EXECUTIVE SUMMARY

UNIFIED DISPERSION MODEL

DATE: December 2023

This technical reference manual describes the Unified Dispersion Model (UDM) implemented into the DNV software packages (Phast, Safeti, SAFET-NL). This technical reference manual includes a detailed description of the theory, verification and validation of the UDM, the UDM thermodynamics, and the pool spreading/evaporation model PVAP included in UDM.

No.	Date	Reason for Issue	Prepared by	Verified by	Approved by
1	June 2011				
2	October 2017	Phast & Safeti 8.0	HARP&Witlox		
3	May 2021	Apply new template	D. Vatier		
4	July 2022	Version update	David Worthington		

Date: December 2023

Prepared by: Digital Solutions at DNV

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1 INTRODUCTION

This technical reference manual describes the latest version of the Unified Dispersion Model (UDM, Version 3) implemented into the DNV software packages Phast and Safeti. The original version of UDM (Version 1) was developed by Cook and Woodward in the early nineties, and underwent major revisions for Phast 6.0 (2000), hast 6.7 (2011 – UDM Version 2) and Phast 8.0 (2017 – UDM Version 3).

This technical reference manual includes a detailed description of the theory, verification and validation of the UDM, the UDM thermodynamics, and the pool spreading/evaporation model PVAP included in the UDM.

Each of the modules in the UDM has been investigated and verified in detail in conjunction with a literature review and a sensitivity analysis. The modules have been validated where possible, and been compared with similar external packages.

Sections 2, 3, 4 contain an overview of underlying theory, verification and validation for the dispersion model, the thermodynamics module and the pool spreading/evaporation model.

2 UNIFIED DISPERSION MODEL (UDM)

2.1 Theory

The UDM models the dispersion following a ground-level or elevated two-phase pressurised release. It effectively consists of the following linked modules (see Figure 1 and Figure 2):

- instantaneous expansion (see Section 3 below)
- jet dispersion
- droplet evaporation and rainout, touchdown
- pool spread and vaporisation
- heavy gas dispersion
- passive dispersion

A single form of concentration profile is used to cover all stages of a release. This allows for anything from a sharp-edged profile in the initial stages of a jet release through to the diffuse Gaussian profile that would be expected in the final passive stage of spreading.

The UDM includes the effects of droplet vaporisation using a non-equilibrium model. Rainout produces a pool which spreads and vaporises. Vapour is added back into the plume and allowance is made for this additional vapour flow to vary with time. In addition to the non-equilibrium model, UDM also allows for an equilibrium model and an equilibrium model specific for HF (including effects of polymerisation).

The UDM allows for vertical variation in ambient speed, temperature and pressure. Another feature of the UDM is possible plume lift-off, where a grounded cloud becomes buoyant and rises into the air. Rising clouds may be constrained to the mixing layer if it is reached.

The UDM allows for continuous, instantaneous, constant finite-duration, and general time-varying releases. For the 8.0 release the UDM has been extensively modified (Version 3) to eliminate dispersion “segments”, allow for continuously varying releases and pools, and to incorporate along-wind diffusion (AWD) and along-wind gravity-spreading effects.

Where possible the model coefficients are obtained directly from established data in the literature (based on experiments), rather than doing UDM simulations and fitting the UDM results to the experimental data.

2.2 Verification

2.2.1 Passive dispersion

The UDM theory and solution algorithm for passive dispersion has been investigated in detail.

The UDM results are shown to be in close agreement with vertical and crosswind dispersion coefficients and concentrations obtained from an analytical Gaussian passive dispersion formula.

A sensitivity analysis has been carried out for a given base-case problem (passive dispersion of ‘air’). Parameter variations have been carried out to the release height, averaging time, surface roughness length, stability class, release rate and wind speed.

2.2.2 Jet dispersion

The UDM theory and solution algorithm for elevated dispersion and ground-level jet dispersion have been investigated in detail.

The UDM results are shown to be identical to the results obtained by an analytical solution for an elevated horizontal jet. Very good agreement has been obtained against the Pratte and Baines correlation for plume rise (no ambient turbulence). Improved predictions are shown against the Briggs correlation (including ambient turbulence).

