

3F02: COMPUTATIONAL AND EXPERIMENTAL INVESTIGATION OF THE INTERACTION OF SOOT AND NO_x IN COFLOW DIFFUSION FLAMES.

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Comment by Hongsheng Guo, National Research Council of Canada, Canada

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We have investigated the interaction between soot and NO formation in counterflow and coflow ethylene diffusion flames previously [1,2]. In your simulation, you identify the contributions of thermal and prompt routes to NO formation by two separate calculations. However, these two routes are closely coupled each other in diffusion flames. Atomic N from $N_2 + CH = HCN + N$ (prompt route) significantly affects the reaction rate of $NO + N = N_2 + O$ (thermal route). By separating these two routes in two calculations, you have neglected the coupling. Do you think if this affects any of your final conclusions?

References:

[1] H. Guo, G.J. Smallwood, *Combust. Flame* 149 (2007) 225–233.

[2] H. Guo, F. Liu, G.J. Smallwood, *Combustion Theory and Modelling* 8 (2004) 475–489.

Reply by Mitchell Smooke

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Thank you for your comment and the references. Yes, the thermal and prompt mechanisms are coupled. This is why we have indicated that when we subtract two computational solutions, this provides only an estimate of the prompt NO_x production simulation, and hence was referred to as an approximate Fenimore solution (Fig. 5 in the paper). The thermal NO_x is computed explicitly by including only the three reactions of the extended Zeldovich mechanism. We are computing the Fenimore only solution by setting to zero the forward rate constant for $O + N_2 = NO + N$ and expect to report the results soon. Similar comments regarding coupling can be made for the nitrous oxide mechanism. To turn it off, the forward rate for $O + N_2 + M = N_2O + M$ must be assigned a zero rate.