Motivation

- Soot formation is a key process in flames and fires
  - Radiative heat transfer
  - Incomplete combustion
  - Environmental and health impacts
- Soot affects radiation, which affects temperature, which affects soot…
- Modeling soot formation is challenging
  - Complex chemistry among many species
  - Representation of the particle size distribution
  - Potentially several PSD coordinates
  - Large range of scales
- Combustion simulations
  - complex chemistry, turbulent flow, multicomponent mass transfer, radiative heat transfer, soot formation
  - Burden on users/developers for submodel expertise
  - Availability of libraries that offload submodels facilitates code development and progress
    - Chemkin, Cantera, etc.

https://energy.sandia.gov/programs/nuclear-energy/nuclear-energy-safety-security/

Soot Processes: Nucleation

Semi-empirical

Leung et al.

- *K. M. Leung, R. P. Lindstedt, W. P. Jones, A simplified reaction mechanism for soot formation in nonpremixed flames, Combustion and Flame 87 (1991) 289–305*
- $C_2H_2 \rightarrow 2C_{soot} + H_2$

Lindstedt

- *R. P. Lindstedt, Simplified soot nucleation and surface growth steps for non-premixed flames, in: H. Bockhorn (Ed.), Soot Formation in Combustion, no. 59 in Springer Series in Chemical Physics, Springer-Verlag Berlin Heidelberg, 1994, pp. 417–441*
- $C_2H_2 \rightarrow 2C_{soot} + H_2$
- ($C_6H_6 \rightarrow 6C_{soot} + 3H_2$)

Detailed

PAH Nucleation, Blanquart & Pitsch

- *G. Blanquart, H. Pitsch, A joint volume-surface-hydrogen multi-variate model for soot formation, in: H. Bockhorn, A. D'Anna, A. F. Sarofim, H. Wang (Eds.), Combustion Generated Fine Carbonaceous Particles, KIT Scientific Publishing, 2009, pp. 437–463.*
- 8 PAH species
- Free molecular PAH collisions to form PAH Dimers
  - $PAH_i + PAH_i \rightarrow$ Dimer
  - Only self-collision assumed
  - Dimers not distinguished
- Dimer coagulation to form soot
  - Dimer + Dimer $\rightarrow C_{soot}$
  - Dimers assumed in steady state, quadratic eqn:

$$\underbrace{\sum_{i}^{n_P} \gamma_i \frac{1}{2} \beta_{P_i,P_i} n_{P_i}^2}_{\text{formation}} = \underbrace{\beta_{D,D} \mathbf{n_D}^2}_{\text{soot nuc.}} + \underbrace{\sum_{k}^{n_s} \beta_{D,C_k} n_{C_k} \mathbf{n_D}}_{\text{condensation}}$$

Soot Processes: Growth

Semi-empirical

Leung et al.

- $C_2H_2 + C_{n,soot} \rightarrow C_{n+2,soot} + H_2$
- $R_g \propto \sqrt{A}$

Lindstedt

- $C_2H_2 + C_{n,soot} \rightarrow C_{n+2,soot} + H_2$
- $R_g \propto A$

PAH Condensation

- Consistent with PAH nucleation
- $D_{CxHy} + C_{n,soot} \rightarrow C_{n+x,soot} + (y/2)H_2$
  - Dimer size computed as weighted average over PAH contributions to PAH nucleation

$$R_{cnd,k} = \beta_{D,C_k} n_{C,k} n_D m_D \ (=) \ \mathrm{kg/m^3 s}$$

Detailed

HACA

- *ABF mechanism: Appel, Bockhorn, Frenklach, Combustion and Flame 121:122-136 (2000).*

$$\text{C-H} + \text{H} \rightleftharpoons \text{C}^* + \text{H}_2$$
$$\text{C-H} + \text{OH} \rightleftharpoons \text{C}^* + \text{H}_2\text{O}$$
$$\text{C}^* + \text{H} \rightarrow \text{C-H}$$
$$\text{C}^* + \text{C}_2\text{H}_2 \rightarrow (3\text{C})\text{-H} + \text{H}$$
$$\text{C}^* + \text{O}_2 \rightarrow 2CO$$

- C* from QSSA over given reactions
- *Reverse reactions from Ken Revzan and Frenklach 02/15/02 code soot.f: combustion.berkeley.edu/soot/codes/routines.html*
- *Rate is proportional to frac. available surf. sites α*

$$\alpha = \tanh\left(\frac{a}{\log_{10}(M_1/M_0)} + b\right)$$

  - a(T), b(T) from *Balthasar and Frenklach, Combust. Flame 140:130-145 (2005)*

Soot Processes: Oxidation

O_2 Global: Leung, Lindstedt, Jones 1991

- $C_{soot} + (1/2)O_2 \rightarrow CO$

O_2 Global: Lee, Thring, Beer 1962

- $C_{soot} + (1/2)O_2 \rightarrow CO$

O_2 Elementary: Nagle, Strickland-Constable 1962

- $C_{soot} + (1/2)O_2 \rightarrow CO$
- Graphite rods

OH Elementary Neoh, Howard, Sarofim 1981

- $C_{soot} + OH \rightarrow CO + H$

$$R = 1290 \times 0.13 P_{OH} T^{-0.5}$$

- R (=) kg/m^{2}s, P_{OH} (=) atm, T (=) K

HACA O_2, OH: Appel, Bockhorn, Frenklach 2000

- $C_{soot} + OH \rightarrow CO + H$; from Neoh
- $C^* + (1/2)O_2 \rightarrow CO$
- Same rate as used in HACA for C* from QSSA

