Development and Implementation of a Model for Predicting the Aerosolization of Agents in a Stack

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Outline

- Project Goals
  - Account for aerosol formation in EMIS scenarios
  - Implement results in atmospheric transport and dispersion and chemistry models
- The "Problem"
- Methodology
  - Aerosol formation algorithms
  - Model assumptions and limitations
  - Integration of STACK into EMIS
- Results
  - Model output
    - Example TEPO scenario
    - SLAM particulate results
- Model Sensitivity
  - Sensitivity Analysis
  - Physical property data
- Future Work

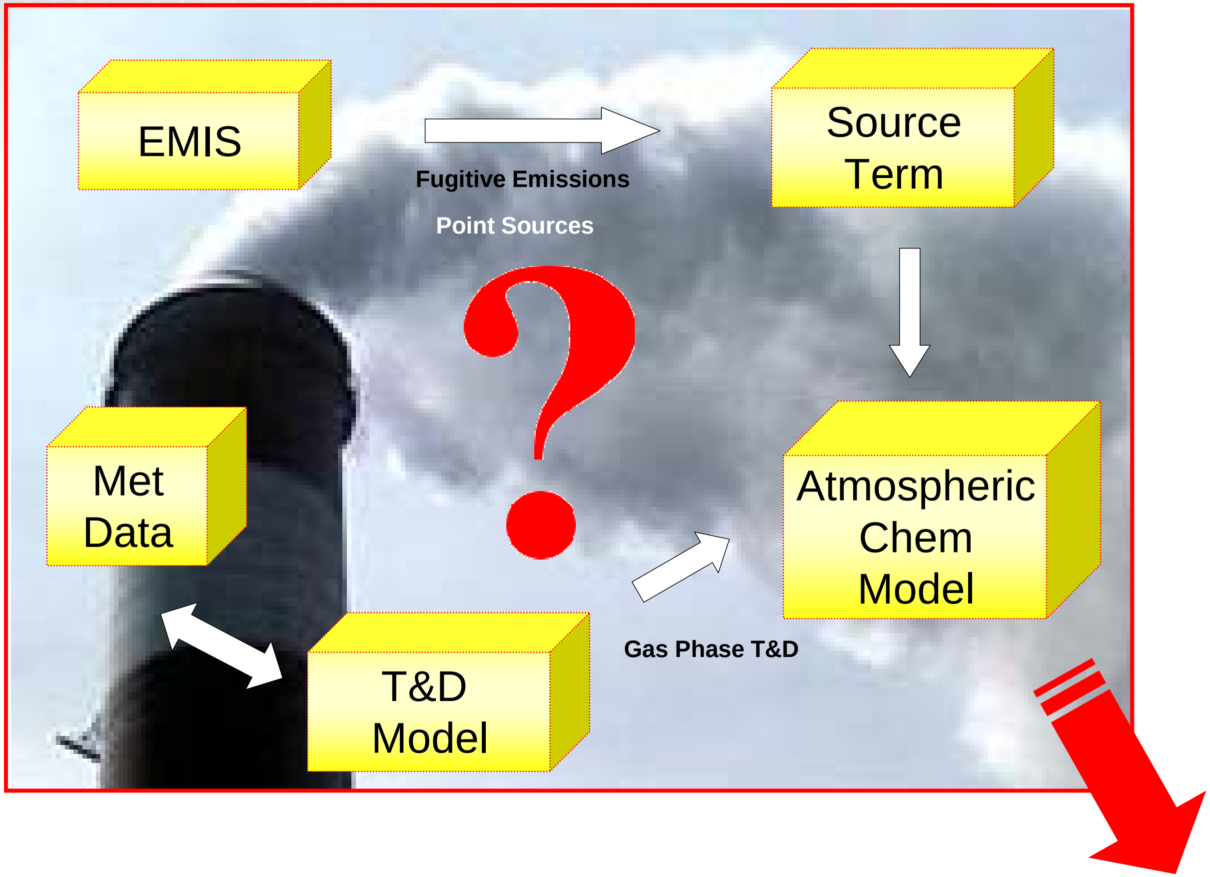
Project Goals

- **Adapt an aerosolization model**
  - Model must run rapidly
  - Code must be fairly "easy" to implement
  - Algorithms must handle streams with multiple components
  - Algorithm must be easily integrated with the EMIS (Emission Model for Industrial Sources) tool
  - Algorithm output must meet requirements for model input to AT&D (i.e., ChemCODE and SLAM)
- **Couple STACK model with EMIS**
- **Formulate output compatible with existing software suite**

