Zero-dimensional model for the prediction of carbon nanotube (CNT) growth region in heterogeneous methane-flame environment

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Abstract

The conventional multi-scale modelling approach that predicts carbon nanotube (CNT) growth region in heterogeneous flame environment is computationally exhaustive. Thus, the present study is the first attempt to develop a zero-dimensional model based on existing multi-scale model where mixture fraction z and the stoichiometric mixture fraction z_{st} are employed to correlate burner operating conditions and CNT growth region for diffusion flames. Baseline flame models for inverse and normal diffusion flames are first established with satisfactory validation of the flame temperature and growth region prediction at various operating conditions. Prior to developing the

correlation, investigation on the effects of z_{st} on CNT growth region is carried out for 17 flame conditions with z_{st} of 0.05 to 0.31. The developed correlation indicates linear (z_{lb} =1.54 z_{st} +0.11) and quadratic (z_{hb} = z_{st} (7-13 z_{st})) models for the z_{lb} and z_{hb} corresponding to the low and high boundaries of mixture fraction, respectively, where both parameters dictate the range of CNT growth rate (GR) in the mixture fraction space. Based on the developed correlations, the CNT growth in mixture fraction space is optimum in the flame with medium-range z_{st} conditions between 0.15 and 0.25. The stronger relationship between growth-region mixture-fraction (GRMF) and z_{st} at the near field region close to the flame sheet compared to that of the far field region away from the flame sheet is due to the higher temperature gradient at the former region compared to that of the latter region. The developed models also reveal three distinct regions that are early expansion, optimum, and reduction of GRMF at varying z_{st} .

Author keywords

Carbon nanotube (CNT); Computational fluid dynamics (CFD); Diffusion flame; Flame synthesis; Zero-dimensional model

Indexed keywords

Engineering controlled terms

Computational fluid dynamics; Diffusion; Flame synthesis

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Carbon nanotube; Carbon nanotube growth; Computational fluid dynamic; Diffusion Flame; Flame-sheets; Methane flame; Mixture fraction; Multiscale modeling; Operating condition; Zero-dimensional models

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