Atmospheric Gas Dispersion Simulator

Technical Operating Manual & Safety Compliance Guide (v10.13)

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1. Executive Summary & Life-Saving Mission

The **QHSE Atmospheric Gas Dispersion Simulator** is an advanced spatial risk assessment and toxic plume modeling engine designed for high-hazard industrial environments, upstream well operations, refineries, and chemical processing facilities. This platform moves beyond basic screening models by simulating real-world, safety-critical rigorous physics. Its fundamental goal is to save lives, prevent community disasters, and enforce compliance with international process safety and hazard management regulations.

Key Operational Strengths:

- **Eliminates False Assumptions:** The engine models realistic atmospheric boundary layers, high-velocity jet dynamics, dense gas slumping, and surface roughness to accurately predict the toxic envelope's true footprint.
- **Protects Critical On-Site Personnel:** Real-time spatial geofencing calculations determine whether control rooms, muster stations, or plant exit gates fall within Immediately Dangerous to Life or Health (IDLH) or Short-Term Exposure Limit (STEL) boundaries.
- **Prevents Off-Site Community Disasters:** By simulating physical touchdown distances, emergency planners can trigger early off-site notifications, municipal coordinate alerts, and crosswind evacuation pathways for neighboring communities.
- **Enforces Scientific PPE Selection:** Generates dynamic, site-specific Emergency Response Action Plans (ERAP) that establish proper respiratory protections, chemical suit classifications, and ignition-isolation protocols.
- **Custom Site Layout Overlays:** Allows users to upload and precisely scale/rotate approved facility blueprints (JPG/PNG) directly onto the map to visualize hazards over internal plant infrastructure.
- **360° Worst-Case Threat Zones:** Computes omnidirectional hazard envelopes to account for variable wind shifts and absolute worst-case scenario planning.
- **Explosion & Thermal Blast Profiling:** Calculates Vapor Cloud Explosion (VCE) and Boiling Liquid Expanding Vapor Explosion (BLEVE) blast overpressure zones for ignited flammable releases.

2. Operational Workflow Pipeline

Before launching any simulation, safety engineers must follow a strict three-phase operational workflow. This pipeline ensures that geographical, meteorological, and chemical variables are correctly aligned before calculations begin. The system executes setup parameters sequentially as illustrated below:

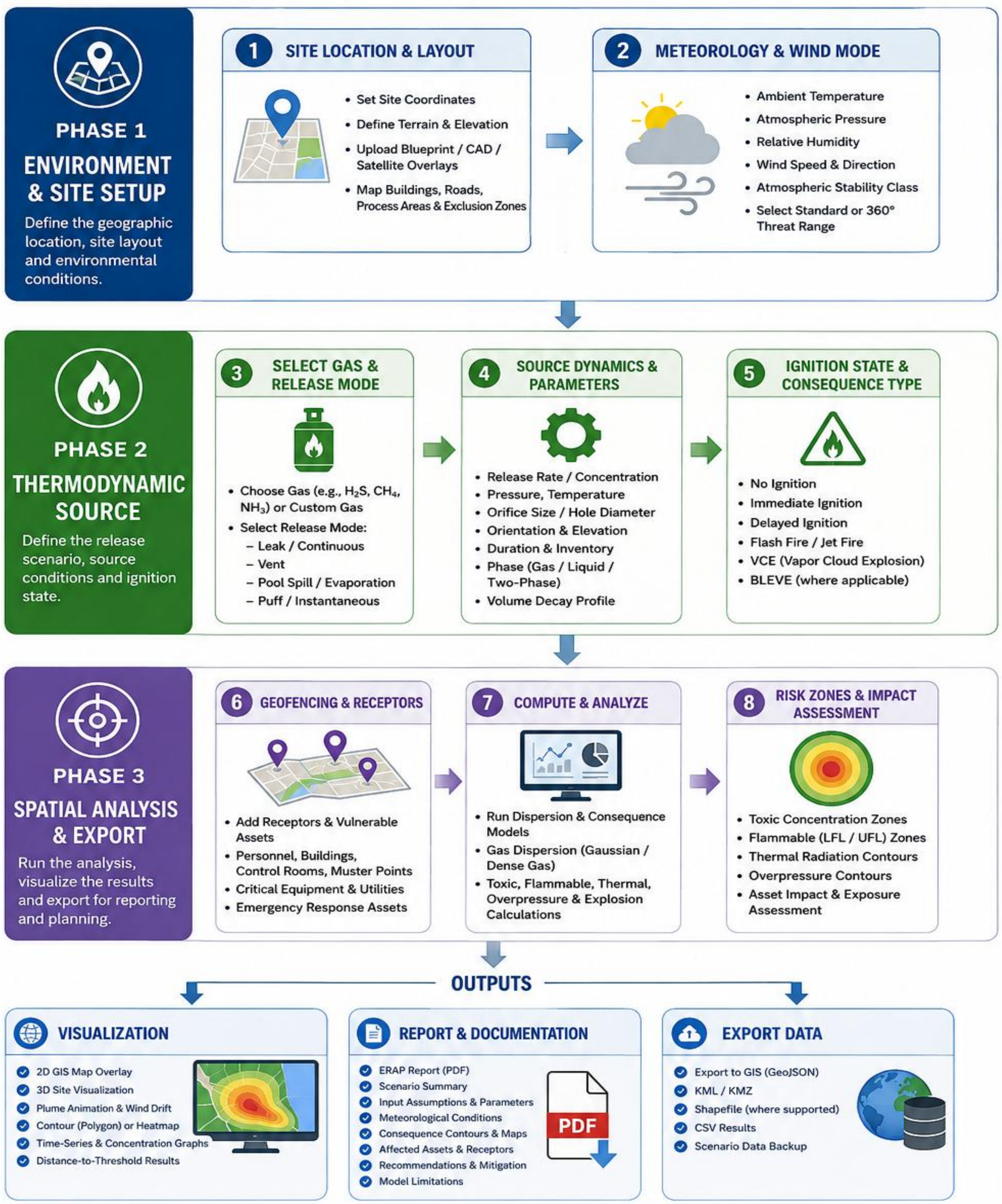

Figure 1.0: Sequential 3-Phase Simulation & Analysis Pipeline

3. Mathematical Foundations & Industry Benchmarks

The calculation core operates in full compliance with international chemical hazard and process safety benchmarks (EPA ALOHA, API 521, and NIOSH standards). Below are the four mathematical cornerstones used to determine toxic transport and concentration limits:

3.1. Ground-Level Gaussian Dispersion Equation

For a continuous atmospheric release under steady-state conditions, including ground reflection and effective emission height (*H*), the downwind ground-level concentration at coordinates (*x, y, 0*) is calculated as:

$$C(x,y,0) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{H^2}{2\sigma_z^2}\right)$$

Where: Q = source release rate (g/s); u = wind speed at release height (m/s); σy, σz = crosswind and vertical dispersion coefficients (m) as functions of downwind distance x.

3.2. Thermodynamic Sonic Choked Flow (API 521)

When upstream pressure exceeds the critical pressure ratio threshold, the gas reaches sonic velocity at the breach orifice. The maximum choked mass release rate (*m*choked) and toxic source release rate (Q) are modeled according to standard thermodynamic gas expansions:

$$\dot{m}_{choked} = C_d A P_{abs} \sqrt{\frac{\gamma M}{R T_k} \left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma+1}{\gamma-1}}}$$

$$Q = \dot{m}_{choked} \cdot \chi_{toxic}$$

Where: Cd = coefficient of discharge; A = hole cross-section area (m²); Pabs = absolute upstream pressure (Pa); γ = specific heat ratio; M = gas molecular weight (kg/mol); R = universal gas constant (8.314 J/mol·K); Tk = upstream temperature (K); χtoxic = molar purity fraction of target toxic chemical.

3.3. Plume Rise & Momentum Jet Rise (Briggs Formulation)

For high-velocity vertical discharges, physical momentum forces the chemical cloud upward, raising its effective release height before vertical dispersion dominates:

$$\Delta h = 3 \cdot d \cdot \left(\frac{v_e}{u}\right)$$

Where: Δh = momentum plume rise (m); d = orifice diameter (m); ve = exit velocity (m/s); u = ambient wind speed (m/s); hstack = physical stack height (m); H = resulting effective release height.

