Title:
Comparison of Different Two-Equation Turbulence Models for Dynamic Effect in HVOF Thermal Spray Process Modeling

Authors:
Jiangzhuo Ren, ren6@ualberta.ca, University of Alberta
Yiming Rong, rongym@sustech.edu.cn, Southern University of Science and Technology
Yongsheng Ma, yongsheng.ma@ualberta.ca, University of Alberta; Southern University of Science and Technology (Visiting Professor)

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Introduction:
High velocity oxygen-fuel (HVOF) deposition is a kind of thermal spraying technology that protects the surface of a workpiece substrate and improves the processed surface performance. During the process, a jet stream of 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 spraying stream. Micro particles of metals, alloys or cermets are accelerated, heated and deposited on the substrate at high speeds [5].

Over the past 20 years, numerical studies have been carried out in the related research fields. During the early development, owing to the sophistication of computational fluid dynamics (CFD), many research works focused on the numerical modeling of flame behavior and particle in-flight characteristics. Due to the high Reynolds number and Mach number of the flame flow, the renormalization group (RNG) k-ε turbulence model [4] or the realizable k-ε turbulence model [6] was used to estimate the turbulent eddy viscosity. However, to the authors' best knowledge, the best fit turbulent model for different industrial scenarios has not been covered. More recently, as movable spray systems were widely applied in thermal spray processes for complex shapes of the substrate components, more and more researchers concentrated on predicting and controlling the dynamic performance of the coating and substrate. Cai et al. [1] proposed a new idea enabling the spray trajectory to be integrated into the finite element method, which realized the prediction of the heat and mass transferred to the substrate during the plasma spray process. Ren and Ma [7] further extended this idea to a feature-based HVOF model, which allows the numerical analysis results of in-flight characteristics to become usable for dynamic analysis of the substrate. However, the validation of the dynamic model has not been covered in that early work.

Therefore, in this paper, the two different turbulence models, the RNG k-ε turbulence model and the realizable k-ε turbulence model, are used to estimate the turbulent viscosity and turbulence kinetic energy in a CFD model of HVOF flame characteristics. And then the results by the models are coupled with spray trajectories to simulate the dynamic behavior of a substrate. For validating these different turbulence models, simulated dynamic temperature fields of the substrate are compared with experimental data. In addition, to develop a robust simulation method, a systematical modeling method to represent the dynamic characteristics of the substrate is proposed.

Main Idea:
The dynamic behavior of the substrate during the torch movement, e.g. thermal field or thermal residual stress, has a significant impact on the coating properties [2]. In order to exactly capture the phenomenon, a robust modeling method is illustrated in Fig. 1, which enables coupling the CFD analysis of HVOF flame jet with numerical analysis of the substrate dynamic physics. The modeling method starts with fuel type selection. According to the equivalence ratio and an assumed reaction chamber pressure, the reaction formula is derived from an instantaneous equilibrium code [3]. Then, the combustion process is modeled by the eddy dissipation model [4]. It is worth noticing that the chamber pressure from the simulation result is very likely different from the preliminary assumed pressure. Therefore, to improve the reaction model accuracy, several iterations of running this part of the algorithm are needed to ensure the convergence between these two parameters up to a certain tolerant difference range. The spray process is solved by Reynolds or Favre-averaged governing equations with a turbulence model. Motivated by generating a robust simulation of the burning gas flow, a set of rules to analyze the stability and convergence status are described in Fig. 1. After obtaining the steady characteristics of the burning gas, the coupling mechanism can convert the steady characteristics to a surface source moving with the spray trajectory, and then the dynamic performance of a substrate is computed at the time steps in CFD tools through discretizing the trajectory. For the detailed interpretation of the coupling algorithm, the reader could refer to our previous publication [7]. Considering the limitation in our previous work, the improvement of the proposed method is that the characteristic of the substrate surface from the dynamic result is extracted and compared with the ideal wall property from a steady CFD model where the substrate surface is set up as the wall boundary condition with a hypothetical physics properties (such as constant temperature). If an error exists between these two models, several iterations will be triggered until an acceptable error is reached. In this way, the dynamic physics of the substrate can be captured accurately.

