

Modelling of Time-Dependent Dispersion for Releases Including Potential Rainout

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Many commonly-used atmospheric dispersion models cannot accurately simulate time-varying releases of hazardous chemicals in the atmosphere. A new version of the Phast dispersion model UDM has been developed to more accurately simulate time-varying effects resulting from a pressure drop in a vessel or pipe and/or from a time-varying pool (following rainout or from direct spill). The new formulation presumes a number of 'observers' to be released at successive times from the point of discharge or the upwind edge of the pool. The UDM first carries out pseudo steady-state calculations for each observer, where the release data correspond to the time at which the observer is released, and where the observer may rain out or pick up vapour while travelling over the evaporating pool. Secondly the model applies a correction to the observer concentrations to ensure mass conservation when observers move with different velocities. Finally effects of along-wind diffusion (due to ambient turbulence) are included by means of Gaussian integration over the downwind distance. This results in reduced concentrations as the cloud disperses in the downwind direction which is particularly relevant for toxic releases.

The above new UDM formulation has been verified against the time-varying HGSYSTEM model HEGADAS-T for the case of dispersion from a pool, and it has been verified and tested for elevated releases without and with rainout.

Keywords: cloud dispersion; rainout; hazards evaluation; risk assessment

Introduction

Many accidents involve releases of hazardous chemicals into the atmosphere. Many commonly used atmospheric dispersion models are limited to continuous or instantaneous releases only. They do not accurately account for time-varying effects following time-varying releases i.e. resulting from a pressure drop in a vessel or pipe, and/or from a time-varying pool (following rainout or from direct spill). These effects include along-wind-diffusion (due to ambient turbulence) resulting in reduced concentrations.

The consequence modelling package Phast includes the Unified Dispersion Model UDM (Witlox and Harper, 2011) for modelling two-phase outdoor releases including potential rainout. The UDM in the current Phast (versions 6.7 and 7.1) only accounts for along-wind-diffusion (AWD) for instantaneous releases or finite-duration continuous releases that do not rain out.

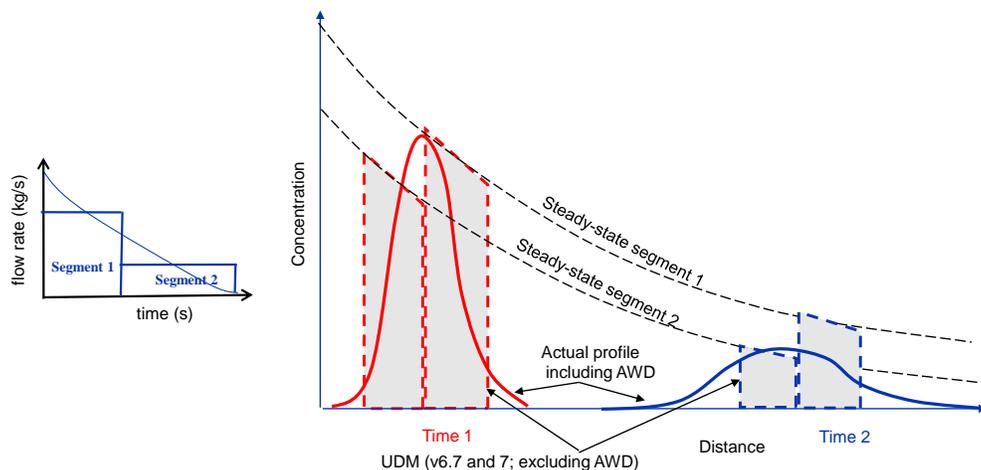


Figure 1. UDM time-varying dispersion – old segment method excluding AWD

For a time-varying release, Phast currently divides the calculated discharge mass into a user-specified number of equal-mass segments (Figure 1). Likewise in case of rainout or dispersion directly from an evaporating pool, the evaporated mass from the pool is divided into equal-mass segments. Subsequently the UDM model carries out steady-state dispersion calculations for each segment, and determines for successive times the concentration as a function of distance from these segment data as shown in Figure 1 by the dashed curves. Thus for time-varying releases or for dispersion after rainout, the current UDM does not apply along-wind-diffusion at the upwind and downwind edges of the cloud, or between segments, which may lead to significant over-prediction of concentration and under-prediction of duration in the far-field (see Figure 1 at time 2). This is particularly important for toxic releases, where dispersion calculations are required to be carried out to small concentration levels such as ERPG levels. It is less important for flammable releases with calculations to relatively high concentration levels only, such as LFL or 0.5LFL.

The Shell consequence modelling package HGSYSTEM 3.0 includes the time-dependent dispersion model HEGADAS-T (Witlox, 1994) for modelling the time-dependent dispersion of a heavy-gas cloud moving with the ambient wind. It can be used to model the dispersion downwind of either a time-dependent ground-level source (unpressurised release) or a transition with a near-source jet model (pressurised

release). The transient behaviour of the cloud is approximated by a quasi-steady-state description in which so-called “observers” are released at the source/transition-plane at a series of times. These observers travel with the cloud. For each observer, the observed concentration is set from steady-state HEGADAS-S calculations using the observed source/transition data. Thus by calculating the position of each observer at a given time t , the concentration c is set for a number of downwind distances. Subsequently the actual concentration is set from Gaussian integration with respect to the downwind distance x of the above observer concentrations as illustrated in Figure 2. This involves a downwind dispersion coefficient σ_x , which allows along-wind diffusion to be taken into account.

The current paper introduces a new enhanced dispersion formulation (Witlox and Harper, 2013; Witlox et al., 2013) accounting for time-varying effects resulting from a time-varying release. It generalises the above HEGADAS-T formulation to account for long-wind-diffusion both for ground-level unpressurised releases (e.g. evaporating pools) and for elevated two-phase pressurised releases including potential rainout. This method has been implemented in a new version of the UDM model, which is to be included in a future version of Phast.

