UNIFIED DISPERSION MODEL

Technical Reference Manual

by

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CONSEQUENCE MODELLING DOCUMENTATION
(UDM Version 6.0, February 2000)

This technical reference manual describes the version 6.0 of the Unified Dispersion Model (UDM) implemented into the DNV software package PHAST 6.0. The original version of UDM was developed by Cook and Woodward in the early nineties. The new UDM 6.0 version represents a significant revision and extension to all parts of the model. This has been carried out in conjunction with a detailed literature review, verification and validation of the model. 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.

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CONTENTS

EXECUTIVE SUMMARY

1. Introduction

This technical reference manual describes the version 6.0 of the Unified Dispersion Model (UDM) implemented into the DNV software package PHAST 6.0. The original version of UDM was developed by Cook and Woodward in the early nineties. The new UDM 6.0 version represents a significant revision and extension to all parts of the model. This has been carried out in conjunction with a detailed literature review, verification and validation of the model.

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.

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 corrected where necessary, 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):

- 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 original UDM Cook and Woodward adopted a tuning process, where the tuning coefficients were obtained by comparison of UDM results against a relatively large set of 'tuning experiments. The problem with this approach was that several code errors and/or unrealistic model physics were masked by the use of tuning coefficients. This type of tuning has largely been eliminated as part of the current work. The model coefficients have now been 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. Several corrections to the UDM 5.2 code have been applied. The density tolerance has been removed from the vertical momentum equation (to ensure cloud elevation does not change), double precision logic has been applied (to ensure more stable dispersion behaviour for small concentrations in the far field), the averaging-time logic has been corrected, and the Schmidt number has been eliminated from the UDM concentration profile. Also other more minor corrections have been applied.

Following the above corrections, 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.

Finally 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. Several corrections to the UDM 5.2 code have been applied, the major ones being: corrected circular spread rate during jet phase, new jet entrainment formulation, adjusted entrainment and airborne drag coefficients, addition of near-field ambient turbulence, and a modified ground drag force formulation.

Following the corrections, 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 evaluation of the Richardson number has been corrected.
2. The top-entrainment function is modified to improve the fit with the experimental data for the entrainment function. This modification is in line with the results of a literature review, and also removes the dependency of stability class on the entrainment function.
3. The new 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). After this change, the validation was redone and similar agreement against the experimental data was shown (but now without tuning to the experimental data).
4. The maximum of jet and heavy entrainment is applied (rather than the sum) to avoid double-counting.
5. In line with the results of the literature review, the side entrainment is ignored for continuous dispersion.
6. A literature review is carried out for the crosswind gravity-spreading formulation. As a result the gravity-spreading parameter has been increased. The new formulation has been validated against the isothermal HTAG wind-tunnel experiments. Future implementation of the collapse of gravity spreading is recommended.
7. For the HTAG experiments, the UDM has also been verified against results of the HGSYSTEM model HEGADAS.
8. 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

Plume touchdown

The original UDM 5.2 method for dissipating vertical momentum during touchdown was incorrect. This lead to erroneous excessive acceleration of the cloud in the downwind direction. In addition it involved an arbitrary 'plume impact parameter' for conversion of vertical into horizontal momentum.

A new plume impact formulation has been included, which applies a plume impact force perpendicular to the plume axis during touchdown (assumption of elastic collision). A sensitivity analysis has been carried out to investigate the new formulation for both cases of continuous and instantaneous dispersion.

Passive transition and averaging-time effects

The UDM theory for transition to passive and inclusion of averaging times has been investigated in detail. Several modifications to the UDM 5.2 code have been applied:

1. The UDM 5.11 passive-transition criterion [cloud density close to ambient density] has been refined:

a. The cloud velocity must be close to the ambient velocity to avoid transitions for high-speed jets
b. The passive type of entrainment must be close to the total entrainment to avoid transition if non-passive entrainment is still significantly large
c. The Richardson number must be sufficiently small for a heavy-gas grounded plume, to avoid transition if the heavy entrainment is significantly different from passive entrainment

2. The UDM 5.2 averaging-time treatment overestimated the averaging-time effect along the transition distance. For averaging time t_{av} larger than the core averaging time t_{av}^{core} this leads to too high width and too low maximum concentration, while for $t_{av} < t_{av}^{core}$ the opposite occurs (even up to the extent of reduction of cloud width and increase of concentration). The UDM 5.2 method is retained as the default option within UDM 6.0 using the fixed core averaging time t_{av}^{core}=18.75 s.

