Modelling of particle impact using modified momentum source method in thermal spraying

K Bobzin, M Öte, M A Knoch, I Alkhasli and S R Dokhanchi*
Surface Engineering Institute, RWTH Aachen University, Germany
*e-mail: dokhanchi@iot.rwth-aachen.de

Abstract. Thermal spraying is a coating process in which the feedstock material is accelerated and impacts on a substrate in form of molten or semi-molten particles. Particle impact simulation is helpful for understanding the coating build-up during thermal spraying. In this study, a computational fluid dynamics (CFD) model, based on the volume of fluid (VOF) approach, is used to model the impact and solidification of nickel particles on a flat substrate in 2D and 3D. Temperature dependent viscosity and momentum source are commonly used for solidification modelling. The former is accurate, but computationally too expensive for multiple particle impact simulations. In the momentum source method, the momentum equation of the particle is manipulated in order to reduce its velocity to zero as it solidifies. ANSYS Fluent employs this method for solidification. However, this method is proven to be inadequate for the simulation of multiple-particle solidification. In the context of this study, a modification to this method has been introduced. Temperature dependent viscosity and validated numerical studies from literature are used to validate the modified method. The developed method is proven to be capable of simulating the deposition of a 60 µm thick coating in a more feasible computational time, in comparison to temperature dependent viscosity method.

1. Introduction
Thermal spraying, as a coating technology, is categorized into three major process variants: flame spraying, electric arc spraying, and plasma spraying. In thermal spraying, the feedstock material in form of powder, wire or rod is heated to molten or semi-molten state. The resultant heated particles are accelerated in a high-temperature free jet and impact on a prepared substrate. Through the impact of subsequently approaching particles, a coating is built up [1].

Plasma spraying is characterized by particle velocities of up to $v = 800$ m/s [2] and high plasma temperatures in the range of $T = 6,000$ to $T = 15,000$ °C, considerably above the melting temperature of any known material [1]. Injected particles are usually in the size range of $20 – 90$ µm [2]. Immediately after impact, the heated particles spread and deform on the substrate. During the spreading of particles, rapid solidification with cooling rates in the range of $\dot{q} = 10^7 – 10^8$ K/s occurs due to the heat transfer from the liquid material to the underlying material and to the ambient atmosphere [3]. Therefore, particle deformation on the substrate, cooling down and solidification occur simultaneously.

The coating microstructure is directly related to the particle impact process. Therefore, it is essential to have a detailed understanding of the dynamics of particle impact on the substrate for a better control of the coating build-up. The deposition of the particles in plasma spraying can be poorly observed experimentally, since the splat formation and solidification occur in a few microseconds [4].
Hence, many studies have been dedicated to numerical and analytical investigation of particle impact, splat formation and solidification [5–9].

The volume of fluid (VOF) method provides a region-following scheme with minimum storage requirements [10]. This method is utilized for modelling two or more immiscible fluids by tracking the volume fraction of each of the fluids in two or three-dimensional meshes. Simulation time is a big challenge in numerical problems based on VOF method, since tracking the fluid phases is computationally expensive. Most of the computational cost of VOF algorithms are ascribed to the cells that form interfaces between different fluids [11]. In case of the presented study, the interfaces are the cells in which coating material and gas coexist.

The solidification and melting problems in thermal spraying are associated with many complex physical phenomena. Among others, heat transfer is an important phenomenon, which can affect the evolution of particle impact process. A comprehensive review on major methods of mathematical modelling of solidification and melting problems was done by Hu et al. [12]. They have reviewed the heat transfer analysis of major solidification methods commonly used in literature, such as the enthalpy method and source term method. The main feature of the enthalpy method is that the evolution of the latent heat is described by the enthalpy. In this method, the energy equation can be defined in terms of the enthalpy as a function of temperature. In the source term method, a heat source or a heat sink is introduced into the energy equation as an additional term. This is a popular numerical method for modelling solidification problems due to its easy implementation and low computational cost. [12]

