CFD Analysis and Optimization of CH_4 Pyrolysis in Commercial Hot Wall Chemical Vapor Deposition Reactor

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By

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CHAPTER 5

CONCLUSIONS AND FUTURE SCOPE

5.1 Conclusions

The use of SVM and the Nelder-Mead algorithm to optimise CH4 pyrolysis in a commercial CVD reactor has important implications for the synthesis of advanced carbon materials. The research presented in this thesis has demonstrated the feasibility of using machine learning techniques to optimize the process parameters and to achieve high-quality pyrocarbon. Two factors, such as average growth rate and uniformity index, were used to define the film quality, acquired by a comprehensive CFD modelling combining accurate gas and surface chemistry. Firstly, the parametric investigation was performed to understand how the deposition and film uniformity vary with the total flow rate, reactor temperature, pressure, and inlet concentration of CH_4. The results revealed that the reactor pressure and temperature remarkably influence the deposition rate and film uniformity. C_2H_2 species was identified as the most dominating carbon-forming species. At high pressure, the film uniformity is severely affected due to the non-uniform distribution of C_2H_2. The total flow rate has a negligible effect on the reactor hydrodynamics. The film performance can be significantly improved using an appropriate choice of the inlet CH_4 concentration. The relationship between various process parameters and film quality was modelled using the SVM otherwise is difficult to obtain through linear regression. The SVM model exhibited high accuracy, saving considerable time and cost of performing actual experiments. Finally, the SVM combined with the Nelder-Mead algorithm was employed to optimise the CVD reactor. It has been found that this methodology is efficient and fast and requires less time to optimise the CVD reactor.

5.2 Future Scope

This research has a broad future reach. This study's CFD model can be used to mimic the pyrolysis of different hydrocarbons, such as C_2H_6 and C_3H_8. It can also be used to investigate the effects on the pyrolysis process of various reactor configurations and operating conditions. Other forms of CVD reactors, such as cold wall reactors and plasma-enhanced CVD reactors, can also benefit from the optimisation process. The optimized design of CH_4 pyrolysis in a commercial CVD reactor has significant future scopes for research and development. These include integration with other technologies, alternative feedstocks, advanced materials synthesis, scaling up for industrial applications, process optimization for other industrial applications, environmental sustainability, process control and automation, integration with renewable energy sources, and new applications and markets. Continued research and development in these areas can enhance the efficiency, sustainability, and commercial viability of the process, opening up new opportunities for scientific and technological innovation. Some of them are:

- **Integration with other technologies**: The optimization of CH_4 pyrolysis in a CVD reactor can be integrated with other technologies such as artificial intelligence and machine learning algorithms to enhance the efficiency of the process and develop a more robust model.
- **Alternative feedstocks:** Currently, methane is the most widely used feedstock for CVD reactors. However, research can be conducted to explore other sustainable feedstocks such as biomass, waste materials, or other hydrocarbons.
- **Advanced materials synthesis:** The optimized CH_4 pyrolysis process can be applied for the synthesis of other advanced materials such as carbon nanotubes, diamond-like carbon, and other functionalized carbon materials.
- **Scaling up for industrial applications:** The optimized process can be scaled up for industrial applications, and commercialized for large-scale production of graphene and other advanced carbon materials.
- **Process optimization for other industrial applications:** The optimization of the CH4 pyrolysis process can be applied to other industrial applications that require high-temperature and gas-phase reactions, such as chemical manufacturing, solar cell production, and semiconductor processing.
- **Environmental sustainability:** It can be further developed to minimize the environmental impacts of the process. For example, research into strategies to reduce energy use, greenhouse gas emissions, and garbage generation can be conducted.
- **Process control and automation:** The optimized process can be further developed to implement advanced process control and automation technologies. This can help to reduce human error, enhance process efficiency, and increase the consistency and quality of the products.
- **Integration with renewable energy sources:** The integration of the optimised process with renewable energy sources such as solar, wind, and geothermal power

can be studied. This can help to minimise the process's carbon impact and improve its overall sustainability.

- **New applications and markets**: The optimized process can be further developed to explore new applications and markets for advanced carbon materials. For example, research can be conducted to explore the potential use of graphene in energy storage, water purification, and biomedical applications.