Finally a sensitivity analysis has been carried out for a given base-case problem (jet dispersion of 'air'). Parameter variations have been carried out to the release height, release speed, release angle and transition criterion.

2.2.3 Heavy-gas dispersion

The UDM theory and solution algorithm for steady-state ground-level heavy-gas dispersion has been investigated in detail:

1. The top-entrainment formulation (Richardson-number calculation and entrainment function) has been validated against the 2-D wind-tunnel experiments of McQuaid (steady-state ground-level dispersion of CO_2). Good agreement has been obtained. Moreover UDM results are shown to be in identical agreement against an analytical solution for a neutral ground-level jet (adopting the heavy-gas logic).

2. The crosswind gravity spreading has been validated against the isothermal HTAG wind-tunnel experiments. Future implementation of the collapse of gravity spreading is recommended.
3. For the HTAG experiments the UDM has also been verified against results of the HGSYSTEM model HEGADAS.
4. In the future, a further sensitivity analysis is recommended to be carried out for a given base-case problem, with a selected number of single/multiple parameter variations.

2.2.4 Plume touchdown and transition to passive dispersion

A sensitivity analysis of plume touchdown has been carried out for both cases of continuous and instantaneous dispersion. The UDM theory for transition to passive and inclusion of averaging times has been investigated in detail.

2.2.5 Instantaneous dispersion

The UDM theory and solution algorithm for an unpressurised instantaneous release has been investigated in detail.

For purely passive dispersion, the UDM results are shown to be in close a close agreement with vertical and crosswind dispersion coefficients and concentrations obtained from an analytical Gaussian passive dispersion formula. For ground-level heavy dispersion, good results have been obtained for validation against the Thorney Island experiments.

As part of further work, the UDM instantaneous model should be extended to allow for along-wind diffusion to be different from cross-wind diffusion. This could involve the instantaneous DRIFT approach and/or the more general HEGADAS-T time-dependent approach. The current approach leads to inaccurate results for [a] unstable conditions in conjunction with large averaging times (too large σ_x, too low maximum concentrations) and [b] stable conditions in conjunction with small averaging times (too small σ_x, too large maximum concentrations).

2.2.6 Finite-duration release

The UDM theory and solution algorithm for finite-duration releases has been investigated in detail. The default approach in the current version is to use the generalised AWD model, and the verification of this is covered under time-varying releases (below). However the quasi-instantaneous (QI) model or the finite-duration correction (FDC) model are still supported.

Quasi-instantaneous model
The QI model models the initial phase as a continuous source (neglect of downwind gravity spreading and downwind diffusion). When the cloud width becomes 'large' with respect to the cloud length, the cloud is replaced by an 'equivalent' circular cloud, and the subsequent phase is modelled as an 'instantaneous' circular cloud. The disadvantage of the QI model is the abrupt transition (sometimes resulting in severe discontinuities, e.g. erroneous significant increase in maximum concentration), and the inaccuracy in along-wind diffusion.

Finite-duration correction model

The FDC model is based on the HGSYSTEM formulation derived from that adopted in the SLAB dispersion model. It has a better scientific basis than QI and is derived from an analytical solution of the Gaussian plume passive-dispersion equations. It takes the effects of downwind diffusion gradually into account including effects of both turbulent spread and vertical wind shear. A limitation of this model is however that it is strictly speaking only applicable to ground-level non-pressurised releases without significant rainout. Moreover it produces predictions of the maximum (centre-line ground-level) concentrations only. The finite-duration correction optionally includes the effect of averaging time because of time-dependency of the concentrations.

The FDC module has been verified against the HGSYSTEM/SLAB steady-state results, and shown to lead to finite-duration results virtually identical to the latter programs.

The UDM, HGSYSTEM and SLAB dispersion models have been compared for predictions in the far field for a steady-state release both without and with time averaging. For the chosen test case the UDM predictions have been shown to be below those predicted by HGSYSTEM and SLAB.

Secondly the models have been compared for predictions in the far field for a constant finite-duration release. The FDC finite-duration correction applied to the UDM steady-state results is shown to produce lower concentrations than the original UDM quasi-instantaneous approach. Moreover it also produces lower concentrations than the finite-duration concentrations obtained by HGSYSTEM and SLAB.