   To avoid the above, a new option has been implemented into UDM 6.0 to allow a variable core averaging time, such that t_{av} can be chosen equal to t_{av}^{core}. This leads to a much smoother transition. This method is, however, more CPU-intensive for a range of user-specified averaging times.

3. Far-field passive spread in now also phased in (consistent with the phasing in of passive entrainment), which leads to smoother transitions.

2.2.5 Instantaneous dispersion

The UDM theory and solution algorithm for an unpressurised instantaneous release has been investigated in detail. Several improvements have been applied. These include:

- consistent assumptions for the cloud shape (concentration profile, effective cloud dimensions)
- improved calculation of the cloud surface area above the ground, and the cloud footprint area
- improved criterion for onset of touchdown
- more physically well-based calculation of near-field dispersion. This includes new formulas for jet entrainment, crosswind entrainment and airborne drag force (proportional to the cloud surface area above the cloud). Moreover near-field passive dispersion has now been included.
- more physically well-based calculation of interaction with the ground. This includes new formulas for ground drag force, ground heat transfer and ground water-vapour transfer (proportional to the cloud footprint area).

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). Finally the model for pressurised instantaneous dispersion needs to be investigated in detail (initial phase of energetic expansion).

2.2.6 Finite-duration release

The UDM theory and solution algorithm for an finite-duration releases has been investigated in detail. The UDM allows for the quasi-instantaneous (QI) model or the finite-duration correction (FDC) model.

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.

The QI model can be applied with or without the 'duration adjustment', where the duration adjustment applies the effect of averaging time because of time-dependency of the concentrations (for averaging times larger than release duration). The current duration adjustment over-estimates this effect downwind of the QI transition.

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 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 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.

First 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; time-varying releases

A description of the link between the pool model PVAP and the dispersion model has been added to the UDM theory manual. A limited assessment has been carried out, and several future improvements to the formulation have been identified.

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 and pool segmentation by the pool model PVAP. The PVAP model returns a number of constant values for the pool vaporisation rate, temperature and radius. This is an average of their continuous time varying values.
2. Addition of pool vapour back to the cloud, while the cloud is above the pool.
3. Initialisaton for plume dispersion from the pool, after the cloud has left the pool behind.

Note that UDM steady-state calculations are carried out for each of the individual pool segments.

Time varying discharge can be modelled by approximating the time varying release rate with a series of constant release rates. Several future improvements to the formulation have been identified.

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 experiments, this validation includes Maplin Sands (LNG), Goldfish (HF), Prairie Grass (passive), Desert Tortoise (Ammonia), EEC (Propane), FLADIS (Ammonia) and Burro 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. Corrections to the averaging time logic and heavy spread formulation have meant that the 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, more realistic UDM simulation for dispersion from a pool and the removal of the passive transition zone through the use of virtual sources.

3. UDM thermodynamics model

3.1 Theory

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.

3.2 Verification

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

The old UDM thermodynamics model contained the following errors:

1. The potential energy change with plume centroid height was not included properly in the old code. For increasing plume centroid height, this may lead to too high predictions for the cloud vapour temperature for neutral and stable conditions. This may incorrectly result in a too light cloud and an (additional) plume rise. In addition this leads to the 'bouncing cloud' bug.

2. The model predicted insufficient non-vapour water and set wrong water enthalpies:

   - The reference water enthalpy was set incorrectly in case of presence of ice or liquid water, leading to a significant underestimate of the heating effect resulting from water aerosol formation.
   - In the equilibrium model, the criterion for water aerosol formation was incorrect. In the case of absence of liquid component, water fog was never included, while in other cases the criterion was too severe leading to discontinuities.
   - In the non-equilibrium model the water phase distribution was also incorrectly set.

