

Computational Heat Transfer and Fluid Dynamics Analysis for Titanium Dioxide (TiO₂) Deposition

Rahul Kumar¹, M.K. Chopra²

¹P.G. Scholar, Dept. Of Mechanical Engineering, R.K.D.F Institute of Science & Technology, Bhopal, M.P., India

²Vice Principal, Dean Academic & Head, Dept. Of Mechanical Engineering, R.K.D.F Institute of Science & Technology, Bhopal, M.P., India

Abstract – This paper suggests the best possible model of Computational Fluid Dynamics to simulate the process of deposition of Titanium Dioxide (TiO₂) over a substrate formed as a result of pyrolysis of Titanium Tetraisopropoxide (TTIP) as a precursor and argon as carrier gas. As a result of pyrolysis of TTIP if the solid particles of TiO₂ gets formed before impinging the substrate then Discrete Particle Model (DPM) has to be applied or else if the formation of TiO₂ is in vapor form and its particles are formed after impinging the substrate where it has to be deposited then Species Transport Model (SPM). After carrying out literature reviews it has been found that SPM is the best model to solve the phenomena of TiO₂ formation as a result of TTIP pyrolysis and for finding the deposition rate thickness.

Key Words: Pyrolysis, Impinging, Titanium Dioxide, Discrete Particle Model, Species Transport Model.

1. INTRODUCTION

Titanium Dioxide (TiO₂) is of much relevance and is used extensively for the industrial purposes due to its optical, chemical and electrical properties. Out of all the applications the water splitting as in the case of electrolysis can be done using TiO₂ as electrode and light as a current source thus we call it photolysis of water [1]. This photolysis of water gives us hydrogen gas which can be further used as energy sources for the various applications. For the proper photolysis of water using TiO₂ as electrode the deposition of TiO₂ over a substrate should be proper. There are several processes of TiO₂ formation and deposition over a substrate but the formation of TiO₂ by the pyrolysis of the Titanium Tetraisopropoxide (TTIP) and its deposition on the substrate using argon as carrier gas is considered to be cost effective, which also allows the controlling of the microstructure [2-7]. This process of pyrolysis can be attempted for various ranges of temperature, pressure and concentration of precursor. The proper combination of all these parameters decides the deposition thickness of TiO₂ over the substrate, so one need to carry out the Computational Fluid Dynamic (CFD) analysis in order to estimate the optimized parameter for achieving the required deposited thickness of TiO₂ over a substrate.

2. LITERATURE REVIEW

Yiyang Zhang *et al* performed experiments and found that Nanoporous TiO₂ thin films are deposited directly onto substrates by a one-step stagnation flame synthesis with organometallic precursors. Intensive study related to deposition mechanism in the stagnation-point boundary layer was carried out by them. The radial profile of nanoparticle deposition flux for the first time was measured using a novel method of concentric collecting rings, which depicted similar trend with the heat flux profile of stagnation-point flows. Then they developed the mathematical model of nanoparticle transport and deposition in the stagnation-point boundary layer for further clarifying experimental results, especially the effects of substrate temperatures and in-situ produced particle sizes. Both thermophoresis in an inner part of boundary layer and thermal compression/expansion of the gas phase are found to play important roles in determining the deposition flux. The contribution of Brownian diffusion, determined by a thermophoretic Peclet number, is inappreciable compared to thermophoresis until particle diameter is as small as 2 nm. The results in this work support a conclusion of size-independence of the thermophoretic velocity, implying that the rigid-body collision assumption of Waldmann's formula is not accurate for small particles especially less than 10 nm. This study can be generally applied to other deposition techniques of thin films [2].

