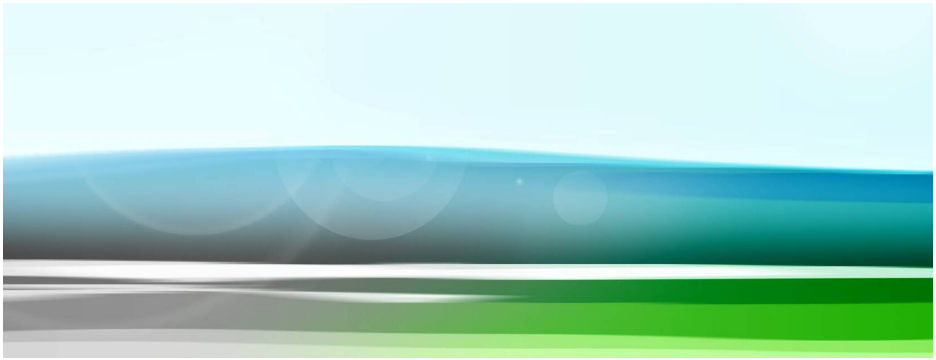

Modelling of time-dependent dispersion for releases including potential rainout

Henk Witlox and Mike Harper – DNV Software

UKELG 50th Anniversary Discussion Meeting
9 – 11 July 2013, Cardiff University

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Modelling of time-varying dispersion for releases including rainout

- 1. Introduction
- 2. Current Phast dispersion model UDM (versions 6.7 and 7.01)
- 3. Improved UDM model including along-wind-diffusion effects
- 4. Testing and verification of new UDM model against HGSYSTEM
- 5. Main conclusions and future work

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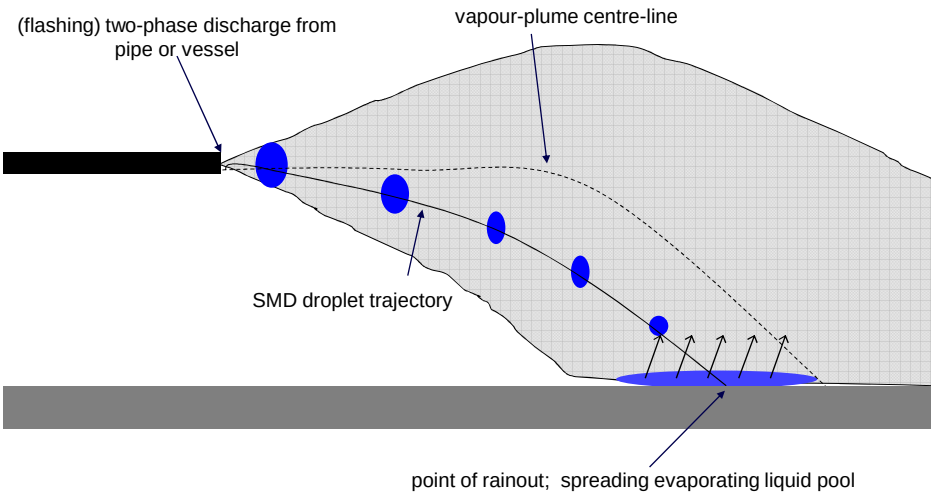
1. Introduction

