IRON CATALYST CHEMISTRY IN HIGH PRESSURE CARBON MONOXIDE NANOTUBE REACTOR

Carl D. Scott
NASA Johnson Space Center, Houston, TX 77058

Alexander Povitsky
ICASE, NASA Langley Research Center, Hampton, VA

Christopher Dateo and Tahir Gökçen
Eloret Corporation, NASA Ames Research Center, Moffatt Field, CA
And
Richard E. Smalley
Center for Nanoscale Science and Technology
Rice University, Houston, TX

POSTER-PLUS ABSTRACT

The high-pressure carbon monoxide (HiPco) technique for producing single wall carbon nanotubes (SWNT) is analyzed using a chemical reaction model coupled with properties calculated along streamlines. Streamline properties for mixing jets are calculated by the FLUENT code using the k-ε turbulent model for pure carbon monixide. The HiPco process introduces cold iron pentacarbonyl diluted in CO, or alternatively nitrogen, at high pressure, ca. 30 atmospheres into a conical mixing zone. Hot CO is also introduced via three jets at angles with respect to the axis of the reactor. Hot CO decomposes the $Fe(CO)_5$ to release atomic Fe. Cluster reaction rates are from Krestinin, et al., based on shock tube measurements. Another model is from classical cluster theory given by Girshick's team. The calculations are performed on streamlines that assume that a cold mixture of $Fe(CO)_5$ in CO is introduced along the reactor axis. Then iron forms clusters that catalyze the formation of SWNTs from the Boudouard reaction on Fe-containing clusters by reaction with CO. To simulate the chemical process along streamlines that were calculated by the fluid dynamics code FLUENT, a time history of temperature and dilution are determined along streamlines. Alternative catalyst injection schemes are also evaluated.

Note: This presentation will not reveal any sensitive information not already published in the open literature.