   The above errors could lead to erroneous oscillations in temperatures etc. The significant error in temperature predictions (too cold plumes) may affect the dispersion predictions. For ground-level plumes this leads to too heavy clouds, slightly too large widths, too small centre-line concentrations, and plume lift-off is less likely. For elevated plumes, it leads to less plume rise.

3. The vapour component was evaluated at the too low partial vapour pressure, instead of the ambient pressure. This results in unrealistic cooling down of the component while mixing with air.

4. Substrate heat transfer was not taken into account, which leads to a too cold/hot plume if the plume is hotter/colder than the substrate. Water transfer from a water substrate was not taken into account for substrate warmer than the plume. This leads to a plume which is too cold and which contains too little water.

5. In the thermodynamics the centroid ambient temperature was applied, which is inconsistent with the use of centre-line mass fractions of component, water and air. Thus the centre-line ambient temperature is applied in the new UDM. This implies that the cloud temperature corresponds to the centre-line temperature.

As a result the equilibrium and non-equilibrium models have been rewritten (not HF, not droplet equations), and heat/water vapour transfer equations have been added.

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.

3.2.2 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.

3.2.3 Droplet model

A brief assessment of the UDM droplet thermodynamics model has been carried out. 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 initial drop size is taken as the minimum of the droplet size by mechanical break-up and flashing break-up. The main conclusions are as follows.

Initial droplet size

1. The adopted formula of the initial droplet size for mechanical break-up incorrectly implements the Weber criterion, which may result in a too high value of the droplet size. This has been corrected in UDM 6.0.
2. The adopted formula of the initial droplet size for flashing break-up is found from an empirical correlation derived against CCPS rainout experiments. The following problems are associated with this:

   2.1. Theoretical objection that droplet correlation is not derived from directly measured droplet size distribution. It is indirectly obtained from the observed capture using flashing, dispersion and pool evaporation calculations. Thus droplet correlation is subject to inaccuracies in flash, dispersion and pool models, which is highly undesirable. In addition it is subject to any inaccuracies in determining the input data to these models.
   2.2. The discharge calculations are not based on PHAST discharge calculations (PHAST leads often to too high post-flash velocities). The adopted post-flash velocities are lower and consistent with those adopted for the RELEASE model. They are however higher those derived from a DIPPR formula. The drag coefficient is adjusted such that the observed release rate is obtained. Moreover there is an uncertainty in the amount of liquid head.
   2.3. The dispersion model assumes rainout at one point, and no liquid remaining afterwards. This is very inaccurate.

   Note that other formulas exist for flashing break-up, and e.g. the TNO formula (Wheatley) may be more suitable for implementation.

3. As a result of the above, it is strongly recommended to carry out further work to develop a robust, well-validated, and well-documented model for flash calculations and droplet correlations, in conjunction with a detailed literature review.

4. The calculations for the droplet diameters needed to fit the CCPS rainout data have been redone using the latest UDM model. The same assumptions were adopted as those that made for developing the original CCPS correlation. Since the new UDM model leads to somewhat more dilution in the near-field, the required droplet diameters are found to be somewhat larger (about 10%).

Droplet equations

5. The vertical droplet momentum equation has been corrected. Also the logic for cloud droplets moving outside the edges of the cloud has been removed.

6. A limited sensitivity analysis has been carried out in which droplet trajectories etc. have been compared. It is confirmed that for reducing droplet size the non-equilibrium model converges to the equilibrium model.

7. The droplet trajectories were calculated incorrectly for instantaneous elevated releases. This lead to erroneous immediate rainout for elevated unpressurised releases, and to a too large reduction of the droplet height after depressurisation for pressurised releases. This has been corrected in UDM 6.0.

4. UDM pool model (PVAP)

4.1 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.

4.2 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, whick 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

5. Conclusions and future work

Summary of work done

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 corrected where necessary, validated where possible, and been compared with similar external packages. This has been carried out in extensive detail for the entire basic continuous model and to some extent also the instantaneous model [phases of dispersion (passive, jet, heavy), equilibrium thermodynamics without rainout]. Following this work the UDM comparison against large-scale experiments improved considerably, despite of the elimination of tuning coefficients.

A detailed assessment and limited corrections have been carried out for the transition to passive, finite-duration releases, HF thermodynamics, and heat/water transfer from the substrate.