New UDM Time-Varying Dispersion Formulation

First Phast discharge calculations are carried out (for release from a hole of a vessel or a pipeline) to determine the time-varying discharge data after expansion to atmospheric pressure and prior to air entrainment [flow rate, velocity, temperature, liquid fraction, droplet size (SMD – Sauter Mean Diameter)].

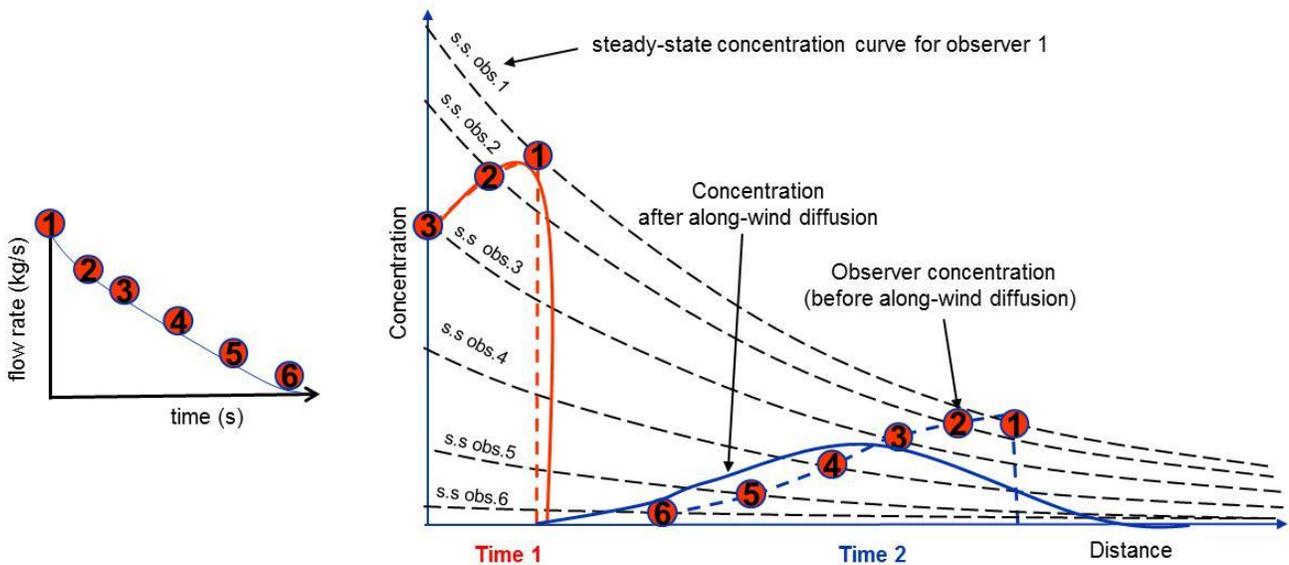
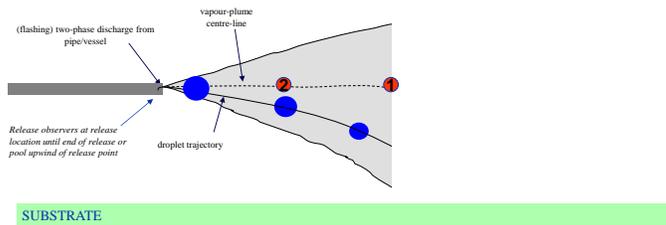
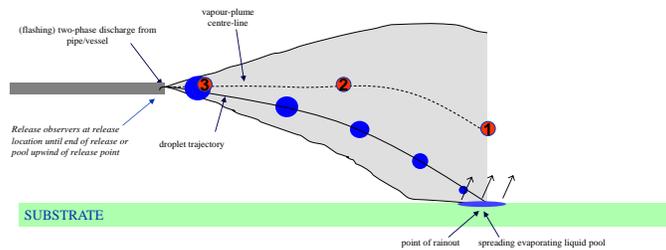


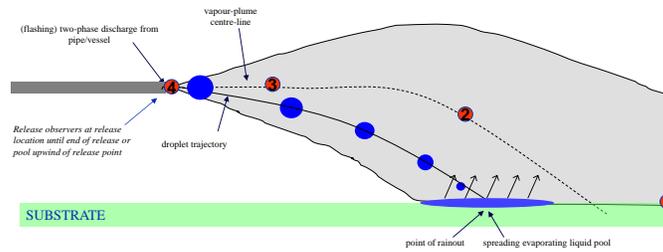
Figure 2. UDM time-varying dispersion –new observer method including AWD



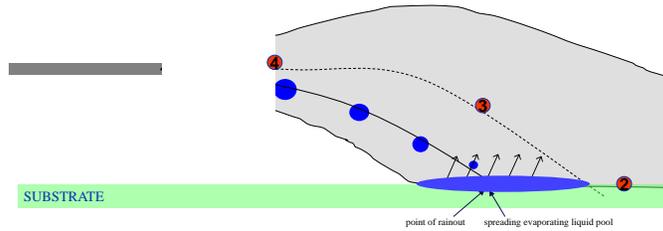
(a) Dispersion before rainout (release observers from release location – no pool effects)



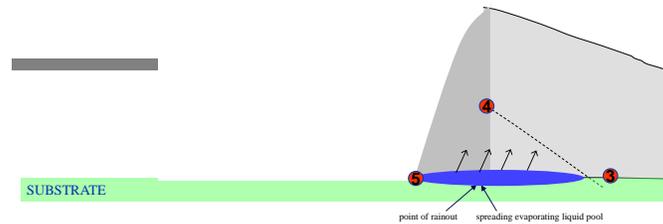
(b) Rainout (adjust observer variables at rainout location; solve pool equations afterwards)



