SCIPUFF Modelling of Dense Gas Dispersion

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DEFENSE THREAT REDUCTION AGENCY

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Approved for public release

SCIPUFF

- **S**econd-order **C**losure **I**ntegrated **PUFF**
- Lagrangian Gaussian puff dispersion model
- Uses second-order turbulence closure to relate diffusion rates to turbulent velocity statistics
- Also uses turbulence closure to predict concentration fluctuation variance in addition to mean concentration

SCIPUFF Buoyancy and Dynamics

- Density differences drive dynamic effects
- SCIPUFF carries velocities and temperature perturbations (from ambient) in each dynamic puff
  - Buoyancy only drives vertical velocity
- Any gas, or vapor, puff can be dynamic
- Buoyancy can be positive or negative
- SCIPUFF uses the Boussinesq approximation
  - Assumes relatively small temperature perturbations, <~ 100ºC
- Also assumes incompressibility
  - Velocities much smaller than speed of sound

Puff Variables

- Basic puff integral quantities are

$$\langle \theta_p \rangle, \langle \overline{u}_{ip} \rangle, \langle \overline{c\,\theta_p} \rangle, \langle \overline{c\,u_{ip}} \rangle, \langle \overline{c\,b_p} \rangle, \langle \overline{c}\,\overline{\theta}_p \rangle, \langle \overline{c}\,\overline{u}_{ip} \rangle, \langle \overline{c}\,\overline{b}_p \rangle$$

  where θ_p is the temperature perturbation, $u_{ip} = (u_p, v_p, w_p)$ is the velocity component perturbation, b is the puff material buoyancy, and c is concentration

  - Angle brackets denote spatial integral over the Gaussian puff
  - Overbar denotes ensemble averaging (turbulent fluctuations)
  - Buoyancy, b, is proportional to material density perturbation (from air) and the local concentration of the material, c

- SCIPUFF carries nonlinear integral quantities representing both the product of the mean quantities and the mean value of the product
  - This enables a description of the turbulent correlation between the two quantities

Puff Overlap Treatment

- SCIPUFF predicts the turbulence-driven variance of the concentration, and therefore needs to calculate overlap integrals for all the puffs
- The concentration-weighted mean quantities are overlap summations over all puffs to account for interactions, e.g.

$$\left\langle \overline{c}\,\overline{\theta}_p \right\rangle_\alpha = \sum_\beta \left\langle \overline{c} \right\rangle_\alpha \left\langle \overline{\theta}_p \right\rangle_\beta G_{\alpha\beta}$$

where α and β are puff indices, and $G_{\alpha\beta}$ is the integral of the product of the two Gaussian shape functions

- This allows dynamic puffs to dynamically move other materials, such as small particles or droplets

Buoyancy-driven Motion

- Conservation of momentum and temperature

$$\frac{d}{dt}\left\langle \overline{u}_{ip} \right\rangle = g_i \left(\frac{\left\langle \overline{\theta}_p \right\rangle}{T_0} - B_{gas} \frac{\langle c \rangle}{1+\hat{B}} \right)$$

$$\frac{d}{dt}\left\langle \overline{\theta}_p \right\rangle = -\frac{d\theta_{amb}}{dz}\left\langle \overline{w}_p \right\rangle$$

- The gas buoyancy is $B_{gas} = \frac{\rho_{gas} - \rho_0}{\rho_{gas}\rho_0}$ and $\hat{B}$ is a

  non-Boussinesq correction factor based on the effective overlap gas density, used to prevent accelerations exceeding the gravity value.

- g_i is the gravitational acceleration (vertical) and T_0 is the ambient temperature

Puff Velocities

- Puff dynamic velocities are obtained from the correlation integrals, e.g.

$$\frac{d}{dt}\left\langle \overline{w_p c} \right\rangle = \frac{g}{T_0}\left\langle \overline{\theta_p c} \right\rangle - \frac{g\left\langle \overline{b_p c} \right\rangle}{1+\hat{B}} - \frac{\left\langle \overline{w_p c} \right\rangle - \left\langle \overline{w}_p \overline{c} \right\rangle}{\tau_c}$$