3.4. Heavy Gas Density Slumping Modifier

Gases with molecular weights greater than standard air (*M* > 28.97 g/mol) resist vertical mixing, causing them to slump and spread wider along the terrain surface. The dispersion coefficients are modified as follows:

$$\sigma_{y,dense} = \sigma_y \cdot \sqrt{\frac{M_{gas}}{M_{air}}}, \quad \sigma_{z,dense} = \frac{\sigma_z}{\sqrt{\frac{M_{gas}}{M_{air}}}}$$

Where: Mgas = molecular weight of modeled substance; Mair = molecular weight of dry air (approx. 28.97 g/mol).

3.5. Thermal & Explosion Radius (BLEVE/VCE)

For flammable gas releases where ignition is present, the simulator calculates the thermal and blast overpressure radius using a TNT equivalence and radiation approximation based on the total mass of the chemical. The exclusion zone radius is calculated as:

$$R = 3.5 \cdot M^{0.333}$$

Where: R = Explosion / Radiant Heat Zone radius (m) and M = Total vessel volume/mass (kg).

4. Step-by-Step Configuration Guide

Users are required to configure two primary software modules within the plugin before running the dispersion model:

Module A: Meteorological & Atmospheric Interface

1. Pasquill-Gifford Stability Class Selection:

- **Class A–C (Unstable):** Applies to bright daytime sun. Strong thermal convective mixing occurs; toxic plumes disperse very rapidly but have highly volatile concentrations close to the source.
- **Class D (Neutral Baseline):** Recommended standard industrial default. Represents high wind speeds or heavy overcast skies.
- **Class E–F (Highly Stable):** Typical of clear, cold nights. Minimal mechanical and thermal mixing. Toxic, high-density clouds glide extensive distances with very low dilution, representing the worst-case scenario.

2. Terrain Surface Roughness Height (z0):

- **Open Rural (z0 ≈ 0.1 m):** Flat grasslands or agricultural zones; creates standard surface friction.
- **Urban / Complex Industrial (z0 ≈ 1.0 m):** Chemical process units, dense piping racks, and tall control structures. Elevates mechanical turbulence and aids localized mixing.
- **Open Water (z0 ≈ 0.001 m):** Extremely low surface friction (offshore platforms, lakes); yields maximum lethal downwind cloud glide distance.

3. Wind Variability & Omnidirectional Modeling:

- **360° Worst-Case Threat Zone:** Enable this setting to evaluate the hazard envelope across all 360 degrees simultaneously, using a defined wind speed range (Min/Current to Max Range) to establish the ultimate safety perimeter regardless of wind shifts.

Note: This is a premium-locked feature depending on user roles or global administrative overrides.

4. Aerodynamic Wake Effect (Building Downwash):

- **Flat Terrain (No Buildings):** Standard dispersion with no structural interference.
- **Building Downwash:** Select this if the release occurs near large structures or dense piping. This modifier forces the plume closer to the ground (increasing vertical grounding) and widens the hazard envelope to account for aerodynamic wake turbulence.

Module B: Source Inventory Setup

This module defines the mechanical source variables and thermodynamics of the chemical leak:

- **Hazardous Gas Database:** Select standard toxic chemicals (H_2S, SO_2, Cl_2, NH_3) or choose the Custom option. If 'Custom' is selected, you must manually enter the chemical name, Molecular Weight (MW), IDLH, STEL, and Vapor Pressure (kPa).
- **Release Mode Model:** Select 'Pressurized Leak' (high-pressure pipe breach modeled as choked sonic flow), 'Direct Vent' (known venting flow rate), 'Evaporating Pool Spill' (continuous boiling of cold liquid), or 'Catastrophic Rupture (Puff)' for instantaneous mass releases.

- **Source Concentration & Vessel Volume:** Set the target chemical concentration in the pipeline (e.g., 100% or ppm). If the release is transient, enter the total Vessel Volume (kg) to calculate the blowdown decay time; leave blank for continuous releases.
- **Jet Orientation:** Choose 'Horizontal' (ground-level jetting), 'Vertical' (applies momentum plume rise aloft), or 'Impinging' (jet shatters against an obstacle, canceling upward momentum and creating localized heavy pooling).
- **Ignition (VCE/BLEVE):** Toggle this checkbox if the flammable gas release is ignited. The system will immediately compute and map the thermal/blast overpressure radius.

Module C: Spatial Analysis, Receptors & Vulnerability Mapping

This module governs the interactive map tools, structural geofencing, and personnel lethality calculations.