Pasandideh-Fard et al. [13] developed a 3D model to simulate the impact and solidification of a molten particle on a flat substrate. They used the fixed velocity approach for solidification, in which the solid is defined as liquid with infinite density and zero velocity. Yet, it is not a physical assumption to consider the material with infinite density. In previous works at the Surface Engineering Institute, the impact and solidification of partially yttria-stabilized zirconia (PYSZ) particles was modelled, both on a flat and a rough substrate, using the temperature dependent dynamic viscosity approach for solidification [14]. In another work at the Surface Engineering Institute, the deposition of multiple particles with diameters between 20 and 60 µm was modelled in 3D, resulting in a 70 µm thick coating using temperature dependent viscosity approach [15]. Here it must be noticed that, this solidification method led to high computational cost in the range of several weeks of computation time. Zheng et al. [16] developed a three-dimensional model to simulate the impact of a single molten droplet on a solid substrate during plasma spraying. They have utilized the momentum source method of ANSYS Fluent, which is based on an enthalpy-porosity technique, for modelling the solidification of a single droplet. While these studies helped to increase the understanding of the particle impact and solidification in thermal spraying, they either only considered the impact of single particles or high computational times were required in case of subsequent impact of a large number of particles.

The goal of this study is to develop a numerical model for simulating the deposition of a Ni-coating in a feasible computation time. First, the temperature dependent viscosity approach was utilized to simulate the particle impact and solidification. Due to its high computational expense, this solidification method is identified to be impractical to simulate an entire coating. However, since the temperature dependent viscosity method is based on a fundamental physical phenomenon, it is used as reference to validate the developed model. For further validation, the results in [8] were reproduced to compare the developed model with a simulation, which was experimentally validated. Afterwards, the solidification model in ANSYS Fluent, which is based on the momentum source method, was used. However, an unphysical phenomenon occurred during the interaction of liquid and solid phases, which made this method inadequate for the simulation of multiple-particle solidification. In this study, a modified momentum source term is introduced which enables the simulation of multiple particle solidification. Chandra and Mostaghimi et al. [8], at the Centre for Advanced Coating Technologies, used nickel as the feedstock material to study the deposition of particles in plasma spraying on a stainless steel surface using both numerical simulations and experiments. In this study, nickel is used as feedstock material to compare the results of a three-dimensional particle impact simulation, using
modified momentum source method, to the results of Chandra and Mostaghimi et al. [8]. Finally, the validated model is employed to simulate the deposition of 100 molten nickel particles on a flat substrate in a 2D domain. Furthermore, the porosity of the simulated coating microstructure is calculated by image processing.

2. Numerical Method
In order to model the particle impact process, Computational Fluid Dynamics (CFD) approach is used. ANSYS Fluent is employed as the simulation tool to implement this method. Feedstock material and gas are the two phases to be considered in the simulation. The Volume of Fluid (VOF) method is employed to study this multiphase problem by tracking the particle and gas phases throughout the domain. Figure 1 shows the boundary and initial conditions of the simulation. In a first run, particle in-flight properties like their temperatures and velocities are taken over from [8], as this work is used as a reference for the validation. Furthermore, the simulations are conducted with different particle velocities as well as with different particle and substrate temperatures in order to analyse the functionality of the model for different processing conditions.

![Figure 1. Schematic diagram of the simulation domain for the particle impact.](image)

The substrate is modelled as a rigid wall with a constant temperature. The material properties of nickel used in the simulation are listed in Table 1. The surface tension coefficient of molten nickel is set to 1.77 N/m as reported in [17].

| Property                     | Unit     | Value  |
|------------------------------|----------|--------|
| Density                      | kg m⁻³   | 7,850  |
| Specific heat                | J kg⁻¹ K⁻¹ | 735    |
| Thermal conductivity         | W m⁻¹ K⁻¹ | 69.2   |
| Viscosity of molten nickel   | kg m⁻¹ s⁻¹ | 0.0055 |
| Latent heat of fusion        | J kg⁻¹   | 292,000|
| Melting temperature          | K        | 1,728  |

2.1. Solidification Model
Solidification depends on splat thickness, thermal diffusivities of both sprayed feedstock material and underlying solid material, and the thermal contact resistance between the flattening particle and substrate. It directly affects the deformation behavior, the splat shape and the coating microstructure [19]. Thus, solidification is an important physical phenomenon during particle impact. Reliable modelling of this complex problem represents the key challenge of particle impact simulation in
thermal spraying. In this study, temperature dependent viscosity and momentum source are considered as the two commonly used solidification modelling methods. Based on the latter, a modified solidification method is developed to simulate the deposition of an entire coating.