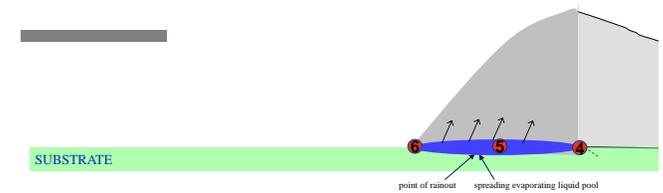
(c) Dispersion after rainout (account for pool vapour pick-up from cloud for observer calculations)



(d) Downwind movement of upwind edge of cloud towards pool (after end of release)



(e) Release observers upwind of pool (after 'release observers' all downwind of upwind pool edge)



(f) Dispersion directly from pool, with residual cloud moving away from pool

Figure 3. New UDM dispersion phases for time-varying release with rainout

Subsequently 'observers' are released from the release location at intervals which can be chosen to correspond to equal-mass increments as for the old UDM method (see Figure 2 for the case of 6 release observers). These observers are assumed to move along the cloud centre-line at the UDM cloud centroid speed. In the case of rainout, additional 'observers' (corresponding to equal pool-mass segments) are released upwind of the pool after the release plume has left the plume behind. This is illustrated by Figure 3, where the first observers (1,2,3,4) start from the release point and subsequent observers (5, 6) start from the upwind edge of the pool.

For each observer steady-state calculations based on the observed source data are carried out to evaluate the observer concentration prior to including effects of along-wind diffusion; see Figure 2. While the observer moves above the pool, the observer dispersion equations (conservation of cloud mass and momentum conservation, cloud crosswind gravity spreading, heat transfer from the substrate, etc.) are modified to account for the pool vapour being added back to the cloud.

Differential observer-velocity cloud mass correction

The above method is based on a quasi steady-state approach based on a steady-state solution for each observer. However, if observers move with substantially different velocities (different curves for observer downwind distance versus observer travel time) the mass of released material is not conserved by simply interpolating between these steady state solutions. Therefore a correction can be applied to the observer concentrations to ensure mass conservation. It reduces observer concentrations when observers drift apart, and increases concentrations when they move to each other; see Witlox et al. (2013) for further details.

Inclusion of effects of along-wind diffusion

The actual plume concentration $c(x,y,z,t)$ including effects of along-wind-diffusion is a function of time t , distance x downwind of the release location, crosswind distance y , and vertical height z ; this function is calculated by means of Gaussian integration of the observer concentration $C(\xi,y,z,t)$,

$$c(x, y, z, t) = \int_0^\infty \frac{C(\xi, y, z, t)}{(2\pi)^{1/2} \sigma_x(\xi)} \exp\left\{-\frac{(x-\xi)^2}{2\sigma_x^2(\xi)}\right\} d\xi \tag{1}$$

In the above equation ξ is the downwind distance from the release point at time t of an observer travelling with the cloud in the downwind direction. At this position the observer observes the concentration $C(\xi,y,z,t)$. In Equation (1) along-wind diffusion is taken into account by assuming that the concentration $C(\xi,y,z,t)$ spreads out around ξ according to a Gaussian distribution with a downwind dispersion coefficient $\sigma_x = \sigma_x(\xi)$. Figure 2 depicts the pre-AWD observer concentration C and the post-AWD concentration c at a short time after the release (time 1; limited AWD effects), and at a larger time after the release (time 2; larger AWD effects).

The downwind dispersion coefficient σ_x consists of two components,

$$\sigma_x(\xi) = \sqrt{\sigma_{xs}^2 + \sigma_{xt}^2} \tag{2}$$

where σ_{xs} is the downwind dispersion due to vertical wind shear and σ_{xt} is the downwind dispersion due to turbulent spread caused by downwind velocity fluctuations; σ_{xs} and σ_{xt} are evaluated as function of downwind distance ξ according to the formulation by Ermak (1986). This assumption is fully consistent with the current finite-duration-correction (FDC) formulation adopted in the UDM to apply AWD effects for finite-duration releases; see Witlox et al. (2013) for further details.

Verification and Testing of New UDM

Verification against HGSYSTEM for dispersion from pool

The case of an instantaneous spill of 10000 kg of butane liquid is considered with both cases of a bund (radius 10m) and no bund (pool on water; dispersion over land). Ambient data applied are stability class D, wind speed at 10m height of 5m/s, temperature 300K and humidity 70%. Furthermore a maximum pool duration of 1 minute is applied, and thus no pool evaporation is assumed to occur after 1 minute.

Figure 4 shows the values predicted by the UDM of butane pool radius and evaporation rate for both cases with and without a bund. It is seen that the immediate butane rainout within the bund results in a virtually steady-state pool of 10 meter radius, 12.3 kg/s evaporation rate and a temperature of 271.8K.