Erik D. Tolmachoff *et al* proposed a new method to fabricate nanocrystalline titania (TiO₂) films of controlled crystalline size and film thickness. The method uses the laminar, premixed, stagnation flame approach, combining particle synthesis and film deposition in a single step. A rotating disc serves as a combination of substrate-holder and stagnation-surface that stabilizes the flame. Disc rotation repetitively passes the substrates over a thin sheet, fuel-lean ethylene-oxygen-argon flame doped with titanium tetra isopropoxide. Convective cooling of the back side of the disc keeps the substrate well below the flame temperature, allowing thermophoretic forces to deposit a uniform film of particles that are nucleated and grown via the flame stabilized just below the surface. The particle film grows typically at ~1 μm/s. The film is made of narrowly distributed, crystalline TiO₂ several nanometers in diameter and forms with a 90% porosity. Analysis shows that the rotation of the stagnation-

surface does not reduce the stability of a stagnation flame, nor does it affect the fundamental chemistry of particle nucleation and growth that occurs between the flame and the stagnation surface [3].

Nkwenti Azong-Wara *et al* developed a new Thermal Precipitator (TP) as a personal sampler for nanoparticle exposure studies. Two parallel 20-mm-long plates with different but uniform temperatures were introduced into the TP with an appropriate gap distance, to achieve a uniform temperature gradient along the length of the plates. Particles are thermophoretically deposited on the colder plate in the TP which acts as the substrate. Analytical calculations were carried out to determine an optimal plate gap distance and temperature gradient in the TP. A simulation grid was created from the resulting geometry which was used for numerical modelling with a CFD Software. Results from the simulations showed a uniform deposition of particles up to the size range of about 300 nm for a temperature gradient of 15 K/mm and a 1-mm gap distance, independent of the orientation of the TP during sampling. In contrast to the old TP where up to 32 SEM images of its non-uniform particle deposition had to be evaluated to obtain an average particle size distribution, an evaluation of the uniform deposition with the new TP is much more simplified, remarkably reducing the time and cost of the evaluation, while providing more accurate results [4].

G.S. McNab and A. Meisen studied that small particles located in stagnant gases with temperature gradients experience a force and consequently, move in the direction of lower temperature. This phenomenon called as "thermophoresis in gases" and has received extensive experimental and theoretical study. No experimental evidence of thermophoresis in liquids has thus far been reported and the present work was therefore undertaken to determine its existence and characteristics. In addition to the purely scientific interest, the phenomenon was also thought to merit investigation due to its possible engineering significance. An example of the latter is the undesirable deposition of particulate matters in heat exchangers [5].

Wes Burwash *et al* performed the experiments and found that an axis symmetric turbulent air jet flow (with vertical and downward orientation) laden with fluorescent solid particles was impinged normally onto a flat surface. The particle deposition efficiency and distribution on the flat surface were measured experimentally using fluorometry and imaging techniques. The fluorescent particles (5.0 μm diameter) were dispersed by a nebulizer and injected into a stream of compressed air, resulting in a steady flow ($Q=111$ L/min). A round nozzle was used to generate a jet characterized by a Reynolds number of $Re = 10^4$, based on the nozzle diameter ($D = 15.0$ mm) and nozzle exit velocity ($u = 10.5$ m/s). Three dimensionless distances from the nozzle's exit to the impact surfaces, $L/D = 2, 4$ and 6 investigated. It was observed that although having similar

total deposition efficiencies (16.5 – 17.8 %), shorter nozzle to surface distances ($L/D = 2$ and 4) show a more pronounced ring-like radial deposition pattern around the stagnation point when compared to the longer distance ($L/D = 6$). Indeed, in moving through $L/D = 2, 4$ and 6 , peak deposition density values of 254, 347 and 685 particles/ mm^2 shift through radii of $2.1D, 0.8D$ and $0.1D$ respectively. In addition to these experiments, numerical simulation was also performed, which showed that the particle deposition was dominated by a turbulent dispersion mechanism for $L/D = 2$, with inertial impaction becoming more important for the $L/D = 4$ and 6 cases [6].

