**ASSESSMENT OF CFD AND ML MODELLING STRATEGIES FOR INDUSTRIAL-SCALE CVD REACTORS**

**P. Papavasileiou1,2,\*, E. D. Koronaki1,2, G. Pozzetti3, M. Kathrein3, C. Czettl4, S. P. A. Bordas2, A. G. Boudouvis1**

1 School of Chemical Engineering, National Technical University of Athens, 9 Heroon Polytechniou str., Zographos Campus, 15780, Attiki, Greece

2 Faculty of Science, Technology and Medicine, University of Luxembourg, Maison du Nombre, 6 Avenue de la Fonte, Esch-sur-Alzette, L-4364, Luxembourg

3 CERATIZIT Luxembourg S.à r.l., L-8201 Mamer, Luxembourg

4 CERATIZIT Austria GmbH, A-6600 Reutte, Austria

*\*paris.papavasileiou@uni.lu*

**ABSTRACT**

In this work a comparison between a Computational Fluid Dynamics (CFD) model and various machine learning (ML) approaches, is presented and assessed for predicting the behavior of an industrial-scale Chemical Vapor Deposition (CVD) reactor used for the coating of cutting tool inserts. The developed CFD model is two-dimensional, time-dependent, includes the transport of mass, momentum, and chemical species, while also incorporating the relevant chemical reactions. Based on the information given by the available production data, various ML regression models have been trained for predicting the produced coatings' thickness. The developed models are compared based on their accuracy, interpretability, and computational cost. The latter is highly important since it is one of the main criteria for implementing such models in everyday production.

The modeled industrial-scale CVD reactor consists of 40-50 perforated trays stacked one on top of the other. Cutting tool inserts of varying geometries are placed on these trays and are coated by a mixture of gas reactants. The gas reactant mixture enters the reactor chamber via perforations on a rotating tube. The reactor geometry (or set-up) changes on a run-to-run basis since the number and geometry of the coated inserts (and the respective trays where they are placed on) vary from run to run. Therefore, conceptually, there is no single model for this production process, since every day, in every run, the geometry and consequently, the computational domain, is completely different, based on the production schedule.

Due to the high variability of the reactor geometry, the proposed CFD model is sufficiently and appropriately simplified. This way it allows for accurate coating thickness predictions at a reasonable computational cost. Coating thickness predictions are also the output of the trained ML regression models. These models utilize several inputs, including but not limited to the production recipe, cutting tool geometry, tray geometry, and year of production. While the implemented tree-based regressors (decision trees, random forests, xgboost) outperform other ML methods while also being more interpretable, they are still unable to provide the same insight as CFD into the interplay of the several complex chemical and physical phenomena occurring inside a CVD reactor.

**KEYWORDS:** CVD, CFD, Machine Learning, Industrial-scale Reactor modelling

**REFERENCES**

[1] Hochauer, D., Mitterer, C., Penoy, M., Puchner, S., Michotte, C., Martinz, H.P., Hutter, H., Kathrein, M. (2012). *Surf. Coat. Technol.* 206 (23): 4771–4777.