The "Problem"

- Current model treats all emissions as gas phase
- Most OPs will condense to at least some extent at ambient conditions
- A TIC may condense at the stack and some may never even 'see' the transport and dispersion model!
- Result: overestimates downwind hazard prediction

The “Problem”



Downwind Hazard Prediction

Methodology: Governing Equations

$$\frac{\partial n_m}{\partial t} = r_A = -r_N - r_C$$

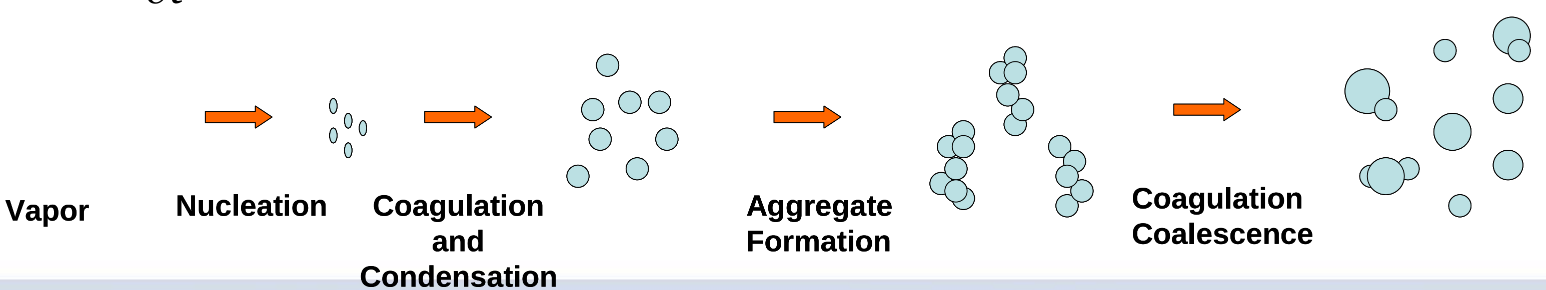
$$r_N = \frac{v_1}{\rho_g}\left[\frac{2\sigma}{\pi m_1}\right]^{\frac{1}{2}} n_{ms}^2 S \exp\left[\theta - \frac{4\theta^3}{27(\ln S)^2}\right] n^*$$

$$r_C = \left[n_m \rho_g \frac{u_m}{4} - n_{ms}\frac{u_m}{4}\right]\left[n_p \pi d_p^2\right] f(Kn)$$

