

VERIFICATION

UDM THERMODYNAMICS: CHAPTER 4

DATE: December 2023

Droplet Model

Reference to part of this report which may lead to misinterpretation is not permissible.

No.	Date	Reason for Issue	Prepared by	Verified by	Approved by
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1	1999	PHAST 6.0	Witlox and Holt
2	Oct 2005	SAFETI 6.5	Witlox and
3	May 2021	Apply new template	D. Vazier

Date: December 2023

Prepared by: Digital Solutions at DNV

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ABSTRACT

The droplet thermodynamic model is used in conjunction with the equilibrium model to set the droplet trajectories and the point of rainout. In conjunction with the non-equilibrium model, it additionally calculates the droplet mass and the liquid droplet temperature. The main conclusions are as follows.

1. Droplet differential equations are now solved in the UDM simultaneously with other cloud differential equations using standard techniques. The old logic of synchronised solution of the droplet equations has been retained.
2. 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.
3. Under equilibrium thermodynamics, the conservation of vertical momentum equation has been corrected to include droplet evaporation rate. Up to PHAST6.42, this term was included only for non-equilibrium thermodynamics.
4. Under non-equilibrium thermodynamics, when individual droplet mass drops below 10^{-12} kg the model switches to assume thermal equilibrium between liquid and vapour phases. When droplet mass drops below 10^{-17} kg no droplet modelling is done and the model switches to a HEM approach.



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4 DROPLET MODEL

Unless stated otherwise, all cases have used the new rigorous droplet solution method.

4.1 Sensitivity analysis

4.1.1 Droplet trajectories and thermodynamics

A sensitivity analysis is performed using the following base-case:

- 70 kg/s propane release at 20 m/s
- liquid fraction 80 %
- droplet size 1mm
- release height 5m
- duration 3600 s
- weather case D5

The following observations were made:

- The horizontal cloud co-ordinate x_{cloud} matches that of the horizontal droplet co-ordinate x_d . This confirms the adopted theory.
- To ensure a converged solution, ODE solver accuracy should be 10^{-4} or lower.
- The aerodynamic drag force F_{drag} acting on the droplet, causes the droplets to be close to the cloud centre line. Figure 1 illustrates the effect of removal of this force.
- As the droplet diameter decreases the cloud liquid and vapour temperature approaches the equilibrium value; see Figure 2 (results are given prior to the rainout distance only)
- The assumption of thermal equilibrium between liquid and vapour is justified below the implemented cut-off for individual droplet mass of 10^{-12} kg. Figure 3 demonstrates that when the cut-off is reached (at ~ 12.7 m in the plot), phase temperatures are much less than 1K different.
- An additional sensitivity analysis was performed for varying release velocities, wind speeds, release rates and release angles.

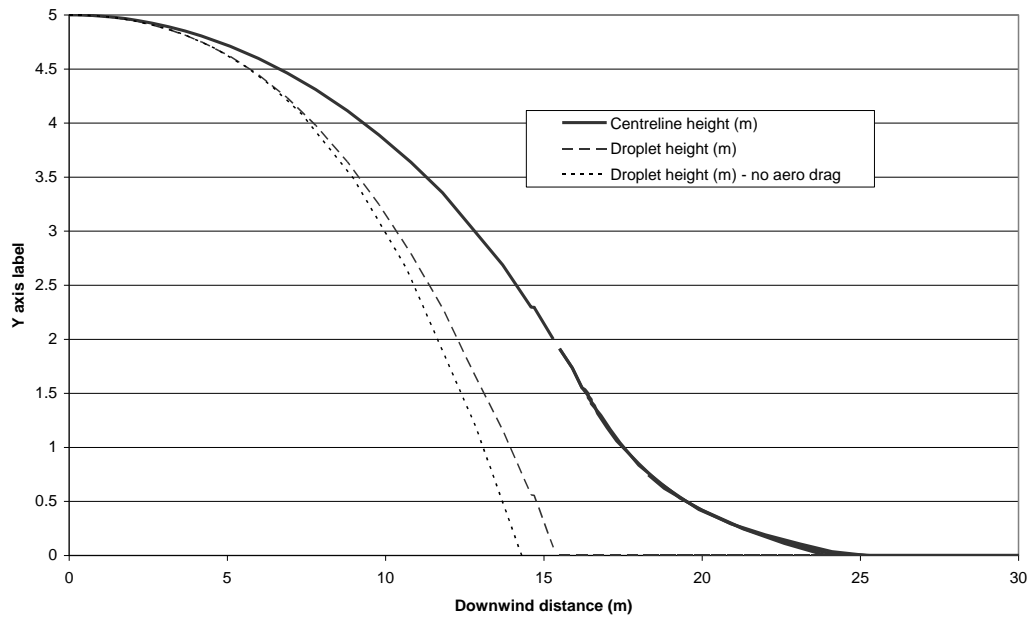
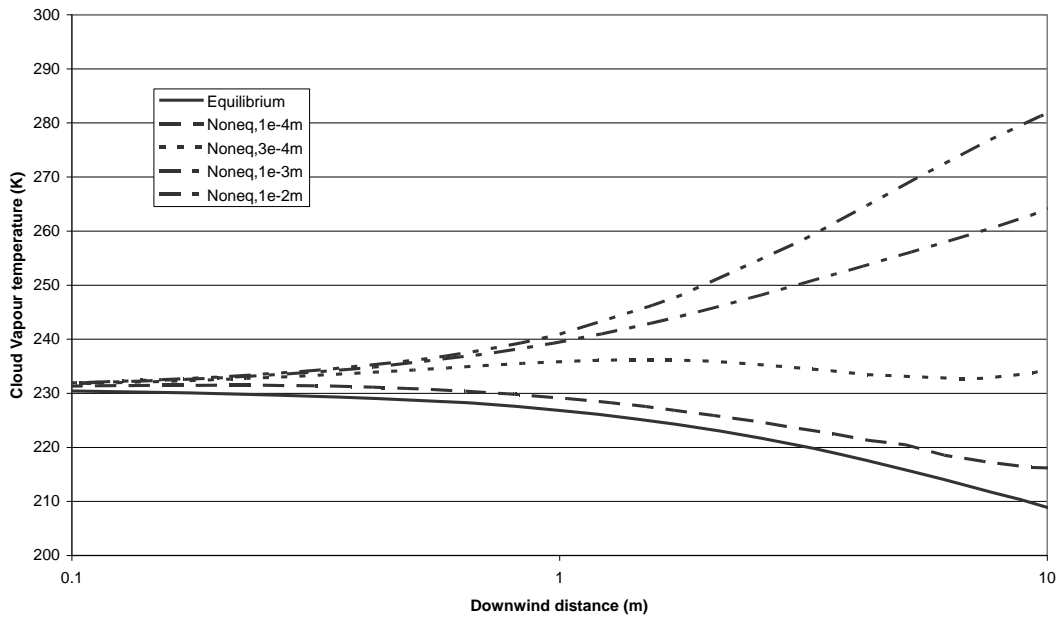
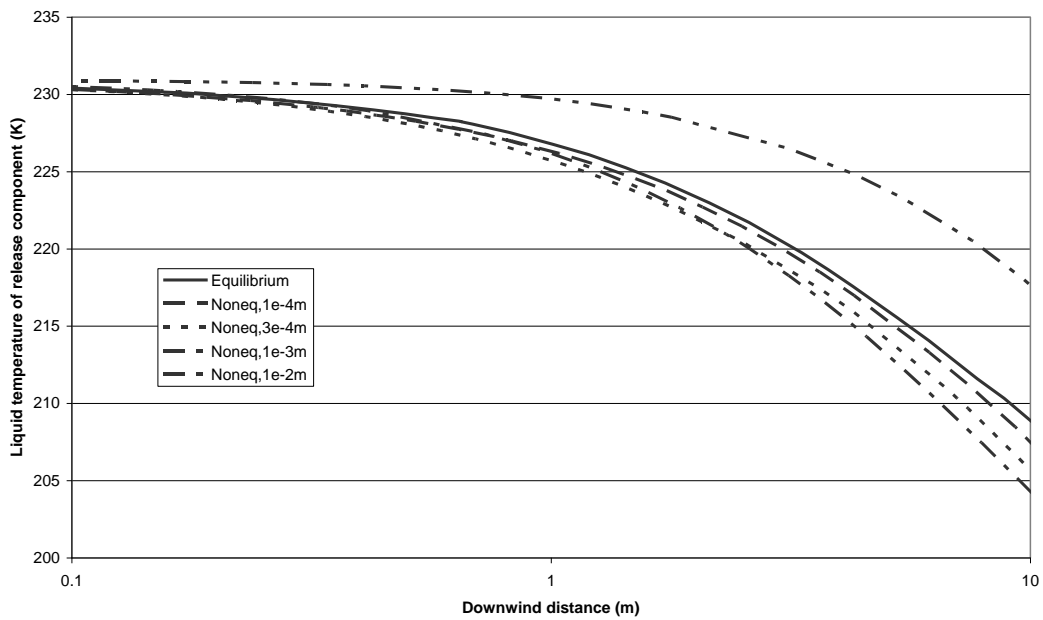