Discharge, droplet dispersion, rainout and re-evaporation

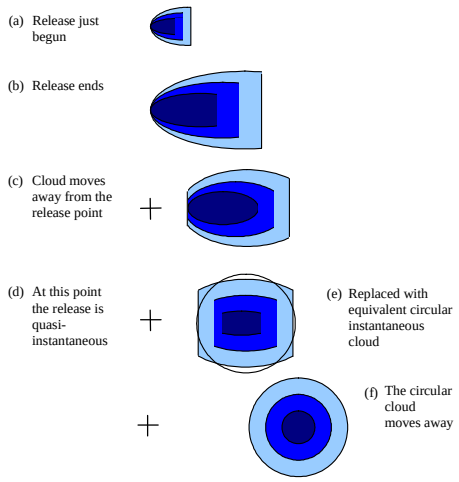


Background – Modelling of time-varying dispersion

- Effects of along-wind-diffusion (AWD): more dilute cloud, increased downwind length
- Early nineties –time-varying heavy-gas dispersion model HEGADAS-T (HGSYSTEM)
  - Dispersion from ground-level area source
  - Release of “Observers” from area source; include AWD effects via integration
  - No rainout modelling, no time-varying dispersion directly from time-varying discharge
- Modelling of time-varying dispersion by Phast model UDM
  - Phast 6.7/7.01: no AWD effects for time-varying releases or time-varying pools
  - (2001) UDM (Phast) validation against Kit Fox experiments (Exxon Mobil)
    - finite-duration release from ground-level source
    - UDM validation based on finite-duration correction (FDC) method
  - (2008-2011) UDM modelling for time-varying releases with or without rainout
    - Sponsors: DNV,RIVM, TOTAL
    - UDM simulation of time-dependent dispersion including along-wind diffusion (observer concept)
    - Verification of UDM against HGSYSTEM (FDC and time-varying)

2. Current Phast dispersion model UDM (versions 6.7 and 7.01)

Finite-duration release: quasi-instantaneous model (Phast default)



- Continuous/instantaneous transition if width/length ratio large
- disadvantages:
  - Abrupt transition
  - Less accurate along-wind diffusion

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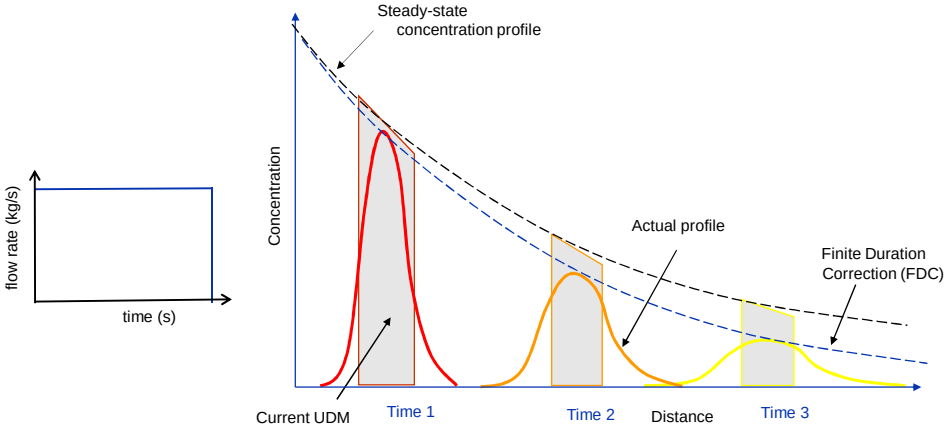
Finite-duration release: finite-duration correction (FDC) method

(Phast alternative option; improved accuracy for validation against Kit Fox experiments)



- Carry out steady-state calculations for single segment
- Apply along-wind-diffusion by finite-duration correction (accounts for wind shear and turbulent spread)
- Disadvantage: predicts maximum concentration only (no cloud width/length, dose)

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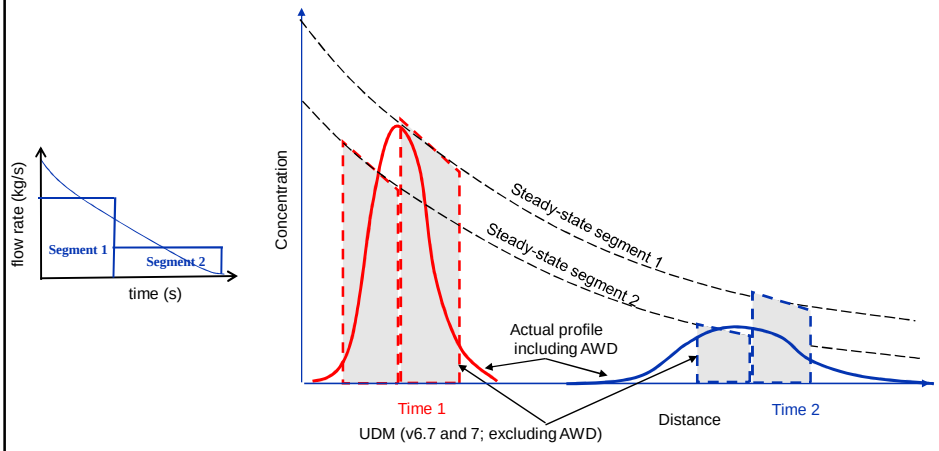
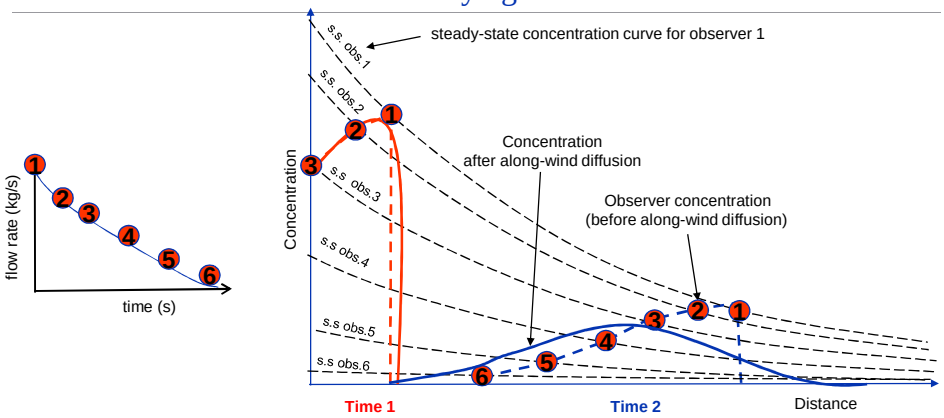
Time-varying release: UDM multi-segment method



