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QUALITY OPTIMIZATION OF THERMALLY SPRAYED COATINGS PRODUCED BY
THE JP-5000 (HVOF) GUN USING MATHEMATICAL MODELING

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INTRODUCTION

Thermal spray coatings have become increasingly important as one of the most advanced coating technologies in modern industry. Production of protective coatings from mechanical wear, excessive heat, and corrosion/oxidation applications has been the goal of thermal spray coatings for a number of years. In particular, the past decade has seen an increased use of various thermally sprayed metal matrix, ceramics and composite coatings. Currently, thermal barrier coatings (TBC) of gas-turbine blades and similar applications have centered around the use of zirconia as a protective coating for such a high thermal application. The advantages of zirconia include low thermal conductivity and good thermal shock resistance, Lugscheider and Rass¹. Moreover, thermally sprayed tungsten carbide hardface coatings are used for a wide range of applications spanning both the aerospace and other industrial markets. Major aircraft engine manufacturers and repair facilities use hardface coatings for original engine manufacture (OEM), as well as in the overhaul of critical engine components. The principle function of these coatings is to resist severe wear environments for such wear mechanisms as abrasion, adhesion, fretting, and erosion, Nerz et al².

The (JP-5000) thermal spray gun is the most advanced in the High Velocity Oxygen Fuel (HVOF) systems. Recently, the (JP-5000) has received considerable attention because of its relative low cost (\$50,000) and its production of quality coatings that challenge the very successful but yet relatively expensive (\$1.5 million) Vacuum Plasma Spraying (VPS) system. The quality of the thermal spray coatings is enhanced as porosity, oxidization, residual stresses, and surface roughness are reduced or minimized. Similarly, higher densification, interfacial bonding strength, hardness and wear resistance of a coating are definitely desirable features for quality improvement. The thermal spraying industry of today is aware of the necessity of well understood, optimized and reproducible coating processes. Therefore, it is essential to progress in the many fields of thermal spray technologies to efficiently determine the set of optimal spraying parameters, Knotek and Schnaut³.

Like all coating processes, HVOF thermal spraying has to be regarded as a system consisting of the substrate, coating material, and coating process (Figures 1,2). All components of the system and their interactions have to be optimized to obtain suitable coatings, Lugscheider et al⁴. The powder characteristics influence the spraying process and the resulting coating properties; two of the most important powder characteristics are flow behavior and particle grain size range. A powder that flows well results in a powder being fed continuously into the HVOF without intermittent or pulsating flow. A narrow particle size range provides homogeneous melting of the particles in the gun barrel. As well, the splat architecture, microstructure, diffusion, phase distribution, and phase transformation at the interface region are of considerable importance to the coating quality and the fundamental understanding of the deposition process, Zimmerman et al⁵. Mathematical modeling of the HVOF process gasdynamics is used to numerically evaluate the particle velocity and temperature immediately before impacting the substrate. These parameters are of prime influence on the coating formation and therefore the coating properties and quality. Numerical solutions and modeling techniques are evidently gaining more importance as tools for optimization of processes, especially in thermal spraying.

The reason is not only their cost effectiveness, but these simulation models are an efficient time saver and provide more insight in the subject matter as compared to the known statistical methods such as Design of Experiments and Taguchi methods, Regression analysis, Knotek and Schnaut³.