N. Anbuhezhan *et al* mathematically solved the problem of laminar fluid flow, which results from the stretching of a vertical surface with variable stream condition in a nanofluid due to solar energy, is investigated numerically. The model used for the nanofluid incorporates the effects of the Brownian motion and thermophoresis in the presence of thermal stratification. The symmetry groups admitted by the corresponding boundary value problem are obtained by using a special form of Lie group transformations, namely the scaling group of transformations. An exact solution is obtained for the translational symmetries and the numerical solutions are obtained for the scaling symmetry. This solution depends on the Lewis number, the Brownian motion parameter, the thermal stratification parameter and the thermophoretic parameter. The conclusion is drawn that the flow field, the temperature, and the nanoparticle volume fraction profiles are significantly influenced by these parameters. Nanofluids have been shown to increase the thermal conductivity and convective heat transfer performance of base liquids. Nanoparticles in the base fluids also offer the potential in improving the radiative properties of the liquids, leading to an increase in the efficiency of direct solar collectors [7].

Jaishree Vyas *et al* performed the experiments and presented experimental results related to generation of anatase TiO_2 nanoparticle film on titanium substrate using CW CO_2 laser. Parameters determining crystalline character of the films were identified and highly crystalline anatase TiO_2 nanoparticles films were generated. Since mixture of anatase and rutile crystalline phase of TiO_2 is better than pure anatase phase for photocatalytic water splitting, CO_2 laser sintering of the films were carried out to transform some anatase to rutile crystalline phase. Anatase to rutile transition of TiO_2 was characterized by GIXRD and Raman spectroscopy [8].

Shalmali Tiwari *et al* presented the various aspects which affect the characteristics of TiO_2 particles films generated by gas phase CO_2 laser based pyrolysis technique. Effect of laser power and precursor concentration has been studied to evaluate their effect on size and crystalline nature of nanoparticles. Other important technical issue related to reproducible TiO_2 film has also been discussed [9].

Graeme M.G. Watson *et al* performed experiment and validated results to further the understanding of nitrogen oxide (NO_x) formation, it is essential to test predictions from existing NO_x kinetics sub-models against reliable, well-defined experiments over a range of fuel compositions and combustion conditions. Such experimental validations require a multifaceted approach whereby burning rate, temperature and species formation are simultaneously measured and compared to numerical predictions. Here, the implementation of particle velocimetry, thermometry and planar laser-induced fluorescence diagnostics is presented for the study of NO pollutant formation in strained, atmospheric pressure, premixed flames stabilized in a jet-wall stagnation flow. The resulting experimental profiles are directly compared to numerical simulations, performed using CANTERA Accurate measurements of premixed gas composition; gas velocity, temperature, and spread-rate yield all necessary inlet boundary conditions. Use of a temperature-controlled stagnation plate allows for first-order temperature (heat loss) effects to be imposed on the numerical simulation, rather than relying on external temperature-corrections. The experiments provide a sensitive test of NO_x sub-models, result in multiple validation targets which do not rely on extrapolations, and allow for accurate specification of measurement uncertainties when comparing experiments to simulations. This work provides a discussion of the diagnostic techniques and compares experimental results for methane flames to numerical predictions using a number of published natural gas kinetics models and their associated sub-models for NO_x formation [10].

M.V. Papalexandris and P.D. Antoniadis developed a thermo-mechanical model for flows in superposed porous and fluid layers with interphasial heat and mass exchange. This model is based on a mixture-theoretic formalism, according to which, the fluid and the solid phases are treated as two coexisting but open thermodynamic continua that interact with each other. As such, each phase is endowed with its own set of thermodynamic variables and conservation laws. In particular, each phase is assigned with its own temperature field, thereby allowing for thermal non-equilibrium between the two phases. Constitutive equations for all dissipative and relaxation phenomena occurring in both phases are derived by exploiting the constraints imposed by the entropy axiom when applied to the entire mixture. This model is valid for both compressible and incompressible flows. Herein we also derive its low-Mach number approximation, which is substantially simpler and, therefore, more convenient for flows where compressibility effects are negligible. The efficacy of the proposed model and the effect of thermal non-equilibrium between the two phases are examined via direct numerical simulations of natural convection in a horizontal channel consisting of a porous layer and a superposed pure-fluid domain [11].