- Divide released mass into equal-mass segments
- Carry out steady-state calculations for each segment
- At each output time set segment concentrations [before along-wind-diffusion]

3. Improved UDM model including along-wind-diffusion effects

New observer method for time-varying release



- Release observers at regular time intervals
- Carry out steady-state calculations for each observer
- At each output time set observer concentrations [before along-wind-diffusion]
- Apply along-wind diffusion and downwind spreading

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UDM along-wind diffusion formulation

(elevated finite-duration or time-varying release with no rainout, or dispersion from pool)

- "Observers" are released from source moving with UDM speed
- Algorithm to set concentration as function of position x and time t
  - Carry out Phast time-varying source-term calculations (flow rate or pool evaporation rate)
  - Divide in equal-mass segments
  - Calculations for each observer
    - Release observer at start of segment
    - Set time-varying observer data (downwind position ξ, concentration $C_o(\xi)$, …) from steady-state UDM run
  - At given time t , apply along-wind-diffusion by Gaussian integration over observer concentrations:

$$c_o(x,t) = \int_0^\infty \frac{C_o(\xi)}{(2\pi)^{1/2}\,\sigma_x(\xi)} \exp\left\{-\frac{(x-\xi)^2}{2\sigma_x^{\,2}(\xi)}\right\} d\xi$$

- Assumptions
  - Ignore along-wind gravity spreading (no gravity shape correction)
  - No automation of observers and output times
  - Use along-wind-diffusion coefficient σ_x consistent with FDC method

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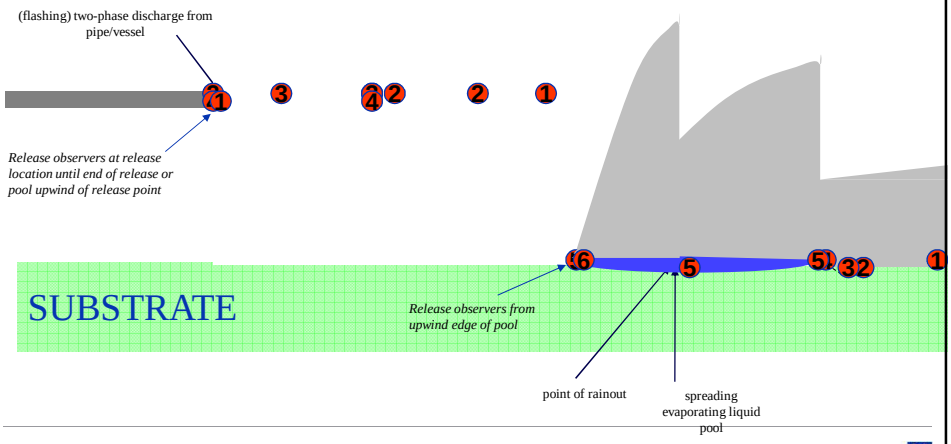
UDM link pool and dispersion (before, during and after rainout)



UDM along-wind diffusion formulation (non-instantaneous release with rainout)

