Modelling in thermal plasma and electric arc column

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Abstract - This paper presents modelling attemps related to atmospheric-pressure thermal plasma with the aim of calculating high-power arcs. It begins with a short presentation of the basic equations, used for the prediction of laminar thermal plasma flows, which account for the electromagnetic source terms. Then, a two-temperature model, assuming chemical (ionization) equilibrium, is applied to the two-dimensional prediction of argon arc columns using full nonequilibrium equations for the cathode sheath region in order to get proper boundary conditions. After a short review of the approaches developed for the turbulence modelling in thermal plasma, the paper presents an exploration, performed for transferred argon arcs, of the capabilities of two-equation turbulence models to account for the laminarization process due to large variations of the viscosity.

INTRODUCTION

The analysis of thermal plasma flows by means of numerical methods has been a growing field of research in the last ten years, as well in the field of plasma jets mixing with cold flows as in the field of plasma flows interacting with electric and magnetic fields. But we must notice that many practical characteristics of such flows increase the difficulty in doing numerical predictions, as for instance :

- large variations of the thermodynamic properties (density, specific heat, viscosity...) ;
- thermodynamic and chimical non-equilibrium situations ;
- presence of both laminar and turbulent regimes in the same flow field ;
- complex geometries with strong wall-plasma interactions ;

- reacting two-phase flows.

The purpose of this paper is to present new developments achieved in our laboratory in the field of the numerical modelling of non-equilibrium situations and turbulent plasma flows, with a special aim of calculating atmospheric-pressure arc column.

BASIC EQUATIONS

At atmospheric pressure, the plasma is generally collision dominated : the mean free path for all species are much smaller than the macroscopic characteristic lengths. Therefore, the plasma can be viewed as a continuum fluid and described by relatively few mixture balance equations obtained by summing over the equations of all individual species.

Mass balance : $\frac{\partial}{\partial t} \rho + \operatorname{div} \rho \stackrel{\rightarrow}{u} = 0$

where ρ the mass density, and u_i (i = 1, 3) are the local instantaneous velocity components.

Momentum balance : $\rho \frac{\partial}{\partial t} \vec{u} + [\rho \vec{u}, \overrightarrow{\text{grad}}] \vec{u} = -\overrightarrow{\text{grad}} p + \overrightarrow{\text{div}} \vec{\tau} + \rho \vec{g} + \vec{j} \wedge \vec{B}$

where p is the local pressure, g is the gravity acceleration and the last term on the right-hand side of the equation accounts for the electromagnetic forces of Lorentz,

 τ_{ii} is the momentum diffusion tensor which is generally written using a single dynamic viscosity µ.

In our approach (Delalondre and Simonin, 1990), the calculation of a non-equilibrium boundary layer is performed on a local one-dimensional subgrid defined at each cathode wall point, in oder to get proper boundary conditions for the full computation of the arc column by coupling with the two-dimensional computation of the heat transfer in the solid.

Thus, the boundary-layer equation for a laminar two-temperature plasma in presence of an electric field perpendicular to the solid wall, are obtained by simplifying the general set of thermodynamic and electromagnetic non-equilibrium equations. As the global neutrality of the plasma is assumed for the derivation of the boundary-layer equations, the model does not not include the simulation of the space charge zone which takes place very close to the electrode, in the order of the electron mean free path length from the cathode surface (Hsu and Pfender, 1983a). However, suitable wall boundary conditions for the subgrid model may be derived from the detailed analysis of the dominating mechanisms occuring in the space charge subzone (Delalondre, 1990).

Electron number density balance :

$$\frac{\partial}{\partial t} n_e - \frac{1}{e} \frac{\partial}{\partial y} j_{ey} = I_e \qquad I_e = k_{re} n_e \Big[n_a K_{eq} - n_e n_i \Big]$$

where I_e is the production rate of electrons which accounts for ionization by electron impact and three body recombination mechanisms, k_{re} is the recombination rate coefficient and K_{eq} the equilibrium constant given by Saha's law in terms of the electronic partition functions. According to the global neutrality assumption, we don't have to solve the balance equation for

According to the global neutrality assumption, we don't have to solve the balance equation for the ion number density $(n_i = n_e)$, and the atoms number density n_a is obtained by assuming a constant pressure in the boundary layer.

