

## Advances in Modeling of the Thermal Spray Process

## 1. Introduction

In past years there has been growing interest in thermal plasma processing of materials, including plasma spraying. In spite of problems in the thermal spray industry in past years, and the associated restructuring, this industry is still growing as the base of existing applications widens and new applications are explored. At the same time, there has been an increasing interest in process prediction by modeling.

Although this editorial will primarily deal with advances in modeling of the thermal plasma spray process, many of the following comments will also apply to other thermal spray processes (for example, HVOF and wire-arc spraying), as well as to thermal plasma processes in general, such as plasma synthesis of fine powders, plasma chemical vapor deposition, plasma metallurgy, or plasma waste destruction.

Conservation of materials and enhanced surface properties have been the major driving forces for developing plasma spray technology. In spite of the attractive properties of plasma sprayed coatings, the growth of this technology has been relatively slow for two reasons: there is still a lack of



E. Pfender

a solid engineering base in terms of control, reproducibility, and optimization of the thermal plasma spray process; and there is only a limited range of applications that appear to be economically viable, based on present technology. It is anticipated that recent advances in modeling of the plasma spray process will not only enhance our knowledge base, but they also should make vital contributions to-wards removing some of the previously mentioned obstacles that hamper the growth of this technology. Realistic models are crucial for establishing control parameters as well as for optimizing the process, eliminating the need for skilled and experienced operators.

## 2. Modeling of the Plasma Spray Process

The thermal plasma spray process may be divided into the following sequence:

- 1. plasma generation
- 2. particulate injection into the plasma and heating and acceleration of the particulates
- 3. coating formation on the substrate.

This editorial will be restricted to advances in modeling related to parts of this sequence.

The most common plasma generation process makes use of an electric arc operated between a stick-type cathode, and a nozzle-shaped anode, which represent the main components of a plasma torch (Ref 1). The plasma gas, introduced from the cathode end of the torch, is heated by the arc and this heated gas emanates from the torch as a plasma jet, which is the processing medium for the injected powder particles. In addition to electric arcs, high frequency, inductively coupled plasma may also be used for heating of the plasma gas (Ref 2, 3). In both cases, the plasmas produced within the torch are classified as thermal plasmas, i.e., the thermodynamic state of the plasma approaches local thermodynamic equilibrium (LTE). This concept of LTE has been extended to subsonic plasma jets operated at or near atmospheric pressure. There is, however, increasing evidence that the existence of LTE even in atmospheric pressure plasmas, is the exception rather than the rule. Both measurements and modeling confirmed deviations from chemical and/or kinetic equilibrium (Ref 1).

Although LTE modeling has been successfully applied under certain conditions (Ref 4-8), its applicability becomes questionable at higher plasma velocities, lower pressures, and in complex chemical reactions. Deviations from both chemical and kinetic equilibrium may become dominant effects in this situation as in supersonic plasma jets, for example (Ref 9, 10). Such departures from LTE will not only affect the characterization of plasmas in terms of temperature and velocity fields, but also particle heating (Ref 11). Studies of ionization and dissociation non-equilibrium in high-speed plasma jets (Ref 12), as well as studies of excited-state kinetics in conventional plasma jets (Ref 13); have been recently initiated. The description of kinetic or excitation non-equilibrium effects in the presence of more complex chemistry, however, remains a challenge. In order to include non-equilibrium effects in modeling work, it is necessary to treat ions, electrons, neutral species, and excited species individually in the mixture, and to treat ionization, dissociation, and excited-state kinetics as separate chemical reactions (Ref 14).

Another complication for modeling of plasma jets is introduced by fluid dynamic effects. As the plasma jet exits the nozzle, it encounters a steep laminar shear at the outer edge of the jet. This large velocity difference causes rolling-up of the shear layer flow around the nozzle exit into a ring vortex, which is pulled downstream by the flow, allowing the process to repeat itself again at the nozzle exit. Adjacently formed vortex rings at the outer edge of the jet have the tendency to coalesce, forming larger vortices; perturbations to these vortices then lead to wave instabilities growing around the entire ring. Next, the distorted vortex rings start entangling themselves with adjacent rings, finally resulting in total breakdown of the vortex structure into large-scale eddies and the onset of turbulent flow, as sketched in Fig. 1.