Optimized O_2, OH: Guo, Anderson, Sunderland 2016

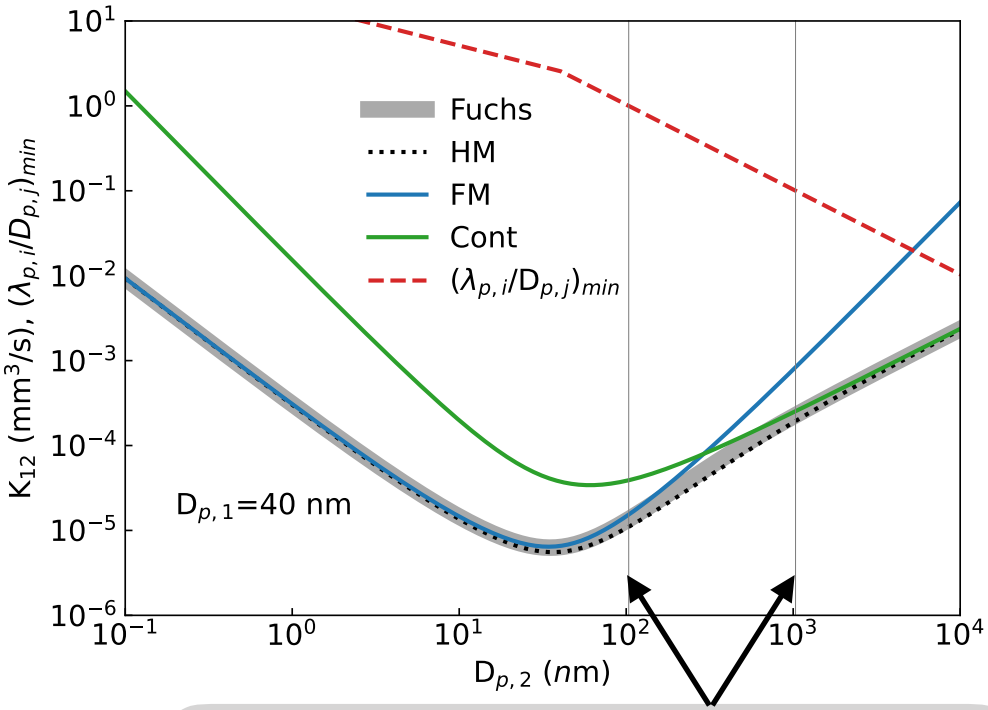
- $C_{soot} + (1/2)O_2 \rightarrow CO$
- $C_{soot} + OH \rightarrow CO + H$
- Optimized among 12 experiments.
    - OH efficiency = 0.1

Optimized O_2, OH: Josephson et al. 2017

- $C_{soot} + (1/2)O_2 \rightarrow CO$
- $C_{soot} + OH \rightarrow CO + H$
- Optimized among 13 experiments using Bayesian statistics.
    - OH efficiency = 0.15

Soot Processes: Coagulation

- Assume spherical particles
- Two regimes
  - Free molecular: small particles
    - D << λ_{mfp}
  - Continuum: large particles
    - D >> λ_{mfp}
  - Note, λ_{mfp} is the mean free path of the particle, *not* the gas.



$$\dot{S}_{\text{coag}}(m) = \frac{1}{2}\int_0^m \beta_{\mu,m-\mu} n(\mu) n(m) d\mu - \int_0^\infty \beta_{\mu,m} n(\mu) n(m) d\mu$$

$$\beta_{m,\mu}^{FM} = c\epsilon_c \left(\frac{\pi k_b T}{2}\right)\left(\frac{6}{\pi\rho_s}\right)^{2/3}\left(\frac{1}{m}+\frac{1}{\mu}\right)^{1/2}(m^{1/3}+\mu^{1/3})^2$$

$$\beta_{m,\mu}^{C} = \frac{2k_b T}{3\mu_v}\left(\frac{C_m}{m^{1/3}}+\frac{C_\mu}{\mu^{1/3}}\right)(m^{1/3}+\mu^{1/3})$$

$$Kn = \left(\frac{\lambda_{p,i}}{D_{p,j}}\right)_{min} \qquad 0.1 \le Kn \le 1$$

Brackets the transition region

Transition Region

- Harmonic mean $HM = \dfrac{C \cdot FM}{C + FM}$
- A more theoretically-based transition by Fuchs is also implemented

PSD: Sectional

- Can't afford to consider all soot sizes
  - 50 nm particle ~ 6 million C's
- Divide the PSD into sections
- Assume uniform size within a section
- Geometrically spaced

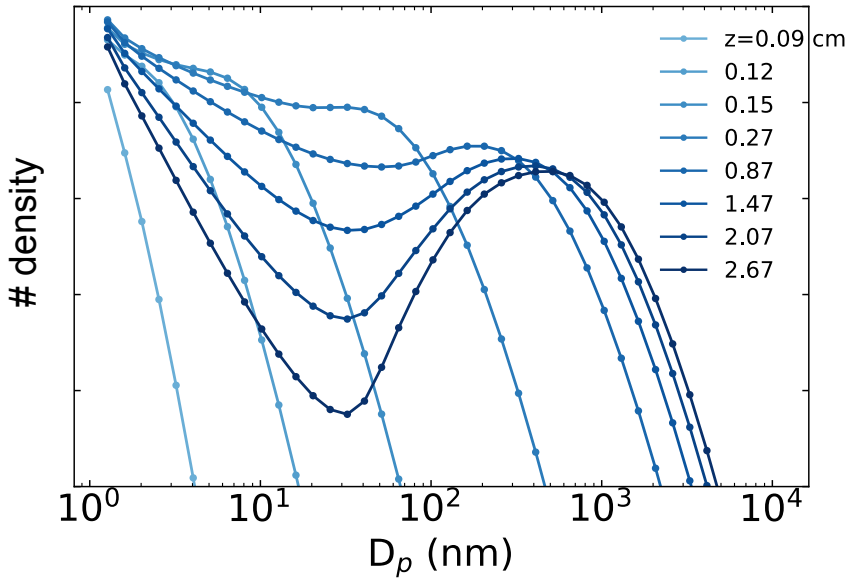
$$m_{min}\left(F^0,\ F^1,\ F^2,\ \ldots,\ F^{N-1}\right)$$

- Nucleation is into the first bin
- Growth and oxidation are transport in the size coordinate, written in n_i.

$$\frac{dn_{i,g}}{dt} = \frac{k_g A_{i-1} n_{i-1}}{m_i - m_{i-1}} - \frac{k_g A_i n_i}{m_{i+1} - m_i}$$

- Coagulation "lands" between bins
  - Assign to neighbors: conserve # and m

Example: premixed flame evolution



PSD: Method of Moments (MOM)

- Sectional models still require many bins
- Instead, solve for moments of the PSD

$$\frac{dn(m)}{dt} = \dot{S}(n(m))$$

$$\downarrow \qquad M_k = \int m^k n(m) dm$$

$$\frac{dM_k}{dt} = \int m^k \dot{S} dm = \dot{S}_k$$

- The moment source term involves integration over the unknown size distribution n(m).
- This requires a method for closure
- For soot growth, the closure of the fractional moments $M_{k-1/3}$ are needed.