Adélio S. Cavadas *et al* carried out an experimental investigation to characterize the flow field in a liquid impinging jet confined by slopping plane walls and emanating from a rectangular duct. The fluids are Newtonian flowing in the laminar (Re=135 and 276) and turbulent regimes (Re=13,750) and the two-dimensional rectangular cell has an aspect-ratio equal to 13. The fully-developed rectangular jet impinging the flat surface (plate) is confined by two slopping plane walls, each one making an angle of 12° relative to the plate. The presence of the impact plate is felt upstream at $y/H = -0.2$ in the laminar regime and at $y/H = -0.4$ in the turbulent regime. The results show that the flow is symmetric relative to the x - y and x - z center planes. Near the plane slopping wall there is separated flow for Reynolds numbers in excess of 208, as was observed in visualization studies. For Re= 275 this small separated flow zone has a normalized length, $x_R/H = 0.25$, whereas for turbulent flow x_R/H is equal to 0.9. In the turbulent flow regime turbulence is very high at the jet impact region due to strong fluid deceleration, but the maximum turbulence is observed in the shear layer formed between the jet along the impinging wall and the separated flow region on the sloping wall. We also report three-dimensional effects due to finite slenderness of the flow geometry [12].

Ming Zhou *et al* performed experiments on PECVD (Plasma-enhanced Chemical Vapor Deposition) process operating at 150 °C has been implemented to prepare micro-columnar porous TiO₂ anatase thin films, performing post-annealing at 300 °C for 5 h. Optimized PECVD conditions have enabled us to obtain homogeneous films with thickness equal to 1–2 μm ± 0.2 μm. An anatase seeding interface deposited prior to the PECVD process has enabled us to reduce crystallization time down to 1.5 h. The size of nano-crystals in prepared anatase thin films has been estimated to be 20 nm by applying the Scherrer equation. Besides, the band-gap energy (E_g) of synthesized anatase thin films on quartz was found to be 3.30 eV [13].

Neyda Bagger *et al* studied the metal-organic (MO) chemical vapor deposition (CVD) of titanium dioxide (TiO₂) films grown using the Titanium Tetraisopropoxide (TTIP) as precursor and nitrogen as carrier gas by means of Computational Fluid Dynamics Simulations. The effects of the precursor concentration, the substrate temperature, and the hydrolysis reaction on the deposition process are investigated. It is found that hydrolysis of TTIP decreases the onset temperature of the gas-phase thermal decomposition, and that the deposition rate increase with the precursor concentration and with the decrease of the substrate temperature. Concerning the mechanism responsible for the film growth, the model shows that at the lowest precursor concentration becomes more important [14].

Siti Hajar Othman studied the 3-dimensional (3D) computational fluid dynamics (CFD) simulation study of metal organic chemical vapor deposition (MOCVD)

producing photocatalytic titanium dioxide (TiO₂) nanoparticle. It aims to provide better understanding of the MOCVD synthesis system especially of deposition process of TiO₂ nanoparticles as well as fluid dynamics inside the reactor. The simulated model predicts temperature, velocity, gas streamline, mass fraction of reactants and products, kinetic rate of reaction, and surface deposition rate profiles. It was found that temperature distribution, flow pattern, and thermophoretic force considerably affected the deposition behavior of TiO₂ nanoparticles. Good mixing of nitrogen (N₂) carrier gas and oxygen (O₂) feed gas is important to ensure uniform deposition and the quality of the nanoparticles produced [15].

3. Discussion

After going through the several published literatures it is inferred that there can be two situations:

- a) TiO₂ particle form immediately after the pyrolysis process.
- b) TiO₂ particles form at the substrate much after pyrolysis.

In the first case (a) the particles are formed immediately and for its deposition on to the substrate it needs to reach the substrate. The particle trajectory while reaching to the substrate is governed by the following equation is as follows:

Particle Trajectory [19]

$$m_p \frac{d\vec{u}}{dt} = \vec{F}_{drag} + \vec{F}_{gravitation} + \vec{F}_{other} \quad \dots\dots\dots (1)$$

In the above equation (1) m_p denotes the mass of the particle formed after pyrolysis and the term $\frac{d\vec{u}}{dt}$ denotes the rate of the change of velocity of the particle.