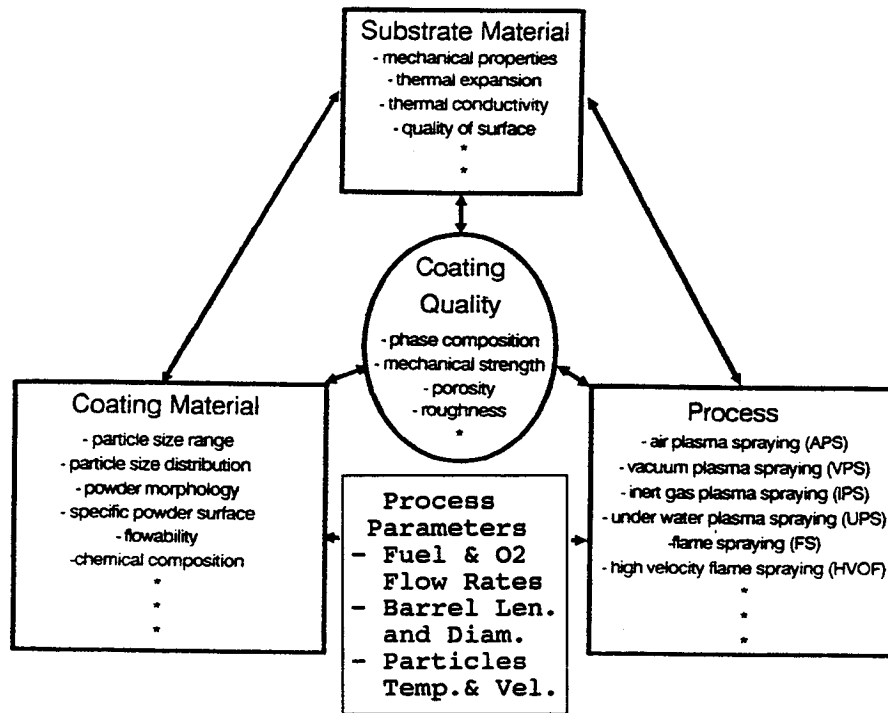


Figure 1: Thermal Coating Quality Diagram

MATHEMATICAL MODEL AND NUMERICAL SOLUTION

A one dimensional single phase flow of combustion gases was assumed in the combustion chamber, conversion-divergent nozzle, and gun barrel. The powder injection at the beginning of the barrel (Fig. 2) represented 10% [powder to (powder + gas), by weight ratio] and negligible volume ratio. For an initial study the effect of the powder on the flow properties was not considered.

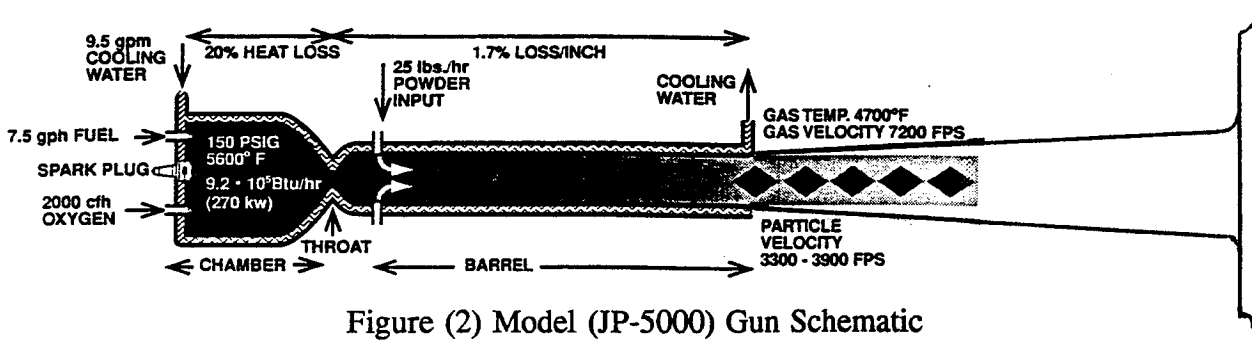


Figure (2) Model (JP-5000) Gun Schematic

Cooling Water Temperature Calculation at the Exit Section:

The model predictions of the cooling water exit temperature from the gun were in good agreement with the measured data provided by Rocketdyne Division. It was assumed that the cooling water absorbed 20% of the kerosene heat value in the combustion chamber and 1.7% of the same amount per unit length of the barrel Fig.(2), Thorpe and Richter⁶.

Modeling of the Combustion Chamber:

The combustion chamber C.C. was modeled through a heat balance equation as described in the following:

Total Heat input to the C.C. = Total Enthalpy Input of Oxygen and Kerosene to C.C. + Low Heat Value of Kerosene - Heat of Evaporation of Kerosene

Total Heat Output From The C.C. = Gases Temp x Gases Sp. Heat x Gases Weight Flow Rate - Heat absorbed by Cooling Water

The weight fractions of the combustion gases were obtained by Chemical Equilibrium with Transport Properties Computer Code, McBirde et al⁷. They were found to read as follows:

CO = 24.5% , O₂ = 12.6% , CO₂ = 16.8% , H₂ O = 27.9% , OH = 9.4% , H₂ = 8.8%

The gas mixture sp. heat was evaluated based on the weighted average of each gas sp. heat using the weight fractions shown above. The sp. heat of each gas was obtained from a correlation as a function of temperature. Due to the dependence of gas sp. heat on temperatures, iteration was necessary to solve for the temperature of the combustion chamber. For the gun specifications and geometry shown in (Fig. 2) a computer program written in the Basic language was developed and the temperature of the (C.C.) was evaluated by this program to read 4440.17 °F which indicated an excellent agreement with the gun manufacturer experimentally measured data.

Modeling of the Convergent-Divergent Nozzle:

Because of the symmetry and small width to length ratio of the HVOF configuration, one-dimensional, friction, diabatic, and steady state flow analysis was considered. The general differential model developed by Shapiro⁸ was modified to allow for four independent variables, namely, Cross-Sectional Area of flow (A), Heat Rejection (Q), Friction (f), and Sp. Heats Ratio (k). The model also incorporated another three dependent variables, they are as follows: Mach No. (M), Temperature (T), and Pressure (P). The working system of differential equations as applied to the control surface defined in Figure (3) is briefly described in Table (1) and in the following equations:

From the convergent-divergent nozzle geometry; $D_{n+1} = D_n - 1.3386 dx$ and $D_{n+1} = D_n +$

0.251 dx respectively.

