



# Modeling Soot Production Using CHEMKIN-PRO

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## Overview

This application note describes how CHEMKIN-PRO can be used to model soot (particle) formation using the Particle Tracking capability. As an example, a JSR/PFR system studied at MIT [1] will be modeled in CHEMKIN-PRO.

## Introduction

Emissions regulations continue to become more stringent concerning acceptable levels of NO<sub>x</sub>, UHC, and CO as well as particulate matter. For particulate matter, focus on controlling particle sizes (as well as total mass) is one outcome of recent studies that show the detrimental impact of nanometer-scale particles to human health. Engineers are faced with the daunting task of developing new designs or modifying current designs to meet these regulations. The ability to accurately model particle chemistry is essential in today's fast-paced design environment.

To model particle chemistry and size distributions, a high-fidelity model is needed that is capable of capturing the different chemical (nucleation and particle interactions with the surrounding gas) as well as physical (coagulation) processes involved. The Particle Tracking option in CHEMKIN-PRO allows users to specify the different chemical processes via a surface chemistry input file, and the physical processes via the reactor model data. Using the Particle Tracking capability, the effects of different operating conditions (temperature, pressure, equivalence ratio, etc.) can be studied to determine their effect on average particle size, particle number density, and total mass/volume of particles, for example.

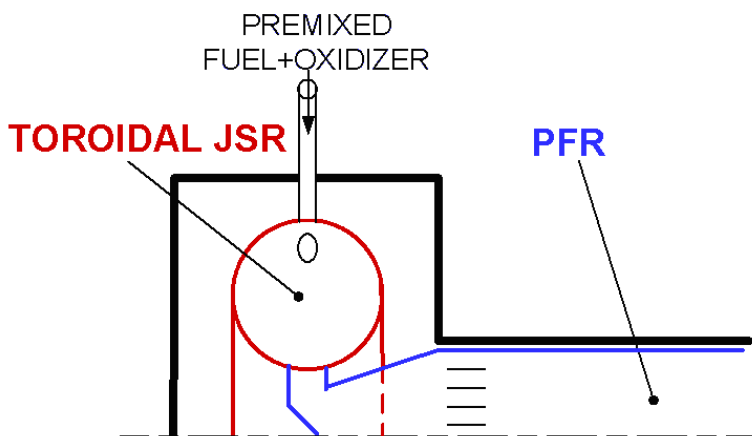
## Application Setup

The Particle Tracking Feature in CHEMKIN-PRO uses the Method of Moments previously applied by Frenklach et. al. [2-4] to describe the average properties of a particle population. This method can provide overall properties of a particle system, e.g., particle number density, total particle volume fraction, total particle surface area density, and average particle size. Using this method, the effects of operating conditions, varying fuel compositions, etc., can be efficiently studied to determine the characteristics of a particle system.

For this example, consider the Jet Stirred Reactor (JSR) / Plug Flow Reactor (PFR) system developed at MIT [1] that provides a good platform for kinetic studies of soot formation and growth. In the model,

the JSR represents a pre-heat and flame zone of a premixed flame and the PFR is used to simulate the post-flame region. A schematic of the configuration is shown in Figure 1.

Figure 1. Schematic of JSR/PFR System



In the example, the Particle Tracking Feature is used to simulate a  $C_2H_4/O_2/N_2$  mixture that is used in the experiments by Marr [1]. The moles for each species are shown in Table 1. The experimental data include mole fractions of major species, PAH's (poly-aromatic hydrocarbons), and soot mass concentration at various locations in the reactor. This data are useful for validating the soot-chemistry model, as well as providing valuable insights on the nucleation and soot growth surface reactions.

The CHEMKIN-PRO reactor network is shown in Figure 2. It consists of a PSR and two PFR's in series. The first PSR is used to represent the flame zone, while the first PFR represents the transition from the PSR to the post-flame PFR region where the measurements are performed. The primary purpose of the transition PFR is to allow the PSR exhaust to cool from 1630 K to 1620 K. To activate the Particle Tracking Feature in CHEMKIN-PRO, the "Dispersed" keyword is included in the surface chemistry input file to indicate that the material is dispersed in the gas, rather than a solid wall boundary condition. This keyword will activate the Particle Tracking option in CHEMKIN-PRO. The inputs to the Particle Tracking Feature are available on the Dispersed Phase tab in the Reactor Physical Properties input dialog and will be available for all reactors in the model.

