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

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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)=1.54z(st) +0.11) and quadratic (z(hb)=z(st)(7-13z(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).

Keywords

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

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