Figure 1. Cloud centre-line and droplet position; (effect of aerodynamic drag)



(a) vapour temperature



(b) liquid temperature

Figure 2. Comparison of equilibrium and non-equilibrium temperatures for a range of droplet diameters

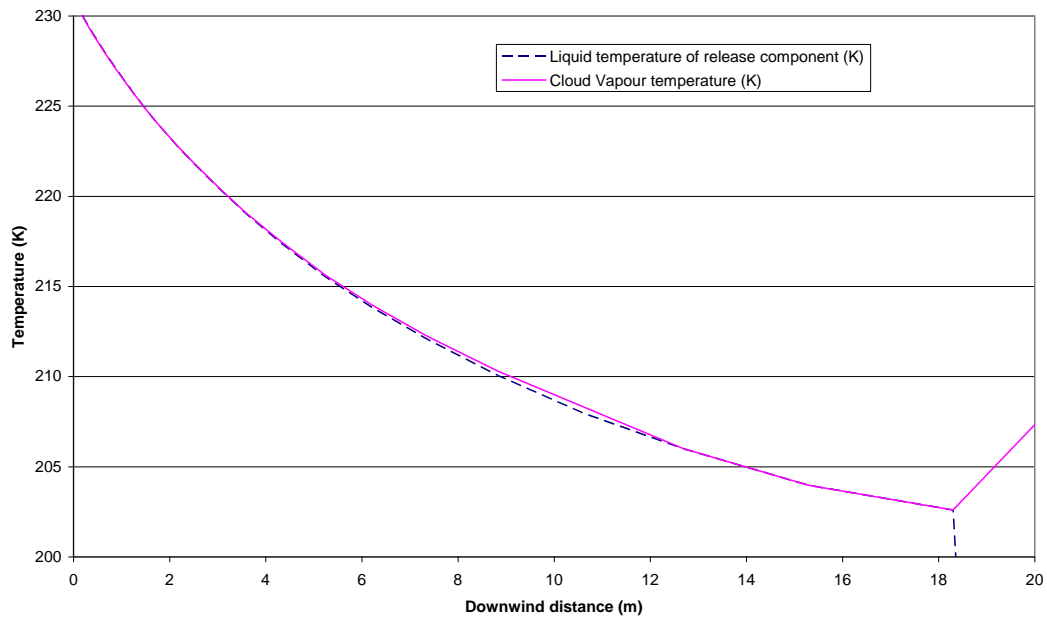


Figure 3. Vapour and liquid temperature for initial droplet size of 1.8×10^{-5} m, showing effect of cut-off for non-equilibrium thermodynamics.