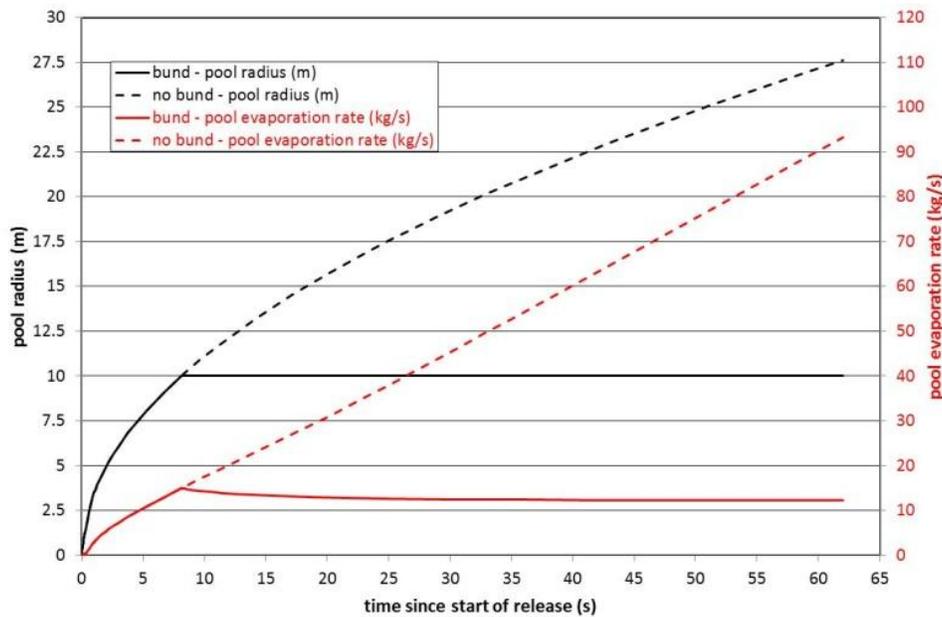


Figure 4. UDM pool predictions (instantaneous 10000kg spill of butane on water)

Figure 5 includes results of the following calculations for the case of a banded pool:

- HGSYSTEM 3.0 calculations (the rectangular HEGADAS source was chosen to be square with the same area as the UDM pool)
 - steady-state HEGADAS-S calculations (ground-level steady-state heavy-gas dispersion from area source) based on the steady-state pool data mentioned above.
 - FDC finite-duration correction (using Ermak's formula) to above HEGADAS-S results (60 seconds duration) using the post-processor program POSTHS
 - HEGADAS-T calculations (ground-level time-varying heavy-gas dispersion from area source). In line with the new UDM model, no gravity-shape correction was applied and the along-wind-diffusion coefficient was chosen to be based on Ermak's formula (non-default HEGADAS-T options)
- UDM calculations
 - Steady-state UDM calculations based on the above steady-state pool data
 - FDC correction to the above steady-state UDM results (60 seconds duration)
 - UDM AWD calculations, with 30 observers released from the upwind edge of the pool

Figure 5a includes the steady-state HEGADAS-S and UDM results of the centre-line ground-level concentrations in the near-field for the case of a steady-state pool. HEGADAS-S assumes a uniform concentration (top-hat profile) above the area source (about 15% mole fraction), which is envisaged to lead to an over-prediction near the source. On the other hand, the UDM model more rigorously solves the dispersion equations across the pool allowing for a variation of the concentration across the pool. The very rapid decrease predicted by the UDM of the concentration near the upwind edge of the pool is a numerical artefact and may not occur in reality. Further downwind from the pool a closer match is observed between the UDM and HEGADAS-S data.

Figure 5b includes results of all the above calculations. It includes results of the time-varying dispersion calculations by UDM AWD and HEGADAS-T at output times 300s, 600s and 1200s. It is seen that the maximum values of these curves correctly touch the maximum centre-line concentration (maximum value over all times) predicted by UDM FDC and HEGADAS-S FDC, respectively. This confirms that the AWD integration is carried out correctly by both programs and is consistent with the FDC formulation. Also adequate agreement between the UDM and HEGADAS FDC results is observed. It is seen that initially the HEGADAS-T cloud is more heavy (larger concentrations) and therefore moves more slowly than the UDM AWD cloud, but this effect reduces in the far-field when the predictions become closer.

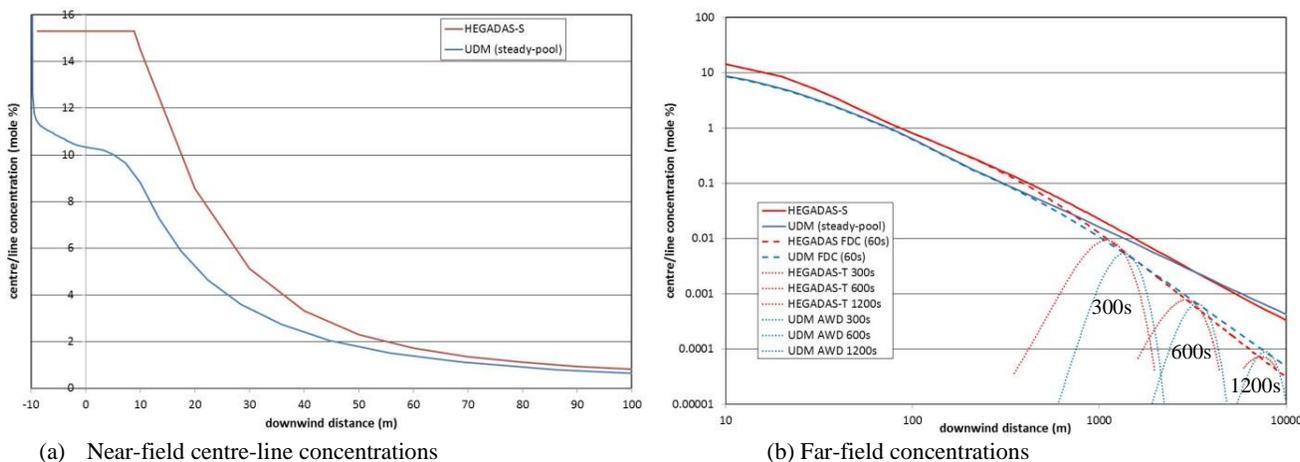


Figure 5. UDM verification against HEGADAS for spill of butane with bund (radius 10m)

Likewise, Figure 6 includes UDM AWD and HEGADAS-T results at times 300s, 600s and 1200s for the case without the bund. Here the UDM calculated pool data were specified as input to HEGADAS-T with a step size of 2 seconds. The observed differences are confirmed to be very similar to that seen for the case with the bund (compare Figures 5b and 6).