2.2.7 Link between dispersion and pool model

A description of the link between the pool model PVAP and the dispersion model has been added to the UDM theory manual.

The link between the dispersion and the pool model consists of the following phases:

1. Rainout of liquid component from the plume, and calculation of pool spreading/evaporation by the pool model PVAP.
2. Addition of pool vapour back to the cloud, while the cloud is above the pool.
3. Initialisation for plume dispersion from the pool, after the cloud has left the pool behind.
4. Post-processing of dispersion results to add AWD and gravity spreading effects to the cloud

Time varying discharge is modelled by approximating the time varying release rate with a series of release observers sampled at different times from the time-varying discharge results. As for rainout cases, AWD effects are added by post-processing UDM dispersion results

The derivation of the FDC model is described in detail, and FDC and AWD models are compared and their differences elaborated. For a simplified ground level passive dispersion case, the FDC and AWD results are verified against each other and against an analytical solution. The UDM FDC and AWD results have also been verified against the equivalent HEGADAS models for dispersion from a pool.

A detailed analysis has been done for a chlorine elevated release with rainout, and for a time-varying sour-gas release without rainout.

The gravity-spreading correction is verified using KitFox experiments (short duration CO_2 area releases) for both URA continuous and URA puff experiments.

2.3 Validation

A comprehensive description of the overall validation of the UDM model is given. This includes a description of each validation experiment, the details of the assumptions made for the UDM simulation plus a detailed discussion of the results obtained from a statistical and graphical comparison against the field data.

The above sections described the verification of the individual modules, whilst this document is concerned with the validation of the overall model. The former involved wind-tunnel experiments whilst the latter is mostly concerned with field experiments. For continuous and finite-duration experiments, this validation includes Maplin Sands (LNG, LPG), Goldfish (HF), Prairie Grass (passive), Desert Tortoise (Ammonia), EEC (Propane), FLADIS (Ammonia), Burro (LNG), Coyote (LNG), Thorney Island (Freon and Nitrogen) Kit Fox and CO_2 PIPETRANS (carbon dioxide) experiments. For instantaneous experiments, the validation includes the Thorney Island experiments (Freon and Nitrogen).

The performance of the UDM in predicting peak centreline concentration and cloud widths is good. Predictions for the neutrally buoyant Prairie Grass experiments and the aerosol releases of Desert Tortoise and EEC are very good.

Recommendations for future work are made in light of the performance of the UDM against the complex Goldfish experiments and the Maplin Sands LNG spill. These centre upon the enhancement of the heavy spread formulation to include a gravity collapse criteria and the removal of the passive transition zone through the use of virtual sources.

3 PRESSURISED INSTANTANEOUS EXPANSION MODEL (INEX)

3.1 Theory and Validation

INEX models the rapid energetic expansion of a pressurised instantaneous release during the earliest stages of a release. Following this stage, the model transitions to the normal unpressurised UDM model (Section 2.2.5).

The current INEX model was introduced in Phast & Safeti 8.0 to replace an earlier version. The previous model did not take into account gravity effects and assumed a single droplet size moving along a fixed upward angle resulting in too little rainout. The new INEX model is based on sounder phyisical principles. It includes gravity effects, and assumes the liquid to move radially away from the cloud centre. In case of a INEX cloud touching down the ground, this results in time-varying rainout.

The report includes a description of the theory, solution algorithm, model verificaton against analytical solutions, and model validation against experimental data.

The correctness of the new INEX numerical predictions has been verified against analytical solutions for ground-level vapor or two-phase releases and elevated non-evaporating liquid releases. It has been validated against experiments for ground-level presurised releases for nitrogen vapour and flashing liquid propylene, and elevated flashing liquid releases for Freon 11, Freon 12, propane and butane. Overall the new INEX model tends to underpredict the cloud radius and cloud speed versus time, while the new model provides larger predictions and more closely agrees against experimental data. In addition, the new model predicts a larger amount of rainout which is again more in line with the experimental data. Therefore when rainout occurs the new model produces smaller concentrations and doses, and is less conservative.

