

GTS/HSE/R003
Issue 2

Rainout Correlations for Continuous Releases

Graham Tickle

GT Science & Software Ltd

QA Sheet

Report Title	Rainout Correlations for Continuous Releases
Report Number	GTS/HSE/R003
Report Issue	Issue 2
Report Date	11 March 2015
Author	Graham Tickle

Document Revision History

Draft A	Initial draft for HSE/HSL comment
Draft B	Corrected typos
Draft C	Incorporating comments received on Draft B from HSE and HSL
Draft D	Incorporating comments received on Draft C from HSE and HSL
Issue 1	Report for issue incorporating client comments
Issue 2	Corrected typos and added addendum

This report covers a work task undertaken by GT Science and Software Ltd under sub-contract from the Health & Safety Laboratory (HSL), Contract No: PSSC 093282. Any opinions expressed are those of the authors and do not necessarily reflect those of HSL or HSE. HSE Copyright 2014.

GT Science & Software Ltd
29 Mount Way
Waverton
Chester
CH3 7QF
Web: www.gtscience.co.uk
email: info@gtscience.co.uk

Registered in England and Wales No: 0791495

Table of Contents

1	Introduction	1
2	Rainout Experiments	2
2.1	CCPS Rainout Experiments.....	2
2.2	Joint Industry Project Experiments	2
3	Rainout Correlations	3
3.1	Kletz.....	3
3.2	DeVaul and King	5
3.3	Lautkaski	8
4	Rainout Models	12
4.1	RELEASE.....	12
4.2	DNV Rainout Model	12
5	New Rainout Correlation.....	14
6	Comparisons with Observations from Large Scale Two-Phase Field Trials.....	16
7	Rainout from Sub-Cooled Releases	18
8	Summary of Comparison Results	20
8.1	Comparisons against CCPS Rainout Data.....	20
8.2	Comparisons with Observations from Large Scale Field Trials	20
8.3	Rainout from Sub-Cooled Releases.....	21
9	Recommendations	22
10	Addendum.....	23
11	References.....	24

1 Introduction

1. Release of pressure liquefied gas may result in the formation of a two-phase aerosol cloud. The hazard range of the dispersing cloud is dependent upon the quantity of the released material that remains airborne in the cloud. Pressure liquefied gas stored at a temperature much higher than the normal boiling temperature (high superheat) will undergo rapid initial vaporisation (flashing) upon release whereby the generated vapour breaks up the liquid into a fine spray of droplets which are sufficiently small that no significant rainout of liquid onto the ground is observed. At lower superheat, in the absence of formation of a fine spray by mechanical break-up¹, rainout of liquid may lead to pool formation. The hazard from a vaporising pool may differ significantly from the hazard from a two-phase jet and therefore it is desirable to be able to estimate rainout of liquid that may lead to a pool hazard in addition to, or instead of, the two-phase jet hazard.
2. Liquid rainout is likely to depend upon many factors which may not be known for accidental releases or are poorly understood. A pragmatic approach to estimating rainout is therefore required which broadly accounts for circumstances under which significant rainout is expected and circumstances in which rainout may be safely neglected.
3. DRIFT [1], [2] models the dispersion of two-phase clouds, but it does not include a model for liquid rainout². For flashing instantaneous releases, the source term model ACE [3] includes an estimate of liquid rainout at the source correlated with superheat and based on observations from experiments of flashing instantaneous releases. We seek a similar approach, if possible, for rainout from flashing continuous releases. Rainout from non-flashing sub-cooled releases in the context of toxic sprays is considered in [4].

¹ Generally, formation of a fine spray by mechanical break-up requires a combination of low superheat, high pressure and small orifice size.

² DRIFT includes a simple model for liquid deposition from a ground based cloud, but this does not allow for rainout from elevated releases.

