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A critical review on the numerical simulation related to Physical Vapour Deposition

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Abstract

Physical Vapour Deposition (PVD) is a process usually used for the production of advanced coatings regarding its application in several industrial and current products, such as optical lens, moulds and dies, decorative parts or tools. This process has several variants due to its strong evolution along the last decades. The process is commonly assisted by plasma, creating a particular low pressure and medium temperature atmosphere, which is responsible for the transition of atomic particles between the target and the parts to be coated into a vacuum reactor. Several parameters are directly affecting the deposition, namely the substrate temperature, pressure inside the reactor, assisting gases used, type of current, power supply, bias, substrate and target materials, samples holder and corresponding rotation, deposition time, among others. Many mathematical models have been developed in order to allow the generation of numerical simulation applications, trying to combine parameters and expect the corresponding results. Numerical simulation applications were created around the mathematical models previously developed, which can play an important role in the prediction of the coating properties and structure. This paper intends to describe the numerical simulation evolution in the last years, namely the use of Finite Elements Method (FEM) and Computational Fluid Dynamics (CFD).

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Keywords: Simulation; Reactor; Physical Vapor Deposition; Coating; Numerical Modelling; Finite Elements Method; Computational Fluid Dynamics;

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1. Introduction

The need to increase the components' lifetime by protecting their surfaces from wear and corrosion has accelerated the development of new surface studies in Mechanical Engineering [1-3].

Initially, some design changes were made to overcome the above mentioned problem. Nowadays, several techniques are used allowing to modify the surfaces' characteristics, such as wear resistance properties through deposition of ultra-hard thin films, usually called coatings [4, 5].

The use of coatings improves surface abrasion, erosion, adhesion or fatigue behavior, protecting it against corrosion, improves the surface appearance, decreases residual stresses and friction coefficients as well as improving wear and chemical stability [6-12]. Due to the importance of these aspects, many researchers have done a large number of studies in mathematical modelling and numerical simulation of coatings. There are also studies on the thermal conductivity of coatings, as the substrates' thermal conductivity is a characteristic that influences the performance of the coatings' mechanical properties [13-17]. In these studies, it is very important the correct interpretation of the thermal and mechanical analysis [18].

Other studies, such as improving the thermal insulation behavior of thermal barrier coatings [13, 19], vapors behavior from materials and gases deposition, plasma improvement by optimizing the vacuum system or study of the collisions process between target and substrate, were also performed using the Computational Fluid Dynamics (CFD) numerical simulation. This tool is widely use together with experiments to understand the real problem, as it is a cost efficient and expeditious tool for solving problems [20]. However, simulation of combustion systems requires large computational efforts, namely, in the mesh and huge equations number [21] therefore, powerful computers are needed. The CFD simulation tool is also widely used to evaluate, improve, predict and/or optimize processes like in Biomass Combustion [20-24], in Fuel Combustion [25], in different Reactors types, namely, a continuous PhotoFuelCell (PFC), solar tubular, fixed biofilm, industrial methanol synthesis, tubular Pd-Ag membrane, steam cracking, industrial Claus and industrial physical vapor deposition reactors [26-35], among others.

The coating deposition can be performed using the most varied techniques. The researcher's desire and interest in achieving better results in the materials' filed has given rise to several variants in the coating technique. To understand the literature review regarding Physical Vapour Deposition (PVD) coatings using 2D and 3D simulation in CFD, a small introduction to the process will be undertaken.

In order to understand the behavior of the sputtering PVD coating process into the reactor, some studies have been carried out using 2D and 3D numerical simulations, Finite Elements Method (FEM) and CFD. Simulation assumes particular relevance when the physical reproduction of the problem becomes very expensive and encompasses in time.

The development of numerical methods as well as digital technology allows elaborating mathematical models to cover the largest practical cases number. Regarding simulation, it is possible to better know all the phenomena occurred in the process. This acquired knowledge allows for its optimization, whereafter validation can be done through a real-scale test [28, 29, 31].

