Nucleation of incipient soot and carbon black affects particle size distribution, morphology and composition. However, nucleation is poorly understood. Clusters of large Polycyclic Aromatic Hydrocarbons (PAH) with physical or chemical forces are often considered as soot nuclei. Here a kinetic model is developed to investigate soot nucleation mechanisms, dominant species and oligomers in a so called “nucleation” premixed flame.

Motivation

For Classic Nucleation, any PAH can be used!

Physical Nucleation is Reversible and Weak

Theory


Small Aromatics Contribute the Most

Chemical Bonding is Required for Nucleation

References

Conclusions

1. Physical nucleation must be modeled reversible and cannot explain soot nucleation at high temperatures.
2. An irreversible nucleation model using a collision factor cannot capture the temperature dependency of nucleation.
3. Only by accounting for a nucleation process that involves chemical bond formation, soot nucleation kinetics can be modeled.
4. Soot nucleation at high temperature has a thermodynamic barrier of 21 kcal/mol.