The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5 – 9 June 2022, Oslo, Norway

A comparison of equation-based and machine learning models of industrial scale deposition processes

Paris Papavasileiou*[1,2], Eleni D. Koronaki[1,2], Gabriele Pozzetti[3], Martin Kathrein[3], Christoph Czettl[4], Andreas G. Boudouvis[2], Stéphane P.A. Bordas[1]

[1] Faculty of Science, Technology and Medicine, University of Luxembourg, Esch-sur-Alzette, Luxembourg
[2] School of Chemical Engineering, National Technical University of Athens, Greece
[3] CERATIZIT Luxembourg S.à.r.l., L-8201 Mamer, Luxembourg,
[4] CERATIZIT Austria GmbH, A-6600 Reutte, Austria

Key Words: *Chemical Vapor Deposition, Computational Fluid Dynamics, Machine Learning, Industrial Process*

This work presents a comparison of a Computational Fluid Dynamics (CFD) model and several machine learning (ML) predictive models of an industrial-scale Chemical Vapor Deposition (CVD) reactor, used for the coating of cutting tool inserts. The performance of the developed two-dimensional, time-dependent CFD model of the reactor that accounts for mass, momentum, species transport, and chemical reactions is compared with that of several ML regression models utilizing the information given by the production data for the thickness prediction of the produced coatings. The proposed models will be compared based on their accuracy and computational cost since the latter is a criterion for their implementation in everyday production.

The studied CVD reactor has a complex geometry that consists of around 45 perforated trays, stacked one on top of the other. The cutting tool inserts are placed on the trays and are coated when a mixture of gas reactants enters through perforations on a rotating central tube. The geometry changes in each production run as the number of inserts is typically big and each one is placed in a different tray with dedicated special design.

The proposed CFD model is appropriately simplified to include the dominant physical mechanism as well as a chemistry model and it can deliver accurate thickness predictions at a reasonable computational cost. The same output is delivered by the ML regression model, namely it can predict the thickness given several inputs including the geometry, chemical recipe, and year of production. The implemented tree-based regression methods (decision trees, random forests, xgboost, etc.) appear to outperform other ML methods for the investigated dataset while also being more interpretable. Nevertheless, the CFD approach can shed light into the relevant importance of the dominant physical phenomena, especially in applications such as CVD where mechanisms such as diffusion and convection compete with each other and with chemical reaction rates.

REFERENCES

[1] Hochauer, D.; Mitterer, C.; Penoy, M.; Puchner, S.; Michotte, C.; Martinz, H. P.; Hutter, H.; Kathrein, M. Carbon Doped α-Al2O3 Coatings Grown by Chemical Vapor Deposition. Surface and Coatings Technology 2012, 206 (23), 4771–4777.

https://doi.org/10.1016/j.surfcoat.2012.03.059

[2] Ruppi, S., 2020. Influence of Process Conditions on the Growth and Texture of CVD Alpha-Alumina. Coatings 10, 158. https://doi.org/10.3390/coatings10020158