Title:
A Feature-based Coupling Model for Dynamic Effect in HVOF Thermal Spray Process

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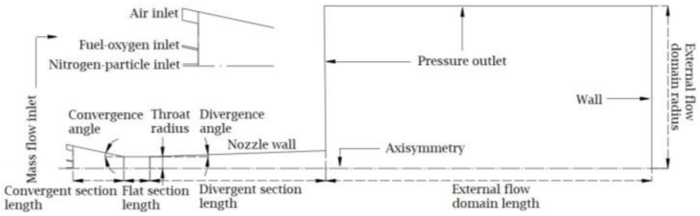
Introduction:

High velocity oxygen-fuel (HVOF) deposition is a kind of thermal spraying technologies protecting or improving the surface performance of a substrate or workpiece [1]. It is a complex physicochemical process involving chemical reaction, turbulence, compressible flow, multiphase interactions, subsonic/supersonic transitions, droplet deformation and solidification [10]. During the process, the thoroughly mixed fuel-oxygen gases (typically hydrocarbon-oxygen) and micro particles are fed into the gun chamber where a combustion reaction takes place. The fuel-oxygen combustion generates a hot-sonic/supersonic gas stream. Micro particles of metals, alloys or cermets are accelerated and heated in the sonic/supersonic combusting gas stream and are deposited on a substrate at high speeds [8]. Due to the complexity of this process, coating quality is influenced by many factors, like gun geometry, fuel/oxygen ratio, and particle sizes. In industry, robots and handling systems are traditionally used in thermal spraying processes to control the relative movement between spray torch and substrate. The parameters of spray distance, scanning velocity, and scanning step also have a significant impact on the coating properties [4]. Computational fluid dynamics (CFD) simulation has reached a high level of sophistication in the field of thermal spray process modeling. Most simulation studies of HVOF are only considered for single disciplinary parameters (e.g. geometric effect or torch path effect). In the paper, a novel modeling system enabling multidisciplinary parameters management in the HVOF thermal spray process is developed which is not existing in previous research works.

Main Idea:

The primary focus of this research is on implementing a feature-based technique [6] to maintain the information consistency among different disciplinary domains and manage the parameters involved in the process. For fulfilling this purpose, the correspondences between the actual parameters and the simulation setups have to be established. Besides, a coupling mechanism needs to be proposed to construct the link between the reactive jet behaviors and dynamic physics of a substrate surface.
Geometric entities involved in the process play an important role in the simulation results [1]. Thus, a complete mechanism of information transfer between computer-aided design (CAD) and computer-aided engineering (CAE) tools is necessary for associating the geometric entities with the CAE modeling. Li et al. [7] proposed a novel CAE boundary feature based on the associative feature concept [10], which fulfills a seamless CAD/CAE integration. In our research, the CAE boundary feature is used in the thermal spray process to manage the relations among geometric entities and CAE boundary condition setups, such as the determination of the fluid domain and CAE configurations for a specified spray gun.

Fig. 1(a) shows the mapping relationship between geometric entities and CAE boundary conditions for the simulation of the combustion and particle-gas jet, which is embedded in the CAE boundary feature. In this way, the CAE boundary condition setups could be automatically completed without redundant model preparations when the geometries are changed. For instance, the external flow domain length will be changed when the spray distance is adjusted.



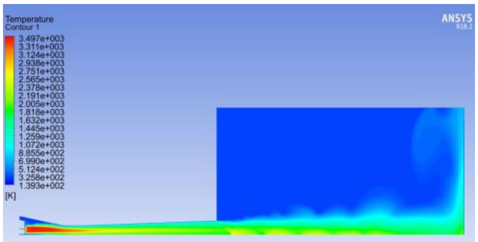


Fig. 1: (a) A template of computational domain and boundary conditions for the particle-gas jet, (b) A temperature field of the gas jet (100 mm length external flow domain).