Soot Growth Source

$$\dot{S}_G = -\frac{\partial}{\partial m}(v_g n)$$

$$\dot{S}_{k,G} = -\int_0^\infty m^k \frac{\partial}{\partial m}(v_g n) dm$$

$$\dot{S}_{k,G} = k \int_0^\infty v_g m^{k-1} n dm$$

$$v_g = k_s A$$

$$A = \pi D^2$$

$$m = \rho_s \frac{\pi}{6} D^3$$

$$v_g = k_s \pi \left(\frac{6}{\pi \rho_s}\right)^{2/3} m^{2/3}$$

$$\dot{S}_{k,G} = k_s \pi \left(\frac{6}{\pi \rho_s}\right)^{2/3} k \int_0^\infty m^{k-1/3} n dm$$

$$\dot{S}_{k,G} = k_s \pi \left(\frac{6}{\pi \rho_s}\right)^{2/3} k M_{k-1/3}$$

PSD: Method of Moments (MOM)

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Closure Approaches

- **Assumed shape n(m)**
  - Monodispersed
  - Lognormal
  - (Power-law + lognormal)
- **Interpolative closure**
  - Interpolate whole order moments to fractional moments
- **Quadrature**
  - QMOM
  - (DQMOM)
  - (CQMOM)

PSD: Assumed Shape n(m)

Monodispersed

- Simplest model
- 2 moments
  - M_0: number density, #/m^3
  - M_1: soot mass density, kg/m^3
    - $M_1 = \rho Y_s$
    - $f_v = M_1/\rho_s$
- $$n(m) = \delta(m - \bar{m})$$
  $$\bar{m} = \frac{M_1}{M_0} = \frac{\rho Y_s}{n}$$
- Direct integration without closure
- Single (but variable) size
- Special case of QMOM

Lognormal

$$n(m) = \frac{M_0}{\sigma\sqrt{2\pi}} \frac{1}{m} \exp\left(-\frac{\log^2(m/\bar{m})}{2\sigma^2}\right)$$

$$M_k = \int m^k n(m) dm$$

$$M_k = M_0 \bar{m}^k \exp(k^2\sigma^2/2)$$

Write for M_1, M_2, solve for $\bar{m}$, σ

$$\sigma^2 = \ln\left(\frac{M_0 M_2}{M_1^2}\right)$$

$$\bar{m} = \frac{M_1^2}{M_0^{3/2} M_2^{1/2}}$$

$$M_k = M_0^{1-3k/2+k^2/2} M_1^{2k-k^2} M_2^{k^2/2-k/2}$$

General fractional moment k

PSD: Assumed Shape n(m)

Free molecular collision coefficient has factor

$$\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^{1/2}$$

- This factor precludes direct integration with closure using fraction moments
- Following Pratsinis (1988), assume

$$\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^{1/2} \approx b\left(\frac{1}{m_1^{1/2}}+\frac{1}{m_2^{1/2}}\right)$$

- b is bounded between 0.707 and 1 when m_1 and m_2 approach the same size, and are widely separated, respectively.
- b=0.854 gives at worst a 15% error.
- FM coagulation:

$$S^{fm}_{0,\text{coag}} = -Kb\left(M_1 M_{1/6} + 2M_{2/6}M_{-1/6} + M_{4/6}M_{-3/6}\right)$$
$$S^{fm}_{1,\text{coag}} = 0$$
$$S^{fm}_{0,\text{coag}} = 2Kb\left(M_1 M_{7/6} + 2M_{8/6}M_{5/6} + M_{10/6}M_{3/6}\right)$$
$$K = c\epsilon_c\left(\frac{\pi k_b T}{2}\right)^{1/2}\left(\frac{6}{\pi}\rho_s\right)^{2/3}$$

Sotiris E Pratsinis. Simultaneous nucleation, condensation, and coagulation in aerosol reactors. Journal of Colloid and Interface Science, 124(2):416–427, 1988.

Lognormal

$$n(m) = \frac{M_0}{\sigma\sqrt{2\pi}}\frac{1}{m}\exp\left(-\frac{\log^2(m/\bar{m})}{2\sigma^2}\right)$$

$$M_k = \int m^k n(m) dm$$

$$M_k = M_0 \bar{m}^k \exp(k^2\sigma^2/2)$$

Write for M_1, M_2, solve for $\bar{m}$, σ

$$\sigma^2 = \ln\left(\frac{M_0 M_2}{M_1^2}\right)$$

$$\bar{m} = \frac{M_1^2}{M_0^{3/2} M_2^{1/2}}$$

$$M_k = M_0^{1-3k/2+k^2/2} M_1^{2k-k^2} M_2^{k^2/2-k/2}$$

General fractional moment k

PSD: Quadrature

General quadrature with function f and weight function W

$$\int_a^b W(x)f(x)dx \approx \sum_{j=1}^{N} w_j f(x_j)$$

- w_j are weight factors and x_j are abscissas (environments)
- Take W(x) = n(m) for soot.

$$\int_0^\infty n(m)f(m)dm \approx \sum_{j=1}^{N} w_j f(m_j)$$

- This is equivalent to assuming

$$n(m) = \sum_{j=1}^{N} w_j \delta(m - m_j)$$

- If w_j and m_j are known, integration is trivial
- Compute w_j, m_j from moments M_k

2 environment Quadrature, 4 moments

$$M_0 = \int m^0 n(m)dm = \sum_{j=1}^{2} m_j^0 w_j = w_1 + w_2$$

$$M_1 = \int m^1 n(m)dm = \sum_{j=1}^{2} m_j^1 w_j = m_1 w_1 + m_2 w_2$$

$$M_3 = \int m^3 n(m)dm = \sum_{j=1}^{2} m_j^2 w_j = m_1^2 w_1 + m_2^2 w_2$$

$$M_4 = \int m^4 n(m)dm = \sum_{j=1}^{2} m_j^2 w_j = m_1^3 w_1 + m_2^3 w_2$$

Efficient and stable evaluation using the Wheeler Algorithm (*uses LAPACK*)

$$\dot{S}_{0,\text{coag}} = \frac{1}{2}\iint \beta(m,\mu)n(m)n(\mu)dmd\mu = -\frac{1}{2}\sum_{j=1}^{N}\sum_{i=1}^{N}\beta_{m_j,m_i}w_j w_i$$

PSD: MOMIC

- Frenklach's MOM with interpolative closure.
- Interpolate fractional moments from whole-order moments
  - Interpolate among $\log(M_k)$
  - Positive moments: interpolate among all integer moments
  - Negative moments: interpolate among M_0, M_1, M_2
- Interpolation is done many times for a given set of integer moments.
  - Use a Newton forward polynomial; O(n) operations vs $O(n^2)$
  - (But Barycentric Lagrange Interpolation is better)
- Interpolation among moments works for nucleation, growth, oxidation, and continuum coagulation.
- But special treatment is needed for the FM regime (including treatment of PAH condensation).