2 Rainout Experiments

2.1 CCPS Rainout Experiments

4. Rainout experiments for continuous releases of a number of fluids were conducted in the early 1990s sponsored by the CCPS. The experiments involved superheated releases of water, cyclohexane, trichlorofluoromethane (CFC-11), chlorine and methylamine. Results from separate Rohm and Haas methylamine experiments are also included. The experimental data and an accompanying rainout model are described in the RELEASE book [5]. The experimental data and RELEASE rainout model are reviewed in [6].
5. The rainout measured in CCPS experiments was affected by incomplete capture of rained out liquid, due in part to
 - vaporisation from the rainout collection trays,
 - incomplete overlap of releases with the collection trays,
 - the atmosphere becoming saturated (in the case of water releases only).

As described in [5] attempts have been made to correct for some of the losses, but, as pointed out in [6], the accuracy of the corrected rainout data is somewhat uncertain.

2.2 Joint Industry Project Experiments

6. More recently a Joint Industry Project (JIP) on liquid and two-phase jets has investigated droplet sizes from sub-cooled (non-flashing) and superheated (flashing) liquid jets. This JIP mainly covers droplet size correlations and is described in references [7], [8], [9], [10]. Most recently, Phase IV of this JIP included an experimental study by the Health and Safety Laboratory (HSL) on rainout from sub-cooled releases [11], validation of DNV software and comparisons of rainout with simple correlations not involving droplet modelling [12].

3 Rainout Correlations

7. We consider here simple correlations, by which we mean models that do not directly determine droplet sizes or trajectories, but instead directly correlate liquid rainout with release conditions. We define a rainout fraction by the mass of material rained out divided by the total release mass.

3.1 Kletz

8. Kletz [13] suggested a “rule of thumb” for the rainout fraction, x_R based upon the isenthalpic flash fraction x_H :

$$x_R = 1 - 2 x_H \quad (3-1)$$

where

$$x_H = \frac{C_{pL}(T_0 - T_b)}{\Delta H_{vap}} \quad (3-2)$$

and

C_{pL} is the specific heat capacity of the liquid

ΔH_{vap} is the enthalpy of vaporisation

T_0 is the stagnation temperature

T_b is the boiling temperature at ambient pressure

9. Figure 3-1 and Figure 3-2 show the prediction using this Kletz rule of thumb compared with the CCPS corrected rainout data. The Kletz rule of thumb provides reasonable agreement with the CCPS water data, but for all other substances it over-predicts rainout. The approximate agreement with water and poor agreement for other substances suggests that vaporisation of droplets is not adequately accounted for.