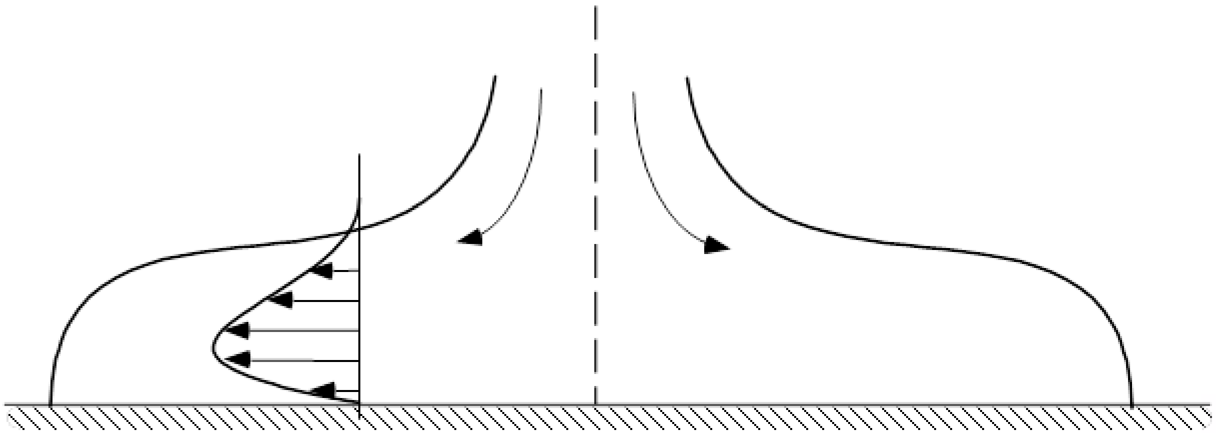
- The dynamic velocities are defined as $\hat{\boldsymbol{u}}_p = \dfrac{\left\langle \overline{\boldsymbol{u}_p c} \right\rangle}{\left\langle c \right\rangle}$

  and a dynamic entrainment velocity is defined by the perturbation velocities and Richardson number, and this defines a dynamic diffusivity, added to the ambient diffusion

- This defines the puff velocity perturbation in the absence of any ground interaction

Dense Gas Effects

- Negative vertical velocities occur due to cold temperatures or dense gases
- When the puff interacts with the ground surface, pressure forces generate lateral outward motion, i.e. slumping.



Dense Gas Flowfield

- We can show that the mean vertical velocity integral is equivalent to the vertical moment of vorticity

$$\left\langle w_p \right\rangle = \left\langle \boldsymbol{e}_3 \bullet \boldsymbol{x} \times \boldsymbol{\omega} \right\rangle$$

and this can be used to define a horizontal flowfield

$$u_X = U_0 \frac{X}{L_X} \frac{L_Y \sqrt{2}}{\sqrt{L_X^2 + L_Y^2}} \exp\left(-\frac{X^2}{L_X^2} - \frac{Y^2}{L_Y^2} \right); \qquad u_Y = U_0 \frac{Y}{L_Y} \frac{L_X \sqrt{2}}{\sqrt{L_X^2 + L_Y^2}} \exp\left(-\frac{X^2}{L_X^2} - \frac{Y^2}{L_Y^2} \right)$$

- Here, principal axes of the puff define the coordinates, and the length scales are related to the puff sigma's. The velocity scale is proportional to $\left\langle w_p \right\rangle$.

Dense Gas Velocity

- Forming the vertical moment of vorticity, we determine

$$U_0 = -\frac{\langle w_p \rangle}{\pi\sqrt{2}} \frac{\sqrt{L_X^2 + L_Y^2}}{L_X^2 \, L_Y^2}$$

which completes the definition of the horizontal flowfield

- Note that the dense gas flowfield is zero at the center of the puff, so the puff does not move itself.
- It does have velocity gradients, so it spreads laterally and slumps vertically
- It also moves and distorts other puffs in its neighborhood

Dense Gas on Terrain

- A dense gas on sloping terrain will move down the slope
- This effect is included using a simplified representation; use the component of the free-field vertical velocity resolved along the slope direction
- Thus

