CFD Simulations of H₂S-Rich Plumes from Oil/Gas Well Blowouts

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October 16, 2014

sandia.gov and noaa.gov
Oil and gas wells under high pressure can inadvertently “blowout” and release significant quantities of oil and gas. Gas in some formations contains as much as 90% H₂S. Blowout releases typically self-ignite or are intentionally ignited. If not ignited, releases can behave as dense gases, and dangerous (toxic or lethal) H₂S concentrations persist for considerable distance.
Setting

• Client involved in oil/gas well exploration in very rugged terrain
• Closest inhabitants a few km distant
• Goal: Design Emergency Response Planning Procedures to protect local populations
• Information uncertain
  – Reservoir characteristics
  – Meteorological data
Available Models and Tools

- U.S. EPA Appendix W Modeling Guidance offers no *recommended* models for dense gas dispersion
- Alternative Models listed on EPA’s Support Center for Regulatory Atmospheric Modeling (SCRAM) website list ADAM, DEGADIS, HGSYSTEM, PANEPR (PANACHE), and SLAB as candidate dense gas dispersion models
- Other options: ALOHA, ERCBH2S, and PHAST
- Of these candidates, only PANEPR is designed for application in complex terrain, and it was selected for this application
PANEPR Model

- Licensed by fluidyn
- Based on computational fluid dynamics (CFD)
  - Not a traditional Gaussian plume/puff approach
  - Solves basic mass, momentum, and energy equations using finite element discretization of a three-dimensional grid
  - Turbulence modeled based on fluid dynamics
- Considerable flexibility, numerous options
Source Modeling

• Based on representative reservoir properties, anticipated production rate, and gas-to-oil ratio (GOR)

• Simplified source parameterization
  – Interest focused on far-field predictions
  – Assume flashing evaporates oil-phase to produce a dense gas mixture
  – Mix the release into an elevated volume source

• Release properties
  – 0.28 kg/s H$_2$S emission rate (12.1% H$_2$S mixture)
  – 144 g/mol average molecular weight
  – Source concentration ~750 ppm (within volume source)
Model Options

- Computational grid
  - Unstructured grid resolved in source region
  - 62 vertical layers (2000 m), 4616 cells per layer (~3 km × 4.5 km)
- Inflow boundary condition at upwind domain edge
- $\kappa-\epsilon$ turbulence model
- Meteorological conditions
  - Specified through surface heat flux and vertical temperature gradient
  - Two simulations
    - Pasquill-Gifford Class D, 10-m wind speed 2 m/s
    - Pasquill-Gifford Class E/F, 10-m wind speed 1 m/s
Topography and Computational Grid

- Source
- Receptor

Wind

~4 km
<table>
<thead>
<tr>
<th>$H_2S$ Concentration (ppm)</th>
<th>Toxicity Guidelines</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ACGIH’s recently revised 8-hour Threshold Limit Value (TLV)</td>
</tr>
<tr>
<td></td>
<td>NRC’s 90-day Emergency Exposure Guidance Level (EEGL)</td>
</tr>
<tr>
<td></td>
<td>NRC’s 24-hour EEGL</td>
</tr>
<tr>
<td></td>
<td>NIOSH’s 10-minute Recommended Exposure Limit (REL)</td>
</tr>
<tr>
<td>1</td>
<td>ACGIH’s former 8-hour TLV</td>
</tr>
<tr>
<td></td>
<td>NRC’s 24-hour EEGL</td>
</tr>
<tr>
<td></td>
<td>NIOSH’s 10-minute Recommended Exposure Limit (REL)</td>
</tr>
<tr>
<td>10</td>
<td>AIHA Emergency Response Planning Guideline (ERPG-3)</td>
</tr>
<tr>
<td></td>
<td>&lt;1 hour exposure not life threatening for most people</td>
</tr>
<tr>
<td>100</td>
<td>NIOSH Immediately Dangerous To Life or Health (IDLH)</td>
</tr>
</tbody>
</table>

$H_2S$ Odor Threshold $\sim 0.001$ ppm
Steady State Plume (Simulation time 2 hours)
Stable (E/F) case, 1 m/s wind speed

- Ground-level plan view (left) and centerline vertical cross-section (right)
- Some influence of terrain on wind field
- Some influence of buoyancy in near field
Example Results (GIS Version)

- Class D simulation
<table>
<thead>
<tr>
<th>Scenario</th>
<th>Maximum Concentration (ppm)</th>
<th>Downwind extent of H₂S concentration (km) at end of simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stable (Class E/F) 1 m/s wind</td>
<td>790</td>
<td>0.35              2.1               3.3               &gt; 4</td>
</tr>
<tr>
<td>Neutrally stable (Class D) 2 m/s wind</td>
<td>202</td>
<td>0.2               0.7               1.2               2.1</td>
</tr>
</tbody>
</table>
**ALOHA Model Predictions**

Similar source parameters

- User-defined chemical with thresholds adjusted to match 100, 10, and 1 ppm H$_2$S levels
- Simulation at left matches stable (Class E), 1 m/s wind speed
## Comparison of PANEPR and ALOHA Models

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Model</th>
<th>100 ppm</th>
<th>10 ppm</th>
<th>1 ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Downwind extent of H_2S concentration (km)</td>
<td></td>
<td></td>
<td></td>
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<td>Stable (Class E/F)</td>
<td>PANEPR</td>
<td>0.35</td>
<td>2.1</td>
<td>&gt; 4</td>
</tr>
<tr>
<td>1 m/s wind</td>
<td>ALOHA</td>
<td>0.46-0.53</td>
<td>1.5-1.7</td>
<td>5.7-6.2</td>
</tr>
<tr>
<td>Neutrally stable</td>
<td>PANEPR</td>
<td>0.2</td>
<td>0.7</td>
<td>2.1</td>
</tr>
<tr>
<td>(Class D) 2 m/s wind</td>
<td>ALOHA</td>
<td>0.28</td>
<td>1.1</td>
<td>4.6</td>
</tr>
</tbody>
</table>
Blowout Parameterization – Larger Source
Minor effects on far field plume (left)
Source size affects peak near-field concentrations (right)

(10 m$^3$) source, peak ground-level $[\text{H}_2\text{S}] = 1,360$ ppm
Blowout Parameterization – Smaller Source

Minor effects on far field plume (left)
Source size affects peak near-field concentrations (right)

(2.5 m)$^3$ source, peak ground-level $[H_2S] = 3,250$ ppm
Effects of Terrain
Side-by-side comparison, with (left) and without (right) terrain

Predicted $[\text{H}_2\text{S}]$ in ppm at 1-hr mark

Peak Values
135 ppm <= left
337 ppm right =>
Conclusions and Observations

• PANER is able simulate plume dispersion to significant distances (several km) in very rough terrain
  – Accounts for highly varying terrain
  – Considers dense gas effects
  – Some evidence of terrain-induced dispersion and gravity channeling effects

• Predictions similar to those of the simple ALOHA model (based on preliminary comparisons)

• Uncertainties to consider
  – Source modeling
  – Grid resolution and boundary condition effects
  – Atmospheric boundary layer characterization
Thanks …

• for your attention – and attending the final session!

Questions or Comments?