# A Model Fuels Consortium to Promote Engine Modeling

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# A Soot Formation Model Based on Surface Chemistry

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## Motivation

- **Particle growth and oxidation modeled as surface processes**
- **Generalized descriptions of particle nucleation and growth required**
- **The ability to use kinetic parameters from surface kinetic studies wanted**
- **Sensitivity and rate-of-production to analyze soot growth pathways needed**
- **A software module that can be linked to various simulation tools desired**

## Modeling Approach

- **Size distribution evolution tracked by method of moments of Frenklach and Harris**
- **Size/class definable by the number of bulk atom/compound in the particle**
- **Average particle properties (diameter, etc.) derived from size moments**

## Surface Chemistry Representation

- **Particle material**
  - Particle composition represented by bulk species of the dispersed material
  - Different particles definable as different surface materials (no interaction)
- **Nucleation reactions**
  - New particle inception class and initial surface coverage defined by nucleation reaction
  - Particles formable by multiple nucleation reactions
- **Particle growth & oxidation**
  - Surface chemical processes expressed as coverage dependent elementary surface reactions (statistical surface coverage same for all particles)
  - Particle growth if the net surface production rate of the bulk species is positive