To provide a tribological improvement, simulation is also used in many mathematical models. They are used to improve the protection of surfaces subjected to wear and corrosion, improve their structure and films composition as well as to optimize the process variables that are involved in PVD coatings [33].

This review will focus on the numerical simulation studies done in the last years, namely with the use of FEM and CFD mainly applied to PVD coating processes.

2. Physical Vapour Deposition Technique

The PVD coating process has brought some solutions to problems associated with the characteristics of metallic and non-metallic materials, for example wear resistance and corrosion protection, among others [1, 36]. The materials technology followed the technological evolution with the appearance of new coating techniques as well as their maturation. The commonly used coating techniques can be seen in the scheme below.

In gaseous state processes, the usually used coating methods are the Chemical Vapor Deposition (CVD) and PVD. Fig. 1 shows a resume of the surface coating methods [37-39].

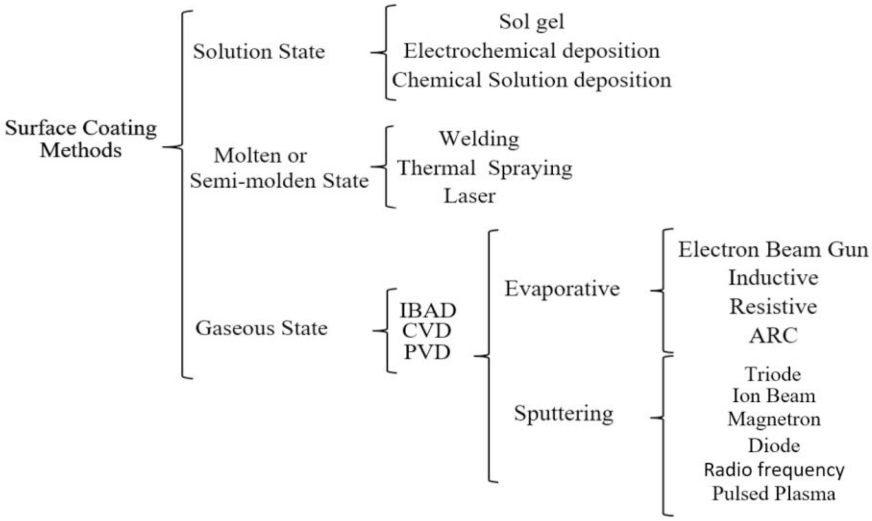

Fig. 1. Surface coating methods [37].

In these cases, the surfaces treatment is through a gaseous phase or vapor before depositing or modifying the surface.

The principle of PVD deposition is based on the projection of material from one or more solid sources, called targets, into one or more substrates within a gaseous plasma or vacuum chamber, as can be seen in Fig. 2 [40, 41].

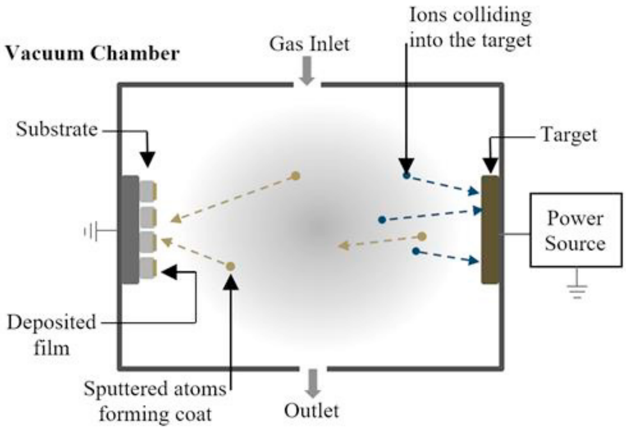

Fig. 2. Schematic diagram of the PVD methods

PVD is a vacuum plasma deposition technique where the material to be deposited is heated through the chamber into the substrate to form a thin film. The coating material chosen is an important element in this technique because it has a great impact on the substrate adhesion and also on the temperature to be used due to the different melting points of the materials. Adhesion to the substrate will depend on the type of material selected.