A brief assessment has been carried out for droplet modelling, pool spreading/evaporation, link between pool and dispersion model, pressurised instantaneous expansion, lift-off and mixing-layer logic, and time-dependent releases. Significant further work may be required for these areas.

Differences in results between PHAST 5.2 and PHAST 6.0

The key resulting differences between PHAST 6.0 and PHAST 5.2.0 are larger concentrations for far-field passive dispersion, lower concentrations for near-field elevated jet dispersion, larger ground-level heavy-gas spreading (wider clouds), often smaller droplet sizes and reduced rainout, and sometimes increased water aerosol formation (hotter clouds). Note however that many other applied changes may also play a role! See table below for a summary of the effect of the PHAST 6.0 enhancements on the UDM model predictions.

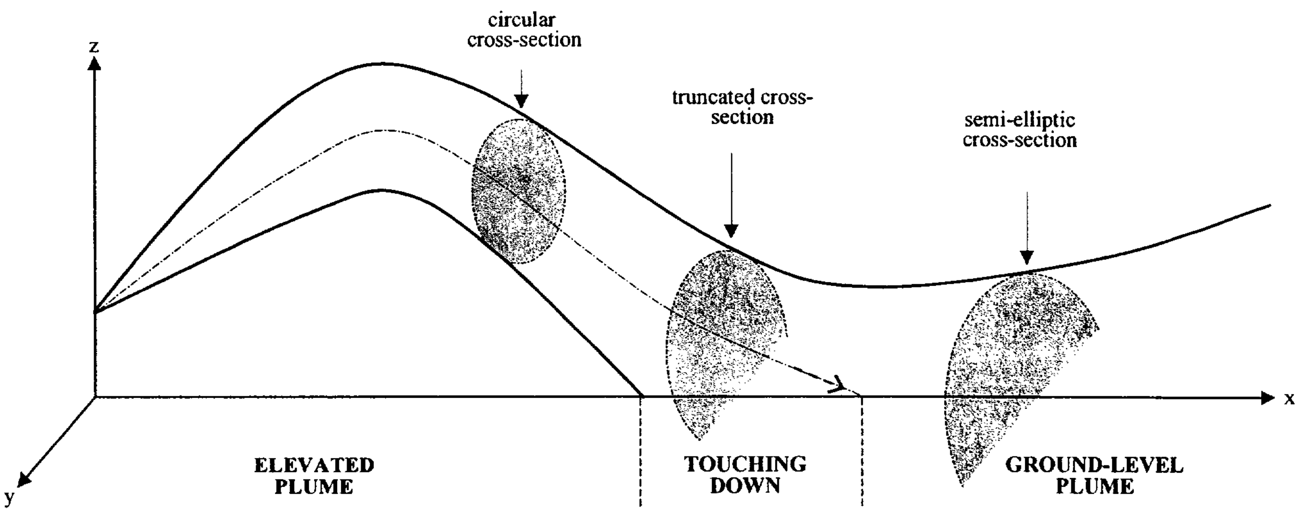
UDM SUBMODEL	PHAST 6.0 ENHANCEMENT	→ EFFECT ON PREDICTIONS	Fix in 5.2 patch
passive	correct σ_y (averaging time) remove Schmidt number	→ 2.26× less wide/dilute → $1.4^{0.5}$× less wide/high, 1.4×less dilute	yes, 5.2.2 yes, 5.2.2
jet	always circular cross-section larger jet/cross entrainment near-field passive entrainment improved ground drag no airborne drag	→ no 'narrow tall' grounded jet → lower concentrations → lower concentrations → often less drag, larger velocity, lower concentration, later passive → less plume deflection (compensated by above changes!)	partly,5.2.2 no no no no
heavy	correct Richardson number entrainment function increase cross-wind spread	→| these errors usually compensate? →| → wider clouds	no no
touchdown **lift-off**	improved ground impact force improved lift-off criterion	→ no erroneous cloud acceleration → less lift-off or lift-off disabled with warning	no partly,5.2.3
passive transition	improved transition criterion also phase in passive spread averaging time at core calcs.	→ no transition if large-speed jet, or if little passive entrainment → more smooth transition → more smooth transition	no no no
instantaneous	improved cloud geometry corrected droplet modelling	→ very different jet/cross entrainment → very different ground drag → lower concentrations in far-field in case of time averaging → no immediate rainout	no no
thermodynamics	potential energy for plume incorrect water aerosol incorrect water enthalpy add heat/water transfer option corrected initial droplet size	→ less plume rise, no bouncing clouds → more water aerosol → more heating if water fog forms → cloud colder if substrate cold, etc. → often reduced droplet-size/rainout	no no no no no
others	double precision no density tolerance	→ not unstable for low concentration → cloud does not become too heavy	no no

