

## Abstract

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Pyrocarbon (PyC) is a kind of carbon that forms on heated surfaces exceeding 900°C due to hydrocarbon cracking. It is generally deposited by chemical vapour deposition (CVD), in which light hydrocarbon gases are pyrolysed over the substrate at high temperatures. PyC CVD successfully fabricates advanced carbon compounds. The ability to control the nanotexture of PyC is crucial for the desired application.

The goal of this thesis is to use machine learning models in conjunction with the Nelder-Mead algorithm to mathematically model and optimise a commercial hot wall vertical reactor for high-quality pyrocarbon coating. To begin, a full 3D CFD model was created by including comprehensive transport reaction kinetics models to explore the effect of various process parameters on the hydrodynamics, temperature, and concentration fields within the CVD reactor. Second, the machine learning model was used in conjunction with the Nelder-Mead algorithm to optimise the CVD reactor to produce a high-quality film. The effect of reactor operating conditions such as temperature, pressure, intake flow rate, and mole fraction on film performance was comprehensively examined. The CVD reactor was then optimised using the model validated by the experimental data. The best film performance can be obtained by selecting the best process parameters. CFD simulations were performed on a vertical hot-wall CVD. The precursor gas mixture of methane and hydrogen enters the reactor through the inlets and pyrolyzes. PyC is deposited on numerous substrates that are placed on the spinning shaft in the reactor's core to ensure uniform coating. The CVD process is made up of several physical and chemical phenomena such as mass, momentum, and heat transfer, as well as chemical reactions. The equations regulating the modelling of physical and chemical events are described in terms of mass conservation, momentum conservation, energy conservation, and species transfer. The reactor geometry was created in Ansys Space-claim and meshed with the ANSYS Workbench mesh generator. A comprehensive CFD model for CH<sub>4</sub> pyrolysis in a commercial CVD reactor is developed. The model's accuracy is improved by integrating detailed gas and surface chemistry as well as temperature-dependent transport characteristics of the gas mixture. A parametric analysis is then used to determine the deposition rate and film homogeneity.

SVMs are utilised to link numerous process parameters with deposition rate and film homogeneity. SVM regression works by mapping the input data points into an n-dimensional

feature space and then converting them to a linear. SVM has been demonstrated to be more accurate than the linear regression model. In the SVM regression model, the optimum point was determined using the Nelder-Mead technique. This algorithm compares triangle vertices inside the domain of the desired solution and then shifts the simplex in the direction of the optimal value. The worst vertex is replaced with a new vertex with the best function values in an iterative process. As a result, a new simplex emerges that tends to reach the function's extreme. This strategy has the advantages of high precision, computational efficiency, and quick convergence over previous techniques. The findings demonstrated that reactor pressure and temperature have a significant impact on deposition rate and film uniformity. The most dominant carbon-forming species was found as C<sub>2</sub>H<sub>2</sub>. The non-uniform distribution of C<sub>2</sub>H<sub>2</sub> has a significant impact on film uniformity at high pressure. The total flow rate has little effect on reactor hydrodynamics. An appropriate choice of input CH<sub>4</sub> concentration can considerably improve film performance. The SVM was used to predict the relationship between different process parameters and film quality, which would otherwise be difficult to achieve by linear regression. This methodology has been found to be efficient and rapid, requiring less time to optimise the CVD reactor.