PVD Sputtering is a plasma deposition method as the evaporation technique, but in this case targets are used, these ones are bombarded by an ionic gas to release nanoparticles that will be deposited on the substrates to create thin films [37-39].

The PVD Evaporation process requires high vacuum pressure and lower atomic energy. The coatings absorb less gases, having higher mass particles compared to sputtering. This results in a lower adhesion to the substrate and a larger coating thickness. This coating process is suitable for industrial applications where the main requirement is not the morphology of the material [39-41].

To study the phenomena that occur in the PVD method, numerical simulation models are used. The most commonly used methods are FEM and CFD. Table 1 shows the focus of each method.

Table 1. FEM and CFD focus.

Numerical simulation	Focus
FEM	Analyses based on product
CFD	Analyses based on reactor's process

In the following chapters these methods will be discussed.

3. Finite Elements Method (FEM)

Projects in the areas of aeronautics, nuclear applications and space travel, among others, are greatly complex due to the demands on safety and reliability. Other projects with requirements of high complexity, for example, acoustics, chemical pollution control and thermal, need to be studied to improve their performances. For this, it is necessary to create mathematical models to simulate the behavior of physical systems. However, some problems have such a high degree of complexity that it becomes very difficult to create a mathematical model [42].

In the last decades the appearance of simulation software based on FEM came to contribute to the modeling of these complex problems [43]. Indeed, in order to understand and solve complex problems in mechanical engineering requires researchers to use numerical methods tools. Some of them, such as FEM, are prepared to help researchers study problems of heat transfer, temperature, fluidity and aerodynamics, mass transport and electromagnetic potential, stress analysis, and others. [44, 45].

The FEM tries to find the solution of a complex problem, replacing it with a simpler problem. This approach allows to come up with only an approximate solution and not the exact solution. The available mathematical tools are not capable enough to find the exact and sometimes approximate solution. After narrowing in on a solution, it is possible to improve or approximate the real solution using more computational efforts [46].

When one uses the FEM it is necessary to go through three phases, pre-processing, analysis and post-processing. The first stage, pre-processing is the most difficult. At this stage, it is necessary to transform the real problem into a mathematical model and to arrive at a numerical solution. The phase of analysis and post-processing will be more effective, the closer the characterization of the problem is to reality. It is necessary to use the appropriate equations, to associate the correct boundary conditions and do an appropriate analysis, for example, linear, nonlinear, stationary, transient, etc.

The finite element mesh must balance the size, that is, it must be refined to obtain good results, but at the same time it can not be exaggerated because it becomes very slow in processing. In the third phase of analysis, the software acquires the data and solves a system of algebraic equations. In the post-processing phase, the researcher has the difficult task of interpreting the results. This interpretation will be influenced by the existing knowledge about the problem, the software, as well as the professional experience of the researcher [47].

Below it can be seen some examples of coatings problems with high complexity solved using FEM.

(a) Śliwa et al. [9] simulated and stutied the multilayers stress distribution evaluation taking into account their deposition conditions on magnesium substrates. This paper studied the difference of internal stresses between the coating and the substrate. They confirmed, with experimental values, that FEM can predict coating properties in surface engineering. So laboratory tests can be reduced to economize time and money. With FEM, is possible to discover the depressions left after the ejected droplets, pores and solidified droplets of the deposited material PVD.

(b) Śliwa et al. [18] studied the internal stresses in coatings obtained by PVD magnetron process under different temperatures (between 460 and 540 ºC) on sintered high-speed ASP 30 steel. It was simulated with FEM in ANSYS® environment. They concluded that simulation results regarding specimens stresses correlate with experimental results. The paper shows a capable model to caracterize the stresses of depositions effects on PVD coatings.