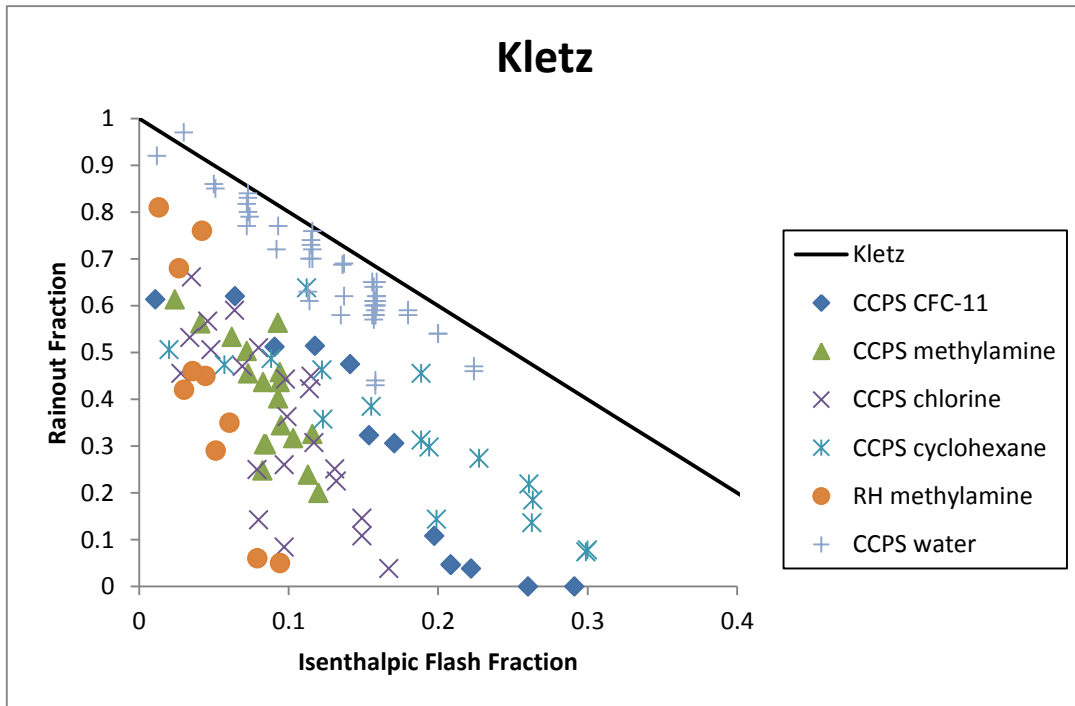


Figure 3-1 Kletz rainout rule of thumb compared with corrected CCPS rainout measurements

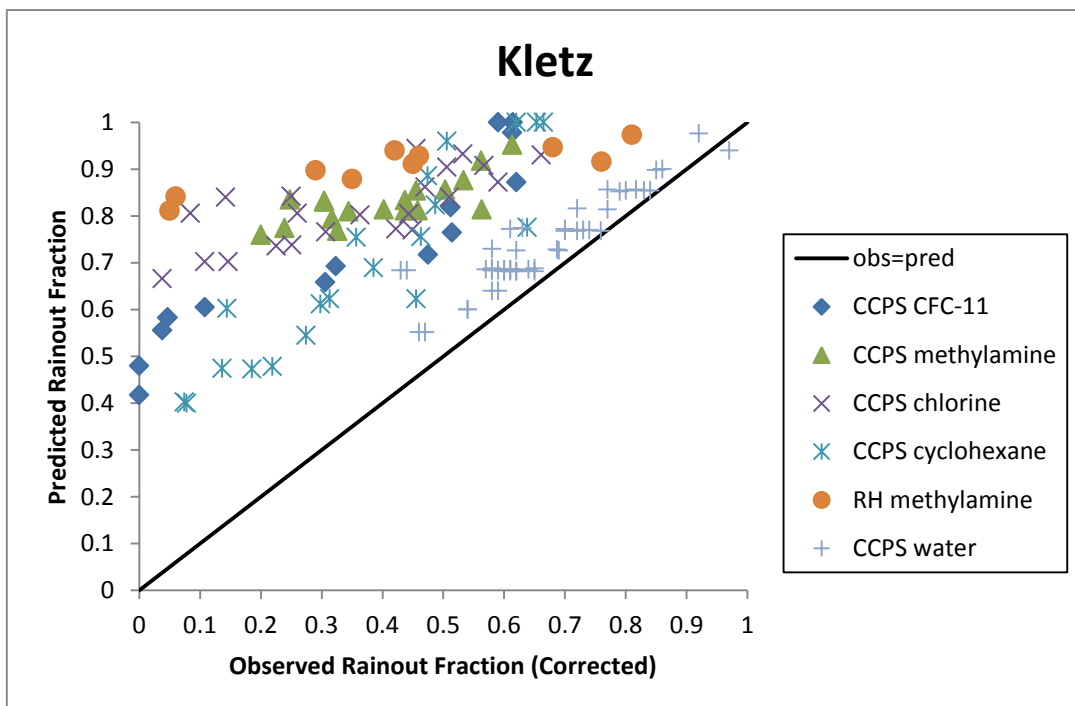


Figure 3-2 Kletz rainout rule of thumb predictions plotted against corrected CCPS rainout measurements

3.2 DeVaul and King

10. DeVaul and King [14] correlate the CCPS rainout measurements uncorrected for losses. Their correlation distinguishes between non-volatile and volatile fluids, using a different correlating parameter for each.
11. DeVaul and King define low volatility liquid as having $(T_a - T_{as})/T_a < 0.14$ where T_a is the ambient temperature and T_{as} is the adiabatic saturation temperature (the temperature corresponding to dry out of liquid when mixed adiabatically with air at temperature T_a). The rainout fraction x_R for low volatility fluids is correlated as:

$$x_R = 1 - \frac{C_{pL}(T_0 - T_{as})}{\Delta H_{vap}} \quad (3-3)$$

12. Figure 3-3 shows this correlation compared with the uncorrected CCPS rainout data for low volatility fluid cases.

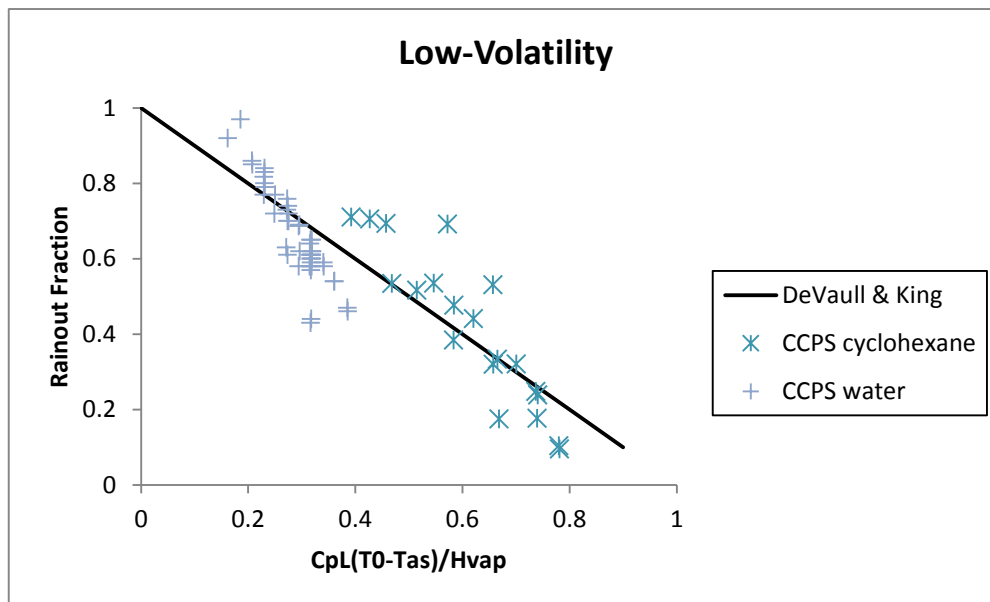


Figure 3-3 DeVaul and King correlation for low-volatility liquids compared with uncorrected CCPS rainout measurements

13. For volatile liquid defined by $(T_a - T_{as})/T_a \geq 0.14$ then DeVaul and King propose

$$\frac{x_R}{x_*} = 1 - \left(\frac{x_H}{0.145} \right)^{1.8} \quad (3-4)$$

for $x_H \leq 0.145$. x_* is obtained from a fit to uncorrected rainout data at low superheats (less than or equal to 10 K) correlated in terms of $(T_a - T_{as})/T_a$:

$$x_* = 1 - 2.33 \frac{T_a - T_{as}}{T_a} \quad (3-5)$$

14. Lautkaski [15] pointed out errors in some substance properties used in the DeVaul and King work. Correcting these errors, the original DeVaul and King correlation for volatile liquid no longer fits the data. Lautkaski refitted the DeVaul and King correlation to the CCPS rainout data. The revised fit is

$$\frac{x_R}{x_*} = 1 - \left(\frac{x_H}{0.224} \right)^{1.69} \quad (3-6)$$

for $x_H \leq 0.224$

15. The original and revised fits at superheats >10 K are shown in Figure 3-4. The fit for low superheats is shown in Figure 3-5.

16. Figure 3-6 and Figure 3-7 show plots of DeVaul and King correlation predictions against CCPS uncorrected measured rainout for the original and refit correlations, respectively. The data points in these figures are corrected for the errors in the substance properties following [15].