In the cathode sheath, the Ohm's law approximation is inaccurate for prediction of the electronic or ionic current density, diffusive contributions must be taken into account, thus for instance the electronic current density is written

$$j_{e,y} = \sigma_e E_y + \frac{\sigma_e}{n_e e} \frac{\partial}{\partial y} n_e k_B T_e \qquad \sigma_e = \sqrt{\frac{\pi}{8 k_B T_e m_e}} \frac{n_e e^2}{\left[n_i Q_{ei} + n_a Q_{ea}\right]}$$

where σ_e is the electronic conductivity calculated in terms of Q_{ei} and Q_{ea} , the electron-ion and electron-atom momentum transfer cross sections. The conservation of the vertical component of the total current density in the boundary layer leads to write the local electric field E_y , from the current densities expressions, in terms of the number densities and the temperatures of the individual species. Finally, we have to solve a single transport equation for the electron number density n_e , whereas n_i , n_a , $j_{e,y}$, $j_{i,y}$ and E_y may be obtained analytically.

Electron energy balance :

$$\frac{5}{2}k_{B}n_{e}\frac{\partial}{\partial t}T_{e} - \frac{j_{ey}}{e}\frac{5}{2}k_{B}\frac{\partial}{\partial y}T_{e} = \frac{\partial}{\partial y}\lambda_{e}\frac{\partial}{\partial y}T_{e} + j_{ey}E_{y} - S_{Rad} - E_{coll} - I_{e}\left[E_{io} - \frac{5}{2}k_{B}\omega_{e}(T_{L} - T_{e})\right]$$

Heavy species energy balance :

$$\frac{5}{2} k_{B} \Big[n_{a} + n_{i} \Big] \frac{\partial}{\partial t} T_{L} = \frac{\partial}{\partial y} \lambda_{L} \frac{\partial}{\partial y} T_{L} + j_{i,y} E_{y} + E_{coll} - I_{e} \Bigg| \frac{5}{2} k_{B} T_{e} + \frac{5}{2} k_{B} \omega_{e} \{ T_{L} - T_{e} \} \Bigg|$$

 E_{coll} is the energy exchange rate between the electrons and the heavy species through elastic collisions, and can be written

$$E_{coll} = -n_{e} \Big[n_{i} Q_{ei} + n_{a} Q_{ea} \Big] \sqrt{\frac{8 k_{B} T_{e}}{\pi m_{e}}} \frac{2 m_{e}}{m_{i}} \frac{3}{2} k_{B} (T_{L} - T_{e})$$

Total radiative dissipation S_{Rad} and energy transfer during ionization/recombination processes (proportional to the ionization rate I_e) are assumed to be mainly lossed from electrons. The term in factor of ω_e represents the thermalisation (at T_e) of electrons emitted from the atoms at the temperature T_L ($\omega_e = 0$ if $I_e < 0$ and $\omega_e = 1$ if $I_e > 0$).

Finally, the previous non-equilibrium equations set is solved on a one-dimensional subgrid defined at each cathode wall point and coupled to the two-dimensional arc column prediction through the input conditions imposed at the top of the boundary layer.

Computations were first performed for free burning and transferred argon arcs under atmospheric pressure, using the L.T.E. assumption in the arc column calculation (Delalondre and Simonin, 1990). Numerical predictions of the temperature in the arc column compare favorably with available experimental data (Hsu and Pfender, 1983b; Coudert and Grimaud, 1989). The subgrid model results correspond to realistic description of the cathode sheath, thus the deviation from kinetic equilibrium is clearly represented on figure 2. The electrons temperature stays nearly constant in the sheath, while the heavy species temperature goes down near the wall with respect to the heat flux transferred to the cathode.

Energy balance :

$$\rho \frac{\partial}{\partial t} h + \rho \vec{u} \operatorname{grad} h = \frac{\partial}{\partial t} p + \vec{u} \operatorname{grad} p - \operatorname{div} \vec{Q} + \Pi$$

where h is the mass enthalpy of the mixture, Π is the enthalpy source term due to radiative transfer and Joule heating,

Q is the thermal diffusion flux which accounts for the macroscopic transport of enthalpy resulting from inhomogeneities in the temperature field, but also from local inequalities of





figure 2 : Laminar L.T.E. prediction of a free burning argon arc (Hsu and Pfender, 1983b)

 $\vec{Q} = -\lambda \overrightarrow{\text{grad}} T - \vec{j} \frac{5}{2} \frac{k_B}{e} T$

where λ is the thermal conductivity, j is the total current density, e is the elementary charge and k_B is the Boltzmann constant.

In order to calculate the electromagnetic field, Maxwell's equations need to be solved. However, simplified equations may be derived according to the global neutrality assumption and by using the Ohm's law approximation.

Electric charge balance :

div
$$j = 0$$
 with $j = -\sigma \operatorname{grad} V$ (Ohm's law)

where σ is the electrical conductivity and V the electric potential.

