Carbon precursor analysis for catalytic growth of carbon nanotube in flame synthesis based on semi-empirical approach

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CARBON LETTERS
DOI: 10.1007/s42823-020-00127-z
Early Access: FEB 2020
Document Type: Article; Early Access
View Journal Impact

Abstract

Although flame synthesis promises economic benefit and rapid synthesis of carbon nanotube (CNT), the lack of control and understanding of the effects of flame parameters (e.g., temperature and precursor composition) impose some challenges in modelling and identifying CNT growth region for obtaining better throughput. The present study presents an investigation on the types of carbon precursor that affect CNT growth region on nickel catalyst particles in an ethylene inverse diffusion flame. An established CNT growth rate model that describes physical growth of CNT is utilised to predict CNT length and growth region using empirical inputs of flame temperature and species composition from the literature. Two variations of the model are employed to determine the dominant precursor for CNT growth which are the constant adsorption activation energy (CAAE) model and the varying adsorption activation energy (VAAE) model. The carbon precursors investigated include ethylene, acetylene, and carbon monoxide as base precursors and all possible combinations of the base precursors. In the CAAE model, the activation energy for adsorption of carbon precursor species on catalyst surface E-a,E-1 is held constant whereas in the VAAE model, E-a,E-1 is varied based on the investigated precursor. The sensitivity of the growth rate model is demonstrated by comparing the shifting of predicted growth regions between the CAAE model and the VAAE model where the CAAE model serves as a control case. Midpoint-based and threshold-based techniques are employed within each model to quantify the predicted CNT growth region. Growth region prediction based on the midpoint-VAAE approach demonstrates the importance of acetylene and carbon monoxide to some extent towards CNT growth. Ultimately, the threshold-VAAE model shows that the dominant precursor for CNT growth is the mixture of acetylene and carbon monoxide. A simplified reaction mechanism is proposed to describe the surface chemistry for precursor reactions with nickel catalyst where decomposition of the ethylene fuel source into acetylene and carbon monoxide is accounted for by chemisorption.

Keywords

Author Keywords: Carbon nanotube (CNT); Modelling; Catalytic growth; Flame synthesis; Carbon precursor
KeyWords Plus: DIESEL-ENGINE; KINETICS; FUEL; DEPOSITION; MORPHOLOGY

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Funding

Funding Agency	Grant Number
Ministry of Education (MOE) through Fundamental Research Grant Scheme	FRGS/1/2019/TK05/UTM/02/8 R.J130000.7851.5F182
Universiti Teknologi Malaysia (UTM) through UTM Fundamental Research	UTMFR: PY/2019/01657 Q.J130000.2551.21H10

View funding text

Publisher

SPRINGER JAPAN KK, SHIROYAMA TRUST TOWER 5F, 4-3-1 TORANOMON, MINATO-KU, TOKYO, 105-6005, JAPAN

Journal Information

Impact Factor: Journal Citation Reports

Categories / Classification

Research Areas: Chemistry; Materials Science

Web of Science Categories: Chemistry, Multidisciplinary; Materials Science, Multidisciplinary

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