$$r_F = 0.5\frac{\beta n_p{}^2 \rho_g}{W_s}$$

$$\frac{\partial n_p}{\partial t} = r_N - r_F$$

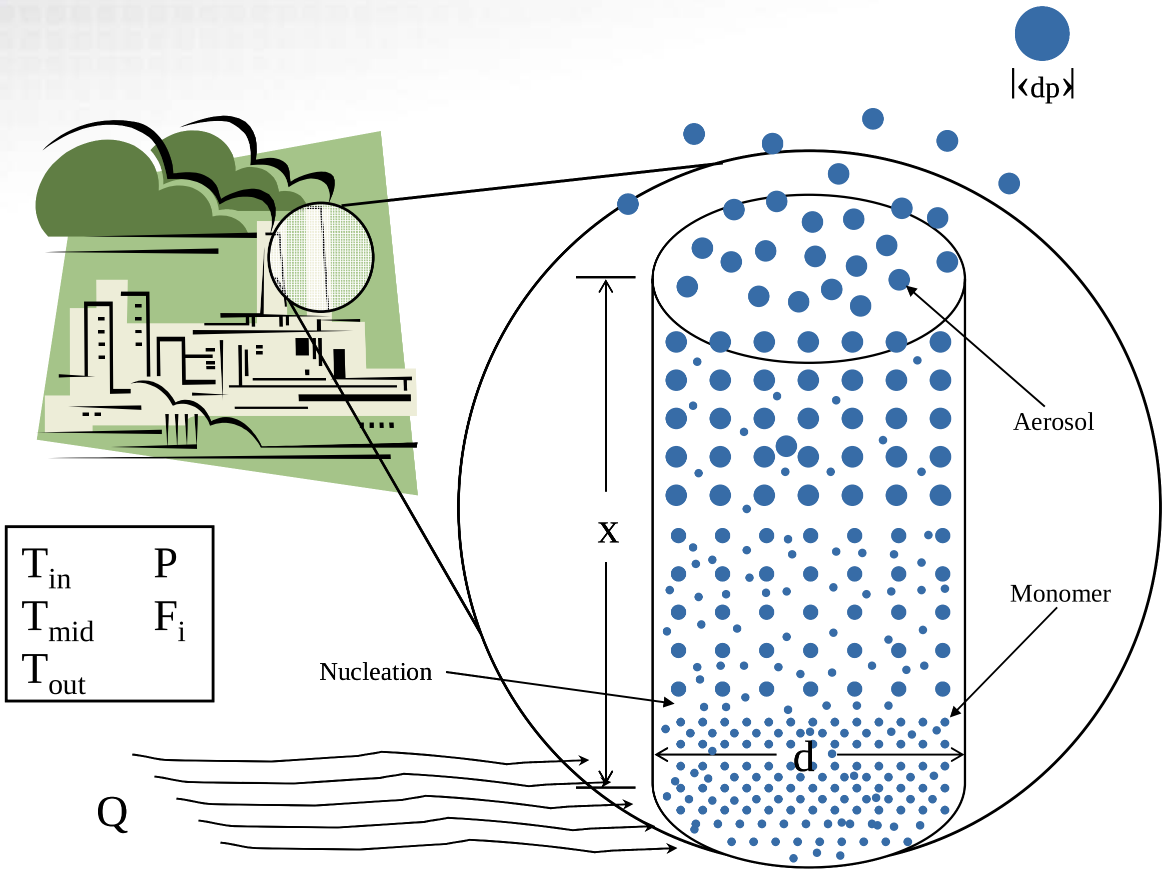
- Change in number of monomer molecules…rate of formation of particles of interest
- Nucleation = *f*(supersaturation ratio, surface tension, etc.)
- Critical nucleus size = point at which particles are stable (Gibbs)
- Coagulation = *f*(Knudsen, supersaturation ratio, flow regime)
- Flocculation = *f*(Number of particles, Knudsen)



Methodology:
Theoretical Model Assumptions/Limitations

- Single condensing component
- Ideal carrier density
- Neglects wall losses
- Produces an average particle diameter (monodisperse)
- Assumes no pair interaction potential between molecules during flocculation

The Stack Model



Methodology: Integration of STACK in EMIS

EMIS Output: process stream and thermodynamic information

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User selection of stack properties

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Physical properties sort and comparison

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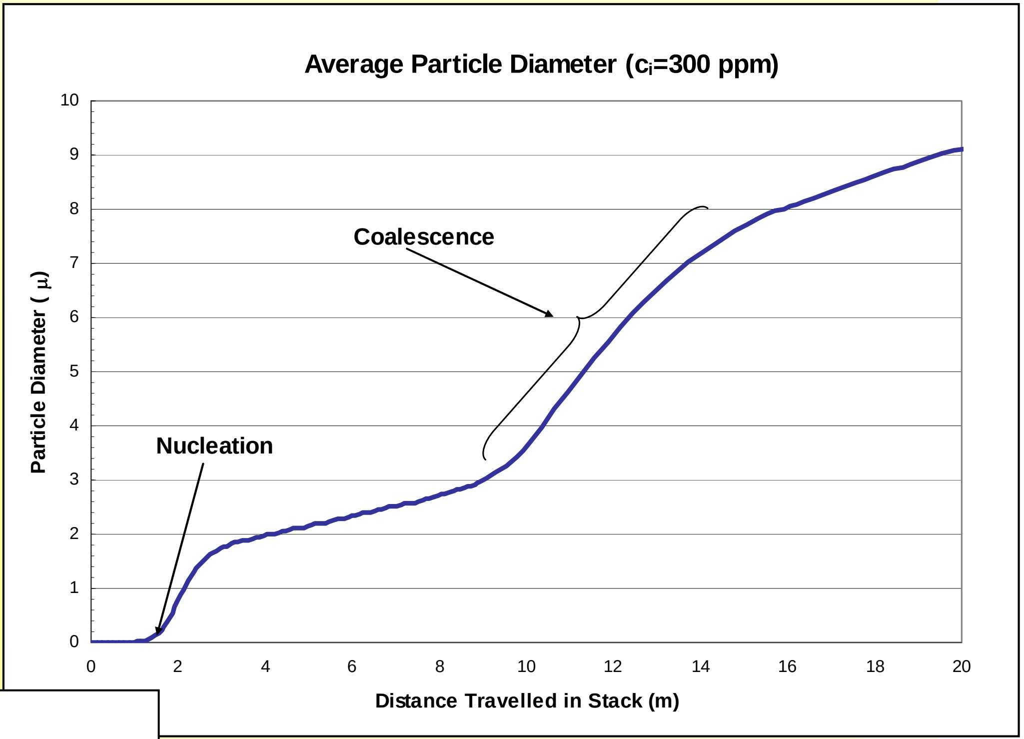
Compound for condensation is selected → **Physical property and stack data passed to STACK algorithm** → **LSODE run on model produces new n_m and d_p**