Figure 2. Schematic of CHEMKIN-PRO Reactor Network

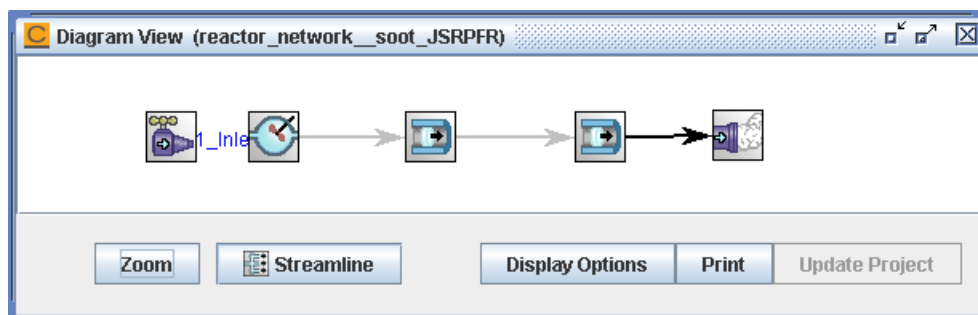


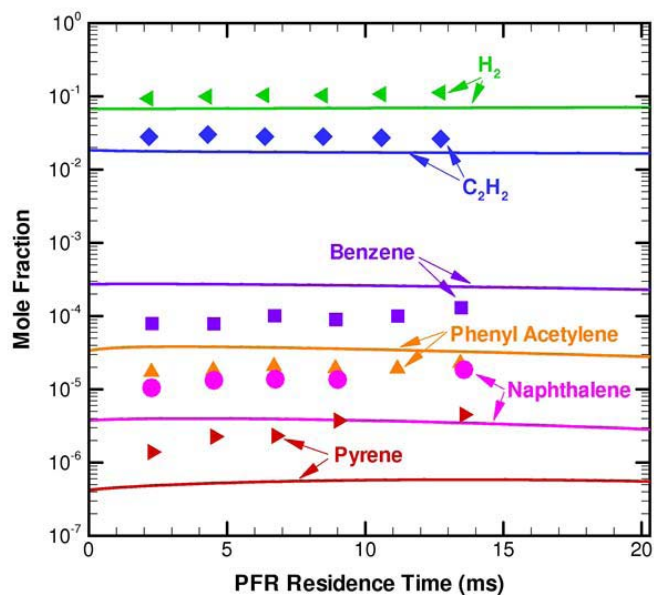
Table 1. Composition of Inlet Gas Mixture

Species	Moles
C <sub>2</sub> H <sub>4</sub>	2.2
N <sub>2</sub>	16.7
O <sub>2</sub>	3.0

## Project Results

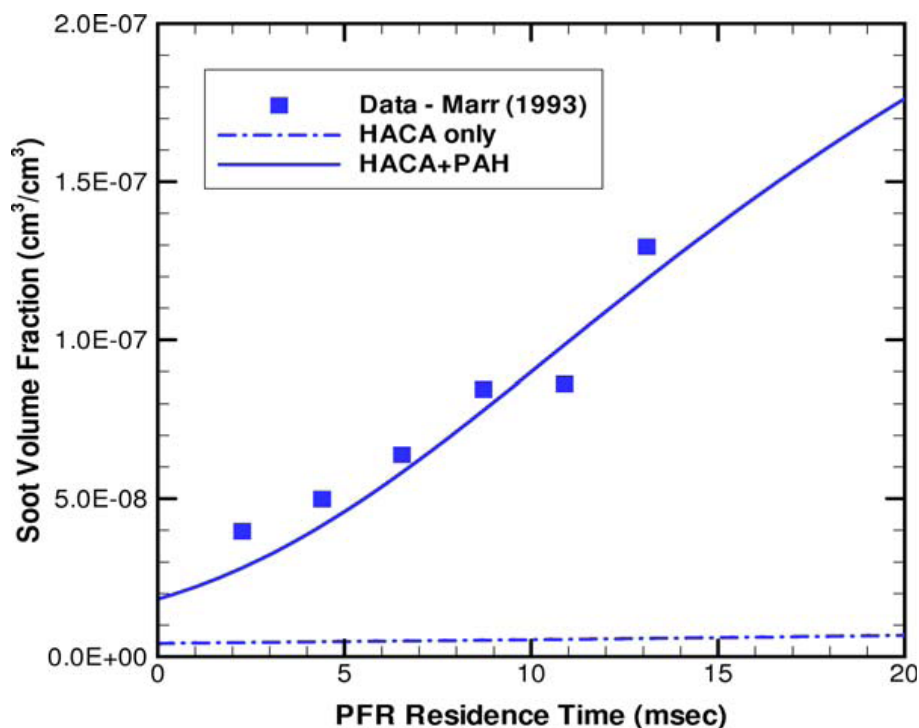
To test different growth mechanisms of soot, two simulations are performed: one with both H-abstraction-C<sub>2</sub>H<sub>2</sub>-addition (HACA) and PAH condensation growth and the other one with HACA growth reactions only. To analyze the results to compare with experimental data, the results of the PFR will be post-processed in the CHEMKIN-PRO Post Processor. The PFR represents the exit of the system, thus we can get outlet concentrations of species such as PAH. The data in Figure 3 show the comparison of Hydrogen, Acetylene, Benzene, Phenyl Acetylene, Naphthalene, and Pyrene gas phase compositions. The experimental data, shown with symbols, compares well with the model predictions, shown as solid lines, of CHEMKIN-PRO.