Michael Frenklach. Method of moments with interpolative closure. Chemical Engineering Science, 57(12):2229–2239, 2002.

$$S_{0,c}^{FM} = -\frac{K_{FM}}{2} \iint n(m)n(\mu)(m+\mu)^{1/2} \left(m^{1/6}\mu^{-3/6} + 2m^{-1/6}\mu^{-1/6} + m^{-3/6}\mu^{1/6}\right) m^0\mu^0 dmd\mu,$$

$$S_{1,c}^{FM} = 0,$$

$$S_{k\geq 2,c}^{FM} = \frac{K_{FM}}{2} \sum_{j=1}^{k-1} \binom{k}{j} \underbrace{\iint n(m)n(\mu)(m+\mu)^{\mathbf{1/2}} \left(m^{1/6}\mu^{-3/6} + 2m^{-1/6}\mu^{-1/6} + m^{-3/6}\mu^{1/6}\right) m^{\mathbf{k}}\mu^{\mathbf{r-k}} dmd\mu}_{f^{j,k-j}_{1/2}}$$

Grid function

Interpolate whole powers to 1/2 power

PSD: MOMIC

$$S_{0,c}^{FM} = -\frac{K_{FM}}{2} \iint n(m)n(\mu)(m+\mu)^{1/2} \left(m^{1/6}\mu^{-3/6} + 2m^{-1/6}\mu^{-1/6} + m^{-3/6}\mu^{1/6}\right) m^0\mu^0 dmd\mu,$$

$$S_{1,c}^{FM} = 0,$$

$$S_{k\geq 2,c}^{FM} = \frac{K_{FM}}{2} \sum_{j=1}^{k-1} \binom{k}{j} \underbrace{\iint n(m)n(\mu)(m+\mu)^{1/2} \left(m^{1/6}\mu^{-3/6} + 2m^{-1/6}\mu^{-1/6} + m^{-3/6}\mu^{1/6}\right) m^{\mathbf{k}}\mu^{\mathbf{r-k}} dmd\mu}_{f_{1/2}^{j,k-j}}$$

Grid function

$$f_0^{x,y} = M_{x-3/6}M_{y+1/6} + 2M_{x-1/6}M_{y-1/6} + M_{x+1/6}M_{y-3/6}$$

$$f_1^{x,y} = M_{x-3/6}M_{y+7/6} + 2M_{x-1/6}M_{y+5/6} + M_{x+1/6}M_{y+3/6} + M_{x+3/6}M_{y+1/6} + 2M_{x+5/6}M_{y-1/6} + M_{x+7/6}M_{y-3/6}$$

$$f_2^{x,y} = M_{x-3/6}M_{y+13/6} + 2M_{x-1/6}M_{y+11/6} + M_{x+1/6}M_{y+9/6} + 2M_{x+3/6}M_{y+7/6} + 4M_{x+5/6}M_{y+5/6} + 2M_{x+7/6}M_{y+3/6} + M_{x+9/6}M_{y+1/6} + 2M_{x+11/6}M_{y-1/6} + M_{x+13/6}M_{y-3/6}$$

$$f_3^{x,y} = M_{x-3/6}M_{y+19/6} + 2M_{x-1/6}M_{y+17/6} + M_{x+1/6}M_{y+15/6} + 3M_{x+3/6}M_{y+13/6} + 6M_{x+5/6}M_{y+11/6} + 3M_{x+7/6}M_{y+9/6} + 3M_{x+9/6}M_{y+7/6} + 6M_{x+11/6}M_{y+5/6} + 3M_{x+13/6}M_{y+3/6} + M_{x+15/6}M_{y+1/6} + 2M_{x+17/6}M_{y-1/6} + M_{x+19/6}M_{y-3/6}$$

- Interpolation using 1, 2, 3, or 4 points
- Many values of x and y
- Exploit symmetry when x=y
- Lots of reused moments
- Create a table: $M_{q/6}$
  - with q = -3, -1, 1, 3, 5 … 55 handling up to 8 moments
- Continuum requires $M_{p/6}$ with p = -4, -2, 0, 2…
- PAH condensation requires similar treatment, but with different grid function (since m_{Dimer} is used)

SootLib

- SootLib: library of soot models for simulation
- Open source, C++, no external libraries besides LAPACK
- Documented
- Examples: simple interface, premixed flame
- Allows consistent model comparison