Turbulence strongly affects all fluid dynamic aspects of plasma jets, including mixing and entrainment. Simple, conventional  $k - \varepsilon$  models have dominated plasma jet modeling, in spite of the fact that such models are not really satisfactory even for simple incompressible flows, and often require ad

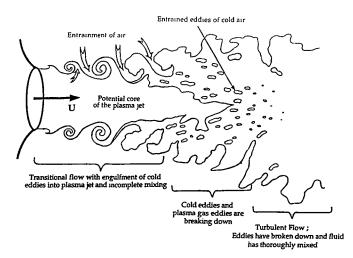


Fig. 1 Main regions of a transitional plasma jet

hoc corrections. Still, such models have provided useful semiquantitative results of fair accuracy (Ref 4, 5, 15, 16).

Attempts have also been made to apply more sophisticated turbulence models to plasmas. For a turbulent argon plasma jet issuing into a stagnant argon environment, a two-fluid turbulence model has been applied (Ref 17). This model has some similarities to models of two-phase flows (i.e., the turbulent plasma jet is treated as a two-phase mixture). The governing equations include transport equations for mass, momentum, and energy for two different fluid parcels (in-moving parcels and out-moving parcels). Auxiliary relations that govern the exchange of mass, momentum, and energy between the fluids are included, along with a description of the mechanisms that control the growth or diminution of the fragment size. The results are usually presented in conditional and unconditional-averaged forms and compared with experimental results from enthalpy-probe measurements (Ref 18). A well known non-dimensional form (a Gaussian error function) can represent the radial distributions of the measured and predicted unconditional mean axial velocity and temperature in consecutive sections (Ref 17). Except in the fringes, the agreement of these measurements with experimental data is excellent.

Previous modeling of the actual plasma spray process with injection of particulates has been primarily based on simple, two-dimensional, steady-state models, assuming that the plasma is in LTE (Ref 4, 5). This approach, however, is limited to low plasma flow velocities and relatively high pressures (atmospheric plasma spraying). As previously stated, the assumption of LTE is no longer valid for high speed plasma flows (Ref 12), especially supersonic flows (Ref 19), for plasmas expanding into low pressure chambers (Ref 9, 10), or for situations with extremely steep gradients of the plasma parameters (Ref 13).

Recently, a comprehensive computational model has been developed at the Idaho National Engineering Laboratories (INEL), which reviews most of the previously mentioned limitations. This model has been incorporated into a powerful computer code (LAVA) (Ref 13, 20, 21) that allows simulation of LTE as well as non-LTE plasma flows with entrained particulates. More specifically, the features of the LAVA code include two and three-dimensional geometries, transient or steady-state simulations, deviations from chemical as well as kinetic equilibrium, generalized ambipolar diffusion for two-temperature plasmas, diffusion, and chemical reactions with arbitrary number of species. Turbulence of the flow in included by using  $k - \varepsilon$  models. Particulate motion with melting employs a stochastic model.

A cooperative program of the High Temperature Laboratory at the University of Minnesota and General Electric has been established for the development of process control methods using simulation data produced by this model. It should be pointed out that the experimentally established instabilities of plasma jets (surging and whipping motion) (Ref 1, 22, 23) must be included in this model in order to facilitate comparisons with experimental data (Ref 24).

**E. Pfender** 

Ernest Eckert Professor of Mechanical Engineering Director of the High Temperature Laboratory University of Minnesota

## References

- 1. E. Pfender, "Plasma Jet Behavior and Modeling Associated with the Plasma Spray Process," *Thin Solid Films*, Vol 238, 1994, p 228-241
- 2. M.I. Boulos, "The Inductively Coupled R.F. Plasma," Pure & Appl. Chem., Vol 57, No. 9, 1985, p 1321
- 3. M.I. Boulos, "R.F. Induction Plasma Spraying: State-of-the-Art Review," J. of Thermal Spray Technol., Vol 1, No. 1, 1992, p 33
- 4. Y.C. Lee, Modeling Work in Thermal Plasma Processing, Ph.D. thesis, University of Minnesota, 1984

