A numerical tool for plasma spraying. Part I: modelling of plasma jet and particle behaviour.

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Abstract.
The current models of plasma spraying are generally complex and time-consuming, especially when they use a 3-D geometry and elliptic solvers. Therefore, these models are difficult to use as a tool to engineer specific coating properties and optimise the operating conditions of the spray systems. However, various clever numerical methods were developed in the past to simulate 2-D parabolic gas flow as laminar boundary layers or jets. For example, the *Genmix* algorithm developed by Spalding and Patankar and known as the *Bikini method* necessitates a very low-cost memory algorithm. This algorithm makes, it possible when using the right thermodynamics and transport properties of plasma gases, to predict in a fast and rather realistic way, the velocity and temperature fields of the plasma jet. The first part of this paper deals with the validation of the predictions for plasma jets obtained with the Genmix 2-D computational fluids dynamics code from experimental results and 3-D predictions obtained with the *ESTET* 3.4 CFD *ESTET* code

1. Introduction

Mathematical models of the atmospheric pressure plasma spray process have existed for almost twenty years [1-3]. Three modelling regions have to be considered [4] i.e. the electrode region, the plasma jet and its plume region where particles are injected, accelerated and heated and at last the region where the coating is generated. The first region is very difficult to model [4, 5] because of the non equilibrium phenomenon at the electrodes and the three dimensional (3D) transient behaviour of the arc connecting column to the anode. The coating generation modelling is still in its infancy even if sophisticated 3D models for a single particle flattening and cooling have been recently developed [6]. The plasma jet region modelling is probably the most developed one. The plasma flow is usually modelled by using low Reynolds k-ε codes to account for the laminar structure of the jet core and its turbulent one in the jet fringes and plume; the particle injection orthogonally to the jet, requires a 3D modelling [7]. In spite of a few problems which are not yet solved such as the engulfment process of the cold surrounding gas, the dispersion of the particles trajectories due to their size and velocity distributions as well as their collision between themselves and the injector wall, the particles parameters at impact are rather well modelled. It is now well recognized that these parameters: diameter, velocity and temperature control coating properties and reproducibility [8]. However the main drawbacks of the existing sophisticated codes is the computing time which is not compatible with industrial needs. That is why there is boom for simplified models able to give quickly (in few seconds) at least good trends. This is the goal of this paper.

Various clever numerical methods were developed in the past to simulate 2-D parabolic gas flows for laminar boundary layers or jets. For example, the *Genmix* algorithm developed by Spalding and Patankar [9] and known as the *Bikini method* requires a very low-cost memory and computing time. This algorithm makes it possible, when using the proper thermodynamics and transport properties of plasma gases, to predict in a fast and rather realistic way, the velocity and temperature fields of the plasma jet. The first part of this paper deals with the validation of the predictions for plasma jet velocity and temperature distributions obtained with the Genmix 2-D axi-symmetric computational fluid dynamics code (CFD) through their comparison with experimental results and 3-D predictions obtained with the *ESTET* 3.4 code.

2. Simulation of the temperature and velocity distributions of the plasma flame

The fast software Jets&Poudres [10] is build on the GENeral MIXing (Genmix) computer code, improved by using thermodynamic and transport properties closely related to the local temperature and composition. These properties are obtained from the T&TWinner data base [11].

2.1 Description of Jets&poudres plasma jet simulation

Genmix handles the two-dimensional, parabolic flows, i.e., those of high Reynolds and Peclet numbers, with not recirculation. "parabolic" flows are:

- steady,

- predominantly in one direction, defined as that in which the velocity vector has nowhere a negative component; and
- without recirculation or diffusion effects in that direction.

These conditions can be used as a first approximation of plasma jets, where the Reynolds and Peclet numbers, based upon the cross-stream dimension are large. Genmix embodies a self-adaptive computational grid, which enlarges or contracts to cover only the regions of interest (hence it explains the relatively small demand on computing power and its nickname, i.e., the Bikini method). The turbulence can be simulated by different models, but in the case of a plasma jet it is the classical mixing length which appears to be the simplest and the fastest.

In Jets&poudres the input data are:

- the mass flow rate m_0^p and the composition of the plasma forming gas,
- the composition of the gas atmosphere far away from the jet,
- the electric current intensity I,
- the electric power P with such previous conditions (obtained from experiments),
- the efficiency of energy transfer to the gas ρ_{th}

Then the specific enthalpy $h = \rho_{th} P / m_0^p$ is calculated from the ratio of effective power $\rho_{th} P$ to the mass flow rate and the enthalpy temperature is obtained from the equilibrium properties at atmospheric pressure. From this temperature the specific volume of the gas is calculated and thus its mean velocity. Uniform radial profiles of temperature and velocity are assumed such as the gas enthalpy and mass flow rate at the nozzle exit are conserved. Whatever may be the profiles at the nozzle exit within a few tenth of mm the code creates its own profile independently of the starting ones.