Further work after PHAST 6.0

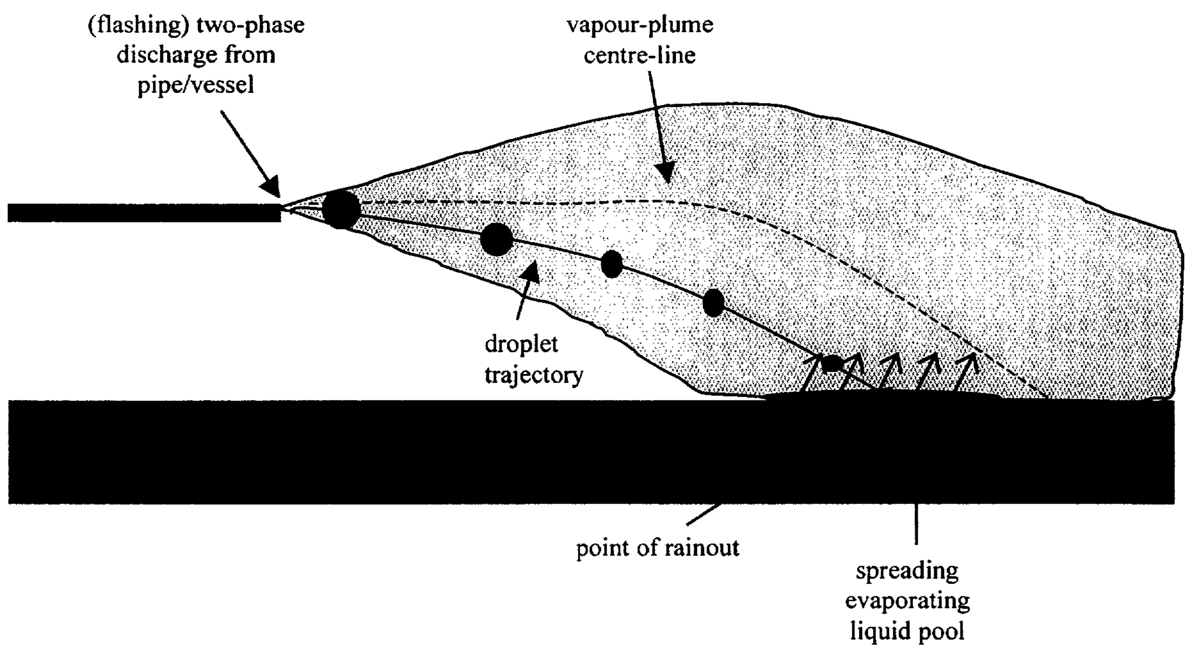
The following items are considered to be the major items for further work before PHAST 6.1 (although some of these items may need to be postponed until after PHAST 6.1):

- remove rather arbitrary passive transition zone, and possibly improve passive formulation
- neat modular code, particularly for droplet modelling, link between pool and dispersion model, and time-dependent releases (ideally also for HF); this would enable further assessment, improvement and detailed testing of these areas of the model and the code. This should correct problems for two-phase instantaneous clouds and reduce numerical problems. It should also easily enable to model dispersion directly from a pool (rather than after rainout only).
- more detailed assessment and possibly improvement for pressurised instantaneous expansion, lift-off and mixing layer logic
- multi-compound dispersion and solid compounds
- more detailed investigation and validation of pool model PVAP, including documentation and improvement of segmentation algorithm
- improved flash calculations

An urgent item after PHAST 6.1 is considered to be the improvement of along-wind-diffusion for non-steady dispersion, e.g. using DRIFT approach for instantaneous dispersion and/or HEGADAS-T approach for time-varying dispersion. The current neglect of along-wind dispersion for time-varying dispersion leads to a significant over-prediction of the concentrations in the far-field.