It is obvious that, from the above description, the turbulence model has a remarkable influence on the simulation result of the in-flight behavior which further affects the accuracy of the substrate dynamic simulation. In this paper, the RNG k-ε turbulence model and the realizable k-ε turbulence model is implemented separately in the above modeling method to investigate the effects on the dynamic behavior of the substrate. According to the Boussinesq hypothesis, the Reynolds stress term representing the effect of turbulence in the governing equations can be related to the mean velocity gradients:

$$-\overline{\rho v_i'' v_j''} = \mu_t\left(\frac{\partial \tilde{v}_i}{\partial x_j}+\frac{\partial \tilde{v}_j}{\partial x_i}\right)-\frac{2}{3}\left(\bar{\rho}k+\mu_t\frac{\partial \tilde{v}_l}{\partial x_l}\right)\delta_{ij} \tag{2.1}$$

where μ_t is the turbulent viscosity and k is the turbulence kinetic energy.

To estimate the effect of turbulence, the RNG k-ε turbulence model has the following form:

$$\frac{\partial}{\partial t}\ \bar{\rho}k\ +\frac{\partial}{\partial x_i}\ \bar{\rho}\tilde{v}_i k\ =\frac{\partial}{\partial x_j}\left[\alpha_k\mu_{eff}\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\bar{\rho}\varepsilon-Y_M+S_k \tag{2.2}$$

and

$$\frac{\partial}{\partial t}\ \bar{\rho}\varepsilon\ +\frac{\partial}{\partial x_i}\ \bar{\rho}\tilde{v}_i\varepsilon\ =\frac{\partial}{\partial x_j}\left[\alpha_\varepsilon\mu_{eff}\frac{\partial \varepsilon}{\partial x_j}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}\ G_k+C_{3\varepsilon}G_b\ -C_{2\varepsilon}\bar{\rho}\frac{\varepsilon^2}{k}-R_\varepsilon+S_\varepsilon \tag{2.3}$$

where ε is the turbulence dissipation rate, G_k is the generation of turbulent kinetic energy due to the mean velocity gradients, G_b is the generation of turbulent kinetic energy due to buoyancy, and Y_M is the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate. α_k and α_ε are inverse effective Prandtl numbers for k and ε. R_ε is the additional term in the ε equation. S_ε and S_k are source terms defined by the user, and $C_{1\varepsilon}$ = 1.42, $C_{2\varepsilon}$ = 1.68.

The transport equations of the realizable k-ε turbulence model are:

$$\frac{\partial}{\partial t}\ \bar{\rho}k\ +\frac{\partial}{\partial x_j}\ \bar{\rho}\tilde{v}_j k\ =\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\bar{\rho}\varepsilon-Y_M+S_k \tag{2.4}$$

and

$$\frac{\partial}{\partial t}\bar{\rho}\varepsilon + \frac{\partial}{\partial x_j}\bar{\rho}\tilde{v}_j\varepsilon = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + \bar{\rho}C_1 S\varepsilon - \bar{\rho}C_2\frac{\varepsilon^2}{k+\sqrt{\nu\varepsilon}} + C_{1\varepsilon}\frac{\varepsilon}{k}C_{3\varepsilon}G_b + S_\varepsilon \tag{2.5}$$

where ε, G_k, G_b, Y_M, S_ε, and S_k has the same definition as the RNG turbulence model. σ_k and σ_ε are the turbulent Prandtl numbers for k and ε, respectively. $C_{1\varepsilon} = 1.44$, $C_2 = 1.9$, $\sigma_k = 1.0$ and $\sigma_\varepsilon = 1.2$.

From the above equations, there are three major differences between the two models: the turbulent Prandtl numbers for k and ε; the generation and destruction terms in the equation for ε; and the method of calculating turbulent viscosity. In the next section, the substrate characteristic properties obtained from the dynamic simulations by these two models will be compared with experimental results.