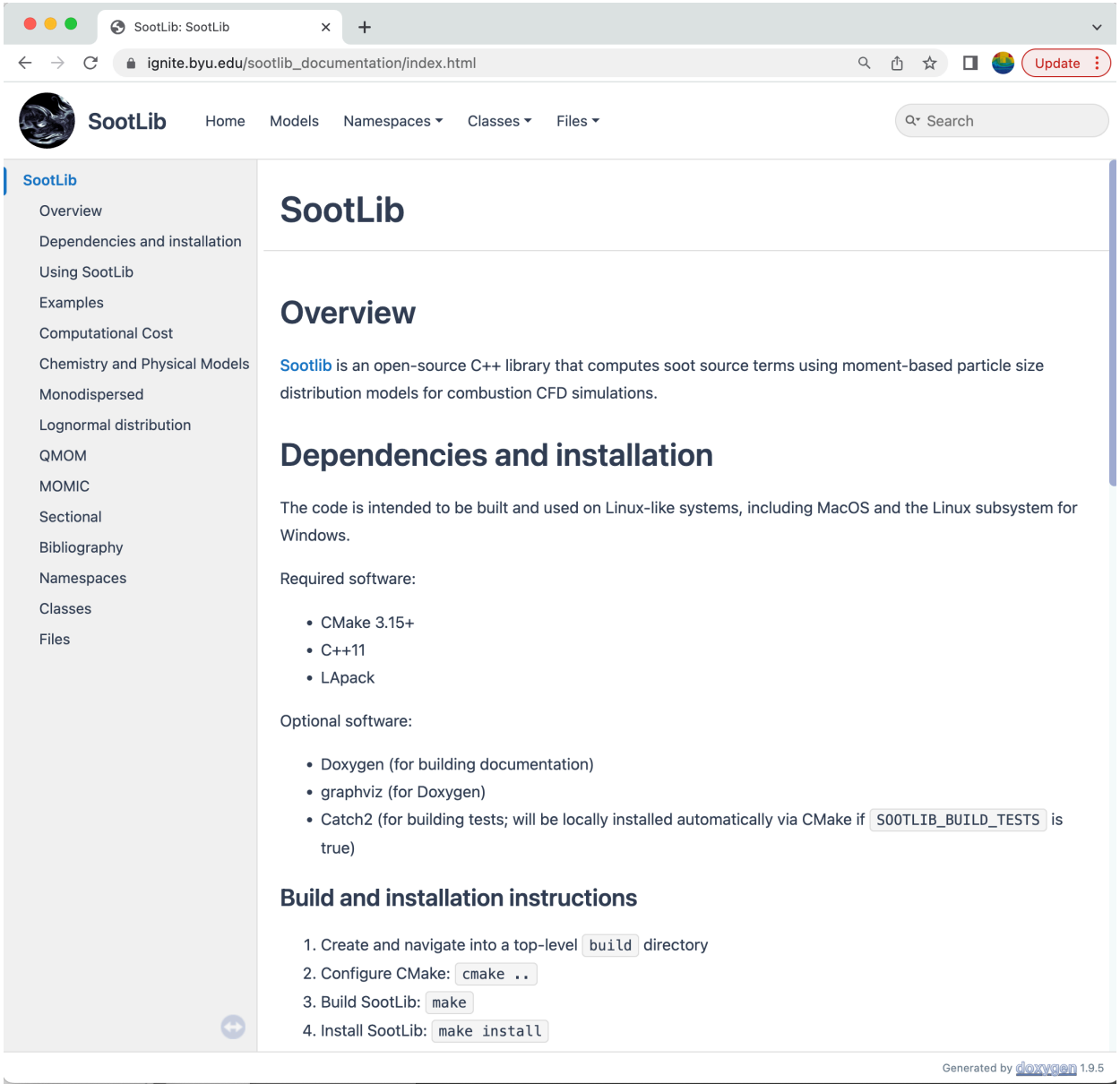
Soot Processes

- Nucleation
- Growth
- Oxidation
- Coagulation
- PAH condensation

Particle Distributions

- Monodispersed
- Lognormal
- Quadrature MOM
- MOM-Interpolative Closure
- Sectional

Documentation



Code Interface

```
#include <iostream>
#include <iomanip>

#include "sootHeaders.h"

using namespace std;
using namespace soot;

int main(int argc, char** argv) {

    //---------- set up and create a soot model

    nucleationModel  *nucl = new soot::nucleationModel_LL();
    growthModel      *grow = new soot::growthModel_LL();
    oxidationModel   *oxid = new soot::oxidationModel_LL();
    coagulationModel *coag = new soot::coagulationModel_FM();

    size_t nsoot = 4;  // number of soot moments (or sections)

    sootModel_QMOM SM(nsoot, nucl, grow, oxid, coag);

    //---------- set up thermodynamic state variables

    state S = state(nsoot);

    double T      = 2100;    // temperature in K
    double P      = 101325;  // pressure in Pa
    double rhoGas = 0.1;     // gas density in kg/m^3
    double muGas  = 1E-5;    // gas viscosity in Pa*s

    vector<double> yGas{3E-4, 0.002, 0.001, 0.05, 0.003, 0.07, 0.1, 0.002};
    vector<double> yPAH{0, 0, 0, 0, 0, 0};
    vector<double> Msoot{0.003, 1.5E-5, 1E-7, 1E-10};

    S.setState(T, P, rhoGas, muGas, yGas, yPAH, Msoot, nsoot);
```

Boiler plate;
Collected soot header files
Namespace

Soot Chemistry, Coagulation Models

PSD model
QMOM, MONO, LOGN, MOMIC, SECT

State object
T, P, ρ, μ
y_i: H, H_2, O, O_2, OH, H_2O, CO, C_2H_4
y_{PAH}: $C_{10}H_8$, $C_{12}H_8$, $C_{12}H_{10}$, $C_{14}H_{10}$, $C_{16}H_{10}$, $C_{18}H_{10}$
Soot variables (M_k or $n_{i,section}$)

Code Interface

```
//---------- calculate source terms

SM.setSourceTerms(S);

//---------- Access soot source terms

double S0 = SM.sources.sootSources[0];
double S1 = SM.sources.sootSources[1];
double S2 = SM.sources.sootSources[2];
double S3 = SM.sources.sootSources[3];

//---------- Access gas source terms

double S_O2   = SM.sources.gasSources[(size_t)gasSp::O2];
double S_O    = SM.sources.gasSources[(size_t)gasSp::O];
double S_H2   = SM.sources.gasSources[(size_t)gasSp::H2];
double S_H    = SM.sources.gasSources[(size_t)gasSp::H];
double S_OH   = SM.sources.gasSources[(size_t)gasSp::OH];
double S_H2O  = SM.sources.gasSources[(size_t)gasSp::H2O];
double S_CO   = SM.sources.gasSources[(size_t)gasSp::CO];
double S_C2H2 = SM.sources.gasSources[(size_t)gasSp::C2H2];
double S_C6H6 = SM.sources.gasSources[(size_t)gasSp::C6H6];

//---------- Access PAH source terms

C10H8  = SM.sources.pahSources[(size_t)pahSp::C10H8];
C12H8  = SM.sources.pahSources[(size_t)pahSp::C12H8];
C12H10 = SM.sources.pahSources[(size_t)pahSp::C12H10];
C14H10 = SM.sources.pahSources[(size_t)pahSp::C14H10];
C16H10 = SM.sources.pahSources[(size_t)pahSp::C16H10];
C18H10 = SM.sources.pahSources[(size_t)pahSp::C18H10];
```