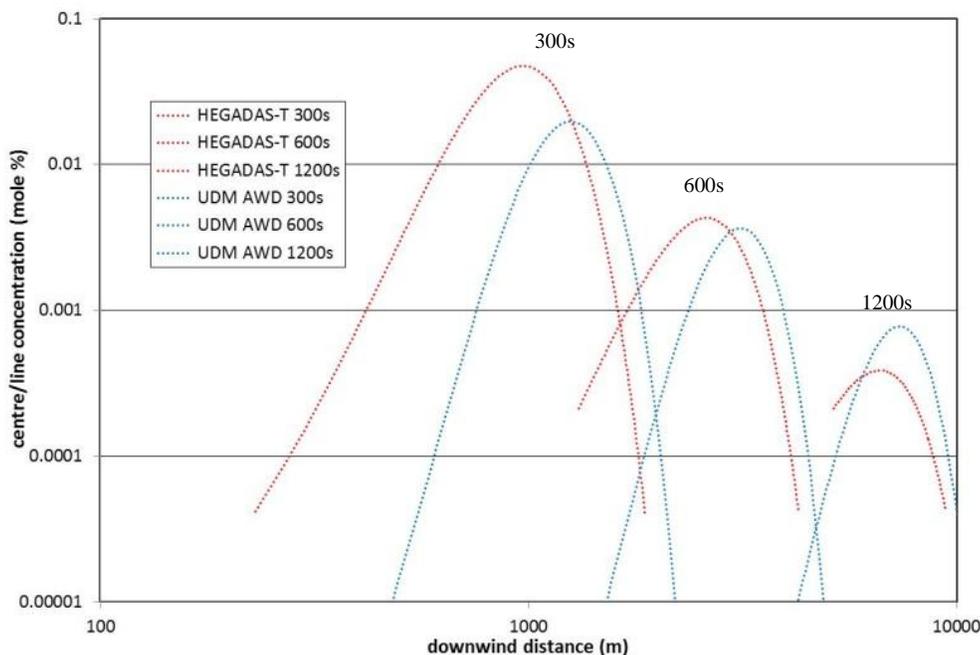


Figure 6. UDM verification against HEGADAS for spill of butane without bund

Elevated chlorine release with rainout

This section includes results for a horizontal chlorine release at elevation height of 1m with a constant release rate of 100kg/s for a duration of 50 seconds. The post-expansion data are chosen to correspond with 100% liquid chlorine at its boiling point (213.9K) with a release velocity of 10m/s and an initially presumed SMD droplet size of 0.001m. Ambient data applied were stability D5, temperature 298K and humidity 70%. Furthermore a maximum pool duration of 500 seconds was applied, and thus no pool evaporation is assumed to occur after 500 seconds. Two observers were released from the release point (at start and end of the release) and subsequently 30 observers were released from the pool.

About 90% rainout was predicted at about 5m downwind distance from the release point. Figure 7a shows the values predicted by the UDM of radius and evaporation rate for the un-banded chlorine pool (pool duration of 500s). The pool radius and evaporation rate are seen to increase rapidly until about 55s at which time the minimum pool thickness is reached. Following this the pool breaks up into wet spots modelled in the UDM by a reducing effective pool radius. The pool evaporation is terminated at the maximum pool duration of 500s.

Figure 7b includes results of both observer concentrations (prior to inclusion of AWD effects; dashed curves) and concentrations after inclusion of AWD effects (solid curves) at output times of 300s, 600s, 1000s and 1500s. Also results are included using the Phast 6.7 UDM segment method (dotted curves). At 300s the release is still on-going, and therefore AWD effects are seen to be only pronounced at the downwind edge of the cloud. With increasing cloud travel times, AWD effects erode concentrations at the upwind and downwind edges of the cloud and increase its cloud length. The pre-AWD observer concentrations predicted by the new UDM observer method are seen to be comparable with the discontinuous segment concentrations predicted by Phast 6.7. Released observers observe a very rapidly reducing discharge rate from the start of the release and this explains the increase of pre-AWD concentration with distance shown in Figure 7b near the downwind edge of the cloud. The new UDM method predicts reduced post-AWD concentrations which are considered to be more accurate. Note that while the AWD cloud at 1500s appears to be much larger than its pre-AWD equivalent, the concentration scale is logarithmic and mass is conserved between the two methods.

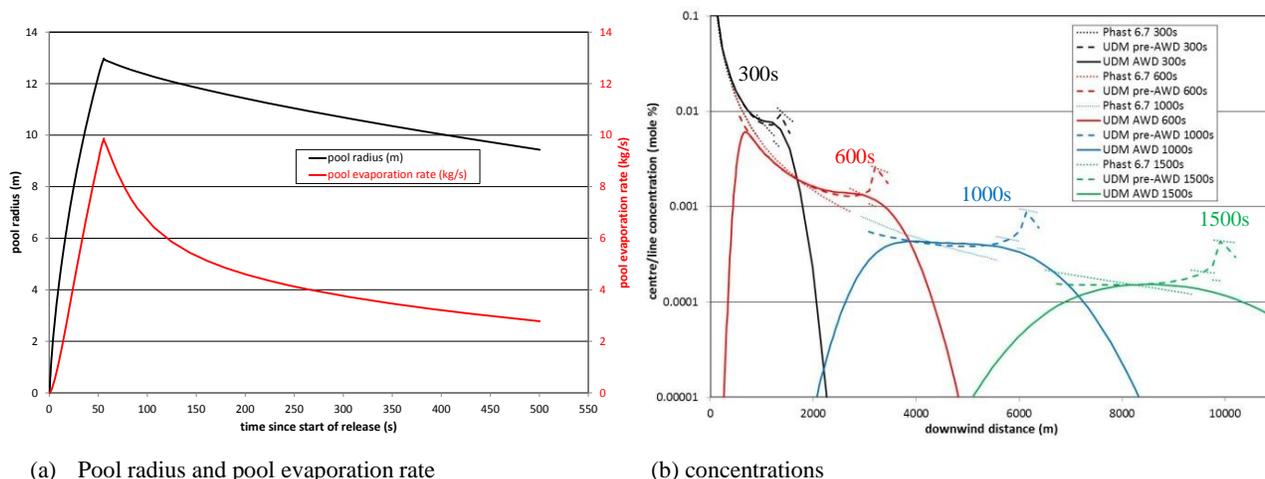


Figure 7. UDM AWD predictions for elevated Cl₂ release with rainout

Elevated sour-gas release from long pipeline without rainout

The example is considered of the time-varying dispersion arising from the time-varying discharge of a sour-gas mixture (including hydrogen sulphide, H₂S) from a long pipeline; see Figure 8.