Experiments identified so far derive the cloud radius and cloud speed from the visible cloud front. This results in added uncertainty since the visible cloud expansion velocity depends amongst others on humidity, and this may e.g. explain some of the discrepancy in results compared to experiments by Schmidli and Pettitt for the measured fraction of kinetic energy. Therefore additional experimental work to measure concentrations is strongly recommended to provide a sounder basis for model validation. In addition experimental data including additional measurements of droplet sizes and rainout would be useful. This may assist in developing improved droplet size correlations applicable for instantaneous releases.

4 UDM THERMODYNAMICS MODEL

4.1 Theory

The UDM invokes the thermodynamics module while solving the dispersion equations in the downwind direction. The module describes the mixing of the released component with moist air, and may take into account water-vapour and heat transfer from the substrate to the cloud. The module calculates the phase distribution [component (vapour, liquid), water (vapour, liquid, ice)], vapour and liquid cloud temperature, and cloud density. Thus separate water (liquid or ice) and component (liquid) aerosols may form.

The liquid component in the aerosol is considered to consist of spherical droplets and additional droplet equations may be solved to determine the droplet trajectories, droplet mass and droplet temperature. Rainout of the liquid component occurs if the droplet size is sufficiently large.

The UDM includes the following types of thermodynamic models:

1. Equilibrium model (no reactions). Thermal equilibrium is assumed, which implies that the same temperature is adopted for all compounds in the cloud (vapour and liquid). The equilibrium model determines the phase distribution and the mixture temperature. Separate droplet equations are solved to determine the droplet trajectories (and the point of rainout).

2. Non-equilibrium model (no reactions). This model allows the temperature of the droplet (liquid component) to be different of the temperature of the other compounds in the cloud. The non-equilibrium model determines the phase distribution of the water and the vapour temperature. Additional droplet equations are solved to determine the droplet trajectories (and point of rainout), droplet mass and droplet temperature.

3. Equilibrium model (HF). The same temperature is adopted for all compounds in the cloud (vapour and liquid). The model includes the effect of HF polymerisation and fog formation.

4.2 Verification

4.2.1 Non-reactive equilibrium model; heat/water transfer from substrate

The following verification has been carried out:

1. In the absence of liquid component, the equilibrium and non-equilibrium model lead to identical results.
2. The equilibrium model is tested for mixing of propane with moist air at 20C. Ambient humidity, propane liquid fraction, propane temperature have been varied. The cooling effect because of component evaporation and the heating effect because of water condensation is shown.
3. UDM predictions are shown to be in very close with HEGADAS predictions for the case of mixing of propane vapour/liquid (at –43/42C) with 0%/100% humid air.
4. The effect of heat and water-vapour transfer has been studied by variation of ground temperature.

4.2.2 Equilibrium model (HF)

A brief assessment of the HF thermodynamics model as implemented into the UDM has been carried out:

1. The HF thermodynamics model is based on the HGSYSTEM thermodynamics model. Therefore the UDM thermodynamic predictions are compared against those of HGSYSTEM, and predictions are shown to be reasonably consistent. This also implies that good agreement is obtained against experiments by Schotte for mixing of HF with moist air. Some small oscillations do occur for the HF simulations, which may be explained by the lower accuracy adopted in the UDM (to reduce CPU time).
2. A limited sensitivity analysis is carried out for mixing of HF with moist air, whereby both humidity and initial liquid mass fraction are varied.
3. The UDM simulation against the Goldfish 3 experiments has been investigated in more detail, and also compared against the corresponding HGSYSTEM simulation. Good agreement is obtained against both the experimental data and the HGSYSTEM predictions.
4. As part of further work a cleaner implementation of the HF thermodynamics is recommended. This could also include extension of the algorithm to allow for the presence of inert gases and/or water in the released HF.

4.2.3 Droplet model

A detailed assessment and improvement of the UDM droplet thermodynamics model has been carried out as part of a droplet modelling joint-industry project (JIP). In conjunction with the equilibrium model, it is used to set the droplet trajectories and the point of rainout only. In conjunction with the non-equilibrium model, it additionally calculates the droplet mass and the liquid droplet temperature.

The originally adopted formula of the initial droplet size was the minimum of a droplet-size based on mechanical break-up (Weber criterion) and flashing breakup (CCPS criterion). The latter empirical correlation was derived by means of a best fit against CCPS rainout experiments (rather than direct measurements of droplet size).