2.2 Turbulence model and gas transport properties

Many models of turbulence with one, two or more equations can be solved with the Genmix code such as the k-ε model (two equations) or dissipation energy of Prandtl (one equation). In general all this models underestimate the surrounding atmosphere entrainment which is in fact of the engulfment type and not well represented by the classical models when the three components of the turbulent velocity are assumed to be equal. However because these models are not satisfactory even in the case of plume flows, a simple standard model of mixing length is used in Jets&poudres. In the mixing length hypothesis, each location in the flow is characterized by a value of the quantity l_m the mixing length, and the turbulent contribution to the effective viscosity, μ_t, is then calculated from the formula :

$$\mu_t = \rho l_m^2 \left| \frac{\partial u}{\partial y} \right|$$

In common applications of the mixing-length hypothesis, l_m is taken as uniform in radial direction but variable longitudinally. It is not the case with the flows described by the Genmix builder where l_m is allowed to vary as described in /9/. To take into account of the laminar behaviour of the jet core at high temperature the mixing length l_m is smoothed by a coefficient computed as $(300 / T(x,0))^{1/n}$ where T(x,0) is the temperature along the jet axis at the distance x from the nozzle exit and n is a factor of adjustment which has been chosen equal to 9 to match the best with the experiments.

The effective viscosity used is $\mu_{eff} = \mu_t + \mu_l$ where the three subscripts denote “effective”, “turbulent” and “laminar” respectively. For the transport properties other than viscosity, the effective ratio of Prandtl to Schmidt numbers σ is assumed to be constant. Further Γ_t may be calculated from $\Gamma_t = \mu_t / \sigma_t$, where σ_t is the turbulent Prandtl or Schmidt number assumed to be constant ($\sigma_t = 0.85$) and $\Gamma_{eff} = \Gamma_t + \Gamma_l$. Then the appropriate expression for σ_{eff} becomes:

$$\sigma_{eff} = \frac{\mu_t + \mu_l}{\mu_t / \mu_l + \Gamma_l}$$

The laminar values of the transport properties are expressed at each point according to the transport properties of the plasma gas and those of the surrounding atmospheric gas using a linear rule for each concentration. The transport properties of the plasma jet and its surrounding atmosphere are accurately forecasted from T&TWinner data base /11/.

2. 3. Comparison of the Jets&poudres plume model with the results of Estet3.4

A plasma jet and its plume has been computed using the sophisticated code Estet3.4 [8] for a flow rate of 45/15 slm Ar-H2, a nozzle internal diameter of ϕ= 7 mm, an effective power of 21.5 kW (65 V, 600 A, $\rho_{th} = 55\%$). The turbulence model of Estet was k-ε RNG and the 3D grid was 71, 88 and 71 according to the x, y, z directions. The Figures 2a, 2b, 2c compare the radial profiles of velocity, temperature and surrounding atmosphere concentration at 0.0004 m, 0.0222 m, 0.0314 m, 0.594m (thin lines) with the same computation with Jets&poudres (thick lines). It can be seen that for temperatures and velocities near the nozzle exit and far away from it the profiles are very close but at the intermediate axial distance (0.0314 m) the profiles are somewhat different. In fig. 3c it can be seen that the dilution of the plume by the surrounding atmosphere is more important in the forecast from Jets&poudres.

However it should be noted that Estet underestimates the experimental results obtained with an enthalpy probe at that distance.

Fig. 2d presents the comparison of the axial profiles for temperature and it can see that Estet code (Estet) or Jets&poudres (J) forecasts a smoother evolution of temperature than Jets&poudres with standard l_m (Jgenuine) in the intermediate axial distance from the nozzle exit. However with the modified mixing length the trend of Jets&poudres is the same as that given by Estet.