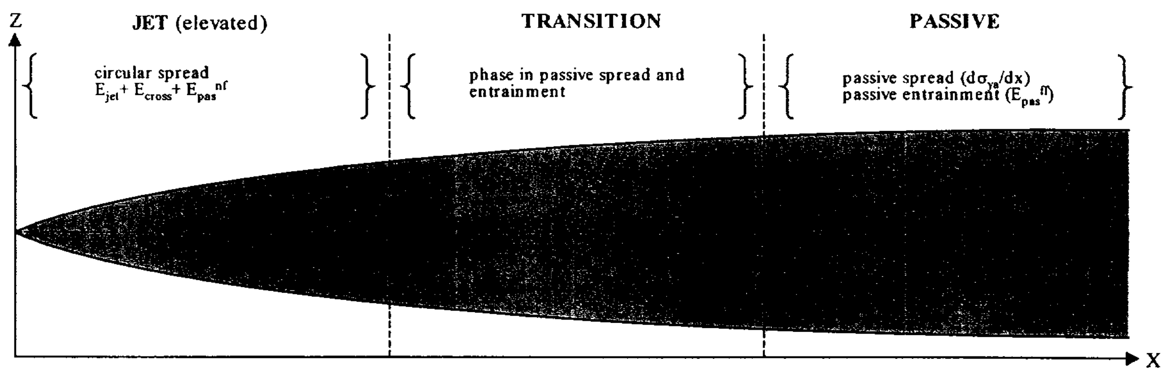


(a) plume dispersion

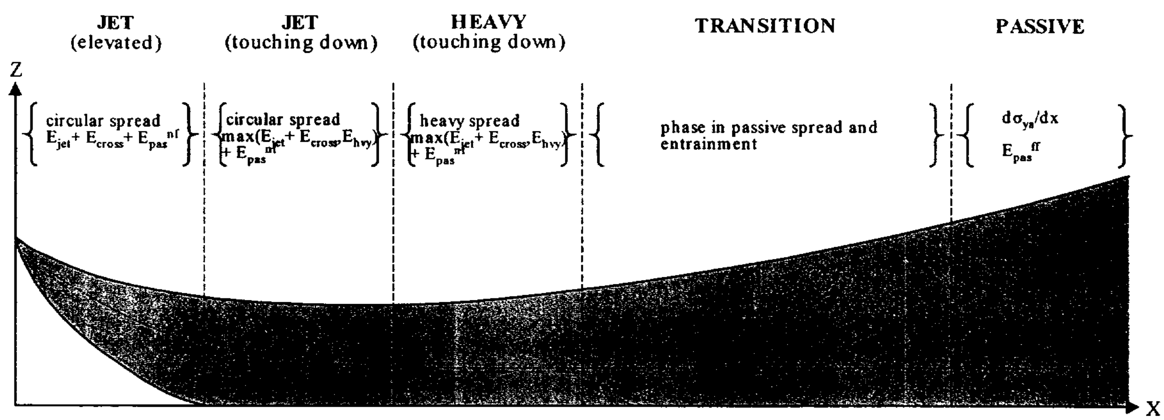


(b) droplet evaporation, rainout, and pool spreading/evaporation

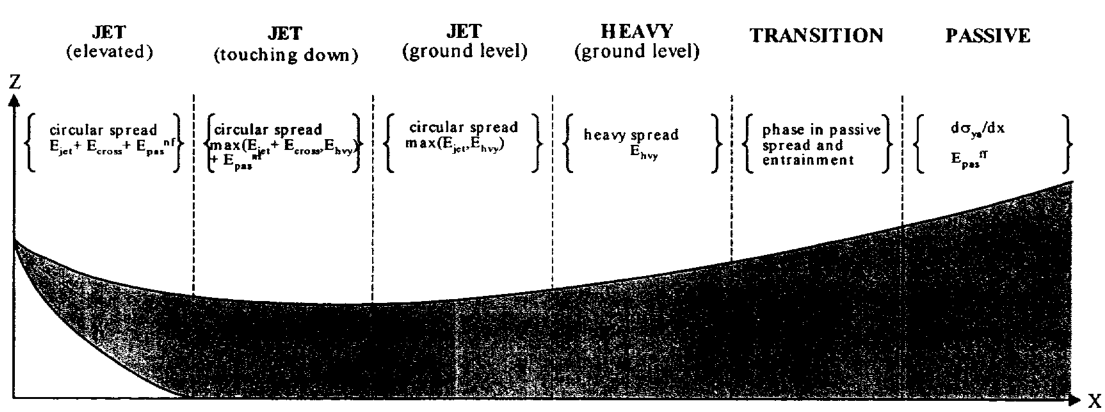
Figure 1. UDM cloud geometry for continuous release