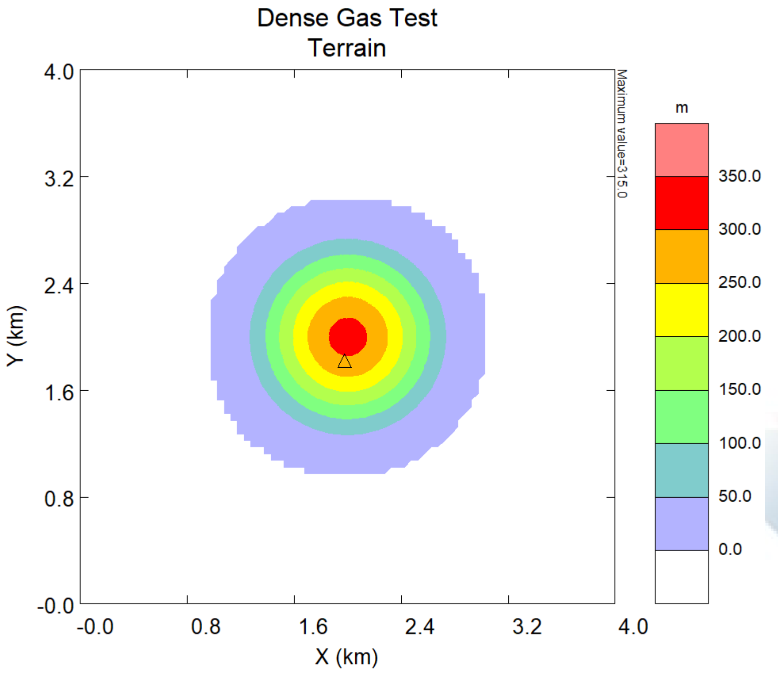
$$\hat{u}_{dense} = \frac{\left\langle \overline{w_p\, c} \right\rangle}{\left\langle c \right\rangle} \frac{h_x}{\sqrt{1+h_x^2}}; \quad \hat{v}_{dense} = \frac{\left\langle \overline{w_p\, c} \right\rangle}{\left\langle c \right\rangle} \frac{h_y}{\sqrt{1+h_y^2}}$$

Where h is terrain elevation, and h_x and h_y are the terrain slopes, i.e.

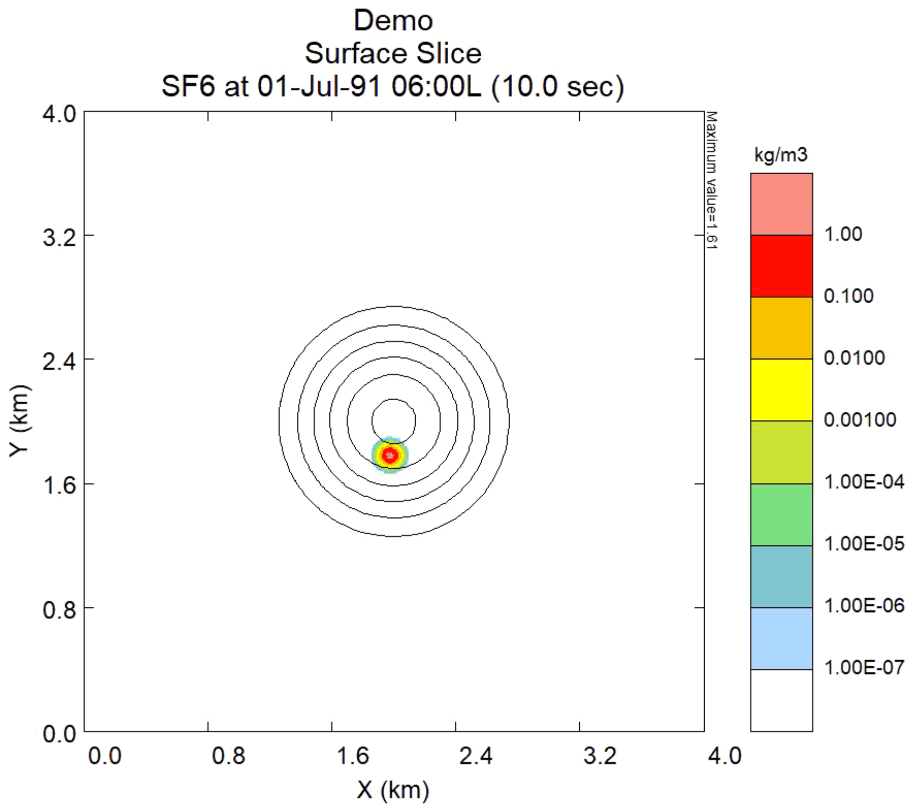
$$h_x = \frac{\partial h}{\partial x}; h_y = \frac{\partial h}{\partial y}$$

Idealized Test Case

- Circular hill, 300m high, no wind
- Instantaneous dense gas release
  - 5 times air density
  - 5m sigma
  - Surface release
  - Pure material