(c) Skordaris et al. [49] developed a mathematical model using FEM to simulate the surface coating fracture caused during the nano-impact test. This model enables simulation for mono or multi-layer. According to the results obtained, this model can be applied to evaluate the effect of several coating structures on their brittleness.

(d) Skordaris et al. [50] studied the contact between the coated tool and the work piece through a FEM simulation. They compared the High Power Pulsed Magnetron Sputtering (HPPMS) with thin coatings on tools in machining processes. It was necessary to give information about film thickness effect on the tool wear evolution. It was found that increasing the film thickness, the tool life is extended almost proportionally with the coating thickness. Thus the higher cost is compensated compared to thin coatings.

(e) Skordaris et al. [6] studied the coating's mechanical properties, cohesion, brittleness and adhesion using nano-impact tests, stress measurements, nanoindentation and FEM calculations. In the investigation, they changed some conditions, such as compressive residual stresses in the film structure that was eliminated by annealing tratment. They concluded that coating residual stresses affect the wear behavior and film properties.

(f) Wang et al., [13] employed the FEM to simulate the heat transfer behavior of thermal barrier coatings (TBCs) based on different interfacial thermal resistance (ITR) models using different conditions. The results of heat flow around the interface presents fantastic changing characteristic. They conclued that the interface roughness also induces a very important effect on thermal conductivity of the as-sprayed TBCs. The investigation helped to creat a powerful guide to design coatings in the future.

(g) In PVD coatings, one of the most used tests to check the film failure mechanisms is the nano-impact test. These tests can introduce local deformations and stresses into the film. Bouzakis et al. [51] developed the 3D-FEM model, to simulate the nano-impact test on a TiAlN PVD coating. This simulation had the conditions equal to the real conditions and describes accurately the film loading and fracture mechanisms, according to the coating mechanical properties.The final results converged with the experimental ones and the FEM model predicts the film failure initiation and evolution.This model can be used with various strength properties and surface treatments.

(h) Michailidis [16] made a study of the temperature-dependent PVD coating properties associated to milling Ti6Al4V varying the shear rate and temperatures from ambient to 400°C. The shear tests were complemented by impact and nano-indentation tests. The obtained results were supported in the FEM, thus allowing the determination of the temperatures and the shear stresses. The study of temperature-dependent properties serves to understand the difference in useful life between coated and uncoated tools.

(i) Skordaris et al. [10] investigated the PVD TiAlN coatings with diverse compressive residual stresses on cemented carbide. They studied the coating's mechanical properties, adhesion, brittleness and cohesion, using nanoindentations, nano-impact tests, as well as FEM. The conclusion revealed some compressive stresses on the film contribute to increase coating mechanical properties and a longer lifespan. However the coated tools' wear increase if residual stresses are greater than the maximum value. This phenomenon deteriorates the film adhesion and increases its brittleness leading to a shorter tool life.

(j) Paiva et al. [17] studied the influence of different machining conditions on the wear and tribological performance of TiB_2-coated cutting tools. For this, they made a FEM modeling to study the friction surface, namely temperature profile, for machining conditions with diferent parameters. The characterization of TiB_2 coated cutting tool wear versus uncoated was done through SEM, EDX and XPS. These results were linked to the FEM modeling. It was then concluded that the TiB_2 coating is more efficient at lower shear rates. For high cutting speeds, the wear performance is identical to the uncoated tool.

(k) Bolot et al. [14] studied the relationships between the microstructure of a coating and its macro-properties with FEM. This study is important to understand the presence of defects, like voids, that origin a decrease in the effective thermal conductivity, so, a study was made regaring the thermo-mechanical properties of a plasma-sprayed composite coating.

(l) Lofaj et al. [52] used FEM combined with nanoindentation and its depth profiles modulus with different radii on hard Tungsten carbide coating steel substrate to study the influence of indenter tip radius on coating. They conclued that if the indenter tip radius increases or the coating thickness decreases, a reduction of the peak of the depth profiles occurs causing fake results.