As part of the modelling JIP a new droplet size correlation was developed, which is known as the ‘Phase III JIP’ droplet size correlation. This correlation was shown to most accurately predict the initial droplet size for a wide range of experimental data. Also developed was a ‘modified’ CCPS correlation, which used the mechanical Weber correlation for sub-cooled liquids, and the CCPS correlation for super-heated liquids. This provides the best rainout predictions against a wide range of experimental data when compared to both the original CCPS and the JIP Phase III methods. As such it is the default correlation in Phast & Safeti.

5 UDM POOL MODEL (PVAP)

5.1 Theory

The source term model PVAP calculates the spreading and vapour flow rate from a pool formed by a spill of liquid onto either land or water. The pool may either boil or evaporate while simultaneously spreading, with different models used for spills on land and on water. Detailed mass and heat balances are kept, permitting variations in the temperature of the pool. For spills on water, solution of the spilled liquid is calculated, and also the reaction with water for ammonia. The model has been validated against experimental data.

When used as a standalone model, it can also predict evaporation from a multi-component pool. The evaporation rate of each component is proportional to its partial pressure

5.2 Review and verification

The pool model PVAP may either be run as a standalone model or may be called during the dispersion calculations following rainout. The PVAP theory was reviewed by David Webber. In addition PVAP results were compared against the SRD/HSE model GASP for a range of scenarios with the aim of testing the various sub-modules. The results and recommendations obtained by David Webber are as follows:

Pool spreading

1. The TNO pool-spreading model on land adopted in PVAP may give the right qualitative behaviour in case of an appropriate choice for the minimum pool thickness h_{min}. An improved formula for the minimum thickness may be considered, e.g. in terms of liquid viscosity etc. PVAP does not allow a zero minimum depth, while GASP recommends a zero minimum depth unless puddles are expected to form. As a result an improved formulation may be considered which does not need a minimum thickness.

2. The 'tuned' model of Dodge adopted in PVAP for spreading on water may not scale properly, particularly because an inappropriate force balance is used.

3. In the long term both above models could be replaced by logic in the GASP pool-spreading model, whic involves the solution of two first-order differential equations (spread rate, force balance) instead of one (spread rate).

Pool vaporisation

1. Unlike GASP, PVAP applies a non-unified treatment for evaporation and boiling. This may result in less smooth results.

2. For a boiling pool on land, the PVAP formula by Shaw and Briscoe for heat flow for conduction Q_{cond} is heuristic, and could be considered to be replaced by the improved GASP correlation introduced by Webber and Jones (1987). However the conduction models are very similar.

3. For an evaporating pool on land, the PVAP formula by McKay and Matsugu for heat flow from evaporation Q_{evap} is dimensionally not sound, and could be considered to be replaced by the more sound and well-validated GASP correlation by Brighton. The GASP correlation leads to significantly less evaporation on land.

4. For an evaporating pool on water, the PVAP formula by Dodge seems to be plausible for including the wind-speed dependent aerodynamic roughness length of the surface but it uses the dimensionally unsound correlation on land. It could be further compared with GASP formulation by Brighton. Note however that the PVAP evaporation rate is usually less than the dissolution rate.

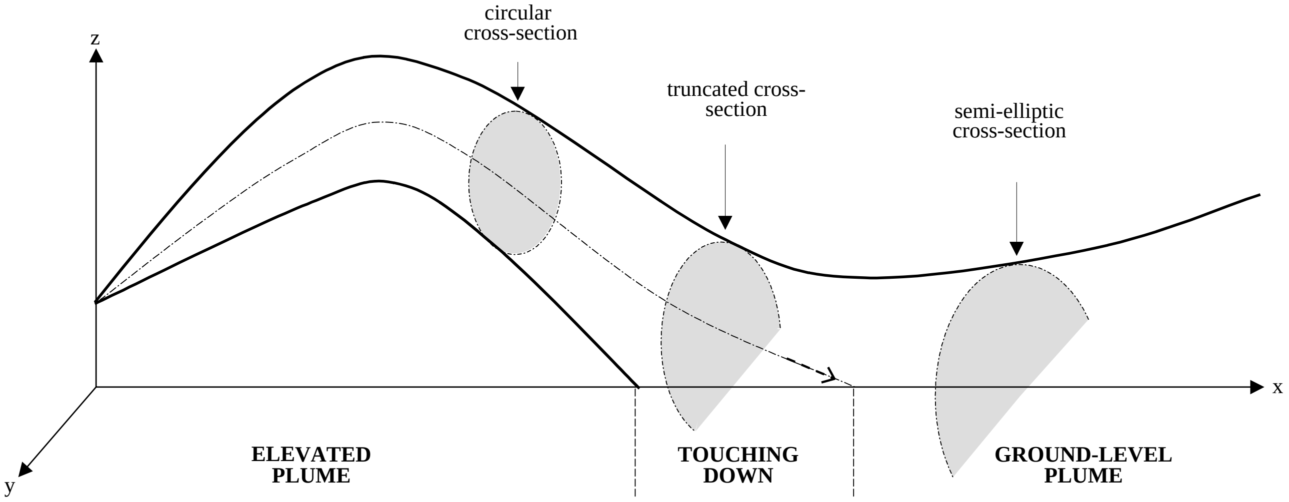
5. No problems have been found for the following existing PVAP sub-models:

   - Boiling on water, although ice formation may be discounted and model for ice formation is complicated
   - The formula by Fleischer for heat convection on land or water
   - The formula for radiation
   - Dissolution on water, although it may be more complicated than necessary
   - Reaction of ammonia pool with water

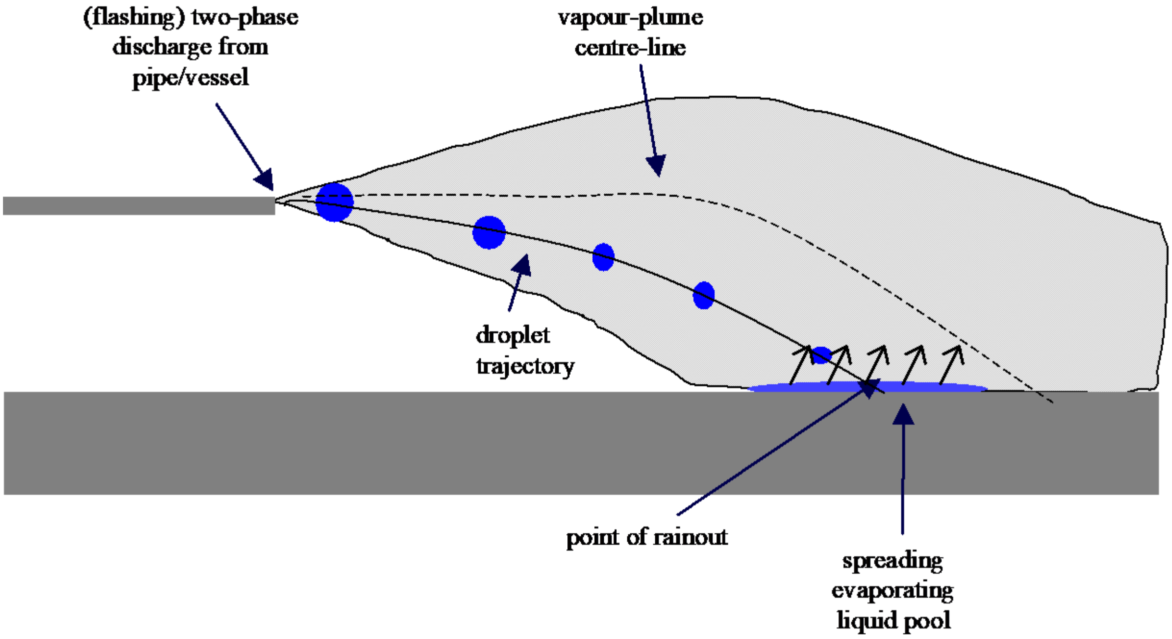
6 FUTURE WORK

The following items are areas of potential further work:

- remove rather arbitrary passive transition zone, and possibly improve passive formulation
- multi-compound dispersion including rainout
- solid compounds (in addition to CO_2)

