

2D01: MODELING TEMPERATURE EFFECTS ON SOOT FORMATION.

*Guillaume Blanquart, Michael Edward Mueller, Heinz Pitsch  
Stanford University, USA*

**Comment by Hai Wang, University of Southern California, USA**

[haiw@usc.edu](mailto:haiw@usc.edu)

It is intriguing that your simulation results suggest that large aggregates tend to be more reactive than small, primary particles. Your argument of a reactive surface density is a good point, but additional factors may have to be considered. For example, it remains unclear how dehydrogenation and carbonization play a role in the overall surface reactivity. One can certainly argue that as soot ages, the graphene size increases, leading to a smaller amount of edge carbons for mass growth.

**Reply by Guillaume Blanquart**

[guillaume.blanquart@polytechnique.org](mailto:guillaume.blanquart@polytechnique.org)

As you point out, processes such as explicit dehydrogenation reactions and graphitization are not included in the model, but these could affect both the surface reactivity and the carbon-to-hydrogen ratio in soot particles. One might speculate that these processes are slow and would have an effect only at long residence times. These reactions would lower the surface reactivity of large soot aggregates. At the same time, the volumetric hydrogen content would be reduced and thus the carbon-to-hydrogen ratio would be increased. However, we have looked at a model extension that also computes the carbon-to-hydrogen ratio. The predicted values are in very good agreement with experimental observations. This could also suggest that the effects neglected in the model are not too important during the time scales considered. But to conclusively answer this question, these processes should be included in further model improvements.