Set source terms, given State S

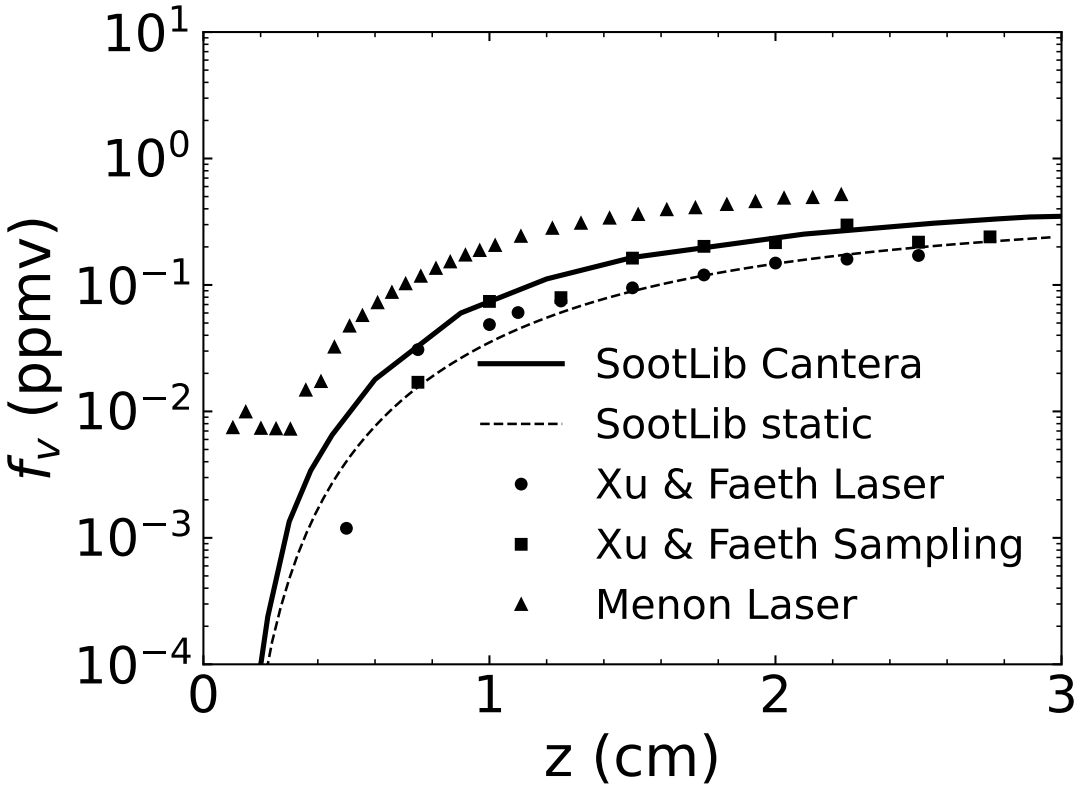
Source terms for soot, gas, PAH in sources object

Soot-gas source term coupling
Species access by name (enumeration)

PAH species organized separately

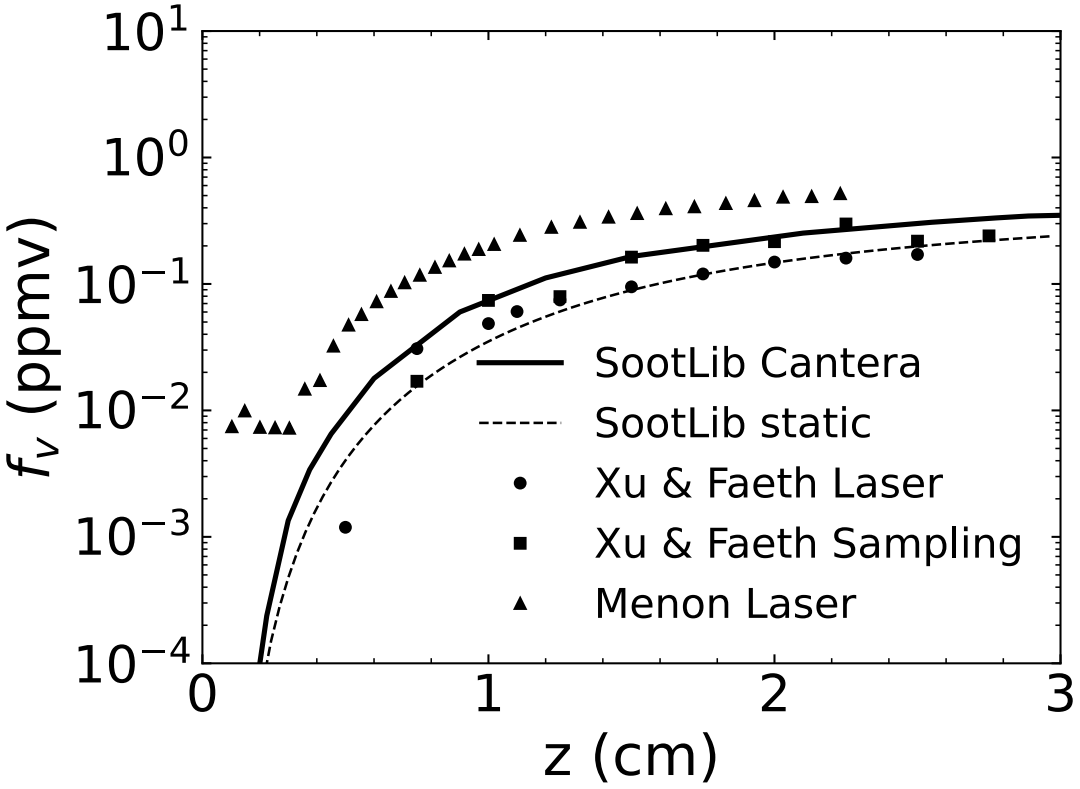
Example: Burner Flame

- Burner stabilized premixed flame
- ISF laminar premixed flame 2
  - C_2H_4-air
  - $\Phi = 2.34$
  - $v_0 = 6.73$ cm/s
- Integrate SootLib into Cantera
  - Modified `flamespeed.cpp`
  - Fixed T(z) profile, experimental
- Models
  - Gas chemistry: gri3.0
  - Nucleation: Lindstedt
  - Growth: Lindstedt
  - Oxidation: Leung
  - Coagulation: FM
  - PSD: Monodispersed