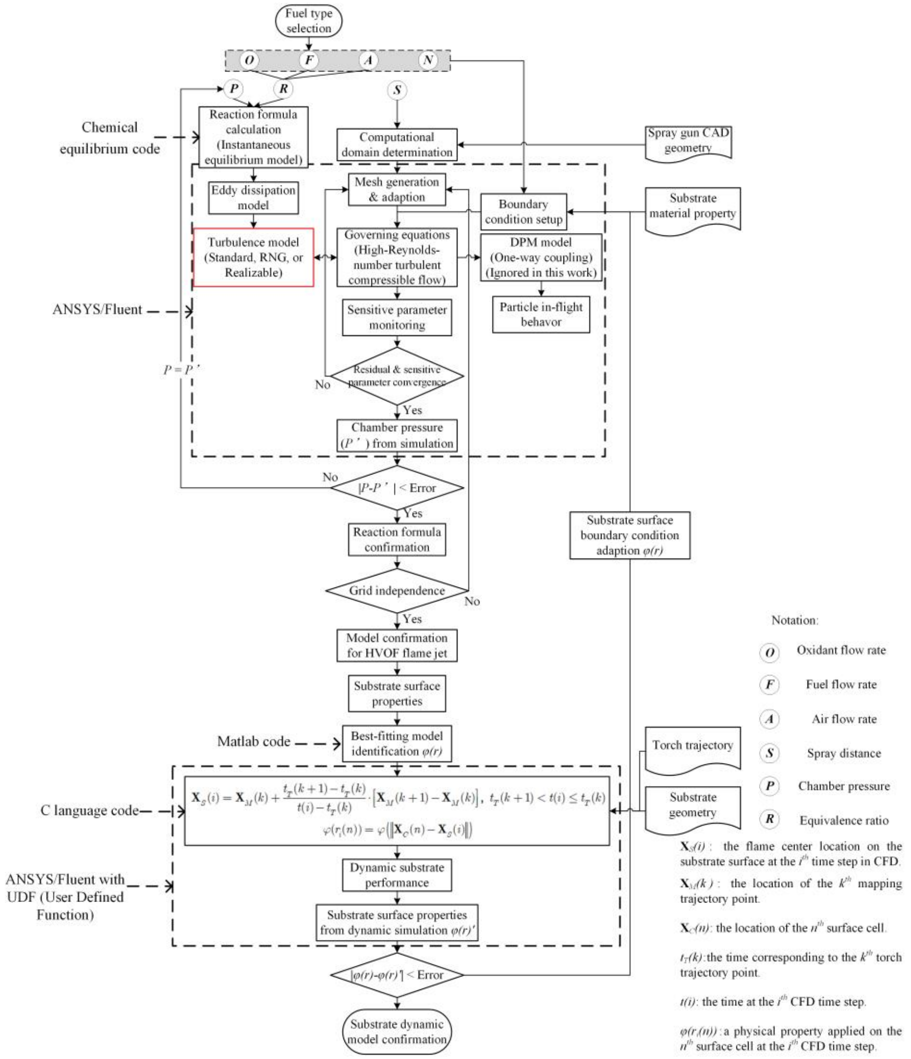

Fig. 1: A robust modeling method for the dynamic behavior of the substrate during HOVF process.

<u>Results and Discussion:</u>

During the HVOF process, the flame is forced to impact on the substrate, which leads to a sharp rise of the substrate temperature. To avoid residual stress due to a sharp change of the temperature, the thermal prediction of the substrate is noticeable. Thus, in this section, the temperature field of the substrate is selected as the representative characteristic to analyze the effect of the two turbulence models. Moreover, the convective heat transfer between the flame flow and substrate surface is related to two important properties of the reactive flow, the velocity and temperature, which are affected by the turbulence model selection.

Based on the proposed modeling method, two sets of gas flow rates as shown in Tab. 1 were performed to calculate the temperature profile at the center point on the top surface of an AISI-1045 steel substrate (300 mm × 300 mm × 30 mm) with two different scanning velocities (5 mm/s and 10 mm/s along the centerline of the top surface). Fig. 2(a) depicts the computational domain of the flame which was acquired from the direct measurement of the real spray gun. Fig. 2(b) presents a temperature contour of the flame flow corresponding to the operation of condition 2 with a 5 mm/s scanning velocity. After obtaining the characteristics of the flame, the dynamic temperature field of the substrate with a spray trajectory was calculated by the proposal coupling mechanism, as shown in Fig. 2(c). Fig. 3 shows the corresponding experimental setup of the substrate, the infrared thermometer (SCIT-3S7, Beijing Sanbo Zhongzi Technology Co., Ltd), and a homemade Diamond Jet spray system with ABB IRC5 M2004 positioning system. It is worth noticing that for sake of the convenience of experimental temperature measurement, the spray velocity used here is quite lower than the real industrial process and all the spray processes were carried out without powder particles.

Condition	*Propane (SLPM)*	*Oxygen (SLPM)*	*Nitrogen (SLPM)*	*Air (SLPM)*	*Spray distance (mm)*
1	334.6	972.0	32.8	758.1	170
2	180.6	625.6	39.0	577.9	180

Tab. 1: Process parameters for model validation.