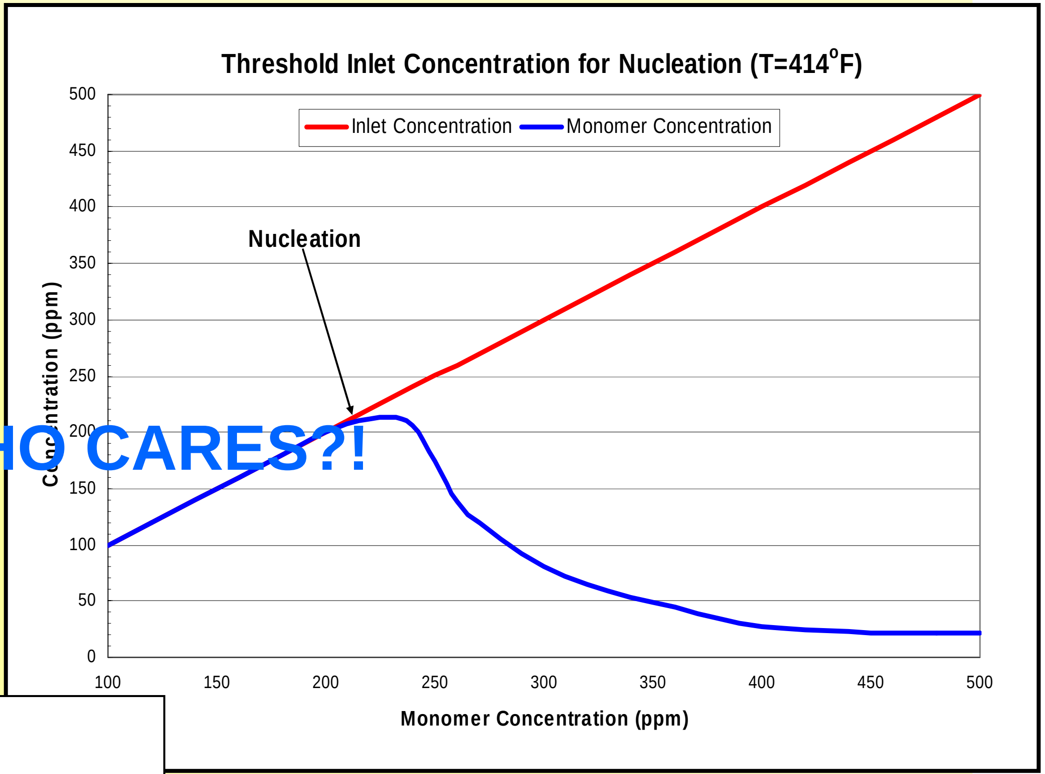
Results: TEPO Particle Size



Example: Parameters

- Compound: **TEPO (Triethyl Phosphate)**
- Carrier Gas: **Air**
- Boiling point: **419°F**
- Stack height: **20 m**
- Stack diameter: **0.3 m**
- Effluent Temperature: **404°F**
- Outlet Temperature: **350°F**

