

FLUID FLOW AND HEAT TRANSFER SIMULATION IN A BARREL TYPE CVD REACTOR

Hamid Nabati¹, Jafar Mahmoudi²

¹PhD Student, School of Sustainable Development of Society and Technology (HST),
Mälardalen University
Västerås, Sweden

²Adjunct Professor, School of Sustainable Development of Society and Technology (HST),
Mälardalen University
Västerås, Sweden

hamid.nabati@mdh.se (Hamid Nabati)

Abstract

Thin-film coating plays an important role in the manufacturing of many cutting and drilling tools. One of the most common types of thin-film coating methods is chemical vapor deposition that is known as CVD in industry. The CVD involves deposition of a thin film from gas phase precursors onto a solid substrate. The uniformity of film thickness is a critical in tools production. To achieve this uniformity, it is necessary to understand the governing transport processes, flow behavior and heat transfer inside the CVD reactor. In the coming paper the aim is numerical modeling of CVD processes using an existing simulation software, Fluent©. A three dimensional model of active part of reactor is simulated. Geometry is simplified to concentrate on flow regime in the whole solution domain. Simulation results show that the gases feeding entrances have great effect on the velocity and temperature field. Based on the results, it is recommended to use same feeding holes diameters to achieve the uniform velocity and temperature field inside the coating domain.

1 Introduction

High quality machining is achieved and accomplished by using high grade cutting tools. All manufacturers continuously apply new manufacturing materials that are lighter and stronger, so the cutting tool makers have to develop tools that can be used for new materials machining at the highest possible levels of productivity. To attain this goal, combinations of better tool material compositions, modern coating techniques and novel geometries are necessary. This development process is continuous and interactive. Among these challenges, coating is one of the most important parameters that has major effects on tools

characteristics like toughness, resistance to oxidation, hardness and resistance to thermal shock. Most steels and cast irons, and also non-ferrous materials such as aluminum alloys are easier to machine than materials such as stainless steels, titanium alloys and super-alloys. So depending on the material which is machined, a given tool material may not perform adequately unless its properties are strengthened. Application of hard coatings by various methods is also used for this purpose. Both single and multiple-coating have been shown that significantly enhance any tooling material, but this is a complex subject that needs careful design to achieve high performance.

There are basically two techniques of hard coating for cutting tools used in the industry[1]: chemical vapor deposition (CVD) and physical vapor deposition (PVD). Each of these methods includes several special techniques that are summarized in Tab. 1.

Tab. 1 Hard coating techniques for cutting tools [1]

CVD	PVD
Conventional CVD	Evaporation
Plasma Assisted CVD (PACVD)	Magnetron Sputtering
Medium Temperature CVD (MTCVD)	Ion Beam Assisted Deposition (IBAD)
Metal-Organic CVD (MOCVD)	Hybrid PVD, Pulsed Plasma PVD
Laser CVD (LCVD)	Laser PVD (LPVD)

A wide range of hard coatings, such as nitrides, carbides, borides, oxides and their mixtures can be deposited by both methods. However, only certain compounds are suitable for cutting tool applications. The main differences between two methods are as following [2]:

- The PVD process is run at lower temperatures (180°C to 500°C) that mean that nearly all tool materials can be coated without concern for softening or deformation. This process does not utilize any harmful materials which makes it environmentally friendly. The PVD process is also very energy efficient and it ensures excellent adhesion.
- The CVD is a high temperature process with typical coating temperature around 1000°C that is used widely in applications requiring resistance to erosion, wear and corrosion over an extensive range of temperatures. The chemical bond that is produced between the coating and substrate, results in excellent diffusion. All surfaces including niche areas and shaded holes are reliably coated. Also thick coatings can be deposited for heavy wear applications.

The CVD method which has been considered for current study generally uses a gas-phase precursor. This precursor is usually a halide or hydride of the element that being deposited. A typical coating system is included an electrical heated furnace; a reaction chamber, special fixtures using for the parts to be coated, a vacuum system with a halide gas generator and gas delivery system that are used for aluminum oxide process, smog neutralization system (or scrubber). These subsystems are controlled by an automated control system[3]. A description of CVD process is presented in section 2.