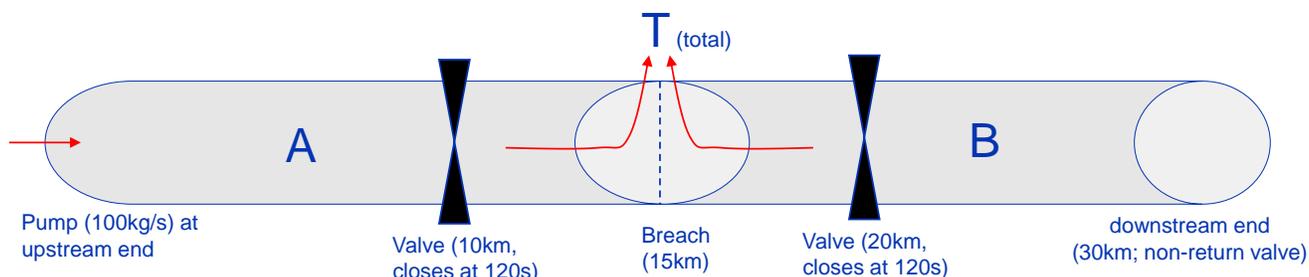


Figure 8. Schematic figure illustrating pipe geometry and breach/valve locations

Input data

Input data are selected corresponding to a long pipeline representative of some extremely sour fields found in the Middle East that are now being developed.

The molar composition of the sour-gas mixture is chosen as follows: CO₂ (10%), H₂S (35%), methane 50%, ethane 1.5%, propane 1.5%, butane 1% and pentane 1%. This corresponds to a molecular weight of 26.77 kg/kmol. The release is presumed to occur following a full-bore rupture at the middle of a 30km long pipeline (inner diameter 30", roughness 45.7µm typical for carbon steel), with a normal production rate of 100 kg/s and with line block valves (LBVs) located at 10km and 20km from the upstream end (closing at 120 seconds). Prior to the breach the mixture temperature inside the pipe is presumed to be 60°C and the upstream pressure 70barg, where the pressure is defined by the receiving plant Acid Gas Removal Unit's ideal operating conditions.

Selected ambient data input to the UDM dispersion calculations are a temperature of 35°C, a pressure of 1 atm., humidity 60% and weather class D5 (neutral conditions, wind speed 5m/s at 10m height). The selected surface roughness is 1.3cm and an averaging time of 600s was adopted for inclusion of effects of wind-meander for far-field passive dispersion.

High-risk sour gas pipelines are normally buried to minimize the risk of external interference and a rupture would create a crater but for simplicity and to demonstrate the difference between the UDM methods the pipeline has been assumed to be routed above ground.

Discharge calculations; evaluation of observer release data

The Phast model GASPIPE was used to calculate the time-varying discharge rate from the pipe. Here the GASPIPE model models the sour-gas mixture as a non-ideal gas; see the GASPIPE theory manual for details (Webber, Witlox and Stene, 2011). Here the total discharge rate (T) is obtained from summing the discharge rates from the upstream branch A and the downstream branch B. It is

conservatively presumed that this results in a single plume with horizontal release direction at 1m elevation height. Default Phast parameters were presumed otherwise for the GASPIPE calculations except that conservation of momentum was assumed (for expansion from breach pressure to ambient pressure) and no velocity cut-off was applied for the post-expansion velocity.

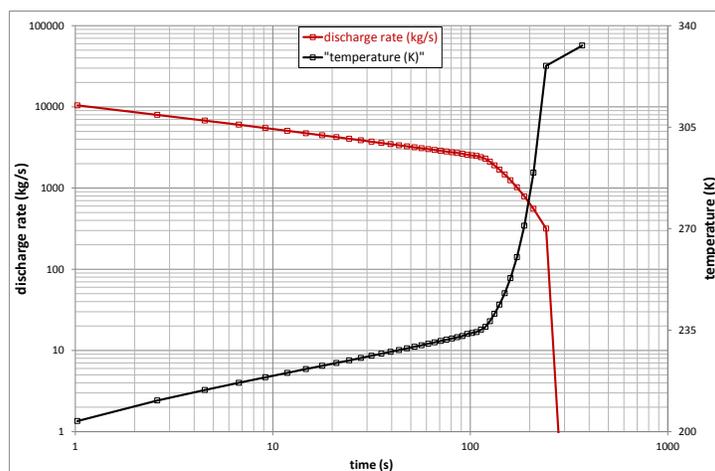


Figure 9. GASPIPE predictions for time-varying discharge from sour-gas long pipeline

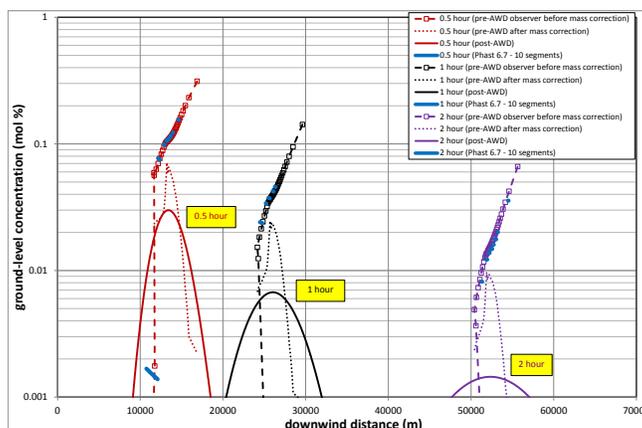
Figure 9 includes results of GASPIPE predictions of the total time-varying discharge rate and the post-expansion temperature. Initially the pressure immediately upstream of the breach is significantly larger than the ambient pressure, and therefore the subsequent depressurization to ambient pressure results in significantly cold plumes (colder than ambient air; touching down on the ground), while for the final times no cooling occurs resulting in a hot plume of 60°C (slightly lighter than ambient air; rising in the air). 41 observers were chosen to be released based on 40 equal discharge mass segments, and the markers in Figure 9 indicate the corresponding observer data.