17. The HSE spreadsheet RAIN Version 1.2 is an implementation of the original DeVaul and King correlation.

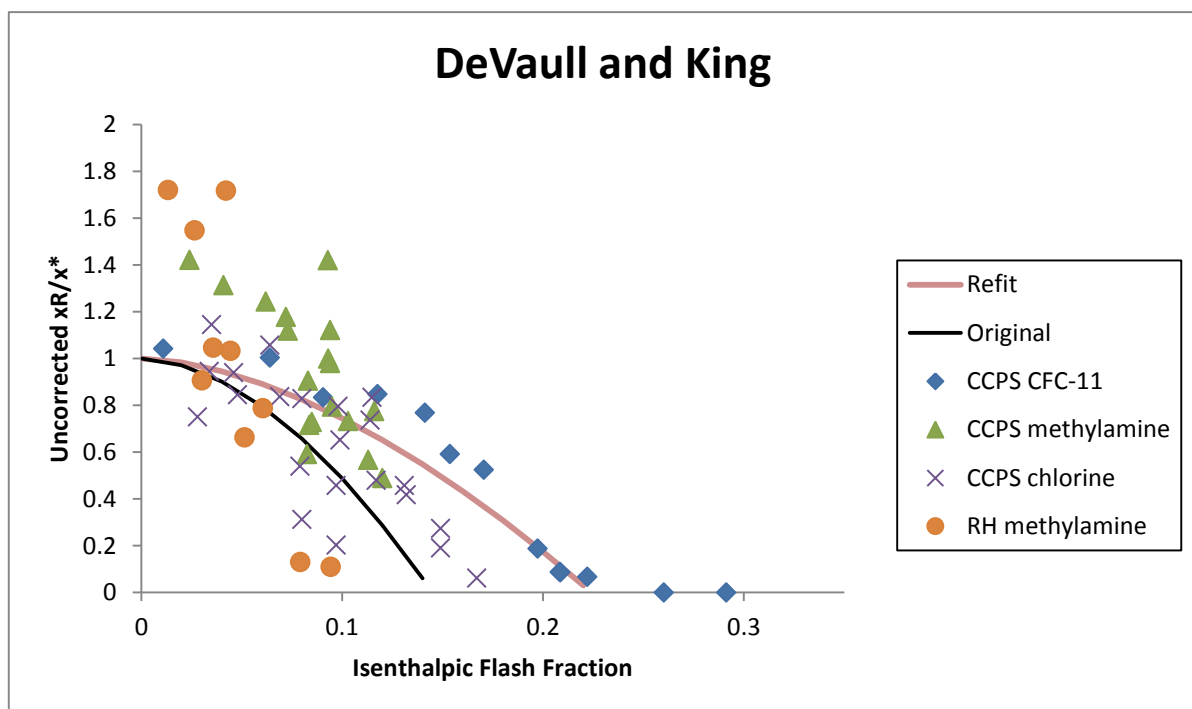


Figure 3-4 DeVaul and King rainout correlation for volatile liquids with high superheat compared with uncorrected CCPS rainout measurements.