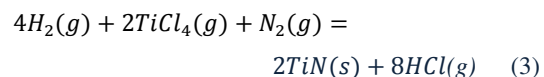
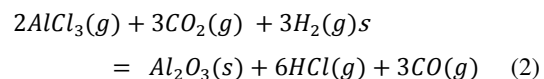
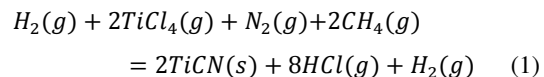
There are few attempting in numerical simulation of CVD reactors. Duverneuil & Couderc[4] and also Moffat[5] have investigated on numerical results for flow field in a realistic CVD geometry in two dimensions. In another study, Park & Pak [6] have worked on the flow, heat and mass transfer in a CVD reactor that its configuration is different from what considered in the present study. Kazunori and coworkers performed numerical simulation to model the heat and mass transfer process that takes place during the growth of CNTs in a CVD reactor. They found that substrate located inside the reactor causes irregular flow field. Based their results, they suggested a new geometry for the reactor [7]. Lu and coworkers simulated the effects of temperature, pressure, concentration of gas, and inlet velocity of gas mixture on the composition of coating and rate of coating growth in a tubular CVD reactor [8].

In this paper a thermal CVD reactor is analyzed numerically. The work is focused on the thermal and flow fields around the multiple substrates inside the reactor. The space between the tools trays is considered as the solution domain and a series of numerical analyses have been performed to attain a reliable solution. The grid independency is checked severely to ensure about final results.

2 Process specifications

The simulation presented in this paper is focusing on multiple-coating CVD process taking place in a vertical CVD reactor with a rotating susceptor. The main material for insert body is cemented carbides (WC/CO). This material is produced by special powder metallurgy methods, lumping grains of WC (tungsten carbide) in a Co (cobalt) matrix which provides toughness property. Coating consists of three different layers: First a layer consisting of titanium carbide (TiC) and titanium nitride (TiN) which is referred as Ti(C, N). The second layer is aluminum oxide (Al₂O₃) and the last layer which covers the insert is TiN. Inserts that are going to be coated are placed in a hydrogen reducing atmosphere reacting chamber with a pressure about 10% of atmospheric pressure. Gases that are containing the coating elements are introduced to the atmosphere and circulated through the reaction chamber and over the inserts.

The coatings are formed on the surfaces of the inserts, by chemical reactions between the gases. Typical temperature for the formation of TiC, TiN and Al₂O₃ on the surfaces of cemented carbides is about 1000°C. The reactions that lead to the coatings are shown in Eq. 1 to Eq. 3.



The total coating thickness is about 5-20µm. A typical photo of coating layers produced by CVD process is also shown in Fig. 1. Schematic representation of CVD coating process is presented in Fig. 2 Fig. 9.

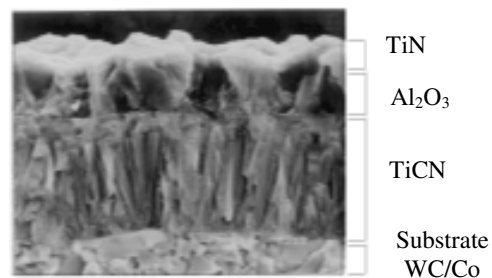


Fig. 1 Typical coating layer in CVD process

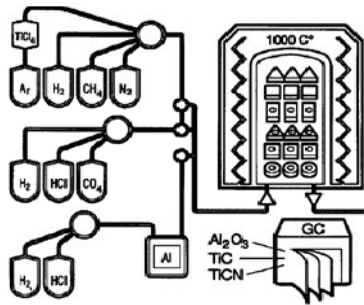


Fig. 2 Schematic of CVD coating process [2]

The reactor chamber consists of a main cylindrical chamber, a circular inlet section, and a circular outlet section. Inserts to be coated placed on trays and these tool trays (Fig. 3) are precisely placed one above another and then loaded onto a central gas distribution column. This column is placed inside circular inlet section. The reaction chamber is heated by an electrical furnace in an inert atmosphere until the coating temperature (1000°C) is reached. An actual photo of reactor chamber in hot condition is shown in Fig. 4 while the electrical furnace is moved up.