The drag force is given as [16] —

$$\vec{F}_{drag} = A_p + \frac{\rho}{2} C_D |\vec{u} - \vec{u}_p| (\vec{u} - \vec{u}_p) \quad \dots\dots\dots (1.1)$$

The gravitational force is given as —

$$\vec{F}_{drag} = \int_{volume} \rho_p \vec{g} dV = \rho V_p \vec{g} = m_p \vec{g} \quad \dots\dots\dots (1.2)$$

In the other forces, \vec{F}_{other} we can consider rotational forces, thermophoretic forces, brownian force, saffman's lift force,

virtual mass force or user defined force as per the physical condition, but in case of pyrolysis we consider thermophoretic forces as other forces. This thermophoretic force is needed to be taken into account because there is a temperature gradient while the TiO₂ particle moves from the pyrolysis centre where the temperature is very high to the substrate where the temperature is much lower.

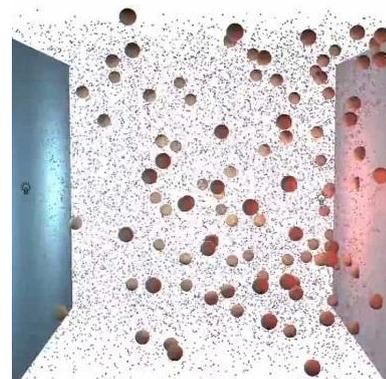


Fig.1 Thermophoresis [19]

In the above figure the blue plate depicts the lower temperature, the red one shows the higher temperature and in between the plates particles are moving. This type of physical phenomena can be modeled using the Discrete Particle Model (DPM). Out of available all commercial CFD software the popular one ANSYS FLUENT which can simulate the process only for the particle size of submicron level, in order to simulate the process for the particle size less than the micron order one needs to include the Fine Particle Module (FPM) together with the Discrete Particle Module (DPM) [4,19,17].

In the second case (b) the process is considered to be happen in the series of reaction in a sequential manner. The pyrolysis of TTIP for the TiO₂ formation is also carried out through the same [14]. The table X shows all the reactions which occurs during the above said process:

Table X: Reactions occurring during the pyrolysis of TTIP

| Reactions | Classification | Ref |
|--|----------------|---------|
| 1 Ti(OC ₃ H ₇) → TiO ₂ (g) + 4C ₃ H ₆ + 2H ₂ O | volumetric | [15] |
| 2 Ti(OC ₃ H ₇) + 2H ₂ O → TiO ₂ (g) + 4C ₃ H ₇ OH | volumetric | [16] |
| 3 Ti(OC ₃ H ₇) → TiO ₂ (c) + 4C ₃ H ₆ + 2H ₂ O | surface | [19] |
| 4 TiO ₂ (g) → TiO ₂ (c) | surface | [17-18] |

In order to simulate the physical process which is occurring in the series of chemical reaction one needs to follow SPECIES TRANSPORT MODEL (SPM). The SPM model takes into account the order of the reaction and all reactant and products as species.

Consider a typical chemical reaction as below –



In the above reaction (2) A, B, C, D have to be considered as the different species and a, b, c, d as their stoichiometric constants. The reaction rate v (also r or R) for a chemical reaction in a closed system under constant volume conditions, without a build up reaction intermediates, is defined as:

$$v = -\frac{1}{a} \frac{d[A]}{dt} = -\frac{1}{b} \frac{d[B]}{dt} = -\frac{1}{c} \frac{d[C]}{dt} = -\frac{1}{d} \frac{d[D]}{dt} \quad \dots\dots\dots (3)$$

For any system the full mass balances taken into account:-

$$F_{A0} - F_A + \int_0^V r dV = \frac{dN_A}{dt} \quad \dots\dots\dots (4)$$

Where F_{A0} is the amount of the substance A that comes into the system F_A is the amount of A that comes out of the system. V is the volume of the system, r is the reaction rate. N_A is the amount of A in the system at any time. It describes the accumulation of substance A in the system.