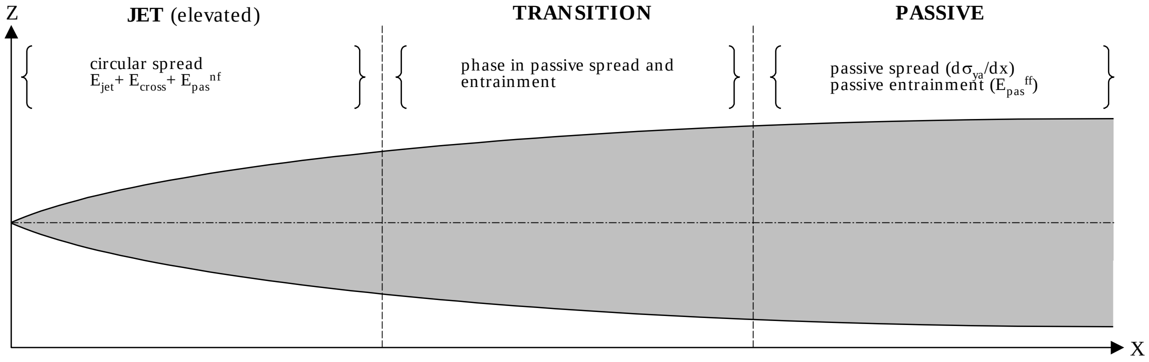


(a) plume dispersion

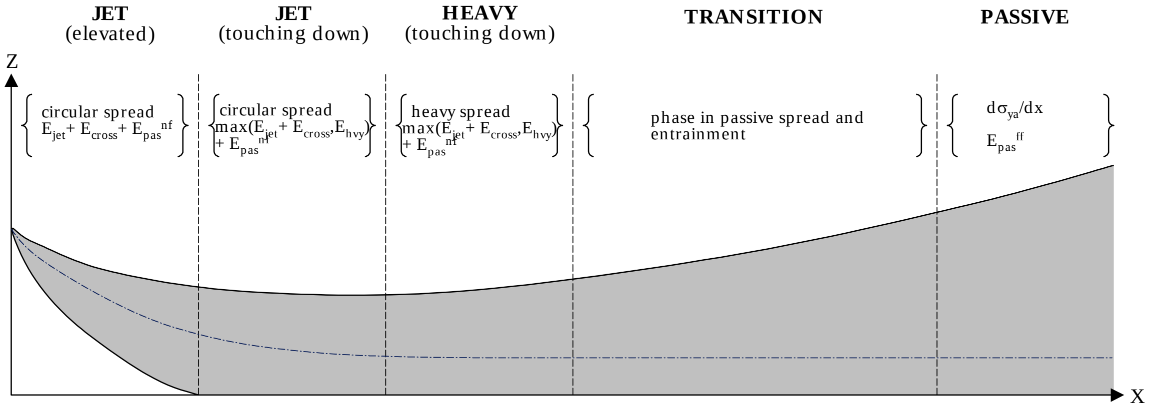


(b) droplet evaporation, rainout, and pool spreading/evaporation

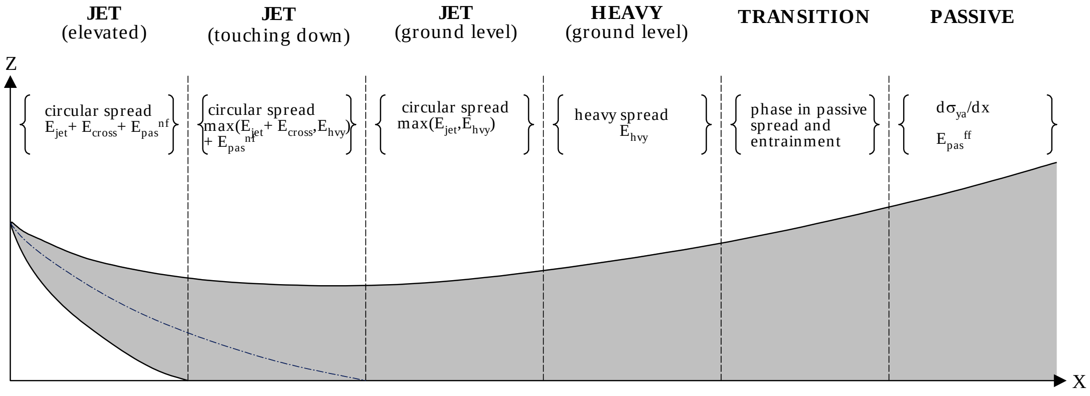
Figure 1. UDM cloud geometry for continuous release