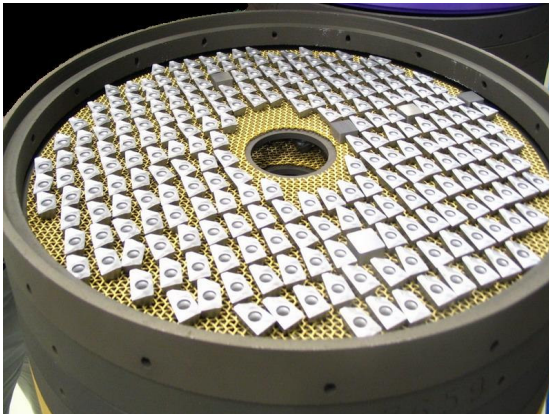


Fig. 3 Tools tray loaded with inserts(SecoTools Co.)



Fig. 4 Reactor chamber for CVD process

The coating cycle is initiated by the introduction of TiCl_4 (Titanium tetrachloride) together with CH_4 (Methane) and Nitrogen (N_2) into the reactor. The TiCl_4 is a cloud of unstable and volatile vapour, so it is transported into the reactor by hydrogen (H_2) as carrier gas. This gases mixture reacts on the hot inserts surfaces and the chemical reaction forms the first coating layer (TiCN). Resulted gases (HCl and H_2) are discharged and other gases that are required for following layers are introduced respectively. The whole process takes place in one cycle taking approximately 14 hours (including heating up, coating and cooling down).

Experimental measurements have been showed that the coating thickness varies inversely with radius distance from gas distribution column at the current configuration of CVD reactor which affects the coating uniformity for inserts. The inserts those are closer to the tools trays center have less coating thickness than inserts that are far from center (Fig. 5). This means that the coating uniformity should be studied considering this parameter beside the other affecting parameters. The thickness of the coating layer is a basically function of various gaseous constituents and their relevant flow rates, coating temperature and the soaking time at this temperature. However velocity profile and flow field inside the reactor are parameters that effect on the particles distribution and residence time and consequently on the coating thickness uniformity.

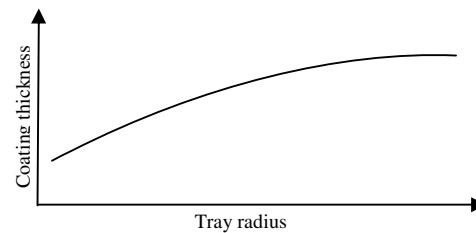


Fig. 5 Coating thickness versos distance from tool tray center

3 Numerical simulation

Governing equations for the problem are continuity equation, general transport equation and energy equation that are solved using Fluent software. The continuity equation is applicable for both incompressible and compressible flows considering one continuous phase without any or phase change and chemical reaction [9].

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0 \quad (4)$$

General transport equation is stated as following:

$$\frac{\partial}{\partial t} \oint_V \rho \phi dV + \oint_A \rho \phi V dA = \oint_A \Gamma \nabla \phi dA + \oint_V S_\phi dV \quad (5)$$

The first term on the left side represent the rate of transport property (ϕ) storage in the control volume. The second term in left hand stands for the net flux of ϕ due to convection from the control volume. The first and second terms on the right hand side represent respectively net flux of ϕ due to diffusion into the control volume and net rate of creation of ϕ inside the control volume. Eq. (5) then expands for momentum equations, energy equating and also turbulence model (like standard k- ϵ).

Built-in discretisation method included in Fluent is used to treat the above transport equations. The Active part of CVD reactor modeled in Fluent is shown in Fig. 6. The solution domain consists of 450630 cells.

A segregated solver is used for simulation that employs the finite volume of discretization process. The governing equations are solved sequentially. As these equations are inherently nonlinear, several iterations loop should be performed before a converged solution is obtained. Second order upwind solution is applied for momentum equation, turbulent kinetic energy, turbulent dissipation and energy equation. Based on available data, "pressure inlet", "pressure outlet" is assumed. The pressure outlet is used to define static pressure at flow outlets. Density and viscosity of gases is a function of temperature and pressure. As the temperature levels are high, these effects are considered for simulation. To investigate the thermal performance of reactor, the energy equation is solved. However, energy of chemical reaction, volumetric heat generation, species diffusion and viscous dissipation terms are not considered in the energy equation. Also the steady state condition is adopted for modeling.