- 5. Y.P. Chyou, Modeling of Thermal Plasma Systems, Ph.D. thesis, University of Minnesota, 1987
- 6. P.C. Huang and E. Pfender, "Study of a Transferred-Arc Plasma Reactor with a Converging Wall and Flow Through a Hollow Cathode," *Plasma Chem. Plasma Process.*, Vol 11, 1991, p 129-150
- 7. S. Paik, X. Chen, P. Kong, and E. Pfender, "Modeling of a Counterflow Plasma Reactor," *Plasma Chem. Plasma Process.*, Vol 11, 1991, p 229-249
- 8. X. Chen and E. Pfender, "Modeling of RF Plasma Torch with a Metallic Tube Inserted for Reactant Injection," *Plasma Chem. Plasma Process.*, Vol 11, 1991, p 103-128
- 9. C.H. Chang and E. Pfender, "Nonequilibrium Modeling of Low-Pressure Argon Plasma Jets; Part I; Laminar Flow," *Plasma Chem. Plasma Process*, Vol 10, 1990, p 473-491
- C.H. Chang and E. Pfender, "Nonequilibrium Modeling of Low-Pressure Argon Plasma Jets; Part II; Laminar Flow," Plasma Chem. Plasma Process, Vol 10, 1990, p 493-500
- 11. C.H. Chang and E. Pfender, "Heat and Momentum Transport to Particulates Injected into Low-Pressure (-80 mbar) Nonequilibrium Plasmas," IEEE Trans. Plasma Sci., Vol 18, 1990, p 958-967
- 12. C.H. Chang and J.D. Ramshaw, "Modeling of Nonequilibrium Effects in a High-Velocity Nitrogen Hydrogen Plasma Jet," *Plasma Chem. Plasma Process.*, Vol 16, No. 1, March 1996 Supplement, p 5S-17S
- 13. C.H. Chang and J.D. Ramshaw, Phys. Plasmas, Vol 1, 1994, p 3698
- 14. C.H. Chang and E. Pfender, "Advances in the Computational Modeling of Thermal-Plasma Processing," JOM, Vol 46, 1996, p 46-48
- 15. C.H. Chang and J.D. Ramshaw, "Numerical Simulations of Argon Plasma Jets Flowing into Cold Air", *Plasma Chem. Plasma Process.*, Vol 13, No. 2, 1993, p 189-209
- 16. J.R. Fincke et al., Int. J. Heat Mass Transfer, Vol 37, 1994, p 1673
- 17. P.C. Huang, J. Heberlein, and E. Pfender, "A Two-Fluid Model of Turbulence for a Thermal Plasma Jet," *Plasma Chem. Plasma Process.*, Vol 15, No. 1, 1995, p 25-46
- 18. W.L.T. Chen and E. Pfender, Enthalpy Probe and Spectroscopic Measurements in Thermal Plasma Jets, High Temperature Laboratory Report, University of Minnesota, March 1990
- 19. C. George, G. Candler, R. Young, E. Pfender, and J. Heberlein, "Nozzle Optimization for Dissociated Species Transport in Low Pressure Plasma Chemical Vapor Deposition," *Plasma Chem. Plasma Process.*, Vol 16, No. 1, 1996 Supplement, p 43S-56S
- 20. J.D. Ramshaw and C.H. Chang, "Computational Fluid Dynamics Modeling of Multicomponent Thermal Plasmas," *Plasma Chem. Plasma Process.*, Vol 12, No. 3, 1992, p 299-325
- 21. C.H. Chang, Proc. International Thermal Spray Conference (ITSC '92), Materials Park, OH, 1992, p 793
- 22. S. Russ, P.J. Strykowski, and E. Pfender, "Mixing in Plasma and Low Density Jets," Exper. Fluids, Vol 16, 1994, p 297-307
- 23. S.A. Wutzke, E. Pfender, and E.R.G. Eckert, "Symptomatic Behavior of an Electric Arc with a Superimposed Flow," AIAA J., Vol 6, 1968, p 1474
- 24. J.H. Park, Y.C. Lau, J. Heberlein, and E. Pfender, "Modeling of Fluctuations Experienced in N<sub>2</sub> and N<sub>2</sub>/H<sub>2</sub> Plasma Jets Issuing into Atmospheric Air," to be presented at the ISPC-13, Beijing, P.R.C., August 1997