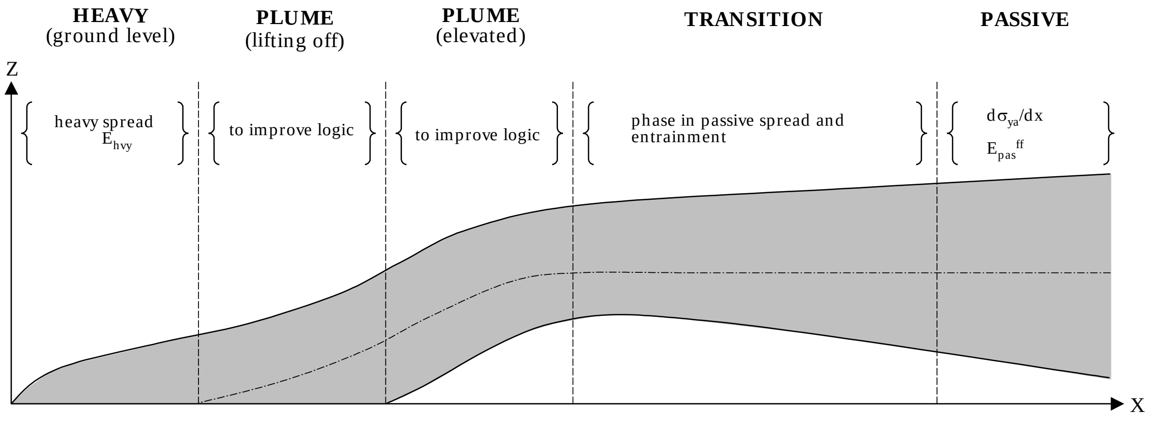
(a) elevated jet/plume (no touching down, no capping)



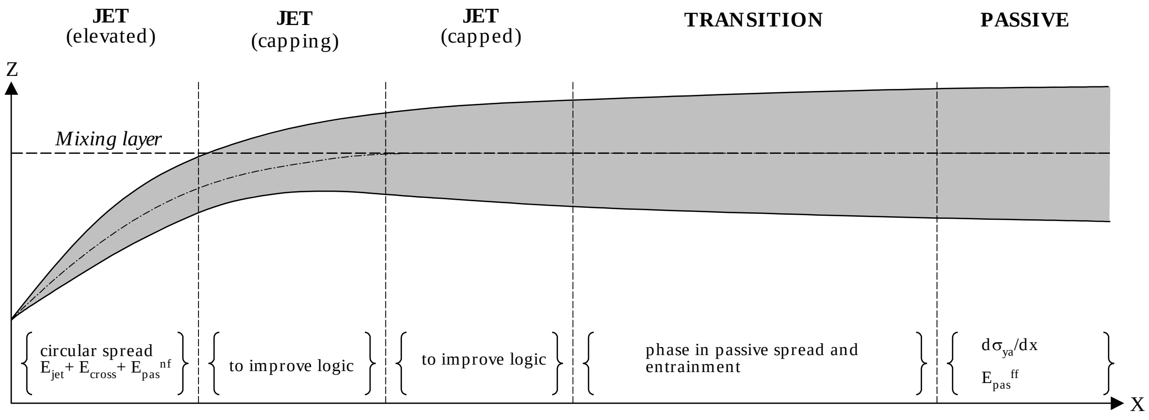
(b) jet/plume becomes passive during touching down



(c) jet/plume become passive after touch down



(d) ground level plume lifts off



(e) jet/plume hits mixing layer

Figure 2. **Phases in UDM cloud dispersion for range of scenarios; (a) no touching down, (b) touching down only, (c) full touchdown, (d) lift-off, (e) capping by mixing layer**

The figures indicate for each phase the type of spreading (circular jet, heavy or passive) and the mechanism of entrainment (E_{jet} = jet; E_{cross} = cross-wind; E_{pas}^{ff} = near-field elevated passive, E_{hvy} = ground-level heavy, E_{pas}^{ff} = far-field passive). Along the transition zone the near-field spread/entrainment are phased out and the far-field spread/entrainment are phased in.

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