A rate law is used to express the relation between the rate and these concentrations. A rate law could be determined by experimental data or may be formulated by a theoretical study. Usually reactions have their rate laws in the following form:-

$$r = k [A]^x [B]^y \dots\dots\dots (5)$$

Where k is the rate constant, feature of a given reaction. The power x , y are the numbers that must be determined experimentally. x is the order with respect to A and y is the order with respect to B. Note that, in general, x and y are not equal to the stoichiometric coefficients a and b . The overall reaction of the order is $(x+y+\dots)$ Orders are usually integers.

For any of the reactions, there may be a lot of factors that affect the rate of reaction, such as concentration, temperature, solvent, pressure, electromagnetic radiation, catalyst and so on. Here we pay our attention to the effect of temperature because it is the most important factor in this study. Rate constants are often found to depend strongly on temperature. It is required to discuss with rate constant together with temperature.

In most case the reaction rate goes up with temperature, but it does not have to. Rate constants are found to have the relation with temperature as follows:

$$k(T) = A \exp \left(-\frac{E_a}{RT} \right) \quad \dots\dots\dots (6)$$

Where the rate constant is written down as $k(T)$ to emphasize its dependence on temperature. R is the gas constant ($8.314 \text{ J.K}^{-1} \text{ mol}^{-1}$). The activation energy E_a , which is the minimum amount of energy required to initiate a chemical reaction, is in unit of energy.mol^{-1} . E_a is usually expressed in kJ.mol^{-1} or kcal.mol^{-1} . A is the pre-exponential factor and it is usually found to be independent on temperature. Besides it must have the same dimensions and units as k . Equation (6) is known as Arrhenius equation. It predicts that the rate constant increases with temperature for a positive activation energy.

Thus the rate of reaction, activation energy and pre-exponential factor needs to be considered for each of the reaction occurring for the process of TiO_2 deposition [14, 15, 19]. The commercial available software ANSYS FLUENT also works in the same manner for SPM.

3. Conclusion

The TiO_2 formation by the pyrolysis of TTIP occurs through a series of reaction and the particle formation takes place at the substrate [14]. So the process can be simulated using Species Transport Model (SPM) instead of the Discrete Particle Model (DPM).

ACKNOWLEDGEMENT

Authors would like to express sincere thanks to Dr. Yogesh Pahariya, Director, R.K.D.F IST, Bhopal (M.P.), India for his continuous support and encouragement during the above study.

REFERENCES

- [1] A. Fujishima and K. Honda, Nature, 238, 37 (1972).
- [2] Yiyang Zhang, Shuiqing, Wen Yan, Qiang Yao; "Nanoparticle transport and deposition in boundary layer of stagnation-point permixed flames"; Elsevier Powder Technology 227 (2012) 24–34.
- [3] Erik D. Tolmachoff, Aamir D. Abid, Denis J. Phares, Charle S.Campbell, Hai Wang; "Synthesis of nano-phase TiO_2 crystalline films over premixed stagnation flames", Elsevier Proceedings of the Combustion Institute 32 (2009) 1839–1845.
- [4] Nkwenti Azong-Wara, Christof Asbach, Burkhard Stahlmecke, Heinz Fissan, Heniz Kaminski, Sabine Plitzko, Thomas A. J. Kuhlbusch ; "Optimisation of thermophoretic personal sampler for nanoparticle exposure studies", Springer Science J Nanopart Res (2009)11:1611–1624.
- [5] G.S. Mcnab, A. Meisen ; "Thermophoresis in Liquids", Department of chemical engineering, The University of