Results: Threshold Nucleation

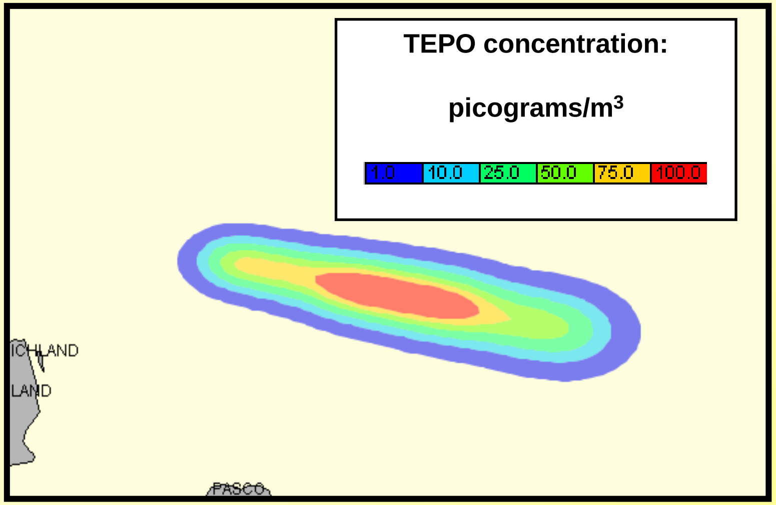


WHO CARES?!

Example: Parameters

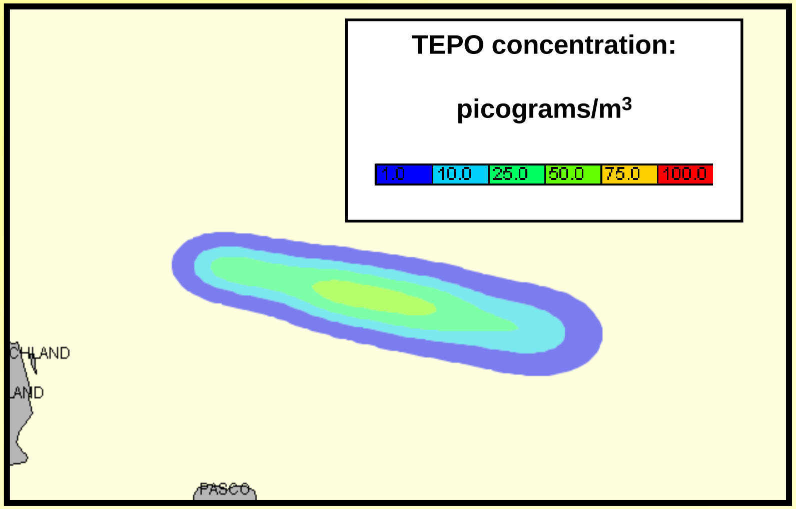
•Compound:	**TEPO (Triethyl Phosphate)**
•Carrier Gas:	**Air**
•Boiling point:	**419°F**
•Stack height:	**20 m**
•Stack diameter:	**0.3 m**
•Temperature:	**414°F**