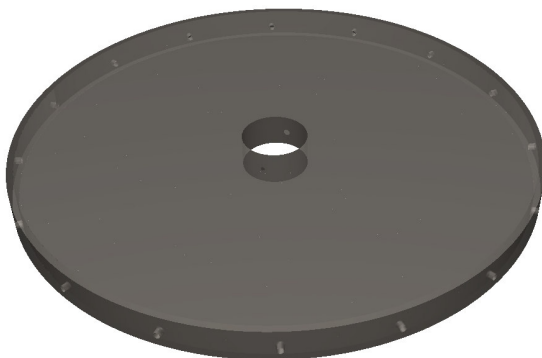


Fig. 6 Active part of coating inside the reactor

4 Results and discussion

Distribution of temperature, velocity magnitude and vectors resulted from numerical solution are presented in the Fig. 7 to Fig. 11.

Fig. 7 shows the temperature distribution a horizontal surface close to inlet passages. Effect of entrance holes diameters is obvious from the figure. The left

entrance has smaller diameter respect to the right side one ($d_{\text{left}}/d_{\text{right}} = 0.6$). The left side of the model has higher temperature level that means inserts in this region placed in the more adequate temperature range than the inserts which are located in the right part. As it was explained in the process specification, typical temperature for the formation of different coating layers on the surfaces of cemented carbides is about 1000°C. So the best regions inside the active part are places with a temperature profile as close as this value. Contour of total temperature in a vertical surface is also illustrated in Fig. 8. Along the height of reactor, again the temperate levels are higher at the left side. Also in the whole domain the temperature is higher at the upper parts. This also can results in different coating characteristics in the bottom and top of inserts. It should be noticed that the illustrated model is repeated in a real reactor. In fact, there are more than 30 numbers of this model that are precisely placed one above another and then loaded onto a central gas distribution column. The bottom of this model represent the top of inserts and the inside section of its roof represents the bottom of inserts that are placing in the next part of CVD reactor.

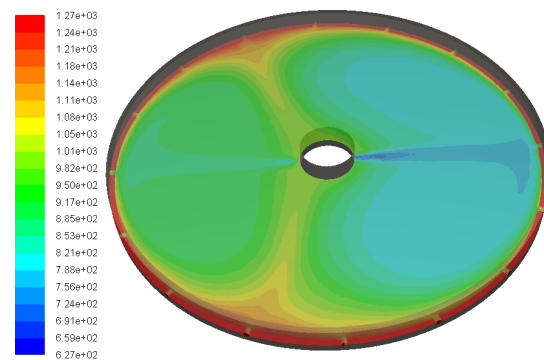


Fig. 7 Contour of total temperature (K) in horizontal surface

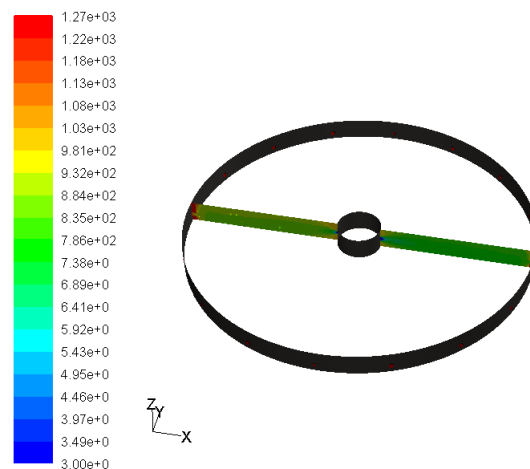


Fig. 8 Contour of total temperature (K) in vertical surface

Fig. 9 illustrates the temperature contour in top and bottom surfaces. Following the above discussion, it confirms that temperature distribution in top and bottom are different. It means that the up and bottom surface of inserts can have different coating thickness, as they face to different thermal condition through the process. Looking to the entrance section, it is seen that the temperature gradient is high. So this is not a good location to place the inserts during the coating process. This is the case again, when we get close to outer edges, where there exists large temperature gradient.