Dispersion results – concentration predictions

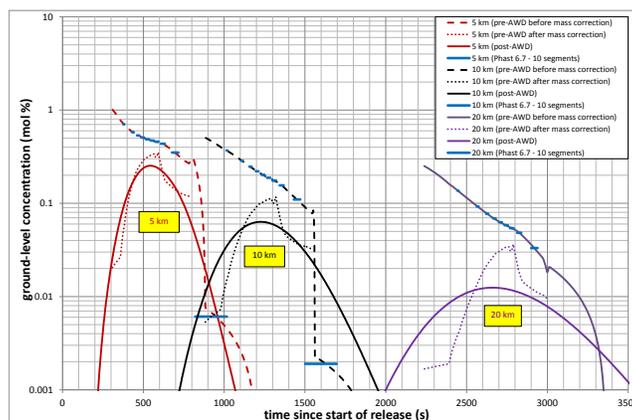
The new UDM AWD algorithm (Section 2) was applied based on the release data for the above 41 observers, while the old Phast 6.7 UDM method (Section 1) was applied based on 10 equal-mass segments.

Figure 10 includes results for the predicted ground-level concentration of the sour-gas mixture versus distance (at times 0.5, 1, 2 hours) and time (at distances 5, 10, 20 km). The old Phast 6.7 results (discontinuous segments) are indicated by blue curves, while the new UDM results are given by red curves (at 0.5 hour or 5 km), black curves (at 1 hour or 10 km) or purple curves (at 2 hours or 20 km). The observer concentrations prior to mass correction are indicated by dashed curves with the markers in Figure 10a indicating the location of the observers. Observer concentrations after inclusion of the mass correction are indicated by dotted curves. The concentrations after inclusion of both AWD and mass correction effects are indicated by solid curves, and these are obtained by means of Gaussian integration over the observer concentrations; see Equation (1).

Figure 10 shows that the Phast 6.7 segment predictions (blue curves) are very close to the new UDM pre-AWD predictions before mass correction. In this example the release rate for consecutive segments reduces rapidly, the cloud segment dilutes faster and therefore moves slower resulting in gaps between segments which increase with time and distance downwind. This gap ensures that mass is conserved, but in reality the cloud would not exist as a discontinuous sequence of segments – concentrations would be lower but continuous and therefore concentrations (and other results sensitive to concentration) will be over-estimated in Phast 6.7. It is this effect that the mass correction factor simulates. Uncorrected observer concentrations are in very close agreement with Phast 6.7, but interpolating continuously between these concentrations will effectively create additional mass in the cloud – it is analogous to having Phast 6.7 segments without the gaps. The mass correction reduces concentrations significantly, and this reflects the along-wind ‘stretching’ of the cloud as early observers travel faster downwind than later ones. It should be noted that the correction illustrated in this example is very large due to the highly time-varying nature of the release.



(a) concentration versus distance at 0.5, 1 and 2 hours



(b) concentration versus time at 5, 10 and 20km

Figure 10. UDM predictions of ground-level sour-gas mixture concentration

The discussion so far has excluded any consideration of along-wind diffusion, shown by the solid lines in Figure 10. It too reduces concentrations and elongates the cloud, but it is important to recognize that it models a different physical process, and frequently will have a much more significant effect than mass correction (e.g. for continuous finite-duration releases). With increasing cloud travel times AWD effects erode concentrations at the upwind and downwind edges of the cloud, and increase cloud length (Figure 10a) or passage time for a particular distance (Figure 10b). AWD is more effective at reducing concentrations as distance increases. AWD effects are not included by the Phast 6.7 segment method and therefore this method produces conservative results.

Dispersion results – dose predictions

Figure 11 includes pre-AWD (before and after mass correction) and post-AWD results of the ground-level dose (toxic load D) which is derived by means of integration of UDM concentrations over time,

$$D = \int (f_{H_2S}c)^N dt \tag{3}$$

Here $f_{H_2S}=0.35$ is the mole fraction of toxic H_2S in the sour-gas mixture, and $c = c(x,y=0,z=0;t)$ is the ground-level concentration (ppm). N is a material-specific probit parameter. Figure 11 also includes doses associated with levels published online by the UK HSE (2013), i.e. SLOD (significant likelihood of death; 50% mortality) and SLOT (specified level of toxicity; 1% mortality); HSE adopts a value of N=4 and therefore this has been applied in the current calculations. In addition Figure 11 includes doses derived from Acute Exposure Guideline Levels AEGL3 (mortality may occur) and AEGL2 (irreversible effects) as issued by the USA EPA (2012).

