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”

- EMIS
- Met Data
- T&D Model
- Source Term
- Atmospheric Chem Model
- Fugitive Emissions
- Downwind Hazard Prediction

Point Sources
Gas Phase T&D
Methodology: Governing Equations

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

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

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

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

\[
\frac{\partial n_p}{\partial t} = r_N - r_F\]

- 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

\[ \frac{d}{dp} \]

Monomer

Aerosol

\( T_{in} \quad P \)

\( T_{mid} \quad F_i \)

\( T_{out} \)

Nucleation

Q

x

d

\( \langle dp \rangle \)
Methodology: Integration of STACK in EMIS

EMIS Output: process stream and thermodynamic information

- User selection of stack properties
  - Physical properties sort and comparison
    - 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

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

WHO CARES?!
Results: Example T&D Runs

Gas Phase SLAM Run

Particulate \((d_p = 5 \mu m)\) SLAM Run

8 hour release starting at noon local time: 1 kg/hr
Model Sensitivity: Analysis, $n_m$

- ±20% Gamma
- ±20% MW
- ±10% Vapor Pressure
- ±20% Vapor Pressure
- ±10% Hvap
- ±20% Hvap
- ±20% Molecular Volume
- ±5% Surface Area
- ±10% Surface Area
- ±20% Surface Area
- ±5% Surface Tension
- ±10% Surface Tension
- ±20% Surface Tension
- ±0.5% Boiling Point
- ±1% Boiling Point
- ±2% Boiling Point

Positive % Change in Input
Negative % Change in Input

% Change in Number of Monomers per kg Gas ($n_m$)
Model Sensitivity: Analysis, $d_p$

- $\pm20\%$ Gamma
- $\pm20\%$ MW
- $\pm10\%$ Vapor Pressure
- $\pm20\%$沸点
- $\pm10\%$沸点
- $\pm20\%$沸点
- $\pm20\%$ Molecular Volume
- $\pm5\%$ Surface Area
- $\pm5\%$ Surface Tension
- $\pm10\%$ Surface Tension
- $\pm20\%$ Surface Tension
- $\pm0.5\%$ Boiling Point
- $\pm1\%$ Boiling Point
- $\pm2\%$ Boiling Point

% Change in Average Particle Diameter

- Positive % Change in Input
- Negative % Change in Input

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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

- **Point Sources**
- **Fugitive Emissions**
- **Gas Phase T&D**
- **Source Term**
- **Met Data**
- **STACK**
- **T&D Model**
- **Aerosol PSD**
- **Atmospheric Chem Model**

**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?