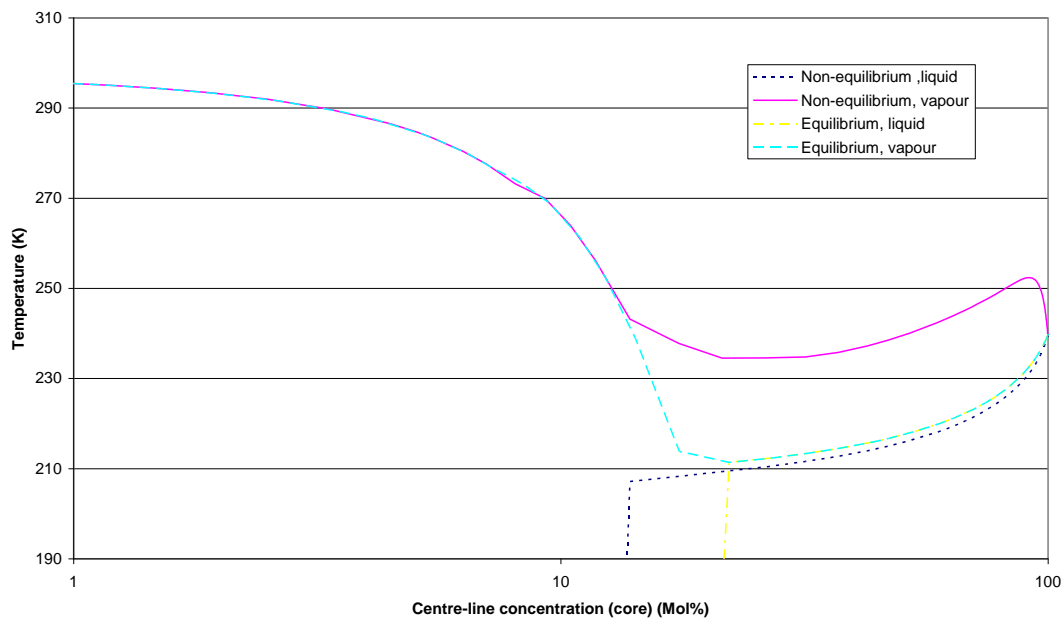
4.1.2 Equilibrium versus non-equilibrium model

UDM runs have been carried out for a range of chemicals, i.e. ammonia, sulphur dioxide and ethylene. The runs were carried out assuming no rainout and heat/water-vapour substrate transfer. Runs were carried out using either the equilibrium model (no droplet equations), or the non-equilibrium model (with droplet equations). A constant temperature profile was adopted. The adopted input data are summarised below.

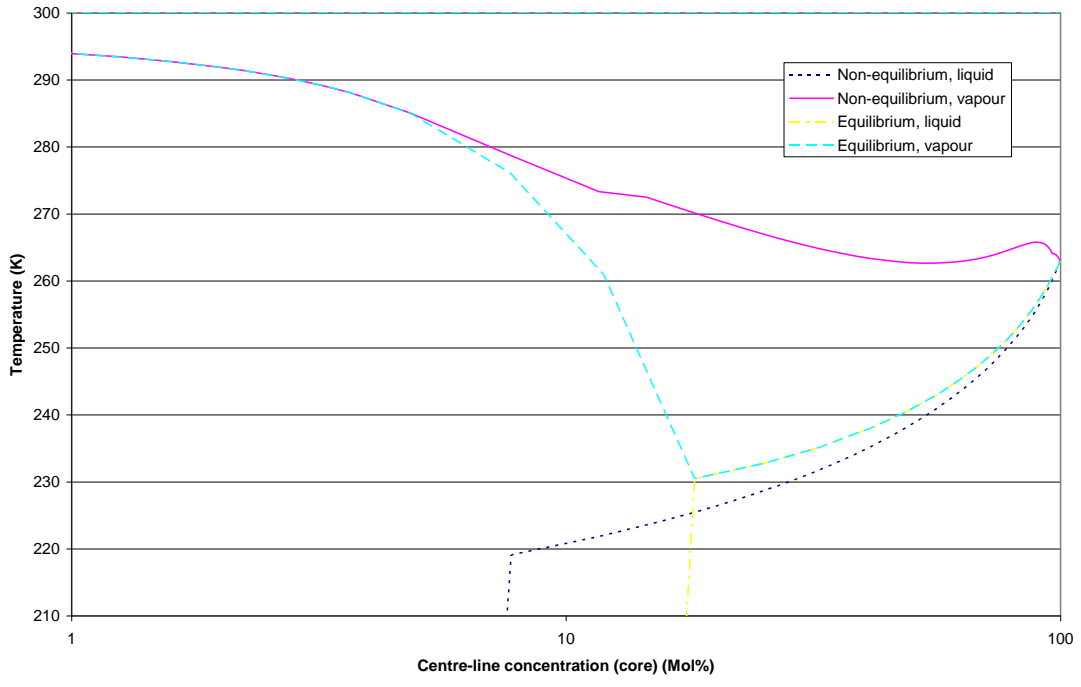
Compound	NH ₃	SO ₂	C ₂ H ₄
release rate (kg/s)	80	5	20
release velocity (m/s)	90.3	10.5	30
liquid fraction	0.83	0.7	0.8
drop size	1E-4	1E-4	1E-4
release height (m)	5	5	10
surface roughness (m)	0.003	0.006	1
stability class	D	D	F
wind speed (m/s) at z _{ref}	7.42	3.3	1
reference height z _{ref} (m)	2	2	10
ambient temperature (K)	302	300.15	298
ground temperature (K)	304.8	300.15	298
duration (s)	126	600	3600

Figure 4 includes the results for the above runs. The following can be observed:

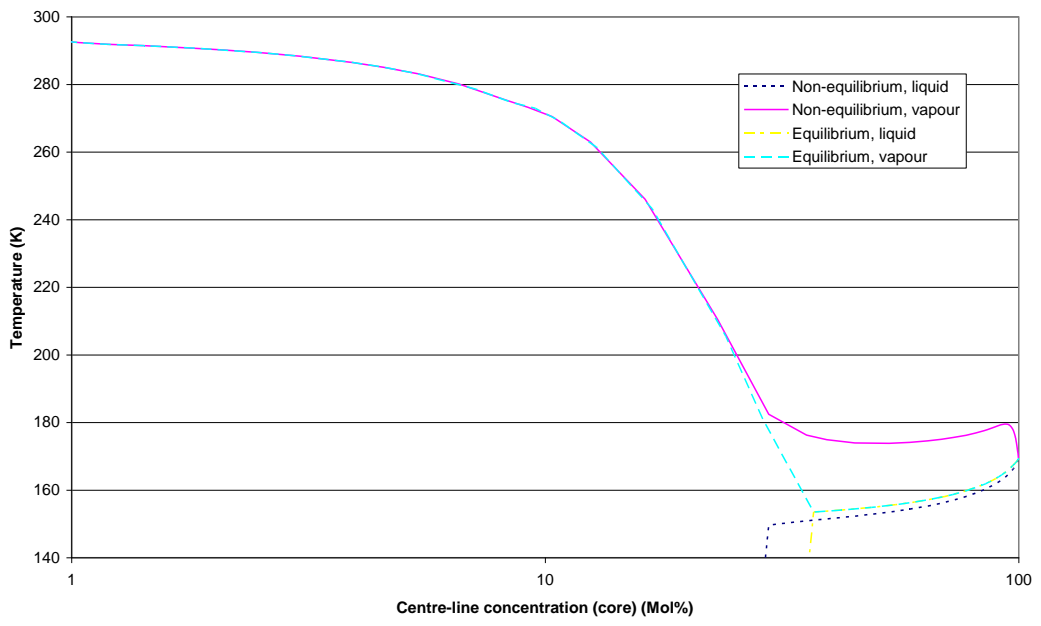
- The liquid temperatures predicted by equilibrium and non-equilibrium models are very close.
- The vapour temperature for the non-equilibrium model is larger for larger concentrations. For reducing fraction of liquid aerosol, the difference in predicted vapour temperature reduces.
- The liquid aerosol for the non-equilibrium model remains present up to significantly smaller concentrations.



(a) ammonia test-case



(b) sulphur dioxide test-case



(c) ethylene test-case

Figure 4. UDM predictions of vapour and liquid temperature for equilibrium and non-equilibrium models

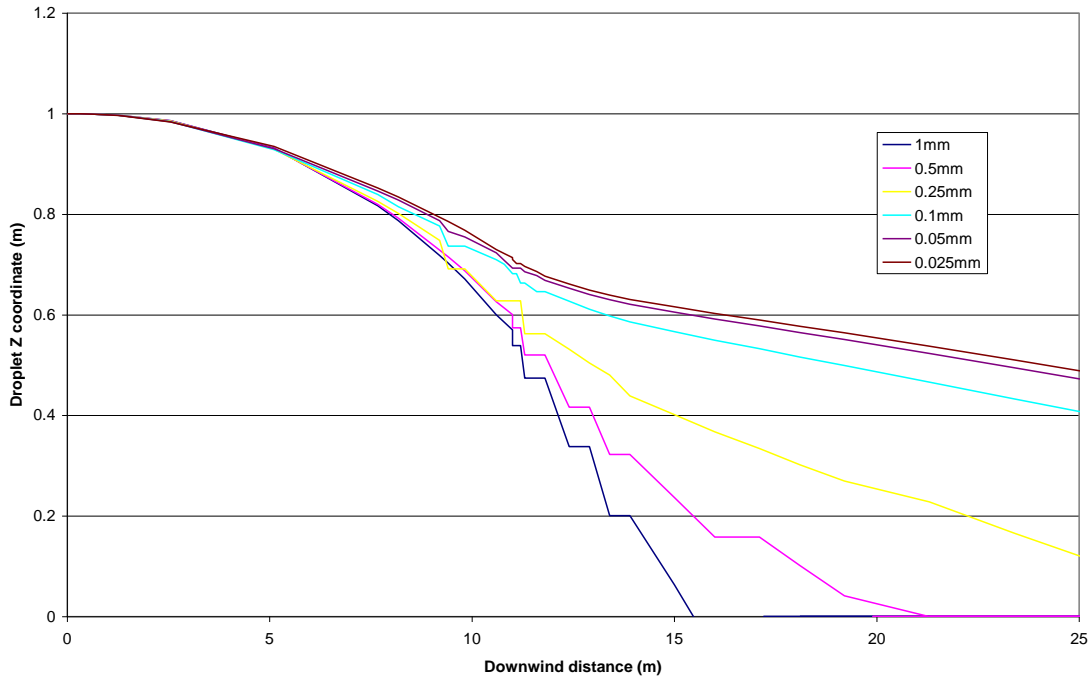
APPENDICES

Appendix A. Effects of using rigorous solver logic on droplet cases

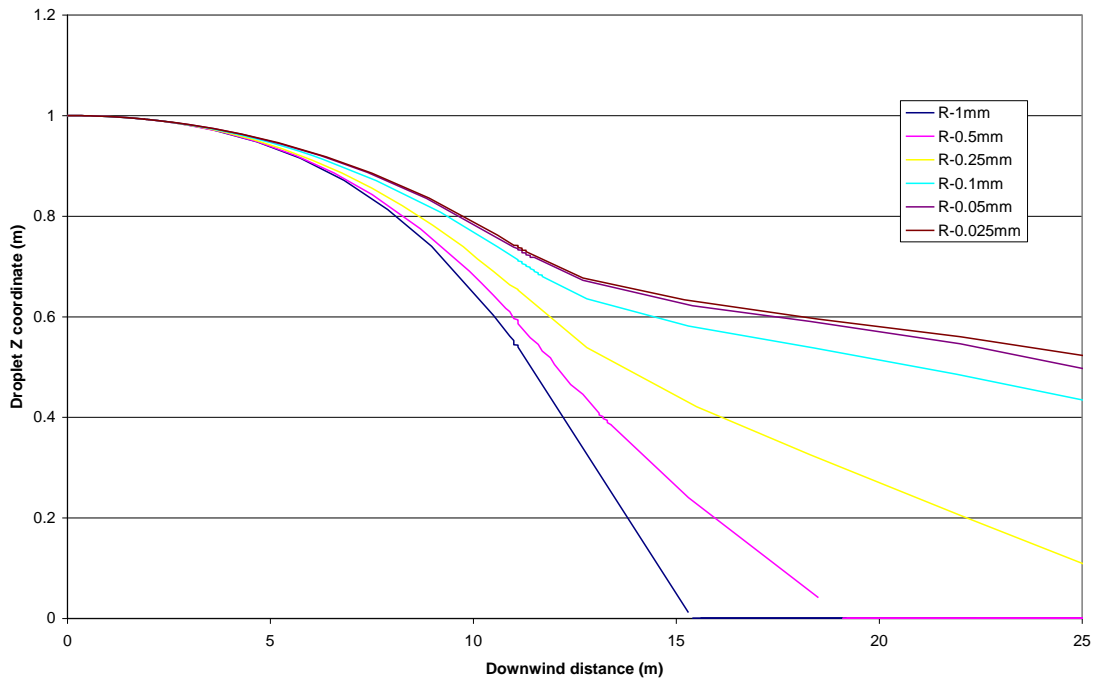
In this Appendix the difference between the new rigorous solver and the old synchronized droplet-equation solver is demonstrated. Two examples are presented to illustrate the improved solution under the modularised code:

- Case A is continuous propane release of saturated liquid at a height of 1m at 50m/s with D10 weather, 70% humidity
- Case B is the base case B from the sensitivity test set (instantaneous propane release, zero expansion energy, 80% liquid, 5m release height).