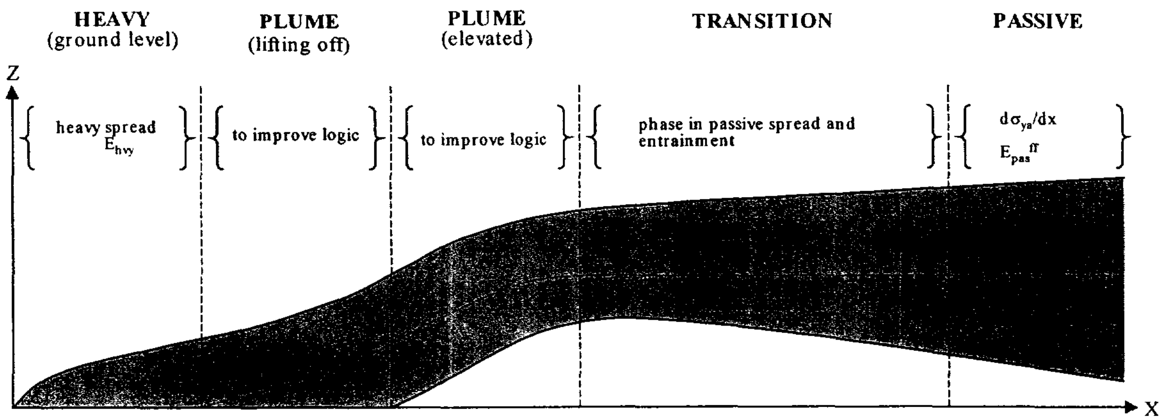
(a) elevated jet/plume (no touching down, no capping)



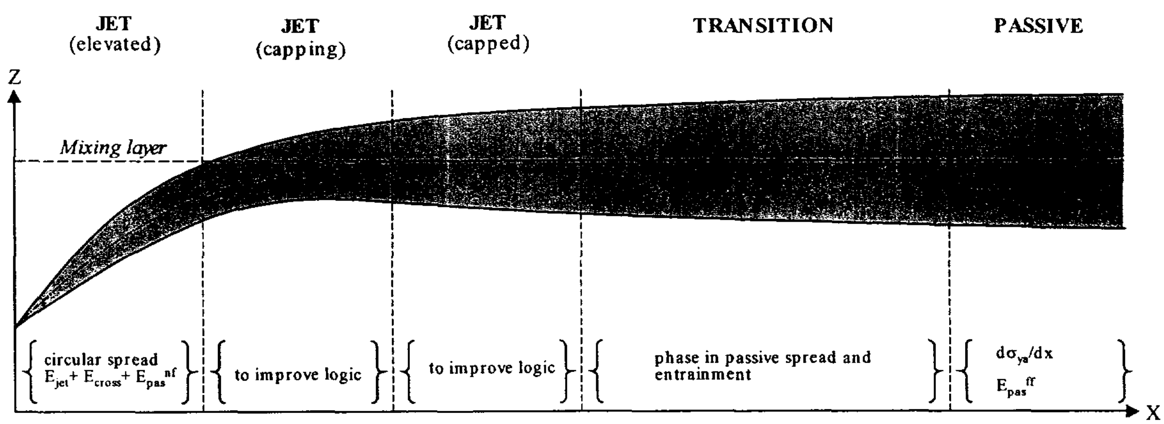
(b) jet/plume becomes passive during touching down



(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.