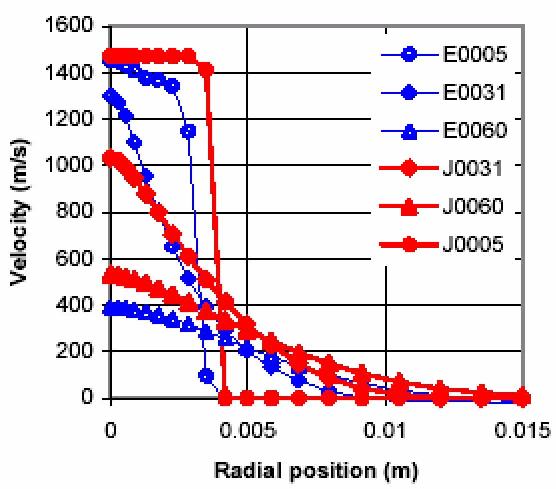


Figure 2a

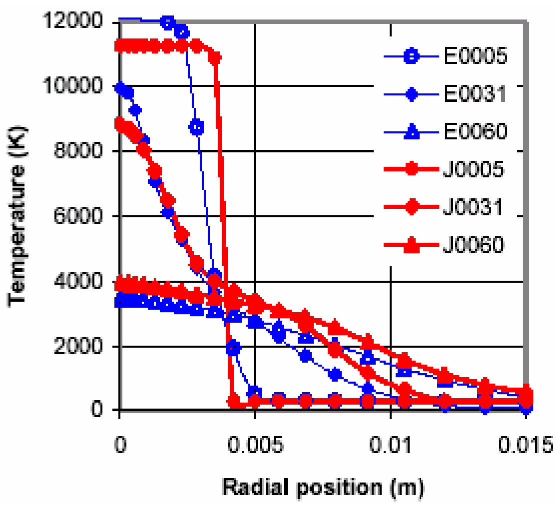
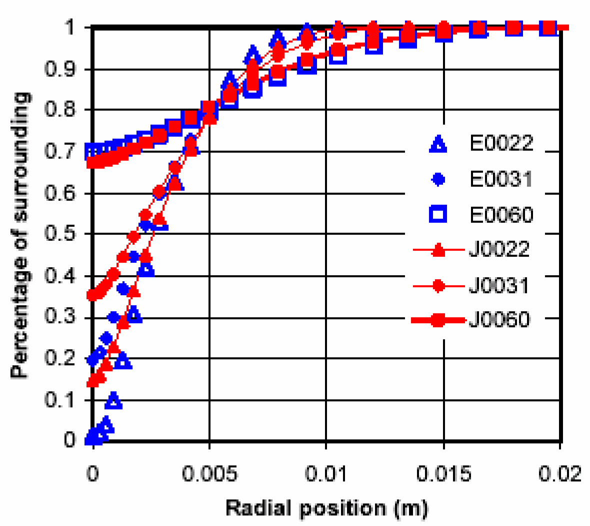


Figure 2b



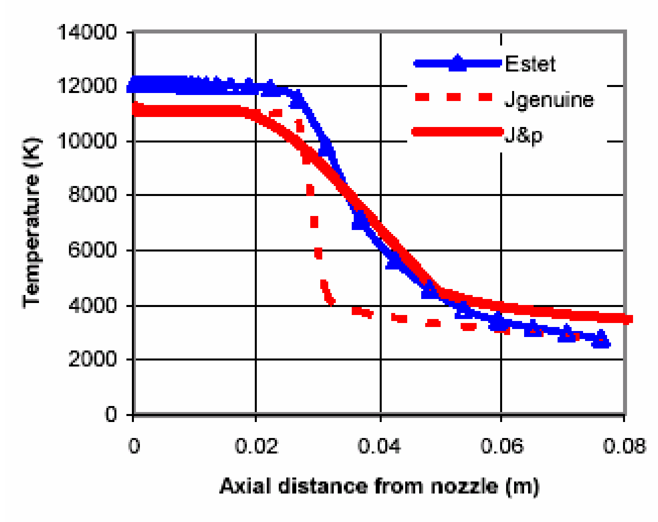


Figure 2c

Figure 2d

Figure 2. Radial distribution of velocity (a), temperature (b) and percentage of surrounding atmosphere (c) calculated with Jets&poudres (J curves) and Estet3.4 computer code (E curves) at different distances from the nozzles exit: E0022, J0022 at 0.0022 m, E0031, J0031 at 0.0031m, E0060, J0060 at 0.0060 m, for an Ar-H2 (45-15 slm, d.c. plasma jet, P= 36300 kW, $\rho_{th} = 0.50$, anode nozzle i.d.=0.0007 m.

(d) Comparison of the axial profile for temperature forecast by Estet code (Estet), Jets&poudres (J) and Jets&poudres with standard l_m (Jgenuine)

2.3 Comparison with other plasma jet plume

Jets&poudres allows to calculate many different plasma jets. In fig. 3a, 3b, 3c are presented the results of the calculations from Jets&poudres, those of the McKelliget's model [12] together with the experimental results for a Miller torch with the plasma jet flowing in air atmosphere with a plasma forming gas argon flow rate of 35.4 slm, an electric power of 7.4 kW and a thermal efficiency of 52 % and 8 mm nozzle diameter. It can be seen that the general tendency of Jets&poudres is to forecast a faster dilution in the surrounding atmosphere than the McKelliget's model. The two models frame the experimental results.