Figure 3. Mole Fraction Profiles of Selected Species inside the PFR at 1630K and  $\phi = 2.2$ . Case of the C<sub>2</sub>H<sub>4</sub>/O<sub>2</sub>/N<sub>2</sub> JSR/PFR experiment by Marr [1]. Symbols: data; Solid lines: predictions with HACA and PAH condensation growth mechanisms.



As further validation of the Particle Tracking Feature, a comparison between measured and predicted soot mass concentration profiles is shown in Figure 4.

Figure 4. Comparisons of Soot Mass Concentration Profiles inside the PFR for the 1630K,  $\phi = 2.2$  case of C<sub>2</sub>H<sub>4</sub>/O<sub>2</sub>/N<sub>2</sub> JSR PFR experiment by Marr [1]. Symbols: data; Solid line: prediction with both HACA and PAH condensation growth mechanisms; Dash-dot line: prediction with HACA growth mechanism only.



The simulation results indicate that the HACA-only (dash-dot line) does not properly capture the slow soot mass growth in the post-flame region. On the other hand, the HACA + PAH mechanism (solid line) shows much better agreement with the experimental data.

## Summary

As regulations on soot become more stringent, it is imperative that modeling tools provide capabilities for accurate prediction of soot particle formation and size distributions. The CHEMKIN-PRO Particle Tracking Feature provides the capabilities to study the fundamental soot formation characteristics, such as nucleation, growth, and agglomeration. The example used in this note demonstrates the capabilities of the CHEMKIN-PRO Particle Tracking Feature to predict these fundamental soot characteristics.

## References

- [1] Marr, J. A. "PAH Chemistry in a Jet-Stirred/Plug-Flow Reactor System," Massachusetts Institute of Technology, 1993.
- [2] Frenklach, M.; Wang, H. In Soot Formation in Combustion: Mechanisms and Models; Bockhorn, H., Ed.; Springer-Verlag: Berlin, 1994.
- [3] Frenklach, M.; Harris, S. J. "Aerosol Dynamics Modeling Using the Method of Moments," *Journal of Colloid and Interface Science* 1987, **118**, 252-261.
- [4] Appel, J.; Bockhorn, H.; Frenklach, M. "Kinetic Modeling of Soot Formation with Detailed Chemistry and Physics: Laminar Premixed Flames of C<sub>2</sub> Hydrocarbons," *Combustion and Flame* 2000, **121**, 122-136.

## About Reaction Design

Reaction Design helps transportation manufacturers and energy companies rapidly achieve their Clean Technology goals by automating the analysis of chemical processes via simulation and modeling solutions. Reaction Design is the exclusive developer and distributor of CHEMKIN and CHEMKIN-PRO, the *de facto* standards for modeling gas-phase and surface chemistry, providing engineers ultra-fast access to reliable answers that save time and money in the development process. Reaction Design also offers the CHEMKIN-CFD software module, which brings detailed kinetics modeling to other engineering applications, such as Computational Fluid Dynamics (CFD) programs. Reaction Design's world-class engineers, chemists and programmers have expertise that spans multi-scale engineering from the molecule to the production plant. Reaction Design serves more than 350 customers in the commercial, government and academic markets.

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