Magnetic field equation :

 $\operatorname{curl} \vec{B} = \mu_0 \vec{j}$

Finally, the equations set must be completed by a state equation, which allows to compute the local mass density, temperature and transport coefficients (such as the dynamic viscosity and the electrical conductivity) in terms of the pressure and the enthalpy of the mixture. However, these direct relations may be established only in the frame of the L.T.E. assumption, when there is a strong collisional coupling for energy exchange between electrons and heavy particles, including chemical reactions such as ionization and recombination. These conditions are generally satisfied, for the case of atmospheric-pressure plasma jets in industrial configurations, according to the large electron number densities and the relatively low velocities encountered in such flows. On the other hand, because of the sharpness of the temperature gradient, substantial deviations from kinetic and ionization equilibrium have to be expected in the fringes of the arc column and near the electrode walls, and must be included in a realistic description of high-power electric arcs.

NON-EQUILIBRIUM MODELLING

The first attempts to model high-power arcs were based on the L.T.E. assumption, and the comparisons of the predicted temperature with experimental results showed a fairly good agreement which indicates that local thermodynamic equilibrium is a valid assumption in the arc column especially in the core of the arc. However, the results are depending on the boundary conditions and the most significant input parameter is the current density distribution at the cathode wall which can not be obtained from measurements. As a matter of fact, near the cathode surface, there is a thin layer which is characterized by steep gradients of temperature, species densities and electric potential. Its thickness is in the order of 0.1 mm and over this thickness a number of important physical processes occur which cannot be taken into account by using the L.T.E assumption.

However, discrepancies between numerical predictions and experimental results may be observed in the fringes of the arc column where the L.T.E. assumption is not valid. And the other hand, results of the subgrid model show that the assumption of L.T.E. at the top of the boundary layer may be inaccurate. Thus, a non-equilibrium model is actually under development for the two-dimensional prediction of the arc column. In a first step, the plasma is assumed in chimical equilibrium and the composition field is determined directly from the multi-temperature Saha equation (Hsu and Pfender, 1983b). Large discrepancies between the electrons and heavy particles temperatures are found in the arc fringes of transferred arc predictions (figure 3) but the differences observed between the heavy species temperature predictions based on the two-temperature model and those derived from a L.T.E. model are not really significant. On the other hand, the separate coupling of the two-temperature computed in the arc column with the ones computed in the subgrid model leads to more realistic treatment of the deviation from kinetic equilibrium close to the cathode.





TURBULENCE MODELLING

In the case of plasma turbulent flows characterized by fluctuations in velocity, temperature and composition, the only properties accessible to the numerical predictions are the averaged ones. In variable density flows, governing equation are generally derived directly from the local instantaneous balance equations of mass, momentum and energy by applying a densityweighted averaging operator (Favre averaging). This averaging process leads to the introduction of further terms in the balance equations, generally diffusive in character, which account for the transport of mass, momentum and energy by the turbulent motion. The possible use for turbulence modelling of methods extended from incompressible flow situations needs to be accuratly validated. And the validation process should account separatly for the main characteristics of such flows. Thus, for instance, in order to analyse the influence of large density variations, experiments are carried out in our laboratory on the mixing of inert gases with large density differences (He-CO₂), and experimental results are compared with predictions of a Reynolds stress transport equation model (Viollet et al., 1990). And the other hand, the k-e model is nowadays extensively used for three-dimensional industrial applications (Lana and Viollet, 1985; Gabillard et al., 1989) and comparisons with experimental results show that the k-e model allows realistic simulations of the threedimensional mixing of fully turbulent thermal plasma jets in cold flows (Lana and Kassabji, 1987).

But turbulence modelling must also account for the transport coefficients dependence on the local temperature as observed in thermal plasma flows. Thus for instance, due to the large variations of the molecular viscosity, both the laminar and turbulent regime may be present in the same flow, when the standard k- ϵ turbulence model must be used in fully developed turbulent flow regimes. In the following, the capabilities of the standard and low Reynolds $k \cdot \epsilon$ turbulence models to account for the laminarization process are studied for transferred argon arcs. We must notice that no turbulent fluctuations in the electrical conductivity are considered at this stage of the investigation, which results in a considerable simplification to the problem.

Both the standard and low Reynolds k-e turbulence model are based on the eddy-viscosity assumption, which writes in a variable density flows :

$$\overline{\rho \, u''_{i} \, u''_{j}} = -\mu^{t} \left[\frac{\partial U_{i}}{\partial x_{j}} + \frac{\partial U_{j}}{\partial x_{i}} \right] + \frac{2}{3} \, \delta_{ij} \left[\overline{\rho} \, k + \mu^{t} \frac{\partial U_{m}}{\partial x_{m}} \right] \qquad \qquad \mu^{t} = -\overline{\rho} \, C_{\mu} \frac{k^{2}}{\epsilon}$$

where $U_i = \overline{\rho u_i}/\overline{\rho}$ is the Favre-averaging of the i-velocity component and u"_i the corresponding fluctuation.