Figure 4.5 shows droplet trajectories for case A. Figure 4.6 and Figure 4.7 show droplet trajectories and vapour temperature respectively for case B. It is seen that the old model fails to produce converged solutions, with numerical artefacts apparent in the plots. Particularly worrying is case B, which under the old model has 10 μm droplets persisting between 10 and 100 times as long before rainout, and with apparently random temperature variations.

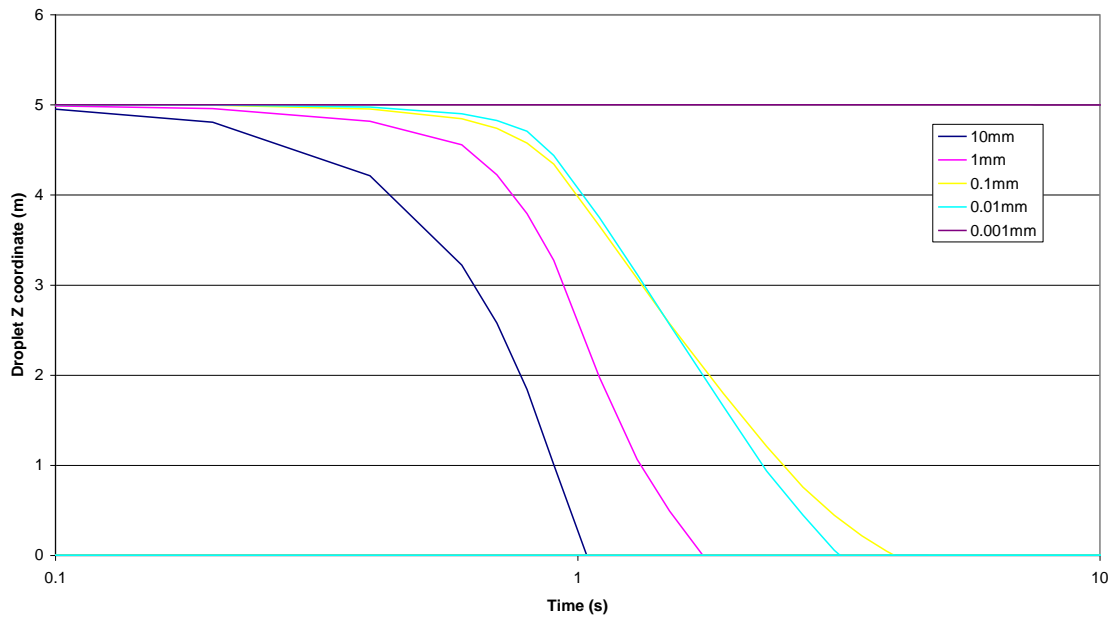