(m) Beblein et al. [15], used 2D FEM to study the thermomechanical properties of coatings necessary for cutting tools. To create a 2D FEM, it was taken into account the coating properties, like physical and technological boundaries of CrAlN. They concluded that adhesion behavior and coating thickness influence the thermomechanical load on cutting and the stresses in the coating are influenced by the Young's modulus, but does not affect the stresses within the substrates. Due to low thermal condutivity, the increase in coating thickness originates heat accumulation. The abrasive wear resistence can decrease because the hardness is temperature dependent.

(n) Rao [12] evaluated the mechanical properties of thin films by FEM, namely in Nylon coatings deposited on the Soda-lime glass substrates. The Young's modulus and hardness was extracted by experimental results. Comparison between the simulation data and the experimental results allows to concluded that they are very similar.

(o) Wang et al. [19] used FEM for calculating the thermal insulation and the fracture failure problems of the thermal barrier coatings (TBCs). With the FEM model created, it is possible to predict the interfacial thermal resistance effect, convection between the environment and coating, the residual stress which is caused by the thermal expansion coefficient between the coating and substrate, or the residual stress which is induced by the plasma spraying process.

(p) Micro-blasting on PVD films can induce material deformation. This can change the superficial mechanical properties of PVD films. For this reason, Bouzakis et al. [11] developed a FEM algorithm to determine residual stresses after micro-blasting. To validate the model, it was taken into account nanoindentation FEM simulations in micro-blasted TiAlN coatings. The FEM simulation results were very similar to the measured values.

4. Computational Fluid Dynamics (CFD)

A tool widely used today to simulate, evaluate and improve engineering problems that involve fluid flow is the CFD. It is possible to find works in the areas of process sciences, pharmaceuticals, biomedical, energy production, nuclear safety, combustion, thermal balance, environmental impact, fluid dynamics, among others [22-25]. The studies in CFD are usually of high complexity due to the problem characterization and the variables to be simulated. The greater the approximation to the real problem, the higher will be the detail needed in the characterization and due to this requirement, the processors used should be effectively powerful. In complex studies with a large number of variables, it is important to simplify the input data to be able to simulate and optimize the problem [54].

CFD, like in FEM, goes through three stages: pre-processing, analysis and post-processing. The pre-processing phase is very important because it will influence the next phases. The investigator must know the problem very well and characterize it at this stage. It is necessary to characterize the boundary conditions, to use the appropriate equations, and to make an appropriate analysis of the problem. The problem mesh has to be well scaled to get a result close to the real one however, it can not be overstated because it will increase the computational effort. In the third phase, post-processing, the researcher has to analyze the results based on knowledge of the problem and the software [55]. Below it can be seen complex studies solved using CFD:

(a) Sen et al. [56] used CFD simulation to describe the self-propagation of the exothermic reaction in Ti/Al reactive multilayer. They showed the time is dependent temperature flow and that CFD presents a huge potential to simulate exothermic reaction in the nanoscale Ti/Al foil. They also founded different reaction modes, for steady state and unsteady state.

(b) The plasma enhanced chemical vapor deposition (PECVD) is the most used method in the manufacture of silicon thin films for solar cells and microelectronic industries because it has lower costs and moderate operating temperatures. Crose et al. [57] developed a multiscale CFD simulation to study the PECVD of thin film solar cells. The 2D-CFD model produced, with accuracy, a plasma chemistry and transport phenomena within the reactor.

(c) Coating processes are very complex and cold spray coating is one of them. When aiming to optimize it, it is necessary to be careful with all parameters, like the input temperature, velocity distribution and pressure in the cold spray nozzle. Adebiyi et al. [58] optimized some of these parameters with a CFD model and achieved coatings with higher hardness and lower porosity.