Results: Example T&D Runs



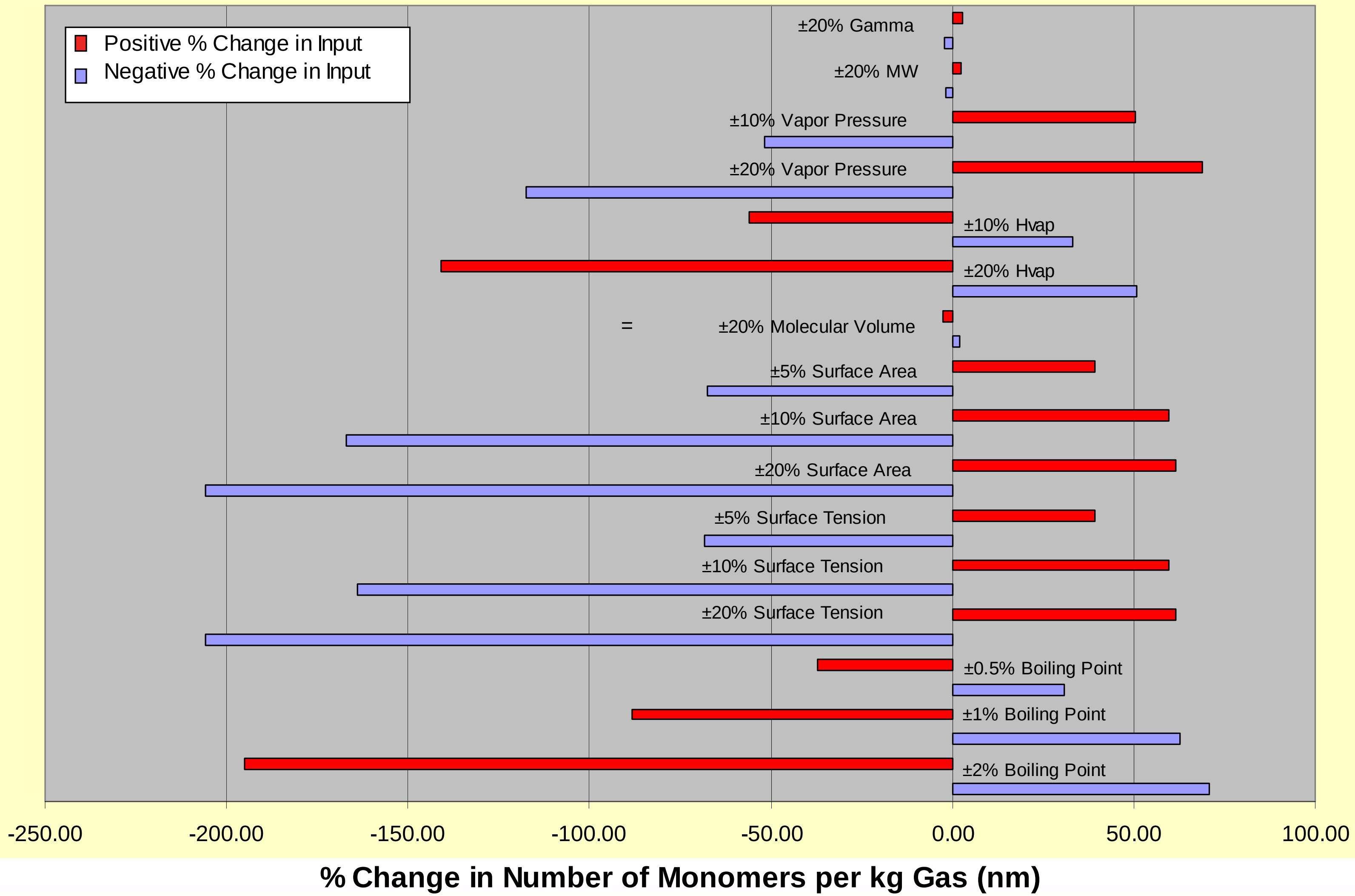
Gas Phase SLAM Run

Particulate (d_p= 5μm) SLAM Run

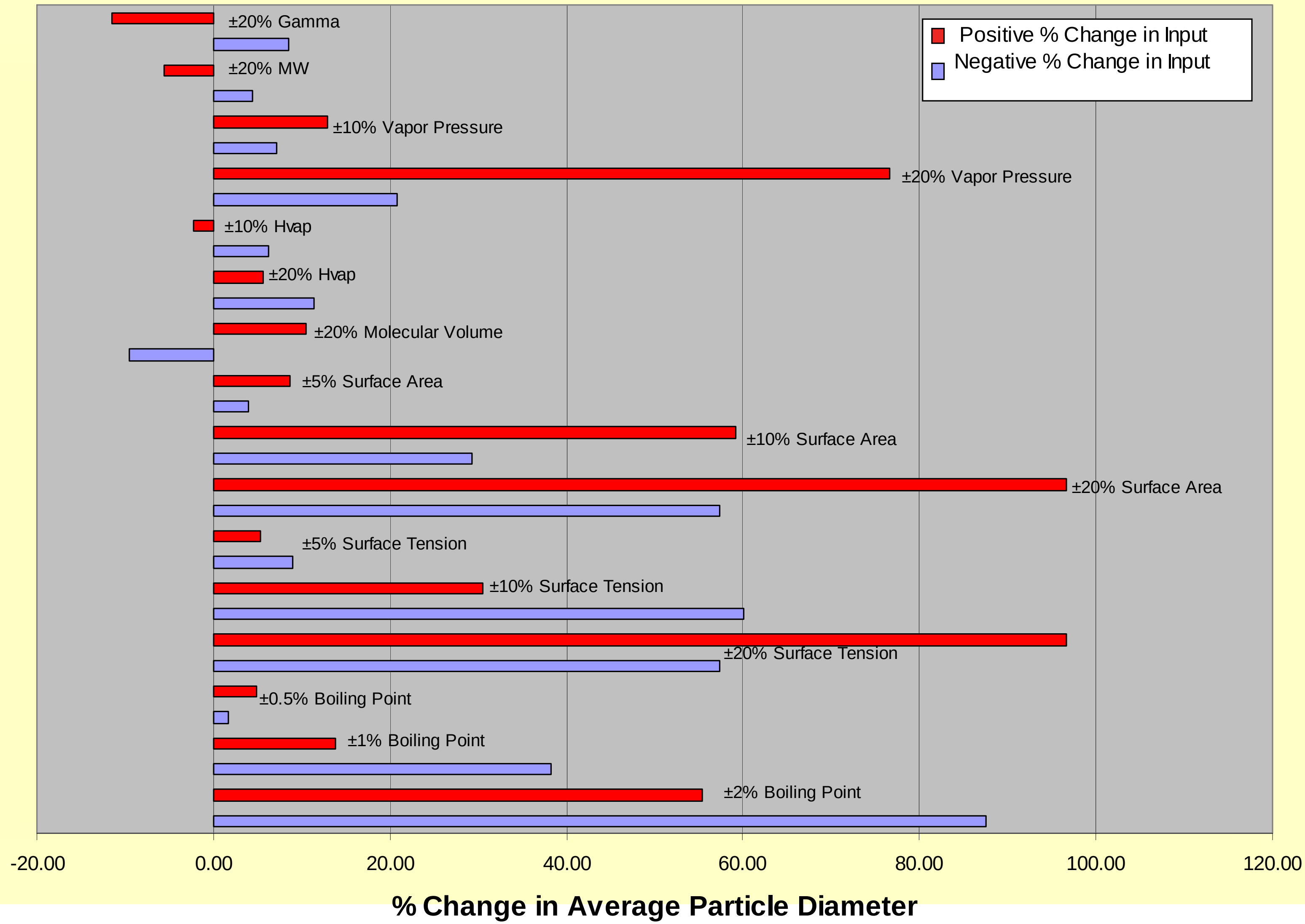


8 hour release starting at noon local time: 1 kg/hr

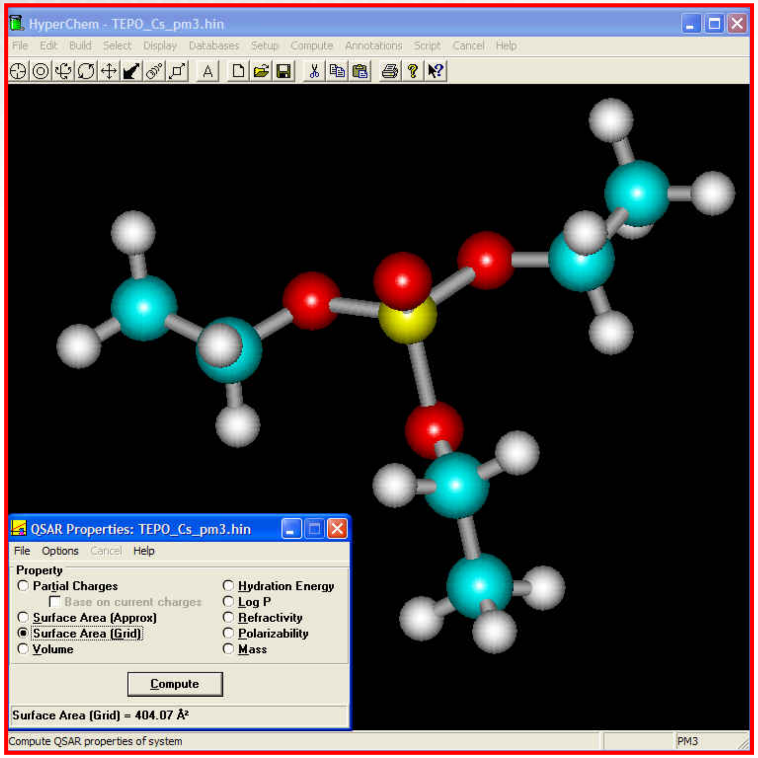
Model Sensitivity: Analysis, n_m



Model Sensitivity: Analysis, d_p

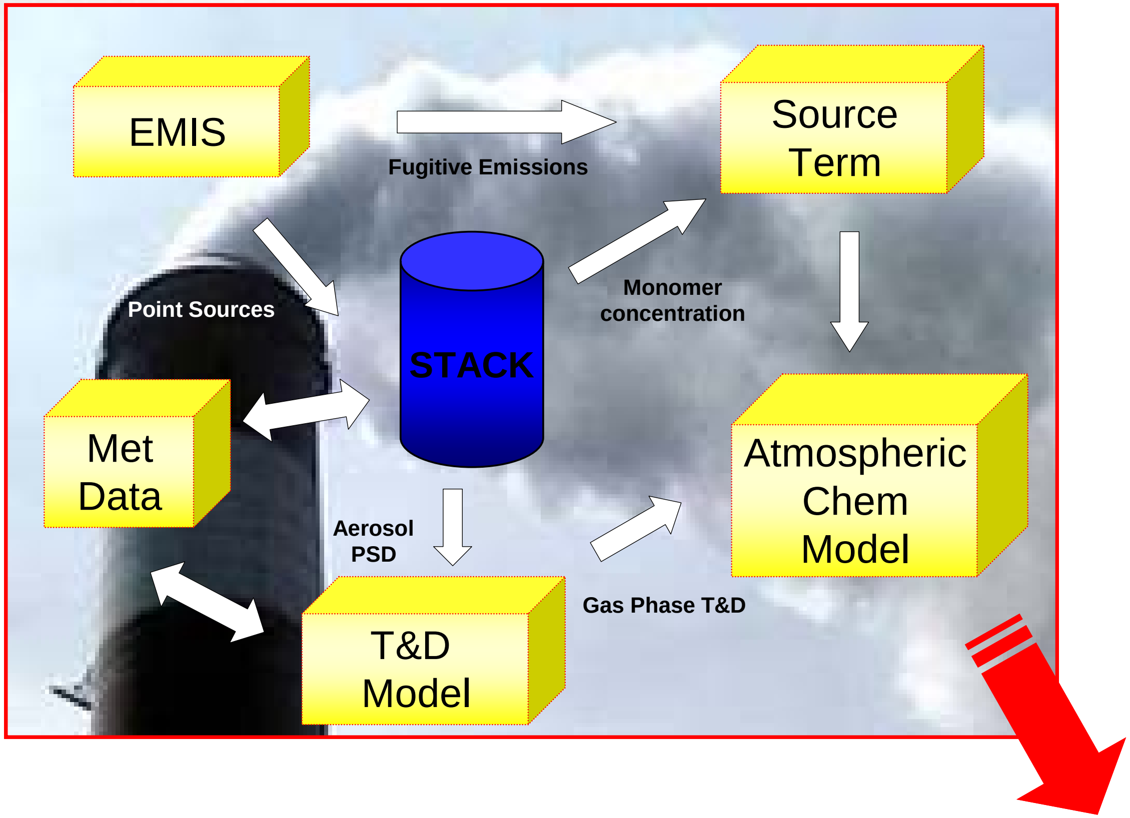


Model Sensitivity: Physical Property Estimation



- **Experimental and literature values**
- **ChemCAD physical property data and thermodynamic information**
- **Molecular surface area and volume estimated using molecular modeling tools (e.g. HyperChem, Gaussian)**
- **Physical property estimations (i.e., gamma from bulk stream viscosity)**
- **“SWAG”**

The Solution



Downwind Hazard Prediction

Future Work

- **Incorporate particle size distribution**
- **Improve handling of multicomponent effects**
- **Model verification and validation**
  - Literature
  - Field study data
  - Experimental data
- **Incorporate mixing effects outside the STACK**
  - Plume rise
  - CFD modeling

Questions?