Figure 4 compares the measurements of Coudert [13] with the Jets&poudres code forecast of the axial temperature of a plasma jet for the following conditions flow rate of 81 slm Ar, 8 slm H2, I=550A, V=64V, efficiency = 58% in an surrounding atmosphere of air, nitrogen and argon respectively. It can be seen that in air atmosphere as it could expected, the temperatures are lower than in nitrogen atmosphere and that in argon atmosphere the temperatures are higher than in air or nitrogen atmosphere. The same tendencies are observed with the experimental data. However with both diatomic gases the Jets&poudres forecasts a much faster axial cooling than shown by the experimental points [14]. This is due to a faster surrounding atmosphere entrainment resulting in a fast cooling of the jet with nitrogen and oxygen dissociations.

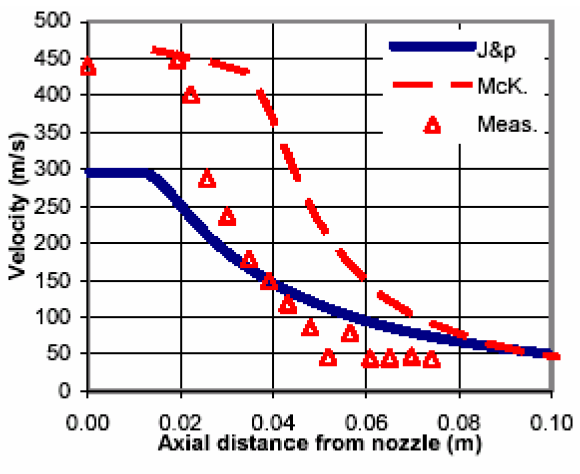


Figure 3a

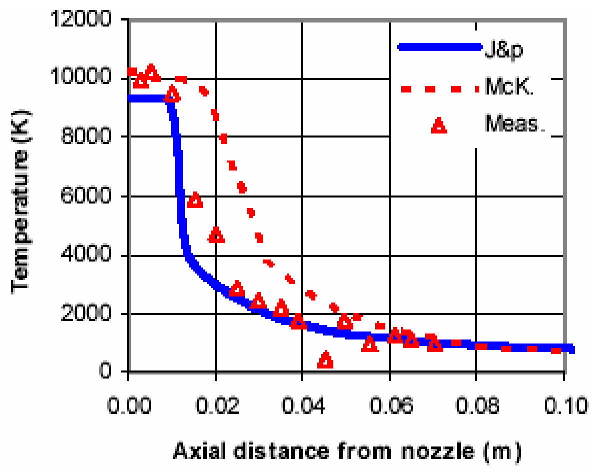


Fig 3b

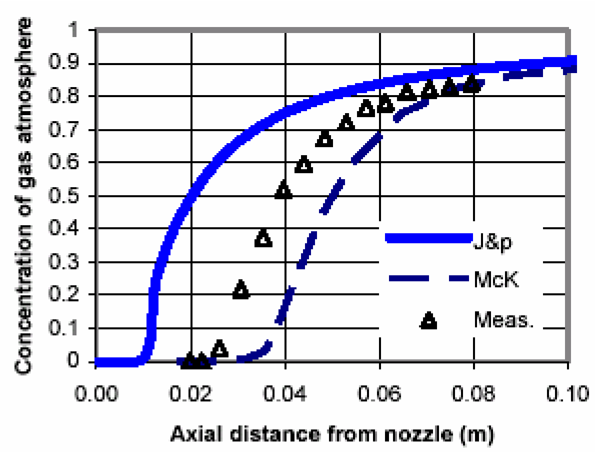


Fig 3c

Figure 3. Comparison of the axial velocity (a), temperature (b) and dilution of surrounding atmosphere (c) calculated by McKelliget's code (McK), Jets&poudres code(J&p) and measured (Mes.) for a Miller torch with a nozzle, d = 8 mm, P=7.4 kW, $\rho_{th} = 52\%$ and an argon flow rate of 35.4 slm in air.