(d) Abdel-Fattah et al. [26] studied an industrial Claus reactor with CFD Simulation help. They built a 3D-CFD model to describe the flow fields and chemical reactions for two different industrial cases. The results obtained are very similar to the industrial data. They proposed the use of the CFD model with different reactor designs.

(e) Tapia et al. [27] developed a thermal CFD model to evaluate the performance of a solar tubular reactor design. They demonstrated that the tool is powerful to identify weaknesses in the solar tubular reactor. In addition, the model can simulate and predict under different operating conditions.

(f) Prades et al. [28] developed 2D bioreactor models with three different tools, AQUASIM, MATLAB, and CFD. They considered ideal flow patterns to more complex fluid dynamics. The goal of the study was to investigate the fluid flow dynamics in the bioreactor models. Simulation results were validated through the measurements obtained by means of high spatial resolution micro sensors.

(g) Mirvakili et al. [29] developed a CFD model to study the temperature decrease occurred at the end of the gas-cooled reactor. The condensation problem occurs after four functioning years and the CFD model was created to find the reasons. The result achieved was validate with the real data. They found that the reasons are improper design of the distributer inside the reactor. This one generates poor fluid distribution inside the reactor.

(h) Phuan et al. [30] created a CFD model to propose and design a PhotoFuelCell (PFC) reactor, namely simulate the events within the PFC reactor. The model created was used to predict the anodic chamber performance. They concluded the simulation is useful to give the conditions of effective water treatment and also give the simultaneous solar hydrogen production in the cathodic chamber.

(i) Ghasemzadeh et al. [31] presented a 2D-CFD isothermal model to investigate a tubular Pd-Ag membrane reactor. They studied an EB dehydrogenation by Pd-Ag membrane reactor and compared the performance of two different flow patterns with respect to traditional reactor. The model provides the local information of pressure, velocity and others for the driving force analysis. The model validation was done with experimental data. They achieved good simulation results compared with real values.

(j) Silva et al. [32] created a CFD using a multi-phase Eulerian-Eulerian approach to study the reaction assessment and fluid dynamics of diesel oil hydrotreating reactors. Some study parameters were pressure, temperature, velocity, gas and liquid flows to know if they influence the reactor performance. They investigated too the porosity influence on fluid velocity and volume fraction of liquid. This model can capture fluid characteristics on the mesh, such as volume fractions, velocities and concentrations. With this information it is possible to calculate reaction and mass transfer rates. Comparing the simulation values and the real ones, the results are very good.

(k) Vandewalle et al. [34] developed a 3D-CFD model to simulate coke formation in 3D steam cracking reactor geometries. The algorithm created is based on dynamic mesh generation. They studied the influence of the growing coke layer with reactor pressure and temperatures. The work concludes that the ribbed reactors overall outperform the other ones. The tubular geometries growth is not uniform, influencing fluid dynamics, coke formation and product yields.

(l) Menon et al. [35] studied Fuel reactor of the Chemical Looping Combustion (CLC) with help of 2D-CFD. In this work Fe_2O_3, CuO and their combination is used. The 2D model simulates the system behavior. They used Indian coal and studied the ash effect performance. When they tested the system without ash, they conclued that the CuO has superior performance than mixed carrier and Fe_2O_3. However, when they included ash, the mixed compost had a better performance.

(m) Guo et al. [59] used a discrete particle CFD model to simulate a Chemical Looping Combustion (CLC) in a packed bed reactor with a metal/metal-oxide oxygen carrier. The reactor has a cylindrical fixed bed with 450 porous spheres. These ones represents the oxygen carrier particles. The CFD model simulation provides very detailed fields of flow, temperature and species because it is a discrete particle methods. The simulation shows apparently improvements with some thicknesses.