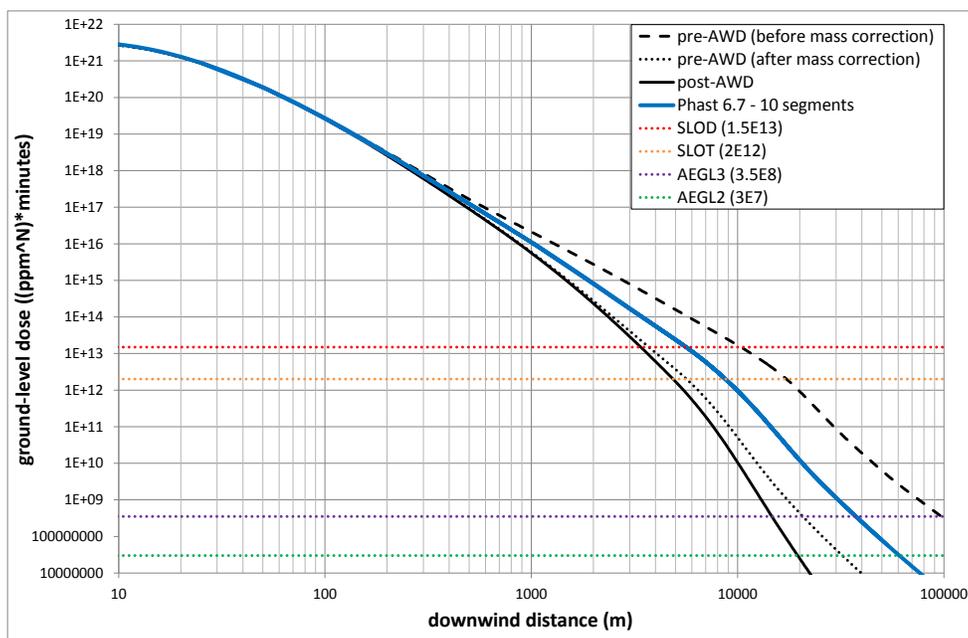


Figure 11. UDM predictions of dose versus downwind distance

Figure 11 demonstrates that in the near-field (up to around 300m), gaps between the Phast 6.7 segments are small and also mass-correction and AWD effects are limited, and therefore all dose results match each other closely.

Further downwind, however, the doses start to diverge. Before the mass correction is applied, the doses are greater than those of Phast 6.7. This indicates that the observers are drifting apart and the cloud elongating. As a consequence additional mass is created which accounts for the increased dose. The mass-corrected dose on the other hand is less than the Phast 6.7 dose. This is because there is a non-linear relationship between concentration and dose – i.e. the N value in Equation (11) is > 1 and dose will be highly sensitive to concentration. The Phast 6.7 approach uses segments with gaps in-between and, as already discussed, this will mean that concentrations and therefore doses are too high since N is larger than 1. Using the reduced value of $N=1$ it was confirmed that toxic dose results are virtually identical between Phast 6.7 and the pre-AWD results after mass correction, since both methods ensure conservation of cloud mass.

Further downwind AWD effects lead to a further reduction in dose, and the magnitude on this effect increases with distance downwind.

For other scenarios where the Phast 6.7 mass release rate reduces less rapidly between subsequent observers and segments and where the duration is relatively short, the mass correction effects would be expected to be less significant and the AWD effects relatively more significant. The authors consider that the newly proposed less conservative UDM approach including mass-correction and AWD effects is preferable for predicting toxic loads associated with toxic releases.

Conclusions and Future Work

The following main conclusions can be drawn:

- The Phast dispersion model UDM has been extended to improve modelling for time-varying ground-level or elevated releases (with or without rainout). The new formulation presumes a number of ‘observers’ to be released at successive times from the point of discharge. The UDM first carries out pseudo steady-state calculations for each observer, where the release data correspond to the time at which the observer is released. Secondly the model applies a correction to the observer concentrations to ensure mass conservation in case of subsequent observers moving with different velocities. Finally the effects of along-wind diffusion are included by means of Gaussian integration over the downwind distance.
- In the new model (Figure 2) the flow-rate and pool-evaporation rate are no longer divided into discontinuous segments. In the old model (Figure 1) the equations were discontinuously modified at the original point of rainout to account for the vapour added back from the entire pool, and no along-wind-diffusion was applied. In the new model the cloud adapts continuously to the presence of an evaporating pool.
- The new method is based on a generalization of the HGSYSTEM model HEGADAS-T or dispersion from area sources. It is fully consistent with the existing UDM finite-duration correction (FDC) method for the case of finite-duration continuous releases. This has also enabled an independent verification between the two formulations to demonstrate correct implementation

of both formulations. Furthermore the FDC formulation has been shown to provide accurate results against experimental data (Kit Fox experiments), and this therefore provides added confidence for the new time-varying formulation.

- The new UDM AWD model has been verified against HEGADAS-T for the case of dispersion from a ground-level area source and good agreement was obtained. In a separate application for source gas releases from a long pipeline (Witlox and Harper, 2008), the new UDM AWD model was verified against HEGADAS-T and good agreement was obtained for application of both the FDC correction method (for finite-duration releases) as well as the application of the observer concept (for time-varying releases).
- For a range of example cases (dispersion from pool, elevated releases with and without rainout) the new UDM calculations are shown to potentially significantly reduce concentrations and doses in the far-field relative to Phast 6.7.

The current further work is being planned:

- More rigorous implementation of mass correction
- Extension of UDM instantaneous model to account for along-wind-diffusion after rainout.
- The current new model includes effects of along-wind-dispersion resulting from ambient turbulence corresponding to passive dispersion. For heavy-gas continuous or time-varying releases, it only takes into account gravity spreading in the cross-wind direction and not gravity spreading in the downwind direction. Thus the model is recommended to be extended to include effects of along-wind gravity spreading, which are particularly relevant in the near-field in the case of small wind speeds
- Validation against experimental data
- Implementation of new UDM AWD model into Phast
- Further refinement of empirical formulas for along-wind-diffusion coefficient σ_x

Reference

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Acknowledgement

Financial support of the work reported in this paper was provided by DNV Software, RIVM (Dutch Government), and TOTAL. The contents of this paper including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect the policy of these organizations.