CFD tools require not only explicit geometry inputs but also complicated solver setups. In the thermal spray process, the solver setup for the combustion needs a precise reaction formula, depending on the fuel-oxygen mass flow rate and the reaction pressure, and the solver setup for the particle-gas interaction is based on the volume fraction. For facilitating an automatic mechanism of the solver setups, *thermal spray physics feature* is defined as an object class with a set of rules for obtaining the setup parameters. Some constant solver setups special for HVOF thermal spray have been verified in the previous studies [1],[8],[9]. Regarding the reaction formula calculation and the interaction model selection, an iteration method [2] and a logical function are programmed separately as FORTRAN subroutines embedded in the rules of the thermal spray physics feature to complete the solver setups.

Fig. 1(b) shows an example of the combustion and jet simulation results by using ANSYS/Fluent.

So far, all physics behaviors of the combustion and the jet can be obtained from the simulation results. Meanwhile, the static physics on the coating surface at an arbitrary spray distance can be obtained as well through extracting the wall properties. The next phase is to establish a coupling mechanism which can associate the simulation results with torch paths to compute dynamic physics of a coating surface. For fulfilling the mechanism, three new features which are specific for thermal spray process, namely *particle-gas jet feature*, *coating dynamic feature* and *spray path feature*, are proposed to maintain the information association during the process. The particle-gas jet feature is defined as a class of physics feature which contains physical properties of the simulation results. For example, temperature and pressure field of the reactive flow adjacent to the wall, and heat flux and particle deposition distribution on the wall are all the attributes of the particle-gas jet feature. In industry, the coating process guided by a handling system is a dynamic process. Therefore, for managing the dynamic behaviors, the coating dynamic feature based on the dynamic feature [7] is proposed to receive the information transferred from the spray path feature and generate the corresponding dynamic features.

The spray path feature is defined as a class of associative feature that contains the mapping relations between physics of the particle-gas jet and associated dynamic physics of the substrate surface.

Fig. 2 shows the semantic associations in the thermal spray process. The function of the spray path feature is to generate trajectories of HVOF flame center point on the substrate surface. Some research works have been dedicated to trajectory generation based on parameters of scanning velocity, scanning step, spray distance, spray angle, and surface normal [2],[3]. After generating the torch trajectories, the mapping trajectories which are defined as the movement of HVOF flame center on the substrate surface can be obtained via the torch orientation as shown in

Fig. 3(a). In this paper, the spray angle between the torch orientation and the tangent plane of the substrate surface is always assumed to be orthogonal to ensure high-quality coatings [2]. For simplification, the flame center trajectories on the substrate surface are intuitively described as surface source trajectories, which distinguishes torch trajectories. The physical properties of the particle-gas jet feature have a rotational-symmetry characteristic due to the axisymmetric shape of the spray gun. Theoretically, such properties can be described by a mathematical function of the radial distance from the center point of the flame through extracting data from the particle-gas jet feature. After obtaining a mathematical expression, an instantaneous physical property applied on each cell surface can be calculated according to the distance from each cell location to the corresponding instantaneous surface source center as shown in

Fig. 3(b). However, the time step in CFD tools may be different from the time interval between torch trajectory points. To overcome this barrier, a FORTRAN subroutine was programmed to calculate the surface source trajectory points at the time steps in CFD tools. Due to the extremely short distance and the time interval between two adjacent torch trajectory points, the torch movement between the two adjacent points is assumed to be uniform-rectilinear. Based on this approximation, the surface source trajectory points at the time steps in CFD tools can be calculated by Eqn. (1), and then the instantaneous physical property applied on each cell surface can be calculated by Eqn. (2):

$$\mathbf{X}_S(i) = \mathbf{X}_M(k) + \frac{t_T(k+1) - t_T(k)}{t(i) - t_T(k)} \cdot \left[\mathbf{X}_M(k+1) - \mathbf{X}_M(k)\right],\ t_T(k+1) < t(i) \le t_T(k) \tag{1}$$

