

2B11: THE IMPACT OF DETAILED MULTICOMPONENT TRANSPORT AND THERMAL DIFFUSION EFFECTS ON SOOT FORMATION IN ETHYLENE/AIR FLAMES.

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We have done a similar study to investigate the effect of thermal diffusion on the prediction of soot formation in coflow ethylene/air diffusion flames [1]. What we found is that although the effect of thermal diffusion is not significant for a pure ethylene/air diffusion flame, it is significant for the prediction of soot formation in a flame with light species (such as helium) added to air or fuel stream. In your soot model, surface growth was calculated by a C₂H₂ based model which has neglected the role of hydrogen abstraction in surface growth. It has been shown recently that hydrogen abstraction plays a key role in soot surface growth [2]. Will you expect any change in your conclusion if hydrogen abstraction is implemented in your soot model?

References:

[1] H. Guo, F. Liu, G.J. Smallwood, Ö.L. Gülder, *Int. J. Computational Fluid Dynamics* 18 (2004) 139–151.

[2] H. Guo, F. Liu, G.J. Smallwood, Ö.L. Gülder, *Combust. Flame* 145 (2006) 324–338.

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Hydrogen abstraction was included in our model. We did not state this explicitly. We only stated that inception depended on hydrogen concentrations. The thermal diffusive velocities of hydrogen have been shown to be significant but it is the cumulative thermal diffusion effect that effects soot formation. When thermal diffusion was only included for H and H₂, and abstraction was included in the model, the effect on soot formation was negligible. This leads us to conclude that for this flame, thermal diffusion has a minimal effect on soot through the hydrogen abstraction pathway.