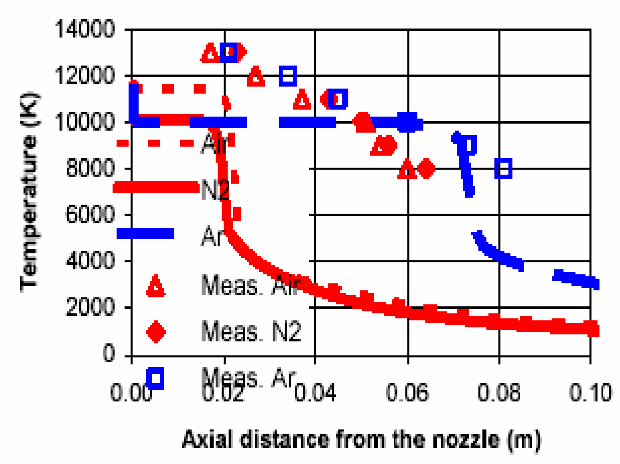


Figure 4. Jets&poudres code forecast of axial temperat Coudert [13] of a plasma jet with an Ar flow rate of 81 : H2, I = 550A, V = 64V, efficiency = 58% in surrou nitrogen an argon.

3. Conclusions

Compared to the 3D Estet code or the 2D code of McKelliget et al. which are elliptical models the simplified 2D parabolic model Jets&poudres gives the same trends for temperature and velocity distributions. However as for the most sophisticated codes its weakness is the way the mixing with the surrounding atmosphere is taken into account. By using a smoothing coefficient of the mixing length the Jet&poudres code match not too badly with the experimental results. Its major advantage compared to the 3D Estet code is its computing time which is three orders of magnitude shorter. As it will be seen in next part the calculation of the heat and momentum transfers to particles in flight are very fast and compare well with experiments which is probably due to the dumping of the plasma jet properties by the particles inertia

4. References

/1/ R. Westoff, G. Trapaga and J. Szekely, Met. Trans. B, 23B (1984) 683-693.

/2/ P. Fauchais, A. Vardelle and B. Dussoubs, J. Thermal Spray Technology **10** (1) (2001) 44-66.

/3/ P. Fauchais and A. Vardelle, IEEE on Plasma Science, **25** (6) (1997) 1258-1280.

/4/ G. Mariaux, E. Lrgros and A. Vardelle, *Modelling of coating formation and heat flux to substrate by particles and plasma jet in plasma spraying,* accepted in ITSC 2003 proc. (pub) ASM int. Mazterials Park, OH, USA (2003) ITSC 2003.

/5/ G. Mariaux, P. Fauchais, A. Vardelle and B. Pateyron, in Progress in plasma processing of materials, (ed. P. Fauchais, J. Amouroux (pub) Begell House, N.Y., USA (2001) 263-287.

/6/ P. Fauchais, M. Fukumoto, A. Vardelle and M. Vardelle, *Knowledge concerning splat formation*: An invited review, J. of Thermal Spray Technology 2003.

/7/ / M. Vardelle, A. Vardelle, P. Fauchais, K. I. Li, B. Dussoubs and N.J. Themelis, Journal of Thermal Spray Technol. **10** (2)(2001) 267-284.

/8/ P. Fauchais and M. Vardelle, *How to improve the reliability and reproducibility of plasma sprayed coating*, accepted ITSC 2003 Proc. (Pub.) ASM int. Material Park, Oh, USA (2003).

/9/ T&TWINner can be downloaded from http://ttwinner.free.fr

/10/ Jets&Poudres can be downloaded from http://jets.poudres.free.fr

/11/ S.V. Patankar & D.B. Spalding (1970) *Heat and mass transfer in boundary layers; 2nd edition*, Morgan-Grampian, London.
See also:
D.B. Spalding (1977),*GENMIX; a general computer program for two-dimensional parabolic phenomena,* Pergamon Press, Oxford.
GENMIX can be downloaded from CHAM's web-site from
http://www.cham.co.uk/website/new/genmix/genmix.htm

/12/ J.W. McKelliget, G. Trapaga, E.Gutierrez-Miravete, M. Cybulski, *An integrated mathematical model of the plasma spraying process*, Thermal Spray Meeting: the challenges of the 21st century (ed. C. Coddet) ASM International USA. (1998) 335-340.

/13/ P. Fauchais, J.F. Coudert, B. Pateyron, *La production des plasmas thermiques*, Rev. Gén. Therm. (1996) 35 543-560.

/14/ A. Denoirjean, O. Lagnoux, P. Fauchais, V. Sember, *Oxidation control in atmospheric plasma spraying: comparison between Ar/H2/He and Ar/H2* 15th International Thermal Spray Conference, Ed C. Coddet IPSE (Pub), ASM int. Oh. (USA) 1998; 809-814