(n) Kapopara et al. [48] simulated the gas flow and mixing behavior within the reactor chamber for TiN thin films deposited by magnetron sputtering. They used the 3D-CFD to study and predict the properties, such as, pressure profiles, velocity and concentration distribution of the process gas species like nitrogen and argon in the sputtering chamber. They concluded two important things: the gas inlet and substrate location influence the gas distribution and substrate where the reactive gas will react to form coating. The CFD modeling has a huge potential for simulating multi-component gas flows and the behavior of gas velocity, pressure and gas species concentration distribution in sputtering chamber.

(o) Kapopara et al. [53] used 3D-CFD simulation to investigate various sputtering parameters, such as, pressure profiles, velocity, mass flow rate, density profiles and concentration distribution of the process gases. This study was based on zirconium nitride films deposited on glass and silica substrates by RF magnetron sputtering. They conclude that the gas inlet location has a huge influence on gas distribution inside the chamber. Here is exactly where the reactive gas will form coating. This information is very important because it is possible to modify the reactor geometry and find a better gas flow to improve the coating.

(p) Bobzin et al. [33] used CFD model to caracterize an industrial scale plasma reactor CC800/9 and simulate a neutral gas flow of argon and molecular nitrogen gas inside. The authors used CFD simulation tools Fluent and dsmcFoam. Their simulation used a fluid model and a kinetic Direct Monte Carlo model. In the first model it was used the Navier–Stokes equations to describe the gas flow, while in the second it was used the Boltzmann equation for the kinetic approach. After checking both models, they found different results of gas flow for the transition regime, only the kinetic model was capable to provide an accurate physical description.

5. Concluding Remarks

After this review it was possible to observe that the FEM and CFD numerical simulation are powerful tools for studying complex problems associated with PVD by reducing R&D costs. After the model creation, it is possible to improve the problem and even extrapolate and apply to other problems. The common research areas of these tools are heat transfer, fluid flow, aerodynamics, temperature, mass transport, electromagnetic potential, however each of them has its specific characteristics. The FEM helps to study the phenomenous related to the product, i.e., substrate and coating, on the other hand the CFD helps to solve problems that arise in PVD processes, such us, gas properties and fluid flow. The table 2 summarizes the application of these two methods that supports research in PVD coating.

Table 2. Overview about FEM and CFD main features and fields of application.

FEM	CFD
Prediction of coating's mechanical properties	Study the plasma-enhanced chemical vapor deposition of thin film used in solar cells
Influence of different machining conditions on the wear and tribological performance of coated cutting tools	Optimization of the input temperature, velocity distribution and pressure in the cold spray nozzle
Contact between the coated PVD tool and the work piece	Prediction of the temperature ramp-down occurred at the end of the deposition process
Presence of defects	Thermal evaluation in a reactor design
Influence of indenter tip radius on coating	Study of the fluid flow dynamics
Material deformation	Prediction of the anodic chamber performance
Prediction of thermomechanical properties of PVD coating	Prediction of the properties of the process gas species into the sputtering chamber
Study of the coating fracture surface	

It is possible to see in the literature analyzed that FEM is generally used to study problems associated with mechanical properties, namely, stresses in the coating, adhesion, wear, influence of coating thickness, among others. On the other hand, CFD is usually used to study problems associated with heat transfer, fluid flow, aerodynamics, temperature, mass transport, electromagnetic potential, among others. All the studies analyzed are focused on understanding, investigating, improving or optimizing the problem. The success of studies regarding other reactor types with the CFD increase the researchers interest in the simulation application of PVD coatings. Initially, the studies had been focused mainly on the materials' properties but now the trend will be to study the PVD reactor in an industrial context using the simulation, and avoiding the cost of stopping. This leads to conclude that there are still many problems to be studied using CFD for PVD reactors, such as improving plasma spraying and its density, optimizing cycle times, making the coating process efficient, studying the gas flow, namely the entering position, the quantity and times of use, substrates position and rotational speed, changes in geometry inside the reactor chamber and gas or gas combinations to assign the desired coating's characteristics.

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