The amount of heat absorbed by the cooling water per unit mass of the gaseous flow (dQ) is evaluated as 1.7% of the total heat value of kerosene per unit inch of the gun length, Thorpe and Richter⁶. Thus, $dQ = -0.017 \times \text{kerosene flow rate} \times (\text{kerosene heat value} - \text{kerosene heat of evaporation}) dx / \text{gas weight flow rate}$. The friction coefficient (f) for subsonic and super sonic flow was given the value of 0.003 and 0.005 respectively.

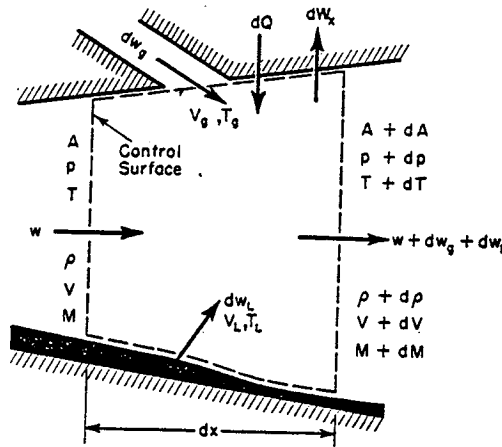


Figure (3) Control Surfaces Definitions

$$\frac{p_2}{p_1} = \frac{w_2 A_1 M_1}{w_1 A_2 M_2} \sqrt{\frac{T_2}{T_1}} \sqrt{\frac{k_1 W_1}{k_2 W_2}}$$

Table (1) INFLUENCE COEFFICIENTS FOR VARIABLE SPECIFIC HEAT AND MOLECULAR WEIGHT

	$\frac{dA}{A}$	$\frac{dQ - dW_x + dH}{c_p T}$	$4f \frac{dx}{D} + \frac{dX}{2kpAM^2} - 2y \frac{dw}{w}$	$\frac{dw}{w}$	$\frac{dW}{W}$	$\frac{dk}{k}$
$\frac{dM^2}{M^2}$	$-\frac{2\left(1 + \frac{k-1}{2}M^2\right)}{1-M^2}$	$\frac{1+kM^2}{1-M^2}$	$\frac{kM^2\left(1 + \frac{k-1}{2}M^2\right)}{1-M^2}$	$\frac{2(1+kM^2)\left(1 + \frac{k-1}{2}M^2\right)}{1-M^2}$	$-\frac{1+kM^2}{1-M^2}$	-1
$\frac{dT}{T}$	$\frac{(k-1)M^2}{1-M^2}$	$\frac{1-kM^2}{1-M^2}$	$-\frac{k(k-1)M^4}{2(1-M^2)}$	$-\frac{(k-1)M^2(1+kM^2)}{1-M^2}$	$\frac{(k-1)M^2}{1-M^2}$	0

NOTES: (1) Each influence coefficient represents the partial derivative of the variable in the left-hand column with respect to the variable in the top row; for example

$$\frac{dM^2}{M^2} = -\frac{2\left(1 + \frac{k-1}{2}M^2\right)}{1-M^2} \frac{dA}{A} + \frac{1+kM^2}{1-M^2} \frac{dQ - dW_x + dH}{c_p T} + \dots - \frac{dk}{k}$$

NUMERICAL INTEGRATION SCHEME

Because of the high nonlinearity of this system of differential equations a numerical integration scheme was conducted to evaluate the flow velocity, temperature, and pressure at various cross-sections of the gun. Both the mach number and temperature differential equations given in Table (1) were modified and integrated over a small element bounded by sections n, n+1 as shown in the following:

$$\int_{T_n}^{T_{n+1}} \frac{dT}{T} = FAT_n \int_{A_n}^{A_{n+1}} \frac{dA}{A} + \frac{FQT_n}{c_p T_n} \int_{Q_n}^{Q_{n+1}} dQ + 4f \frac{FFT_n}{D_n} \int_{x_n}^{x_{n+1}} dx$$

$$\int_{M_n^2}^{M_{n+1}^2} \frac{dM^2}{M^2} = FAM_n \int_{A_n}^{A_{n+1}} \frac{dA}{A} + \frac{FQM_n}{c_p T_n} \int_{Q_n}^{Q_{n+1}} dQ + FFM_n \frac{4f}{D_n} \int_{x_n}^{x_{n+1}} dx - \int_{k_n}^{k_{n+1}} \frac{dk}{k}$$