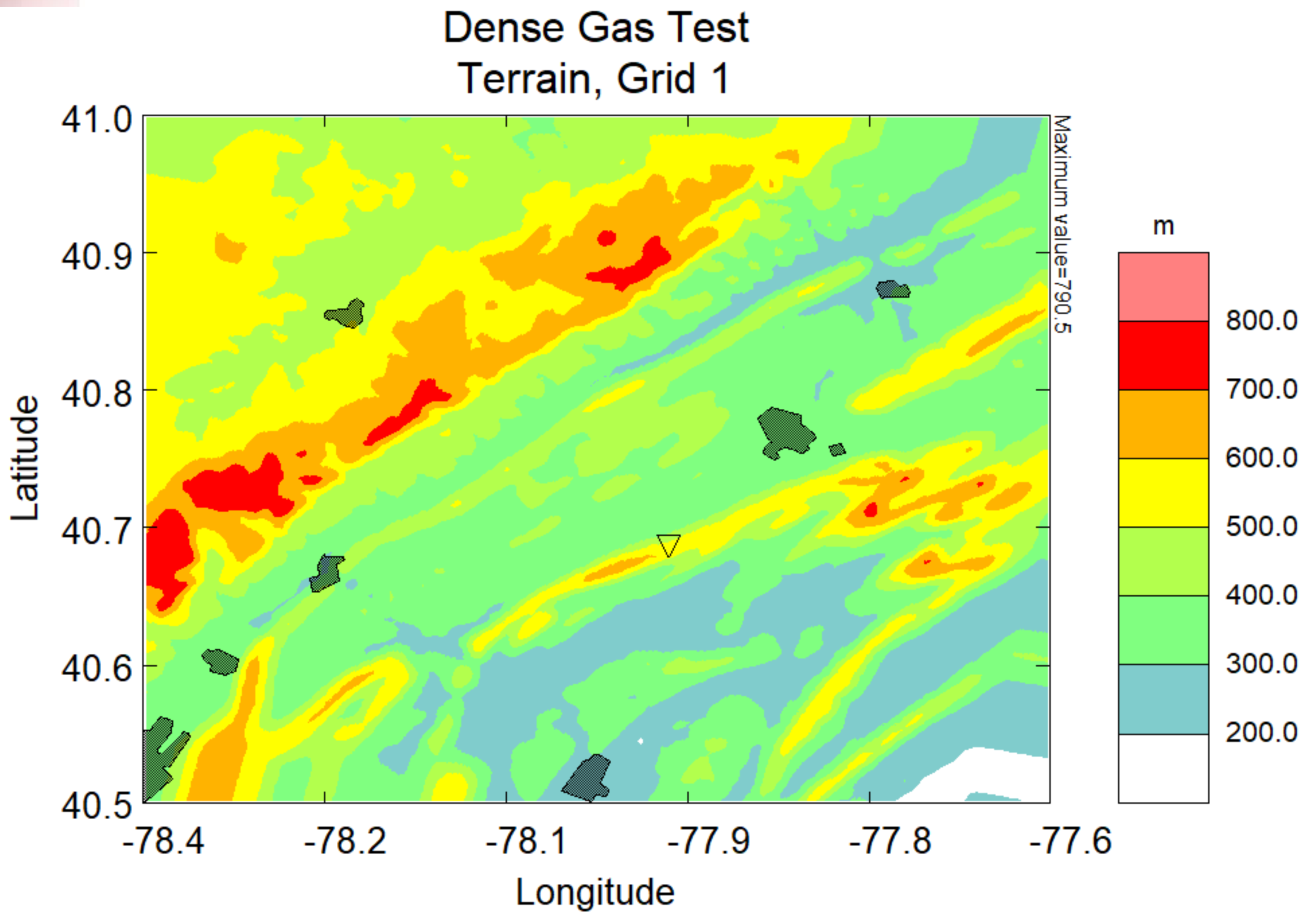
Idealized Test Case



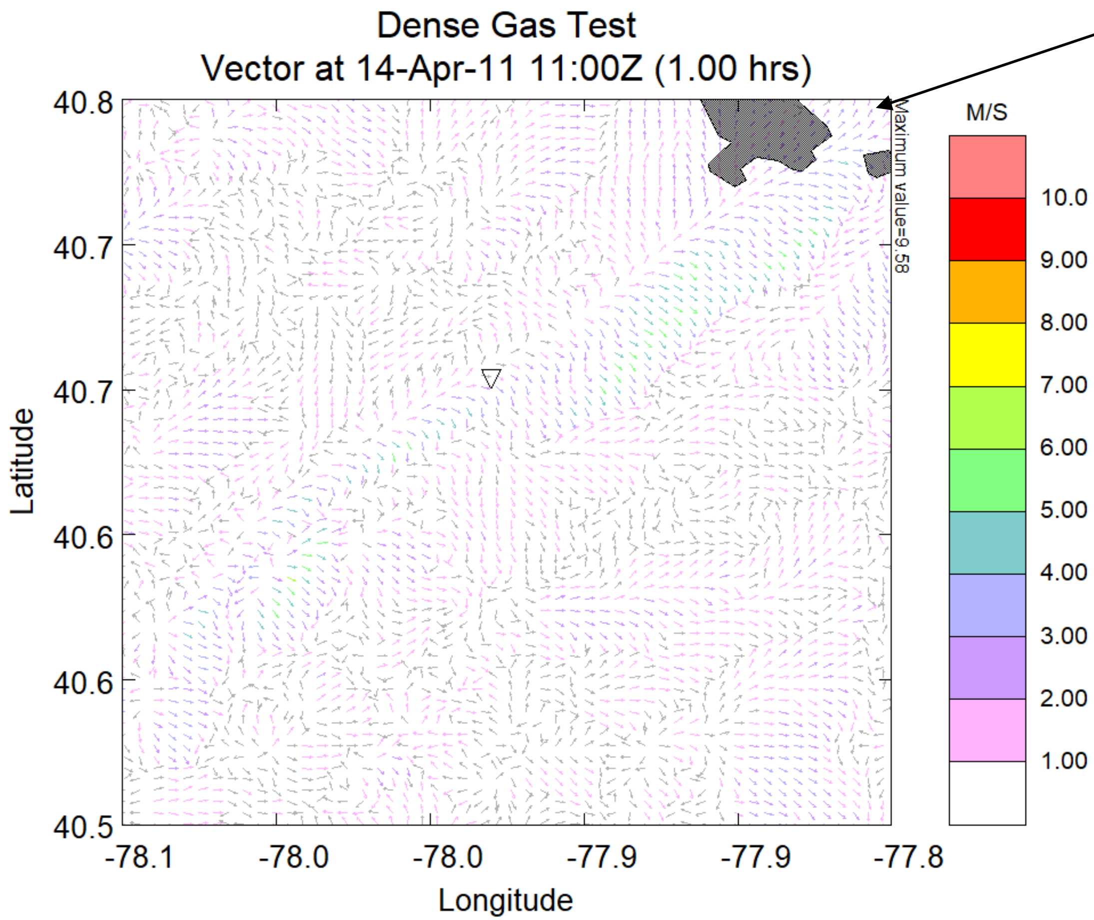
Real-world Example

- CO_2 release
  - 1000kg/min for 12min
- High resolution stable boundary layer meteorology from Penn State Univ
- Note that dense gas effects are most significant under light wind conditions
- High winds rapidly dilute the concentration and eliminate dynamic effects