1. Interactive Pin Tools:

- Place Receptor (Target Concentration): Click "Place Receptor" and drop the green pin on the map to measure exact parts-per-million (PPM) dosages at a specific coordinate.
- Place Asset (Vulnerability Geofencing): Click "Place Asset", drop the pin on critical infrastructure (e.g., Control Room, Exit Gates), and assign it a name. The engine will automatically flag if these assets fall within Critical (IDLH) or Precautionary (STEL) zones.

Note: Click an existing Asset pin on the map to safely remove it.

2. Receptor Toxicity Parameters:

When a receptor pin is placed, the engine calculates the Probit Lethality percentage based on two critical variables:

- **Personnel Exposure Time:** Set the anticipated exposure duration (10 mins for emergency escape, 30 mins for rescue, or 60 mins for standard exposure).
- **Worker PPE Protection Level:** Select the active respiratory protection (None, Half-Mask APF 10, Full-Face APF 50, or SCBA APF 10,000) to determine the actual physiological dose received by the worker.

3. Wind Variability Sectors (Windrose):

Toggle the "Wind Variability" tool to project dispersion probabilities across a spread of adjacent wind angles (±22.5 degrees), accounting for dynamic wind shifts over a 24-hour period.

4. Custom Site Layout Overlays:

Upload approved site blueprints (JPG/PNG/WEBP). Use the blue pin to drag the layout and the red pin to scale and rotate the overlay to match real-world map coordinates.

5. Render Engine Mode & Drift:

- **Render Mode:** Toggle between 'Standard Polygons' for sharp boundary lines or the 'Multi-Tier Isopleth Heatmap' for gradient concentration mapping.
- **Simulate Drift:** In 2D mode, click to animate the real-time downwind trajectory of the toxic plume based on current wind speeds.

Module D: Scenario Management & Reporting

The interface includes built-in tools for saving configurations and generating compliant documentation.

- **Browser State Memory:** Use the **Save** and **Load** buttons in the top header to store your current meteorological and chemical configuration locally within your browser, allowing you to instantly resume complex scenario planning.
- **Operations & Site Metadata:** Before generating a report, fill in the Facility Name, Project/Work Order, and Operational Scope notes. You may also upload a custom Client/Company Logo that will automatically render in the header of the exported PDF.
- **Export Safety PDF:** Clicking this action button captures the map state, geofenced assets, receptor calculations, and the site-specific ERAP protocol, compiling them into a formal two-page safety directive.

5. Emergency Action & Manpower PPE Matrix

When a chemical release occurs, the plugin automatically evaluates the geofenced boundary levels and generates an Emergency Response Action Plan (ERAP). The table below dictates the mandatory on-site engineering actions, tactical safety responses, and required PPE:

Chemical	Thresholds	Immediate Tactical Action & Required PPE
Hydrogen Sulfide (H2S)	**IDLH: 100 ppm** STEL: 15 ppm	Evacuate crosswind immediately. Deploy supplied-air respirators (SCBA / Level B). Initiate automated plant shutdown.
Chlorine (Cl2)	**IDLH: 10 ppm** STEL: 1 ppm	Heavy gas hazard. Evacuate to high ground. Deploy Level A fully encapsulating vapor-tight chemical suits and SCBA.
Sulfur Dioxide (SO2)	**IDLH: 100 ppm** STEL: 5 ppm	Respiratory acid-gas irritant. Mandate SCBA and full-face acid gas canisters for secondary perimeter teams.
Methane / Flammable VOCs	**IDLH: 10% LEL** STEL: 2% LEL	Flammable & Asphyxiation hazard. Eliminate all ignition sources immediately. Prohibit ungrounded electrical equipment.
Ammonia (NH3)	**IDLH: 300 ppm** STEL: 35 ppm	Toxic, corrosive vapor. Deploy Level A/B PPE. Apply water fog knockdown spray. DO NOT spray water directly into liquid pools.

6. Mandatory Fence-Line Safety Directive

⚠ CRITICAL COMPLIANCE DIRECTIVE: FENCE-LINE EXCURSIONS

If dispersion modeling indicates that an IDLH or STEL boundary extends beyond the site property line into local residential or commercial areas, on-site HSE teams must immediately initiate emergency off-site mutual aid agreements. Local municipal safety authorities must be notified instantly, and emergency response teams must initiate crosswind community evacuation procedures. There is zero margin for delay.