(a) synchronised

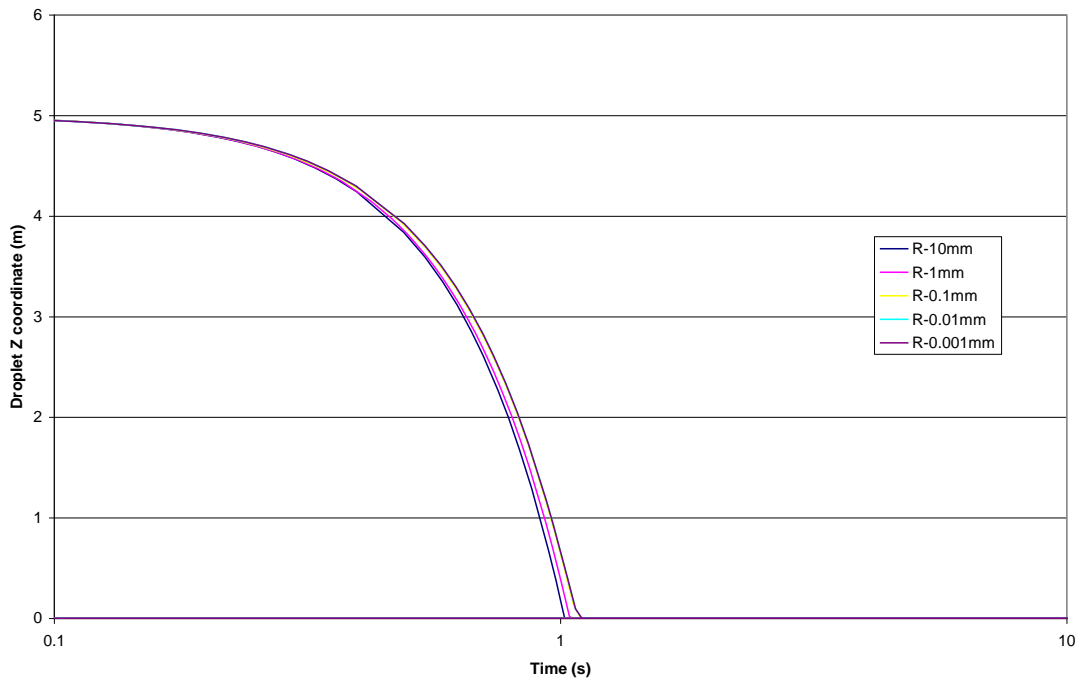


(b) rigorous

Figure 4.5. Case A - Droplet trajectories as a function of droplet diameter

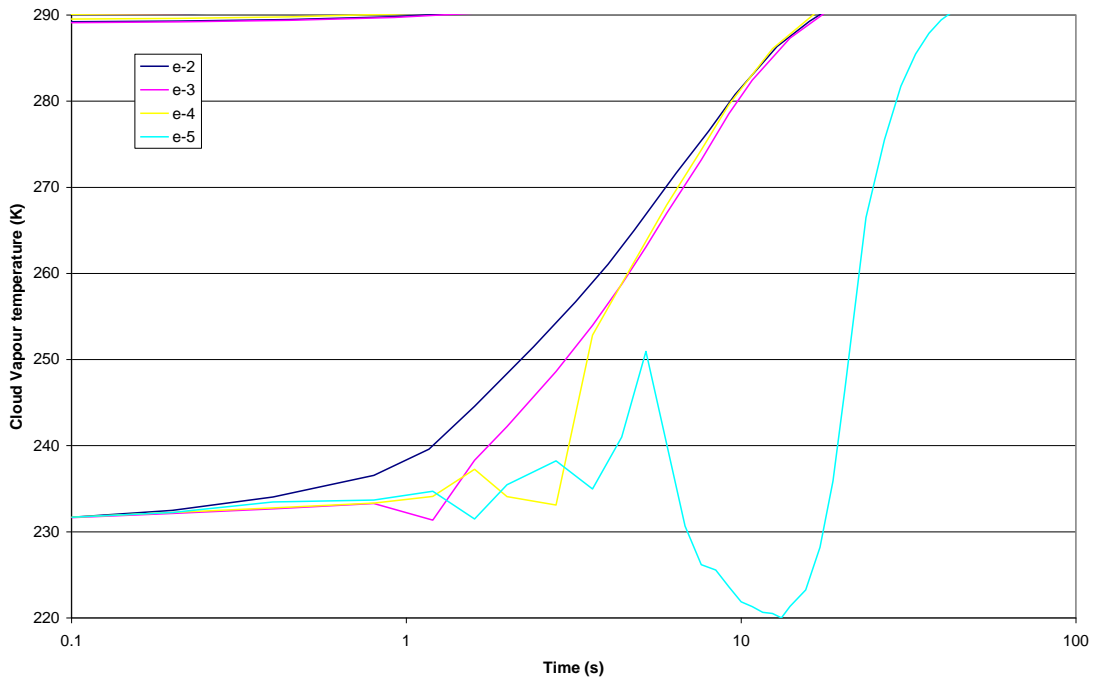


(a) synchronised

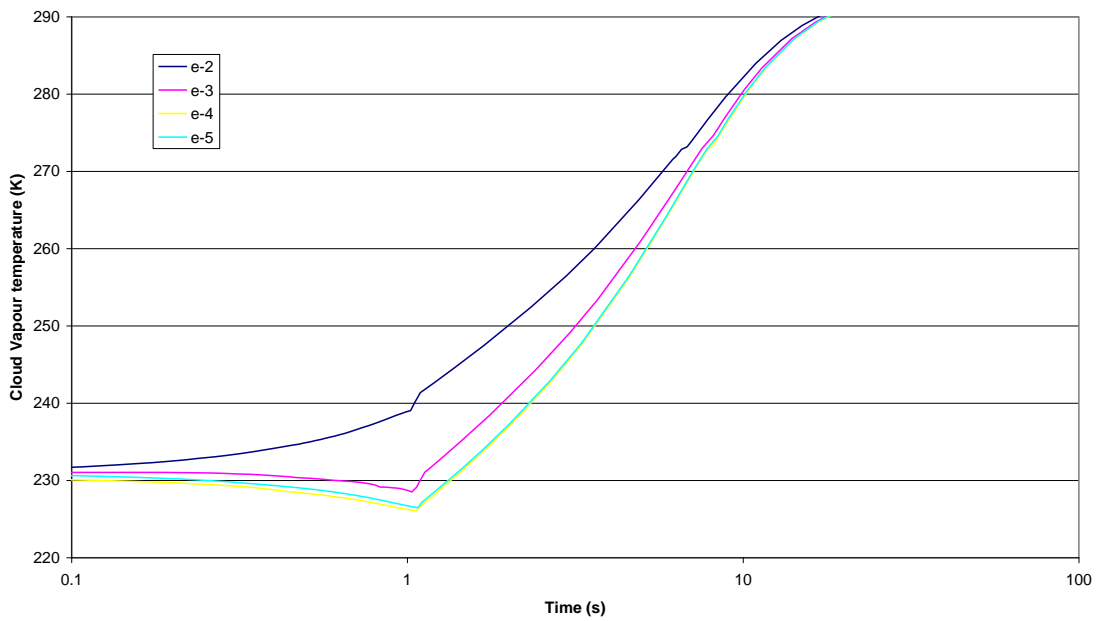


(b) rigorous

Figure 4.6. Case B - Droplet trajectories as a function of droplet diameter



(a) synchronised

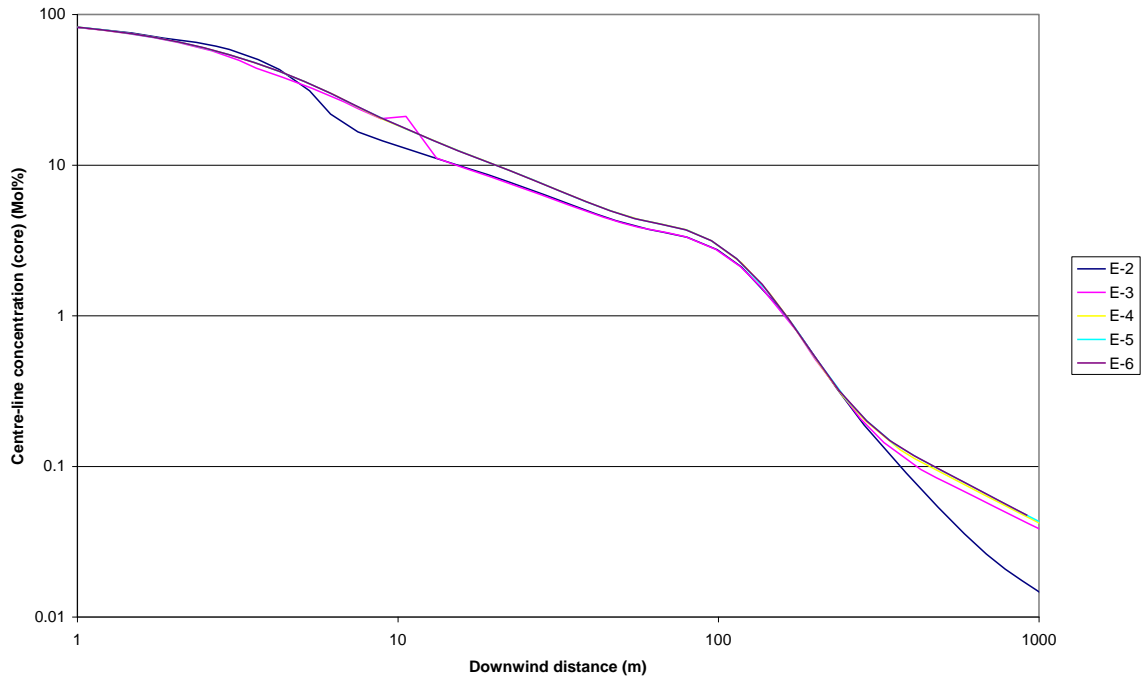


(b) rigorous

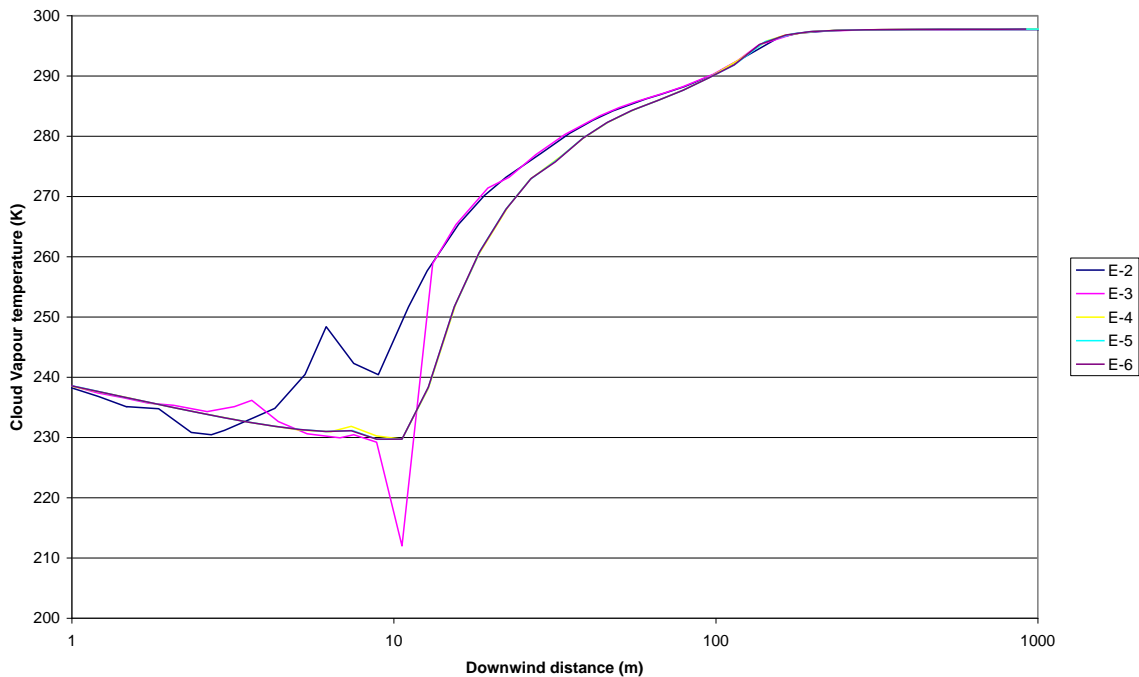
Figure 4.7. Case B – Vapour temperatures as function of droplet diameter

Appendix B. Effects of solution accuracy of ODE equations

The effect of the solution accuracy of the rigorous ODE equations was studied using the chlorine liquid release from the PHAST/SAFETI example cases under 1F weather conditions¹. In all cases droplets evaporated fully in the plume². The results for the four runs are presented in figure 7 below, and show that a converged solution is only achieved in this case for accuracies of 10^{-4} and below.