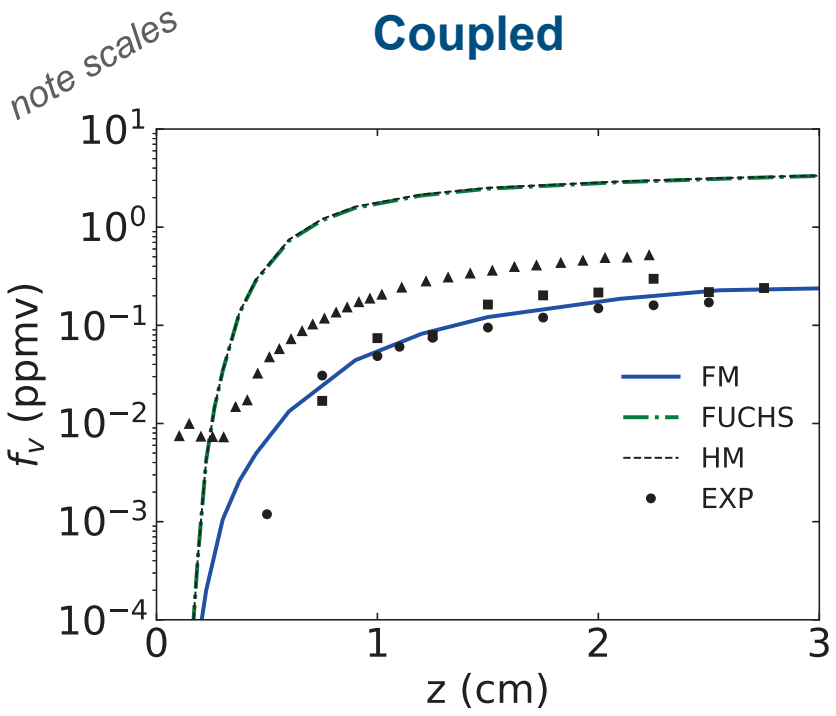


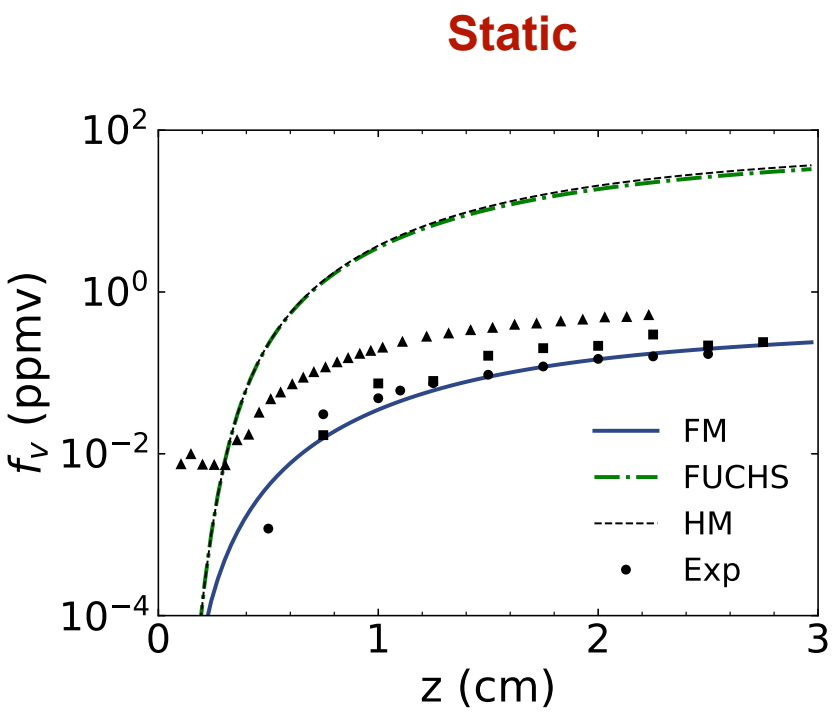
Example: Burner Flame

- Two cases
  - Coupled gas-soot in Cantera
  - Static calculation
- Static calculation
  - Evolves soot using fixed profiles from the (coupled) Cantera run
  - T, ρ, μ, v, y_i
  - $$\frac{d\hat{M}_k}{dz} = \frac{S_k}{\rho v}$$ $$\hat{M}_k = M_k/\rho$$
  - 2nd order integration
  - Included as a simple code example
- Reasonable agreement with the coupled simulation



Coagulation



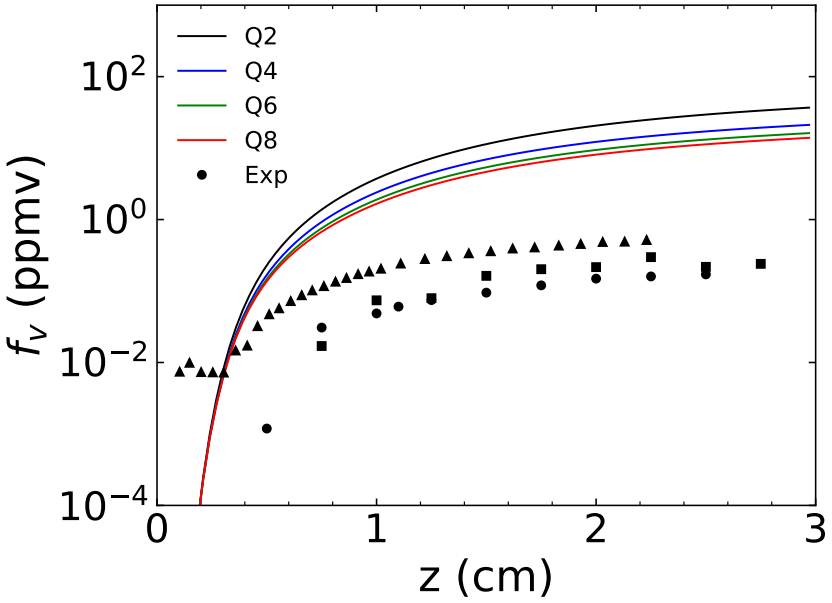


- Large variation with coagulation models used
- Only simple models considered here: Monodispersed, semiemperical chemistry
- HM and Fuchs give nearly identical results
- Lower FM f_v from fewer particles → lower surface area for growth
- Soot models should consider effects of all model components