2.1.1. Temperature dependent viscosity. In this approach, the solid material is modelled as liquid with high viscosity. It assumes that as the particle cools down, it rapidly becomes more viscous and as a result, the particle velocity decreases. A user defined function (UDF) is used to implement this method. The temperature is calculated in every iteration and based on this, the appropriate value of viscosity is set. Temperature dependent viscosity is an accurate method for solidification modelling, since it is based on an underlying physical phenomenon. However, this method is extremely computationally expensive. In this method, the time step size of the simulation calculations decreases exponentially as the viscosity of the particle increases, respectively as the particle solidifies. This increases the total simulation time dramatically. Therefore, the method is impractical for simulating the deposition of an entire coating.

2.1.2. Momentum source method of ANSYS Fluent. ANSYS Fluent employs a momentum source which is based on an enthalpy-porosity technique [20]. In this method, the appropriate momentum sink terms are added to the conservation of momentum equations and hereby, the velocity of the particle is reduced to zero as it solidifies. The momentum source (S) is defined as:

\[ S = \beta^2 \left( \frac{\beta^3 + \varepsilon}{\beta^3 + \varepsilon} \right) A_{\text{mush}} v \]  

In equation (1), \( \beta \) is the liquid volume fraction which is defined here as the volumetric proportion of the fluid phase consisting of the liquid particle phase together with the gas phase in a cell, \( \varepsilon \) is a small number (0.001) to prevent division by zero, \( v \) is the fluid velocity and \( A_{\text{mush}} \) is the mushy zone parameter which is a constant number. \( \beta \) is computed based on an enthalpy balance at each iteration. In the mushy zone, the liquid volume fraction (\( \beta \)) lies between 0 and 1. \( A_{\text{mush}} \) determines the rate at which the source term reduces the velocity. The higher \( A_{\text{mush}} \), the more the source influences the momentum equation. However, very large values may cause the solution to diverge.

In case of a fully molten material, the liquid fraction is one. Thus, according to equation (1), the source term would be zero. In fully solidified regions, \( \beta \) is zero. Thus, the source stops the particle motion.

When using the momentum source method in ANSYS Fluent, an unphysical interaction between solidified particles and molten material of another particle was observed. Upon contact between two such particles, the motionless solid particle is accelerated and thrown out of the simulation domain. This behavior is only observed when simulating the subsequent impact of several particles. The unphysical behavior is assumedly caused by an unknown numerical error in implementation of the method. This study is focused on solving this problem by modifying the momentum source term as explained in the next section.

2.1.3. Modified momentum source method. To circumvent the problem described above, a modification to the momentum source method for solidification modelling is introduced. Equation (2) is the developed function, which replaces equation (1) to manipulate the conservation of momentum equations of the particles.

\[ S = -C V F_p K(p) v \]  

In equation (2), \( C \) is a constant, \( V \) is the volume fraction of the particle, \( F_p \) is the particle function, \( K(p) \) is the kernel function of the particle and \( v \) is the particle velocity.
In equation (2), \( C \) is a numerical constant, \( \text{VF}_p \) is particle volume fraction which is the volumetric proportion of particle phase under or above the melting temperature, \( K(\rho) \) is a function of mixture density and \( \mathbf{v} \) is the velocity vector.

The numerical constant used in equation (2) is adjusted iteratively based on the viscosity method to assure a physically valid implementation. The momentum source is proportional to the velocity and is directed in the opposite direction. Therefore, when the velocity of the particle is positive, a negative momentum source is added to the momentum equation as well.

In the momentum source term of the Fluent, the volume fraction of the fluid phase (\( \beta \)), consisting of the liquid particle phase and the gas phase, is considered. For the particular application of particle impact in thermal spraying, it would be seen favorable to distinguish between the liquid particle phase and the gas phase. For this purpose, the parameter \( \text{VF}_p \) has been introduced instead of \( \beta \). The particle volume fraction in equation (2) could be liquid or solid. Therefore, a temperature condition is implemented to apply the momentum source only on the solid phase. If the temperature is below or equal to the melting temperature, the source is computed according to equation (2) to stop the particle deformation. If the temperature is above the melting point, the source is set to zero. In equation (1), there is no temperature condition and the momentum source depends on the liquid volume fraction (\( \beta \)).