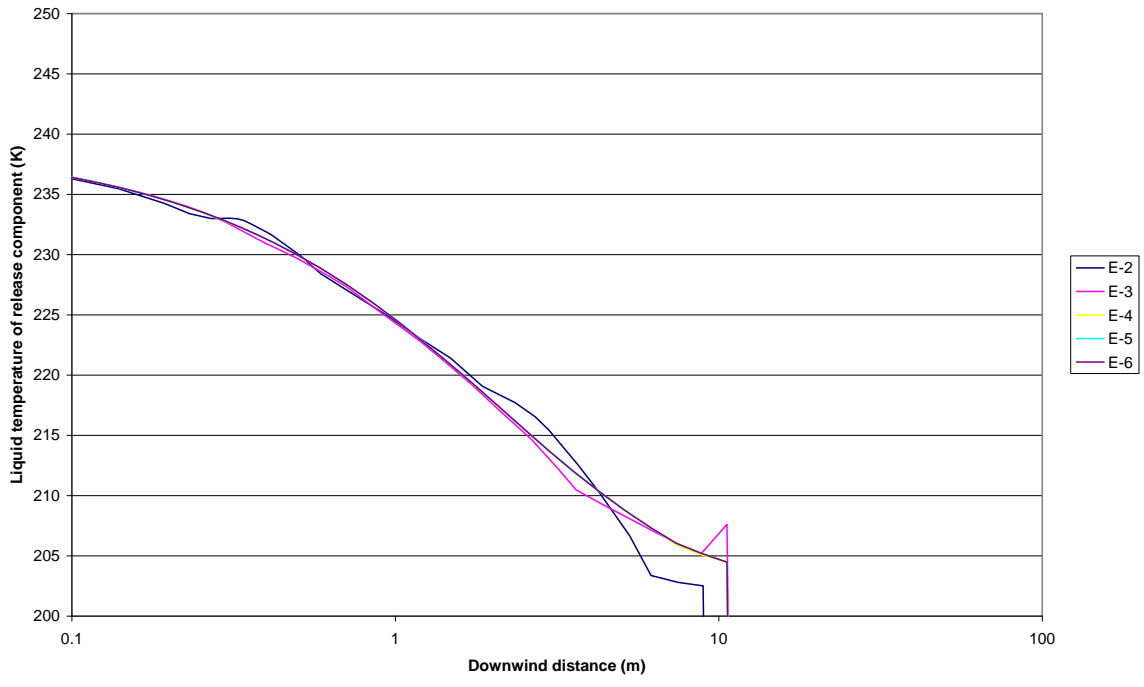
(a) Centreline concentration



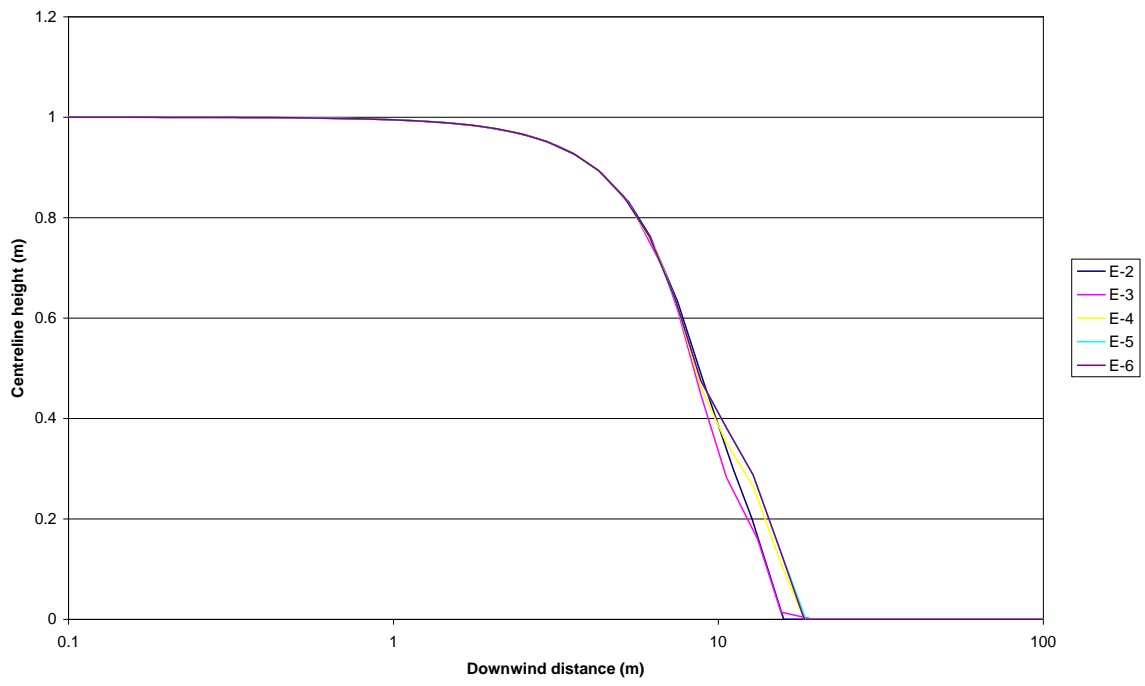
(b) Vapour Temperature

¹ Not strictly true for 6.5 – I have used Adrian's old UDM inputs (from 6.0?), which are different to those produced by 6.5. Adrian's case proves to be a better illustrative one on the effect of accuracy.

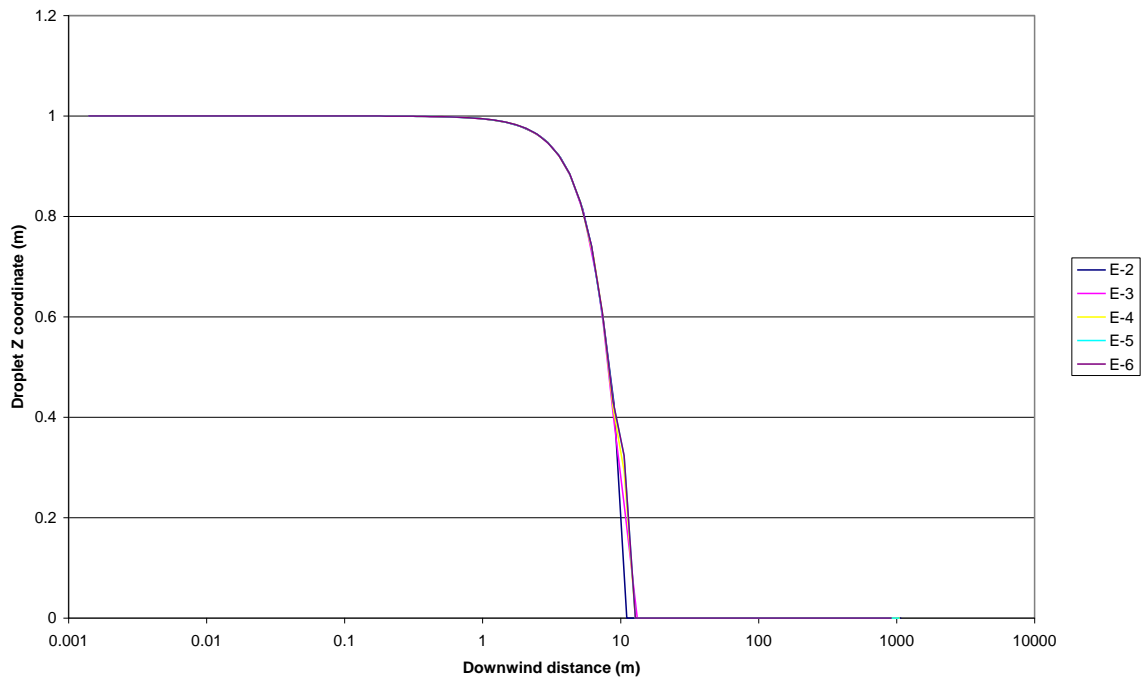
² For the old synchronised solution there was an erratic amount of rainout, between 6 and 14%.



(c) Liquid Temperature



(d) Cloud centreline position



(e) Droplet position

Figure 4.8. Effect of ODE solver accuracy for chlorine liquid release



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