All the influence coefficients were considered constant with their section (n) values in the elements between sections (n), (n+1). Further manipulation and re-arrangement of the last two eqn(s) were performed and an approximate numerical solution was achieved, it read as follows:

$$M_{n+1}^2 = e^{\ln M_n^2 + FAM_n (\ln A_{n+1} - \ln A_n) + FQM_n \frac{\Delta Q}{c_p T_n} + FFM_n \frac{4f \Delta x}{D_n} - (\ln k_{n+1} - \ln k_n)}$$

Similarly

$$T_{n+1} = e^{\ln T_n + FAT_n (\ln A_{n+1} - \ln A_n) + FQT_n \frac{\Delta Q}{c_p T_n} + FFT_n \frac{4f \Delta x}{D_n}}$$

NUMERICAL ITERATION SCHEME

To enhance the accuracy of the numerical integration and hamper the instability of the solution due to the discontinuity in the sonic speed at the throat cross-section, a numerical iteration scheme was developed. This iteration scheme was based on the assumption of linear variation of the coefficients and flow properties within the small integration elements. Therefore each influence coefficient and flow property were considered to be at their average value at the (n+0.5) cross section. The iteration scheme to minimize the errors in the temperature (ET) and Mach No. (EM) is described as shown in the following:

$$EM = \ln M_n^2 - \ln M_{n+1}^2 + FAM_{n+.5} (\ln A_{n+1} - \ln A_n) + FQM_{n+.5} \frac{\Delta Q}{c_p T_{n+.5}} + FFM_{n+.5} \frac{4f \Delta x}{D_{n+.5}} - (\ln k_{n+1} - \ln k_n)$$

$$ET = \ln T_n - \ln T_{n+1} + FAT_{n+.5} (\ln A_{n+1} - \ln A_n) + FQT_{n+.5} \frac{\Delta Q}{c_p T_{n+.5}} + FFT_{n+.5} \frac{4f \Delta x}{D_{n+.5}}$$

The numerical solution was carried out by dividing the convergent and divergent parts of the nozzle and the barrel to a total of 280 small increments. They were distributed as 40,40, and 200 respectively.

RESULTS AND ANALYSIS

The obtained results from the computer program for the flow's gas dynamics properties, pressure, velocity, and temperature calculated at different sections along the gun X-axis were exhibited in table (2). The pressure showed considerable expansion and sharp drop along the nozzle. Meanwhile, the gas velocity reached Mach No. of 1.9 or 8507 FPS, and the temperature dropped from 4440 °R at the C.C. to 3066 °R at the exit of the nozzle. The flow also showed a slight increase in pressure and decrease in velocity in the barrel due to friction. These changes were accompanied with a moderate decrease in temperature due to the cooling water effect.

Table(2) Computer Program Predictions of Flow Gas Dynamics Properties

X - Axis inches	Pressure psi	Velocity Feet/sec	Temperature Degrees R	Comments
0.0	100	194	4440	Comb. Chamber
3.4	100	194	4440	Exit of C.C.
4.28	65.26	4785	4193	Throat
4.78	17.9	8507	3052	Exit of Nozzle
6.78	18.76	8153	3066	Barrel Sec. @ 1.5"
8.78	19.50	7815	3067	Barrel Middle Sec.
10.78	20.34	7493	3055	Barrel Sec. @ 4.5"
12.78	21.05	7181	3031	Barrel Exit Sec.

CONCLUSIONS

- (1) The current model predicted the cooling water exit temperature as well as the gas flow properties, velocity, pressure, and temperature along the X-axis of the JP-5000 Thermal Spray Gun with an overall numerical accuracy of 96%.
- (2) These predictions are in excellent agreement with measurements at the combustion chamber and the barrel exit section.
- (3) The developed numerical iteration scheme succeeded to hamper the brief model instability due to the discontinuity of the sonic speed in the near vicinity of the throat cross-section.
- (4) In the area of thermal spray, the current model presented a unique and a successful beginning towards a more comprehensive simulation model of the JP-5000 to yield the necessary information for the control of the gun parameters on a real time basis to continuously provide optimum quality coatings

WHAT SHOULD BE DONE?

Recommendation #1:

Further development of the current model is recommended to account for the powder (10% by weight) flow in the barrel and in the free plume before impacting the substrate. The study and simulation of such a two phase gas-particle flow will enhance the model prediction accuracy.

Recommendation #2:

Further analysis is recommended to rectify the slight numerical instability in the current model in the very closed vicinity of the throat due to the discontinuity of the speed of sound in this area.

Recommendation #3:

After the incorporation of recommendations #1 and #2 above, the current simulation model should be used to conduct a detailed and comprehensive study on the influence of the thermal spray system parameters on the coatings quality. This model should then be used in cooperation with a neural network system to provide active and real time control on the coatings quality and provide a complete optimization of the HVOF thermal spray process.

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