The parameter \( K(\rho) \), according to equation (3), controls the rate of increase in the momentum source with respect to the inertia of the existing materials in a single cell. In equation (3), mixture density is the average density of a single cell in which both coating material and gas coexist. The mixture density is equal to the density of feedstock material in cells in which the particle volume fraction corresponds to one. In mushy zone, the amount of mixture density is proportional to the volume fraction of the coexisting phases.

\[
K(\rho) = \frac{(\text{mixture density} - \text{gas density})^n}{(\text{feedstock density} - \text{gas density})^{n-1}}
\]  

(3)

Figure 2 shows the plot of \( K(\rho) \) versus mixture density for different \( n \) values. The value of feedstock density is taken from Table 1 and gas density is set to 1.225 kg m\(^{-3}\). In mushy zone, the cells with lower mixture density have less inertia. The amount of momentum source for these cells should be lower in comparison to the cells with higher mixture density. The parameter \( K(\rho) \) adapts the amount of momentum source to the inertia of the cells exponentially. For higher \( n \) values, the effect of the momentum source is reduced for the cells containing lower mixture density. However, by choosing a very high \( n \) value, the rate of stopping deformation decreases because the source will act only on highly pure particle phase. After running several simulations with increasing \( n \) in the momentum source, \( n = 5 \) was selected to add an appropriate momentum sink term to the momentum equation of the particle.
Figure 2. Plot $K(\rho)$ versus mixture density for different values of $n$.

Furthermore, both the particle volume fraction ($V_{FP}$) and the parameter $K(\rho)$ in equation (2) contribute to eliminate the effect of momentum source on the gas phase. Without considering these parameters, the particle does not touch the substrate and deforms in the air as shown in Figure 3-a. The lack of contact between the substrate and particle influences the cooling down of the particle and consequently the spreading and flattening behavior cannot be modelled properly. This problem is due to the significant influence of the momentum source on the gas phase. To simulate the particle solidification, the momentum source should be applied only on the particle phase. However, Fluent applies the momentum source to the mixture of phases. Together with high values of $A_{mush}$, this leads to an unphysical outcome of simulation as shown in Figure 3-a. Hence, in the presence of $V_{FP}$ and $K(\rho)$, as introduced in Figure 2, this undesired affect could be eliminated (see Figure 3-b).

Figure 3. a) Problem in case of acting momentum source on the mixture phase. b) Minimizing the effect of momentum source on the mixture phase.

It should be noticed that the modified momentum source term presented in equation (2) is one of the alternative approaches to adjust the source term in equation (1) for particle impact in thermal spraying. The possibility of using other parameters to modify the momentum source term to be well-functional in thermal spraying applications is not excluded.

3. Results and discussion

In order to validate the developed model, the results of a 3D particle impact simulation using the modified momentum source are compared to the results of Chandra and Mostaghimi et al. [8] (see Figure 4). The model presented by Chandra and Mostaghimi et al. was also experimentally validated [8]. Therefore, it is a suitable validation case for this study. In both simulations, nickel is used as the feedstock material. Small variations might be attributed to the nickel material properties, since this information is not provided in [8]. The particle diameter, impact velocity, particle and substrate temperature are set to $D = 60 \mu m$, $v = 73 m/s$, $T_p = 1,873 K$ and $T_s = 673 K$ respectively. In Figure 4,
the splats exhibit a similar disk-shaped morphology, which shows a good agreement of both splat length and the development of splat morphology with the investigations in literature [3, 8].

![Figure 4](image-url)

**Figure 4.** Particle impact model in 3D using a) modified momentum source and b) fixed velocity method reported in [8].

As a further validation, the results of the simulation, which follows the temperature dependent viscosity approach, is used as a reference. Figure 5 shows the results of the impact of a 60 µm diameter molten nickel particle using the modified momentum source (a) and the temperature dependent viscosity approach (b). In this case, a higher particle velocity of v = 200 m/s and a slightly lower particle temperature T_p = 1,750 K are considered in order to analyse the functionality of the method for different particle in-flight properties. In this simulation, the substrate temperature is set to T_s = 300 K. As the simulation time increases, the particles spread and deform on the substrate. In Figure 5, t = 0 corresponds to the time point of the first contact of the particle to the substrate. The particles still deform at the time shown in the figure. The splat deformation in both cases are compared visually by making an animation sequence with the volume fraction contours. The splat length of both cases are in the same order of magnitude. Therefore, the results of temperature dependent viscosity can be replicated by the modified momentum source method. The main motivation of using momentum source, instead of temperature dependent viscosity for solidification modelling, is that the momentum source allows the use of significant larger time steps. In this case, the time step size in the momentum source simulation was ca. 10^4 times larger than the simulation using the temperature dependent viscosity approach. Consequently, the computation time was reduced approximately by the factor of 100.
Figure 5. Particle impact model in 2D using a) modified momentum source and b) temperature dependent viscosity.