- "Release observers" are released from source until upwind pool upwind of observers
  - Solve original UDM equations before rainout and upwind of pool
  - Adjust observer variables at observer rainout, and solve additional pool equations after rainout
  - Solve extended UDM equations to account pool-vapour pickup for observer above pool
- "Pool observers" released from upwind edge of pool afterwards
- Set AWD concentration as function of position x and time t:

$$c_o(x,t) = \int_0^{\infty} \frac{C_o(\xi)}{(2\pi)^{1/2}\,\sigma_x(\xi)} \exp\left\{-\frac{(x-\xi)^2}{2\sigma_x^{\,2}(\xi)}\right\} d\xi$$

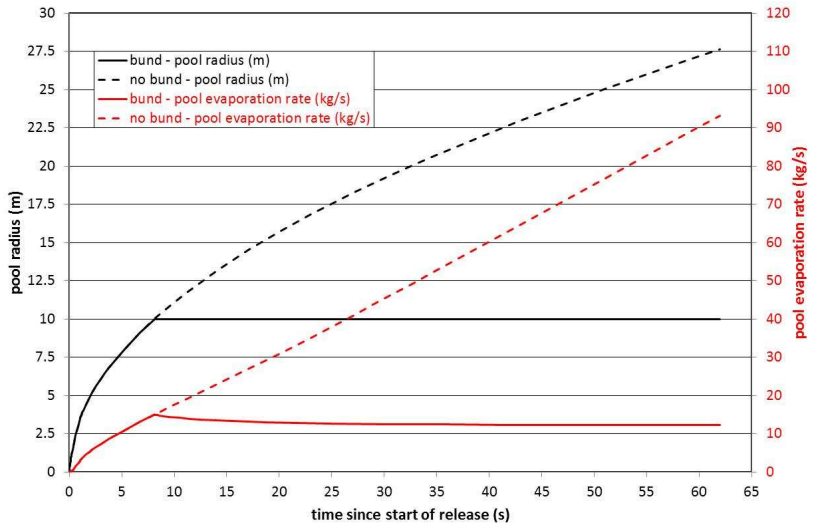
4. Testing and verification of new UDM model against HGSYSTEM

- steady-state/FDC release - CO2 area source (Kit Fox)
- time-varying release without rainout (Kashagan)
- time-varying release from butane pool

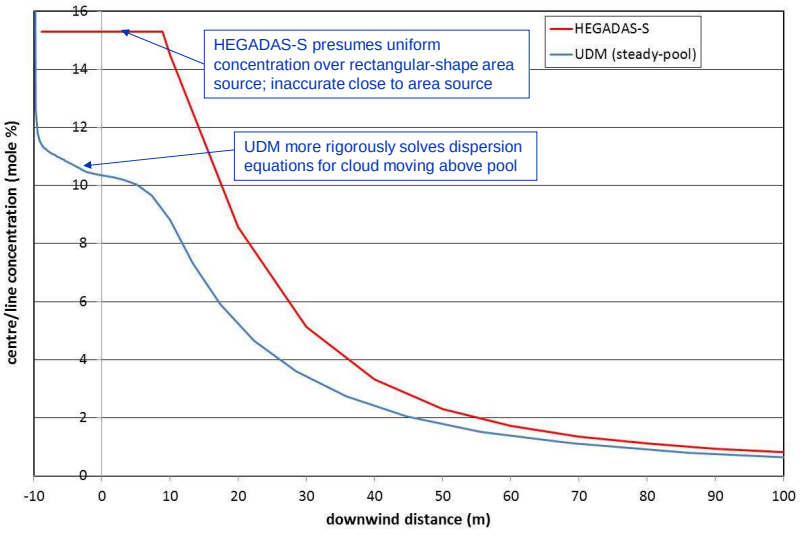
Verification against HGSYSTEM (dispersion from butane pool without or with bund)

- Problem
  - Immediate spill of 10000 kg butane onto ground
    - With bund of 10m radius
    - Without bund
  - Pool on water and dispersion on land; 1 minute maximum pool duration
  - Ambient data: 300K, weather D5, humidity 70%
- HGSYSTEM 3.0 calculations (DOS)
  - HEGADAS-S: ground-level steady-state heavy-gas dispersion from area source
  - POSTHS: post-processing (for FDC calculations)
  - HEGADAS-T: ground-level time-dependent heavy-gas dispersion from area source
- Selection of HEGADAS input
  - No gravity-shape correction (non-default)
  - Along-wind-diffusion coefficient based on Ermak's formula (non-default)
  - HEGADAS-S rectangular source – chosen as square with same area as UDM pool
- Results
  - HEGADAS results very consistent with UDM results

