An Assessment of the Discrete Reaction Model for Calculating the Composition of Sooting Flames

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The emission of particulate matter, or soot, can be considered a side effect associated with a combustion process characterized by high temperature and rich conditions. The production of these carbon nanoparticles entails a reduction in the efficiency of the combustion devices, as well as a detrimental effect on climate change and human health. A drastic reduction in emissions is mandatory, demanding a deeper understanding of the formation process than is currently known.

Calculating the formation and transient composition of sooting flames associated with the combustion process is challenging. Currently solution is by computer-intensive numerical techniques ranging from empirically based correlations through to employing conservation equations coupled with probability density functions, which attempt to address the detailed stochastic mechanism of soot formation and oxidation. These methods are difficult to both comprehend and also require computers with high performance.

The engineering community really requires an easy-to-use, affordable and reasonably accurate calculation method to model combustion problems arising from combustion in under-ventilated environment and fuel enriched operating conditions of many real-life flames. What is assessed here is a discrete reaction model [1, 2] of sooting combustion based on multi-stage representation of oxidation chemistry.

The use of the discrete reaction model was found to be easy-to-use and with realistic and reasonably accurate results ensuing. The algebraic nature of the model relationships makes it easy to integrate the model into the computational loops of available predictive tools.

[1] D. B Spalding. Int. J. Heat Mass Transfer 1 (1960) 192-207.
[2] S. V. Zhubrin. Int. J. Heat Mass Transfer 52 (2009) 4125-4133.