$$\varphi(r_i(n)) = \varphi\ \left\|\mathbf{X}_C(n) - \mathbf{X}_S(i)\right\| \tag{2}$$

where $\mathbf{X}_S(i)$ is the flame center location on the substrate surface at the i^{th} time step in CFD tools, $\mathbf{X}_M(k)$ is the location of the k^{th} mapping trajectory point, $\mathbf{X}_C(n)$ is the location of the n^{th} surface cell, $t_T(k)$ is the time corresponding to the k^{th} torch trajectory point, $t(i)$ is the time at the i^{th} CFD time step and $\varphi(r_i(n))$ is a physical property applied on the n^{th} surface cell at the i^{th} CFD time step. With this treatment, the source center can move with CFD time steps to obtain a dynamic physics field of the substrate surface.

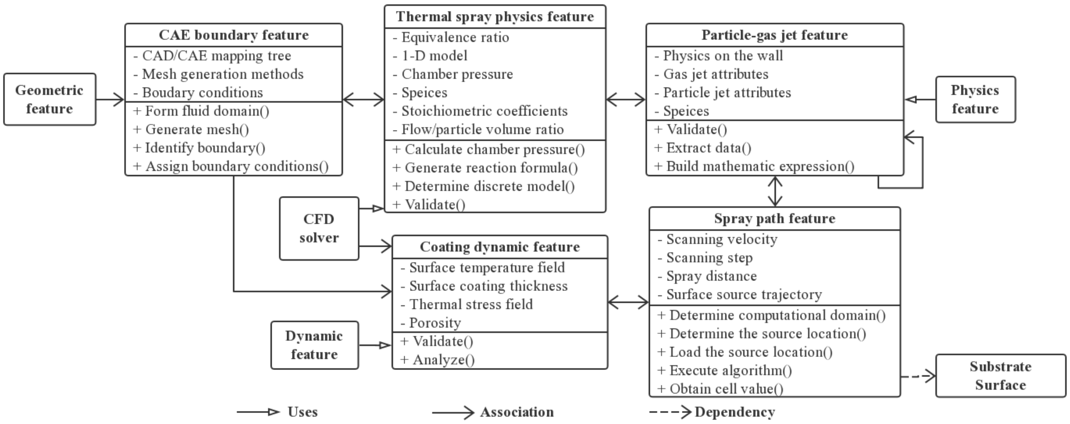


Fig. 2: UML diagram representing semantic associations in the thermal spray process.

The thermal prediction and control of the coated surface are important for improving the coating quality [1],[8],[9]. The application of the proposed feature-based modeling scheme is illustrated by the following case study of the thermal history of a B-spline substrate for the gas jet only (no particle spray, just the reactive flow). The mechanism of the modeling was verified by using ANSYS/FLUENT. The association function of the spray path feature was implemented by Visual C in ANSYS/FLUENT. The first step for the modeling is to set up boundary conditions. Propylene-oxygen combustion is considered in this case. Spray gun geometries and mass flow rates are provided from [9]. The external flow domain length corresponding to the spray distance is 100.00 mm and the external flow domain radius is 50.00 mm which is much greater than the radius of the torch exit. The temperature of the nozzle wall during the process is always assumed as 300 K. The material setup for the wall at the right end of the external flow domain always keeps consistent with the substrate material. According to the above descriptions, the boundary condition setups for the jet simulation were completed based on the CAE boundary feature concept.