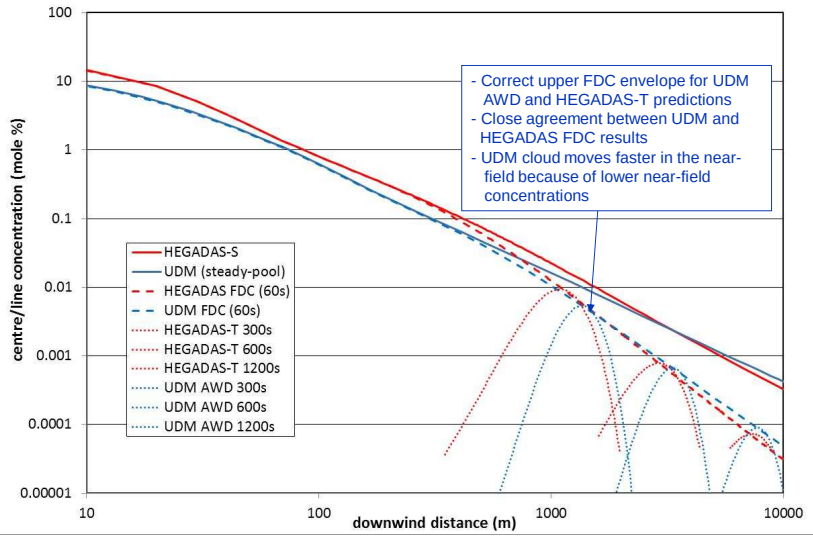
UDM butane pool results (input to HEGADAS-T)



Butane pool with bund –maximum concentration (steady-state, in near-field)



Butane pool with bund – maximum concentration (steady-state, FDC, time-varying)



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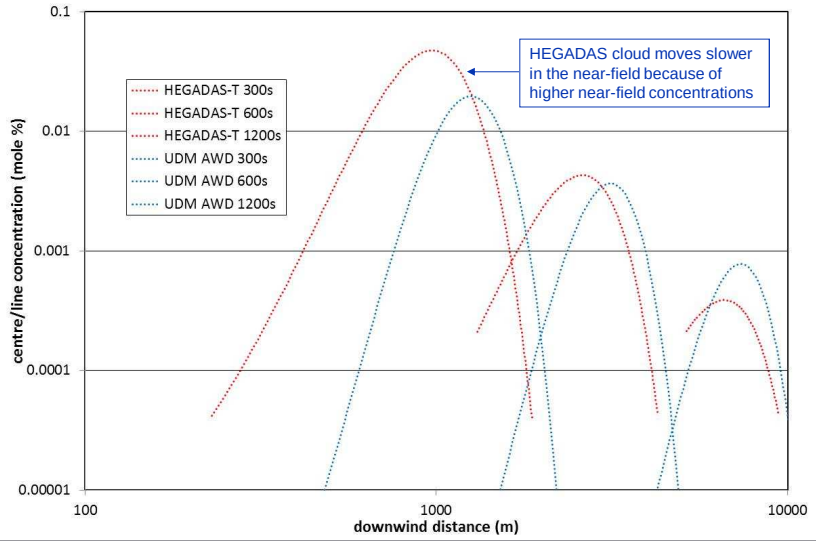
Butane pool without bund - maximum concentrations (time-varying)



