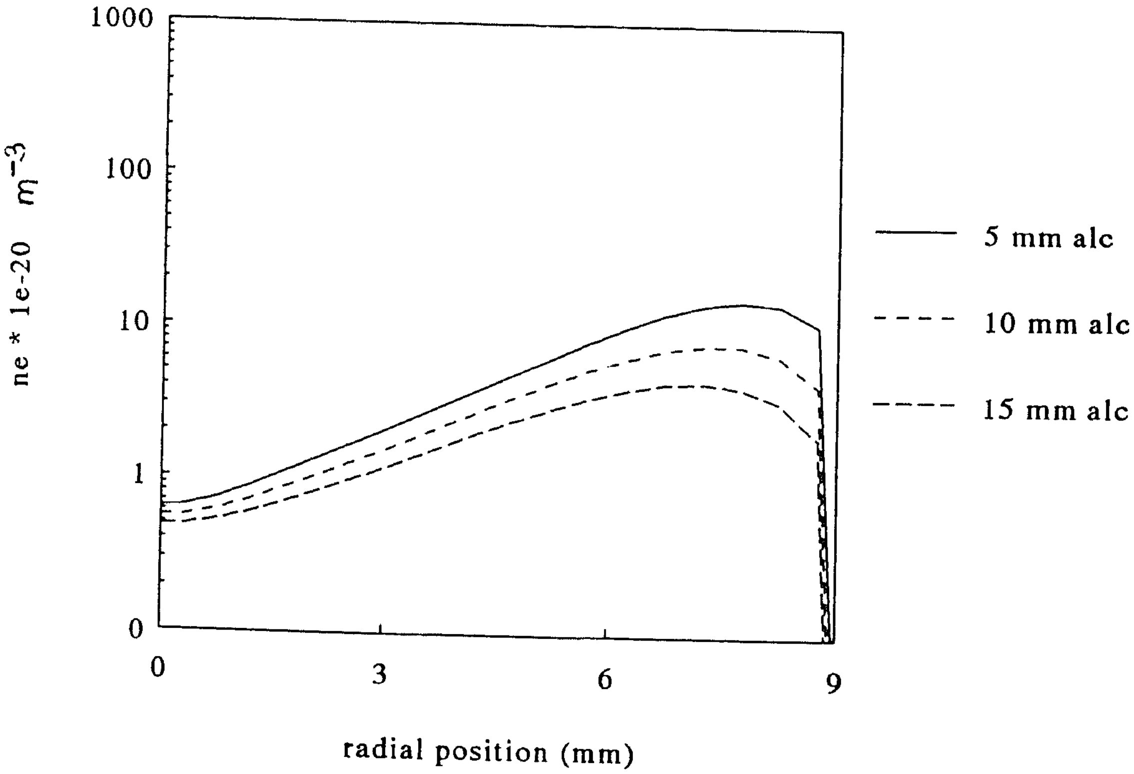

Figure 3. *Radial* n_e *profile*

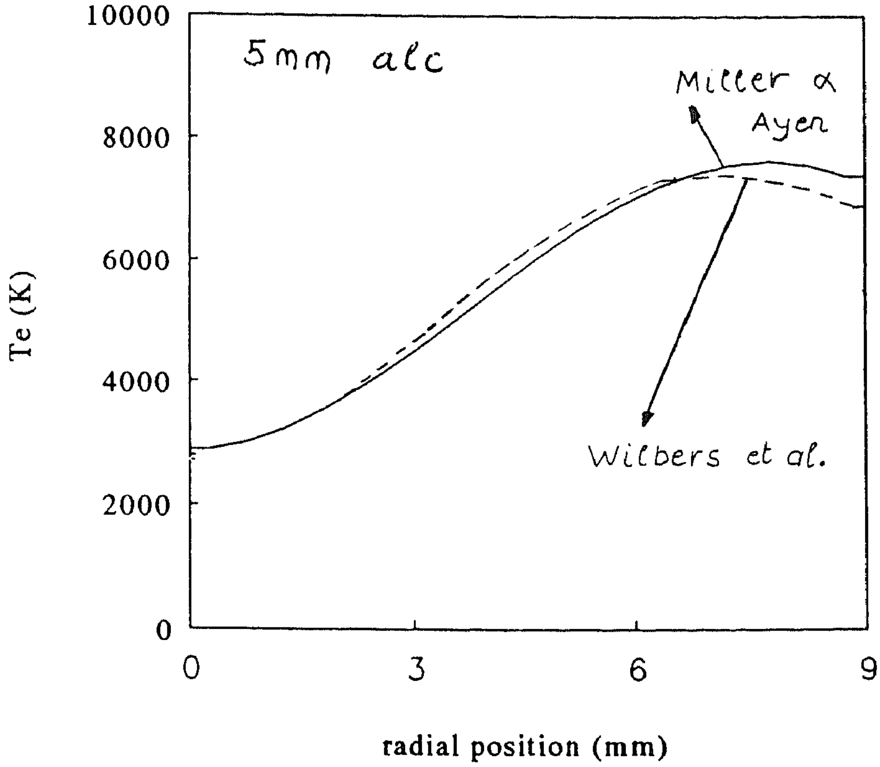

Figure 4. *Radial T_e profile. A comparison between /9/ and /14/*

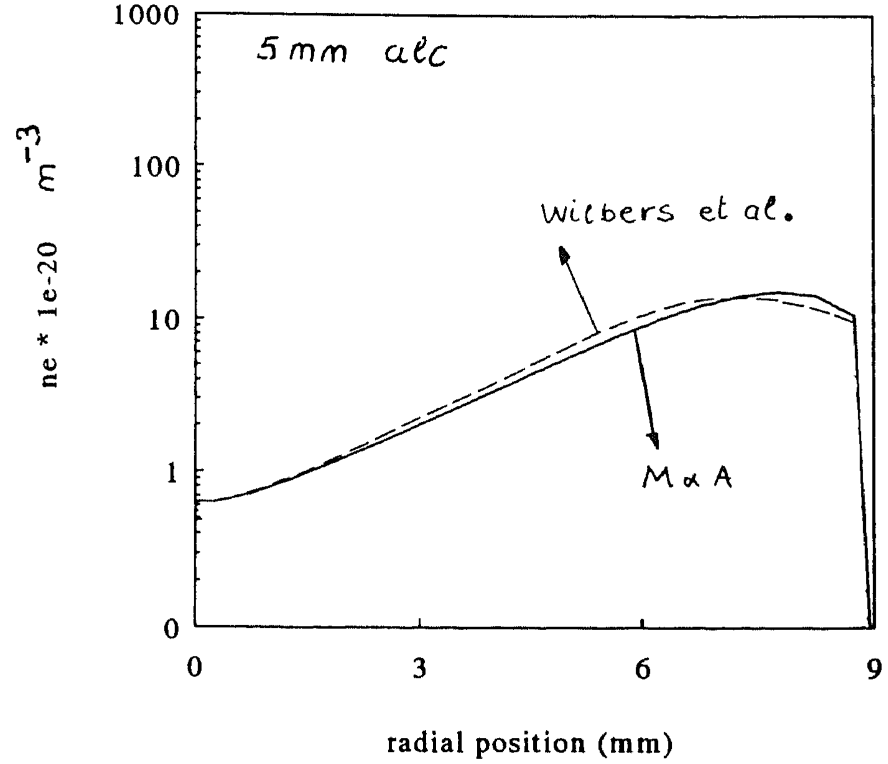

Figure 5. *Radial n_e profile. A comparison between /9/ and /14/*

model. We will focus on the effect of radiative losses on the cooling of the plasma. In the data of /9/ the radiative losses are extended to the lower temperatures (3000 K) while in /14/ the radiative loss has a cut-off at much higher temperatures so that more energy will be lost when data of /9/ are used. In figures 4 and 5 the radial profiles of T_e and n_e are shown, calculated with the radiative losses according to /9/ and /14/ at the axial position 5mm alc. As expected the overall temperature field is decreased and the profile maximum is moved towards a smaller radius. The same effect can be seen for the electron density profile.

4. CONCLUSION

For a 100MHz driven ICP the typical maxima in the T_e and n_e profiles are too close to the plasma wall due to the small skindepth when radiative data of /14/ are used. When data of /9/ are used the maxima are located at smaller radii but still too large compared with experimental values of /15/.

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