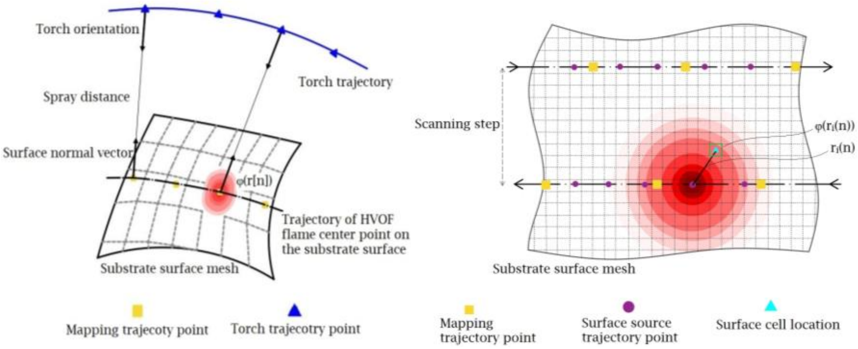


Fig. 3: (a) Trajectories of HVOF flame center point on the substrate surface, (b) Surface source trajectory.

Some research works [1],[9] have illustrated that a one-step reaction developed by Gordon and McBride [5] enables to describe the combustion in HVOF thermal process. As mentioned in the thermal spray physics feature, the reaction formula at this equivalence ratio was calculated via the FORTRAN subroutine. As the particle influence was not considered in this case, the interaction solver setups were skipped. After configuring the solvers, the heat flux transferred to the wall at the spray distance of 100 mm was extracted from the wall properties of the simulation results which are the attributes contained in the particle-gas jet feature. And then the mathematical function based on the extracted data was obtained via the curve fitting of Gaussian distribution with 95% confidence bounds:

$$f(r) = a_1 * exp(-((r-b_1)/c_1)^2) + a_2 * exp(-((r-b_2)/c_2)^2) \tag{3}$$

where, a_1=4.388e+06 (4.363e+06, 4.414e+06), b_1=-1.725e-15 (-2.296e-05, 2.296e-05), c_1=0.005226 (0.005188, 0.005265), a_2=1.914e+06 (1.899e+06, 1.929e+06), b_2=5.122e-14 (-0.0001391, 0.0001391), c_2=0.03497 (0.03471, 0.03522).

Fig. 4 shows the primal parameters for generating the surface source trajectories. According to the parameters, a dynamic temperature field of the substrate was obtained by implementing the coupling mechanism in the spray path feature.

Fig. 5 shows the coating dynamic feature of the computed substrate temperature field at three different times under the predefined conditions. The maximum temperature during the dynamic process is 560 K around 1.5 s.

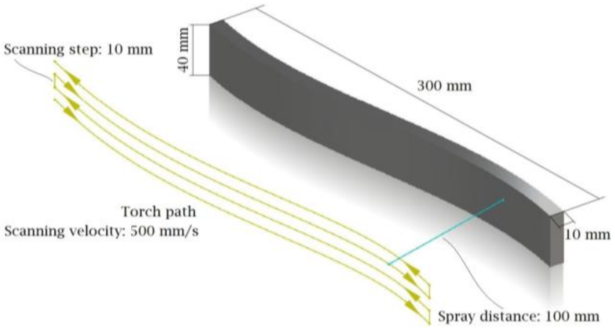


Fig. 4: Schematic representation of the torch path and the substrate.

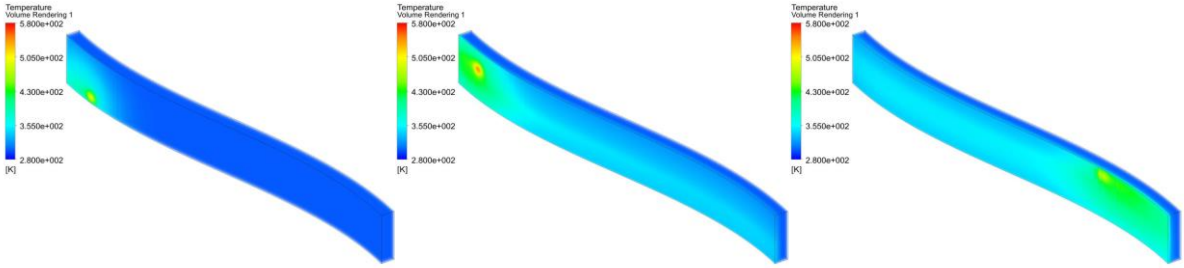


Fig. 5: (a) Temperature field at 0.1 s, (b) Temperature field at 1.5 s, and (c) Temperature field at 2.3 s.