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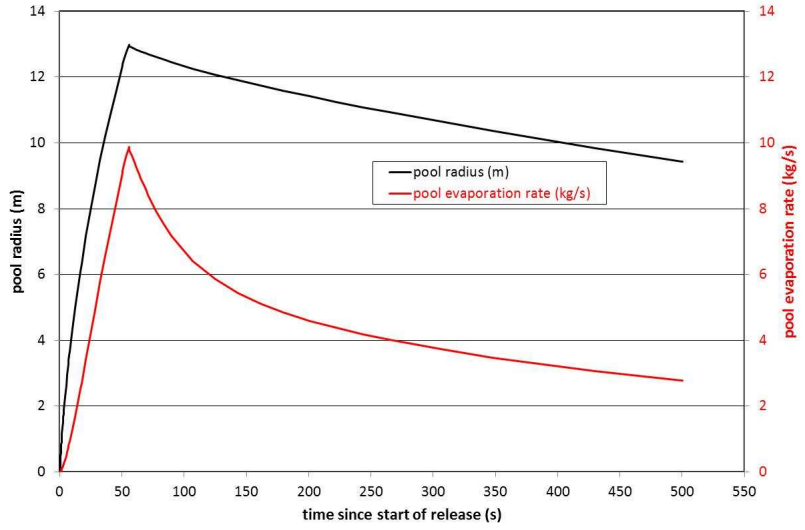
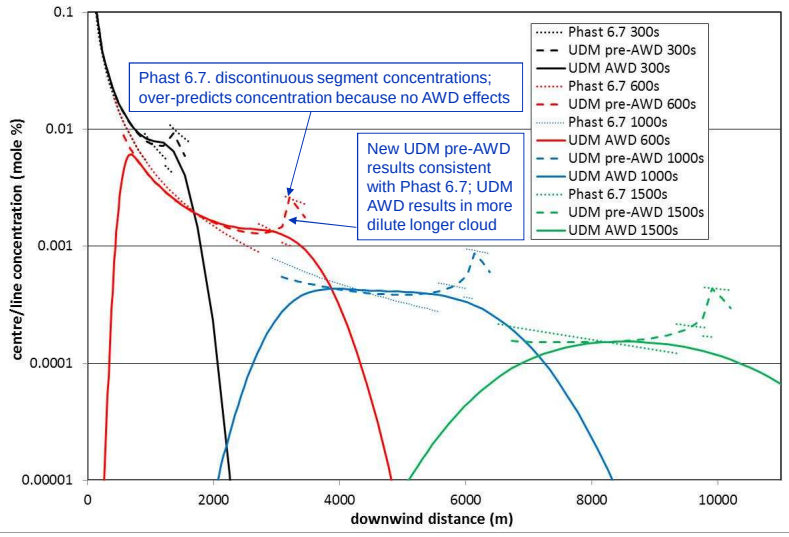
UDM AWD modelling for elevated chlorine release with rainout

- Input data
  - Release data:
    - Horizontal 100kg/s chlorine release with 50s duration
    - Post-expansion data: 100% saturated liquid at its boiling point of 214K, 10m/s, drop size 100μm
  - Pool and dispersion on land; 500 seconds maximum pool duration (no bund)
  - Ambient data: 298K, weather D5, humidity 70%
  - Runs
    - Old Phast 6.7 without AWD effects: multiple pool segments
    - New UDM: 2 observers from release point at 0s,50s and 30 subsequent observers from pool
- Results
  - 90% rainout at 5m downwind distance
  - pool spreading/evaporation
  - Centre-line concentration versus downwind distance (at different output times 300s, 600s, 100s, 1500s)
    - Old Phast 6.7 results (4 pool segments; no effects of along-wind diffusion)
    - New UDM (before and after effects of along-wind-diffusion)

Time-varying pool data: pool radius and evaporation rate



Concentration predictions (old Phast 6.7, new UDM before and after AWD)



5. Main conclusions and future work

Main conclusions

- Algorithm to define observer release data from time-varying discharge or pool models (based on equal-mass segments)
- Time-dependent UDM model including along-wind diffusion (AWD)
  - Scenarios
    - Dispersion from time-varying pool
    - Time-varying elevated release without rainout
    - Time-varying or finite-duration elevated release with rainput
  - Algorithm
    - Sets pre-AWD observer concentrations from steady-state runs (no discontinuous segments)
      - Solves dispersion, droplet and pool equations simultaneously
      - Avoids previous pool segmentation
    - Sets AWD concentrations by integration over downwind distance
  - No longer segments and unrealistically high far-field concentrations
  - Verification against HGSYSTEM
    - Steady or time-varying area source, elevated vapour release
    - consistency with FDC
  - Additional testing for elevated releases with rainout

Future work

- Gravity shape correction to include along-wind gravity spreading
- Implementation into Phast (Safeti)
- Refine formula for along-wind-diffusion coefficient
- Validation against experimental data