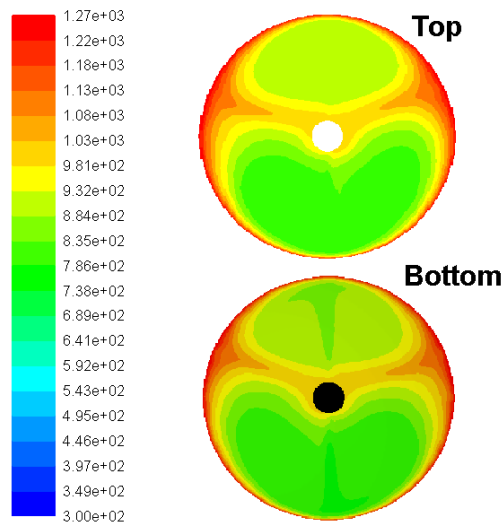


Fig. 9 Contour of total temperature (K) in upper and lower surfaces

Velocity vectors are shown in Fig. 10. There is relatively uniform velocity distribution through the domain except for regions close to right side edge and also locations that are in front of entrance holes. The uniformity is more better in the left side. High velocities causes decrease in residence time of gases mixture in the reactor and subsequently results in decrease in coating thickness in high velocity regions.

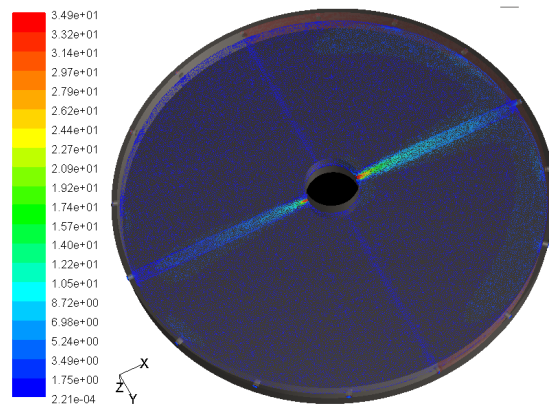


Fig. 10 Velocity vector colored by velocity magnitude (m/s)

A better illustration of velocity distribution among the radius is shown in Fig. 11. It is clear that the left side has a more uniform temperature distribution. Also again it shows that it's better to place the inserts in the middle section of the tools tray.

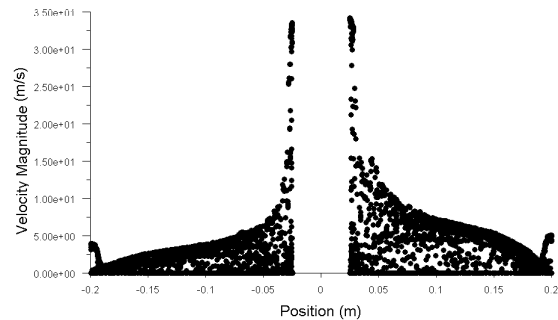


Fig. 11 Velocity magnitude along the vertical plane (m/s)

Simulation results declare that for current running conditions, a distribution column with smaller holes perform better. So one design improvement can be change of current distribution column with a new one containing smaller drilled holes.

5 Conclusion

The flow regime and heat transfer was studied numerically for the tools tray installed in a CVD reactor with respect to diameters of gas feeding holes in the distribution column. The following results were obtained:

- 1) The smaller diameter causes the more uniform temperature distribution over the tools tray.
- 2) At current configuration of tools tray and reactor, the best place for inserts arrangement is the middle part of tray. It's better to avoid placing the inserts in region close to distribution column and also to edges of the active part.
- 3) The temperature gradient is much higher than the velocity. Velocity gradient gets sharp in region close to edges and also in the way straight in front of feeding holes.
- 4) The top side of the inserts could have different coating parameters than the bottom side, as the temperature profiles are different in the ceil and floor of the active part.
- 5) Average temperature of space over the tools tray is less than the amount which is required for efficient coating process. It means that to achieve the optimal coating reactions, it is better to increase the temperature of thermal energy source.

This approach to thin-film manufacturing control opens the door to a new generation of CVD reactor designs, allowing precise thickness uniformity control in a single reactor design. The numerical results offer the possibility of developing CVD reactors with more uniform thickness coating with low investment.

6 Acknowledgments

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