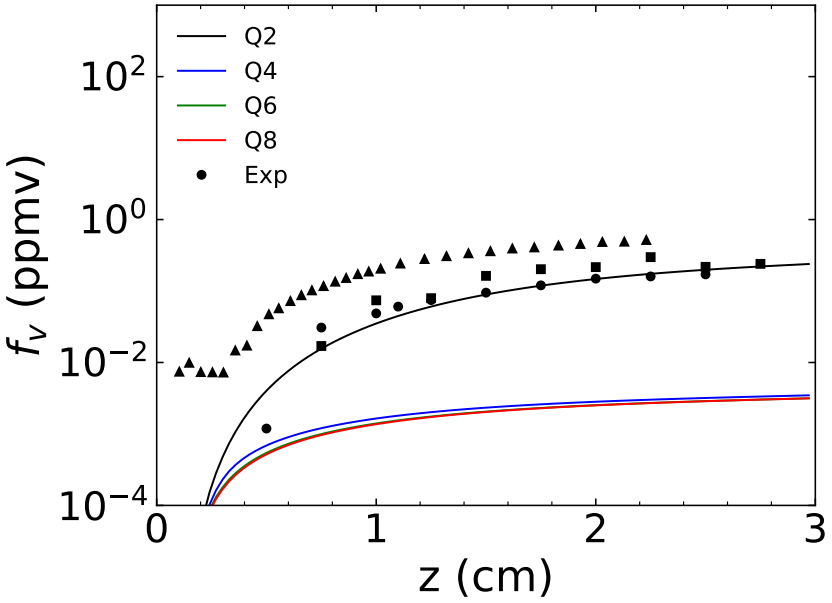
QMOM

Static

HM Coagulation



FM Coagulation

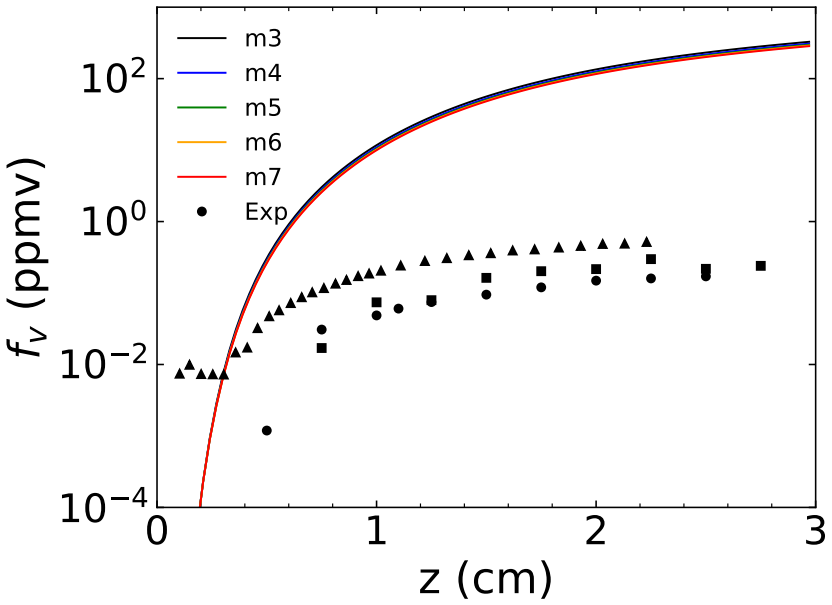


- QMOM shows convergence with increasing environments
  - Q2 has 2 moments, 1 quadrature node (equivalent to monodispersed)
  - Q4 has 4 moments, 2 quadrature nodes
  - Q6 has 6 moments, 3 quadrature nodes
  - Q8 has 8 moments, 4 quadrature nodes
- Q2 → Q8 at z=3 cm

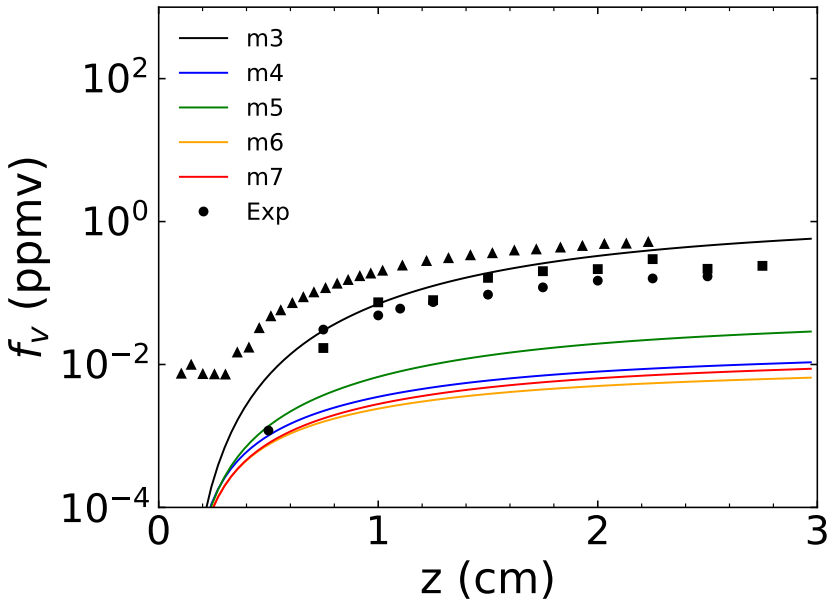
MOMIC

Static

HM Coagulation



FM Coagulation



- FM results show interleaving curves for even and odd number of moments as convergence is approached
- QMOM and MOMIC approach similar converged value for FM.
- MOMIC is higher for HM than QMOM, has less spread.
  - Application of HM is less clean in MOMIC than in QMOM since it is applied on the moment source not “pre-convolution”.
- QMOM is simpler, easier to code, and faster to run.

Github

https://github.com/**BYUignite/sootlib**