Conclusions:

Thermal spray process is modeled as four major domains, geometry, HVOF jet physics, torch path, and coating-dynamic behaviors. The parameters involved in different domains are classified and controlled by using feature technology. For obtaining and controlling dynamic behaviors of a substrate, a coupling mechanism embedded to spray path feature is proposed. Finally, the behaviors of the substrate surface can be parametrically predicted and controlled. So far, the proposed coupling mechanism is not available yet for sharp-shape substrate surfaces, and the torch orientation angle has not been considered. To overcome future application barriers, the coupling mechanism will be further developed and described in the cylindrical coordinate. The concept of thermal physics feature can be further developed to integrate an intelligent solver for different thermal spraying processes.

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References:

[1] Baik, J.-S.; Kim, Y.-J.: Effect of nozzle shape on the performance of high velocity oxygen-fuel thermal spray system, Surface and Coatings Technology, 202(22-23), 2008, 5457-5462. https://doi.org/10.1016/j.surfcoat.2008.06.061

[2] Candel, A.; Gadow, R.: Trajectory generation and coupled numerical simulation for thermal spraying applications on complex geometries, Journal of Thermal Spray Technology, 18(5-6), 2009, 981-986. https://doi.org/10.1007/s11666-009-9338-x

[3] Cai, Z.-H.; Liang, H.; Quan, S.-H.; Deng, S.-H.; Zeng, C.-N.; Zhang, F.: Computer-aided robot trajectory auto-generation strategy in thermal spraying, Journal of Thermal Spray Technology, 24(7), 2015, 1235–1245. https://doi.org/10.1007/s11666-015-0282-7

[4] Gadow, R.; Floristán, M.: Manufacturing engineering in thermal spraying by advanced robot systems and process kinematics, Future Development of Thermal Spray Coatings: Types, Designs, Manufacture and Applications, Elsevier, Cambridge, England, 2015. https://doi.org/10.1016/B978-0-85709-769-9.00011-7

[5] Gordon, S.; McBride, B.-J.: Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman–Jouguet Detonations, National Aeronautics and Space Administration, Washington, D.C., 1976.

[6] Li, L.; Lange, C.-F.; Jiang, P.-Y.; Ma, Y.-S.: Feature-based intelligent system for steam simulation using computational fluid dynamics, Advanced Engineering Informatics, 38, 2018, 357-369. https://doi.org/10.1016/j.aei.2018.08.011

[7] Li, L.; Lange, C.-F.; Ma, Y.-S.: Association of design and computational fluid dynamics simulation intent in flow control product optimization, Proceedings of the Institution of Mechanical Engineers, Part B, Journal of Engineering Manufacture, 232(13), 2018, 2309-2322. https://doi.org/10.1177/0954405417697352

[8] Li, M.-H.; Christofides, P.-D.: Computational study of particle in-flight behavior in the HVOF thermal spray process, Chemical Engineering Science, 61(19), 2006, 6540-6552. https://doi.org/10.1016/j.ces.2006.05.050

[9] Li, M.-H.; Christofides, P.-D.: Multiscale modeling of HVOF thermal spray process, IFAC Proceedings Volumes, 38(1), 2005, 327-332. https://doi.org/10.1016/j.ces.2005.02.043

[10] Ma, Y.-S.; Chen, G.; Thimm, G.: Paradigm shift: unified and associative feature-based concurrent and collaborative engineering, Journal of Intelligent Manufacturing, 19(6), 2008, 625–641. https://doi.org/10.1007/s10845-008-0128-y.