The modified momentum source method yields comparable results as the temperature dependent viscosity method, as well as the numerical and experimental studies in literature [8]. Hence, the developed model is suitable to simulate multiple particles in 3D and also the deposition of an entire coating.

The substrate temperature is vital for the spreading and final shape of the impacted particles [8]. The effect of substrate temperature on the spreading and final shape of the impacted particles was investigated. Typically, during a plasma spray process, the splats result in disk-like shape when the substrate temperature is above 300–400°C [3]. Figure 4 shows the simulation results of disk-shaped morphology of splats, where the impact occurs on a hot substrate. In a further simulation, successive impact of two particles is simulated in order to analyse the functionality of the developed model in a slightly more complicated model setup. In this case, the substrate temperature is reduced to $T_s = 300$ K. Figure 6 shows the successive states of two nickel particles during the impact on a non-heated substrate in a three-dimensional simulation. The initial temperature of the particles is set to $T = 1,750$ K. Thus, the particles are fully molten prior to the impact. The particles have a diameter of $D = 60 \mu m$ and an impact velocity of $v = 200$ m/s. The parameters were changed in comparison to Figure 4 to investigate the possible splash development for faster particles impacting on a cold substrate. Although, an apparent splashing behavior cannot be triggered for the chosen particle in-flight properties and a disk-shaped flattening of the particles is evident, the model is obviously capable of resolving the interaction between two successively impacting particles. Nevertheless, a partial splashing of the second particle in the region of the interaction with the underlying particle can be resolved using the developed model. It is assumed that, a radial jetting takes place at the regions depicted as splashing area in Figure 6, as a result of the altered spreading velocity and solidification rate of the second particle due to the interaction with the underlying one.
Figure 6. 3D model of particle impact using modified momentum source method for solidification.

In a further step, the developed model is utilized to simulate the deposition of a higher number of particles. Figure 7 shows a coating microstructure resulting from the impact of 100 nickel particles with the diameter, temperature and velocity of $D = 60 \, \mu m$, $T = 1,750 \, K$ and $v = 200 \, m/s$ respectively. In this simulation, the substrate temperature is set to $T_s = 300 \, K$. In a real APS process, the particles have different velocities, temperatures and sizes. The aim of this study was to develop a numerical model for simulating the entire coating in a feasible computation time. To demonstrate the feasibility of the developed model, the result of a coating simulation with constant particle parameters is presented. Here, an average time interval of 5 microseconds is chosen between two consecutive particles. The particles are introduced to random locations in the simulation domain. The porosity ($\phi$) of the simulated coating microstructure is calculated to be $\phi = 3.52 \%$ by processing of the dark and light grey pixels of the coating image in MATLAB. The thickness of the coating is 63 $\mu m$. The developed model can be further used to understand the development of the particles deposition and also predicting the porosity of a coating microstructure in thermal spraying. In order to predict the porosity with a reasonable accuracy, different velocities, temperatures and dimensions of successively impacting particles need to be considered in the simulations. The developed model is capable of conducting simulations with different particle in-flight properties as well. The results of these simulations will be addressed in the further publications.
Summary and conclusions
Since the splat formation and solidification in thermal spraying occur in a few microseconds, it is extremely difficult to observe the dynamics of particle impact experimentally. Hence, modelling of particle impact process is of great interest.

The aim of this study was modelling and simulation of the deformation, cooling down and solidification of multiple nickel particles on a solid substrate during thermal spraying. A Computational Fluid Dynamics (CFD) model, based on the volume of fluid (VOF) method, was utilized in ANSYS Fluent as the simulation tool to model the particle impact both in 2D and 3D. In this respect, two common solidification models, temperature dependent viscosity and momentum source method, were presented. The advantages and limitations of each solidification model were further studied. Finally, a modified method for particle solidification was introduced to eliminate the implementing limitations of previous methods. The developed model has been validated with the results of the temperature dependent viscosity method as well as other numerical and experimental studies in literature. The modified method is able to simulate a coating microstructure in a feasible computation time.

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