Real-world terrain



Real-world 10m velocity field

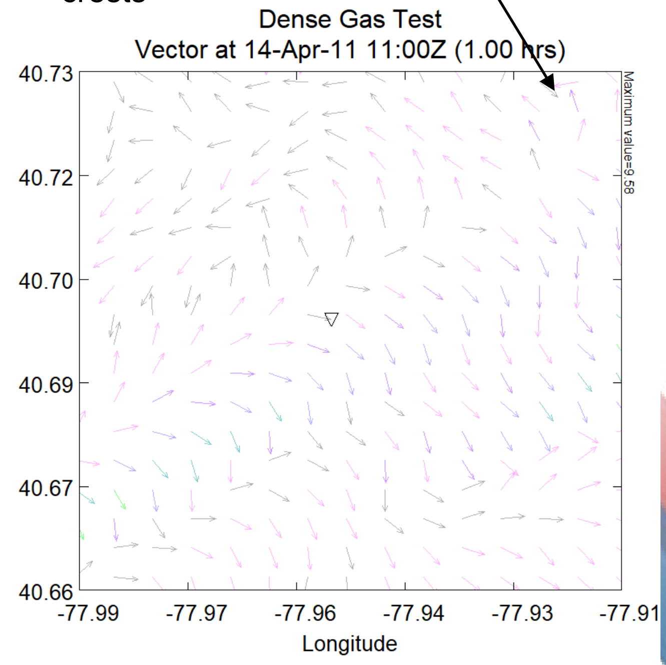


300m area near source

80m zoomed area

Note that 10m wind speed
Is roughly 2-3m/s near the source

Faster speeds over ridge crests



Dense Gas Dosage – 80m domain

Color shading is CO_2, black contours are for same release of a passive trace