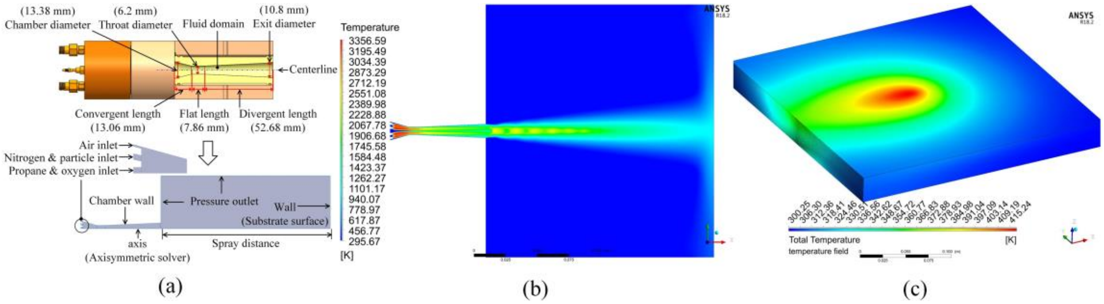

Fig. 2: Schematic representation of the key steps during the modeling of condition 1: (a) the computational domain of the flame flow, (b) the temperature contour of the flame flow corresponding to condition 1, and (c) the instantaneous temperature field corresponding to the moment when the torch moves to the center point of the top surface.

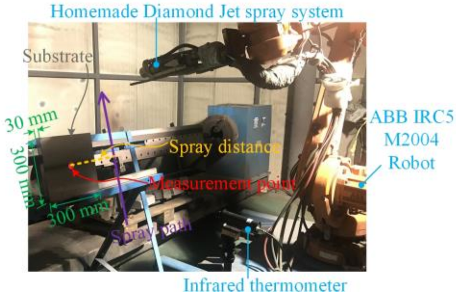

Fig. 3: Experimental temperature measurement of the substrate surface.

Fig. 4 shows the temperature of the center point changes over time. The two sets of operation conditions with different scanning velocities present the same trend that the simulated temperature profiles by the RNG *k*-*ε* turbulence model agree with the data experimentally measured by the infrared thermometer,

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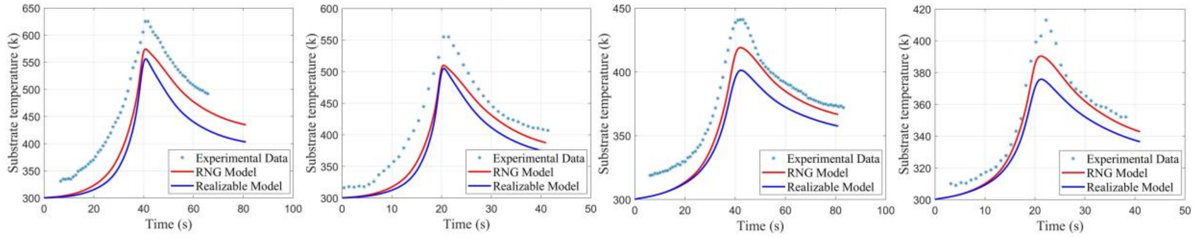
and the realizable *k-ε* turbulence model generated lower temperature distribution than the experimental results.



(a) (b) (c) (d)

Fig. 4: The temperature of the center point versus time: (a) condition 1 with a 5 mm/s velocity, (b) condition 1 with a 10 mm/s velocity, (c) condition 2 with a 5 mm/s velocity, and (d) condition 2 with a 10 mm/s velocity.

Conclusions:

In this paper, an iterative method is used to realize a coupling between HVOF in-flight physic model and the substrate dynamic model. Further, a systematic modeling method is proposed to obtain the substrate dynamic performance with the spray torch trajectory by integrating the coupling mechanism. For testing the effects of turbulence models on the dynamic behavior of the substrate, the RNG *k-ε* turbulence model and the realizable *k-ε* turbulence model are separately used in the modeling method. Temperature filed simulation of the substrate is selected for this purpose under two sets of operation conditions with different scanning velocities. Through comparison with experimental measurement, it can be concluded that the RNG *k-ε* turbulence model generates a more accurate dynamic simulation result than the realizable *k-ε* turbulence model. The realizable *k-ε* turbulence model tends to generate a relatively low-temperature distribution.

In the future, powder particle behaviors will be simulated and the effect of the particle on the substrate dynamic simulation will be analyzed to overcome future application barriers.

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