The equations for the turbulent kinetic energy k and its dissipation rate ε writes under the following general forms valid for both models.

Turbulent kinetic turbulent energy balance :

$$\overline{\rho}\frac{\partial}{\partial t}k + \overline{\rho}U_{j}\frac{\partial}{\partial x_{j}}k = \frac{\partial}{\partial x_{j}}(\overline{\mu} + \frac{\mu}{\sigma_{k}})\frac{\partial}{\partial x_{j}}k + \mathcal{P} - \overline{\rho}\varepsilon + \Pi_{k} \qquad \qquad \mathcal{P} = -\overline{\rho}\frac{u''_{i}u''_{j}}{\partial x_{j}}\frac{\partial U_{i}}{\partial x_{j}}$$

where \mathbf{P} is the turbulence production rate by the mean velocity gradients.

Turbulence dissipation rate balance :

 $\overline{\rho}\frac{\partial}{\partial t}\varepsilon + \overline{\rho}U_{j}\frac{\partial}{\partial x_{j}}\varepsilon = \frac{\partial}{\partial x_{j}}(\overline{\mu} + \frac{\mu}{\sigma_{\varepsilon}})\frac{\partial}{\partial x_{j}}\varepsilon + \frac{\varepsilon}{k}\left[C_{\varepsilon,1}\mathcal{P} - C_{\varepsilon,2}\overline{\rho}\varepsilon\right] + \Pi_{\varepsilon}$ Finally, the turbulence model contains five empirical constants which are assigned the values

given in Table 1.

Table 1 : The standard values of the empirical constants

in the high-Reynolds number form of the k- ϵ turbulence model.

Cμ	C _{ε,1}	C _{ε,2}	σ _k	σ_{ϵ}
0.09	1.44	1.92	1.	1.3

According to Launder and Sharma (1974), the form of the standard k- ε model can be enlarged by making the empirical constants functions of the Reynolds number of turbulence R :

$$C_{\mu} = 0.09 \exp \left[-3.4/(1. + R/50.)^{2} \right] \qquad C_{\epsilon^{2}} = 1.92 \left[1. -0.3 \exp \left(-R^{2} \right) \right] \qquad R = \bar{\rho} k^{2} / \left[\bar{\mu} \epsilon \right]$$

And in order to provide predictions of the turbulence within the viscous layer adjacent to the wall, further empirical terms Π_k and Π_{ε} are added in the k- ε transport equations :

$$\Pi_{k} = -2\overline{\mu} \left[\frac{\partial \sqrt{k}}{\partial x_{i}} \frac{\partial \sqrt{k}}{\partial x_{i}} \right] \qquad \qquad \Pi_{\varepsilon} = 2\overline{\mu} \frac{\mu^{t}}{\overline{\rho}} \left[\frac{\partial^{2} U_{j}}{\partial x_{i}^{2}} \frac{\partial^{2} U_{j}}{\partial x_{i}^{2}} \right]$$

First computations were performed for transferred argon arcs under atmospheric pressure using both k- ε turbulence models in order to analyse the laminarization process. Boundary conditions set is nearly identical to the one used for previous laminar computations, except for the treatment of the mean velocity, the turbulent kinetic energy and the dissipation rate at the solid boundaries where a classical wall function method was used. Figure 4 shows the increase, along the vertical axis, of the eddy cinematic viscosity predicted by the standard k- ϵ model, with a maximum in front of the anode. On the contrary, low Reynolds number model predictions are fully laminar. Major discrepencies between the two computations correspond to an over-estimation by the high-Reynolds $k - \varepsilon$ turbulence model of the predicted temperature, just downstream the cathode (figure 4), and the computed heat flux transferred to the anode.



figure 4 : Turbulent L.T.E. prediction of a transferred argon arc (Coudert and Grimaud, 1989)

CONCLUSION

This paper presents modelling attemps related to atmospheric-pressure thermal plasma with the aim of calculating high-power arcs. According to comparisons with experimental results, the non-equilibrium description of the electrode sheath regions allows to get proper boundary conditions for two-dimensional modelling of electric arc column coupled with the heat transfer computation in the solid. And the other hand, further developments and validations are needed in order to improve the turbulence modelling in thermal plasmas since large variations of density and viscosity are observed in such flows. Thus, a laminarization process is observed in transferred argon arcs which cannot be taking into account by the conventional high-Reynolds number form of the k- ε turbulence model.

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