- British Columbia ,Vancouver 8,B. C.,Canada December 29,1972
- [6] Wes Burwash, Warren Finlay & Edgar Matida; "Deposition of Particles by a Confined Impinging Jet onto a Flat Surface at $Re = 10^4$ ", *Aerosol Science and Technology*, 40:147-156, 2006, ISSN: 0278-6826 print / 1521-7388 online.
- [7] N.Anbuezhian , K. Srinivasan, K. Chandrasekaran, R. Kandasamy; "Thermophoresis and Brownian motion effects on boundary layer flow of nanofluid in presence of thermal stratification due to solar energy", Shanghai University and Springer-Verlag Berlin Heidelberg 2012, *Appl. Math. Mech. -Engl. Ed.*, 33(6),765-780 (2012).
- [8] Jaishree Vyas, Shalmali Tiwari, Manoj Kumar, Alka Ingle, L.B. Rana, M S Bhagat, B Singh and L.M Kukreja - "Synthesis of TiO_2 nanoparticles films by CO_2 laser pyrolysis technique and effect of laser sintering on Anatase to Rutile transformation", 24TH DAE BRNS National Laser Symposium (NLS-24) ISBN 978-81-903321-6-3.
- [9] Shalmali Tiwari , Jaishree Vyas, Manoj Kumar, L.B. Rana, M S Bhagat, B Singh and L.M Kukreja - "Various aspects of gas phase synthesis of TiO_2 nanoparticles films by CO_2 laser pyrolysis technique" ,24TH DAE BRNS National Laser Symposium (NLS-24) ISBN978-81-903321-6-3.
- [10] Graeme M.G. Watson, Jeffrey D. Munzar, Jeffrey M. Bergthorson; "Experimental diagnostics and modeling of jet-wall stagnation flames for NO_x sub-model validation", 8th US National Combustion Meeting Organized by the Western States Section of the Combustion Institute and hosted by the University of Utah May 19-22, 2013, Paper # 070LT-0186.
- [11] M.V. Papalexandris, P.D. Antoniadis ; "A thermo-mechanical model for flows in superposed porous and fluid layers with interphasial heat and mass exchange", *Elsevier International Journal of Heat and Mass Transfer* 88 (2015) 42-54
- [12] Adélio S. Cavadas, João B. L. M. Campos and Fernando T. Pinho; "Flow Field In A Liquid Impinging Jet Confined By Stopping Plane Walls", 13th Int Symp on Applications of Laser Techniques to Fluid Mechanics Lisbon, Portugal, 26-29 June, 2006
- [13] Ming Zhou, Stéphanie Roualdès , Jie Zhao, Vincent Autès, André Ayrál; "Nanocrystalline TiO_2 thin film prepared by low-temperature plasma-enhanced chemical vapor deposition for photocatalytic applications", *Elsevier Thin Solid Films* 589 (2015) 770-777.
- [14] Neyda Baguer, Erik Neyts, Sake Van Gils and Annemie Bogaerts; "Study of Atmospheric MOCVD of TiO_2 Thin Films by Means of Computational Fluid Dynamics Simulations", WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, *Chemical Vap. Deposition* 2008, 14,339-346; DOI: 10.1002/cvde.200806708.
- [15] Siti Hajar Othman, Suraya Abdul Rashid, Tinia Idaty Mohd Ghazi, and Norhafizah Abdullah; "3D CFD Simulations of MOCVD Synthesis System of Titanium Dioxide Nanoparticles", Hindawi Publishing Corporation, *Journal of Nanomaterials*, Volume 2013, Article ID 123256, 11 pages, <http://dx.doi.org/10.1155/2013/123256>.
- [16] Z.Nami, O. Misman, A. Erbil, G.S. May, *J. Cryst. Growth* 1997,171,154
- [17] E. Neyts, A. Bogaerts, M. De Meyer, S. Van Gils, *Surf. Coat. Technology* 2007,201, 8338
- [18] A. Rathu, M. Ritala, *Chem. Vap. Deposition* 2002, 8,21
- [19] ANSYS FLUENT, <http://www.ansys.com>
- [20] <https://support.ansys.com/staticassets/ANSYS/staticassets/partner/Chimera/software-particulates-chimera.pdf>