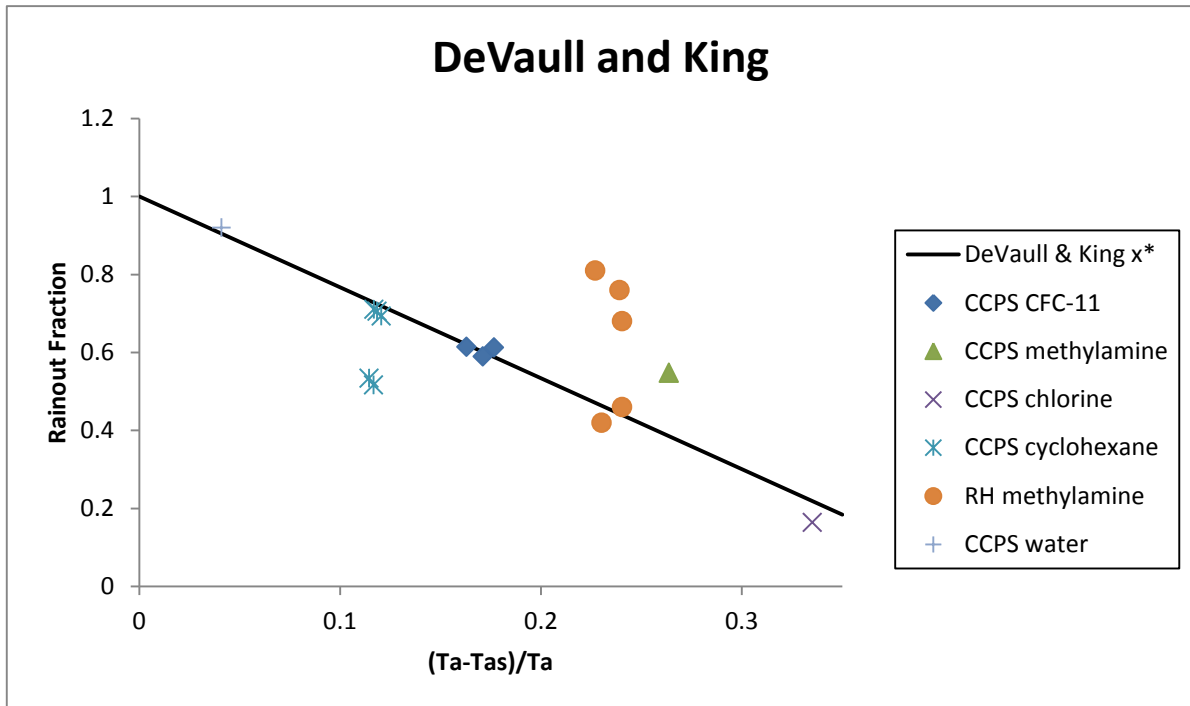


Figure 3-5 DeVaul and King rainout correlation for volatile liquids with low superheat compared with uncorrected CCPS rainout measurements

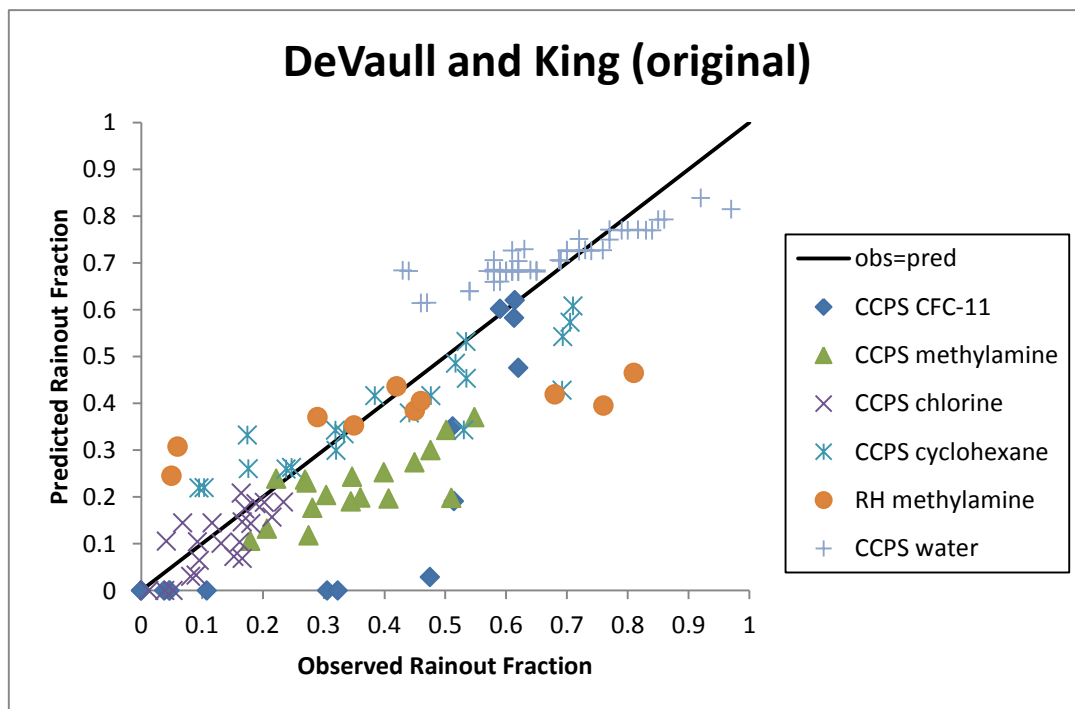


Figure 3-6 DeVaul and King original correlation plotted against uncorrected CCPS rainout measurements

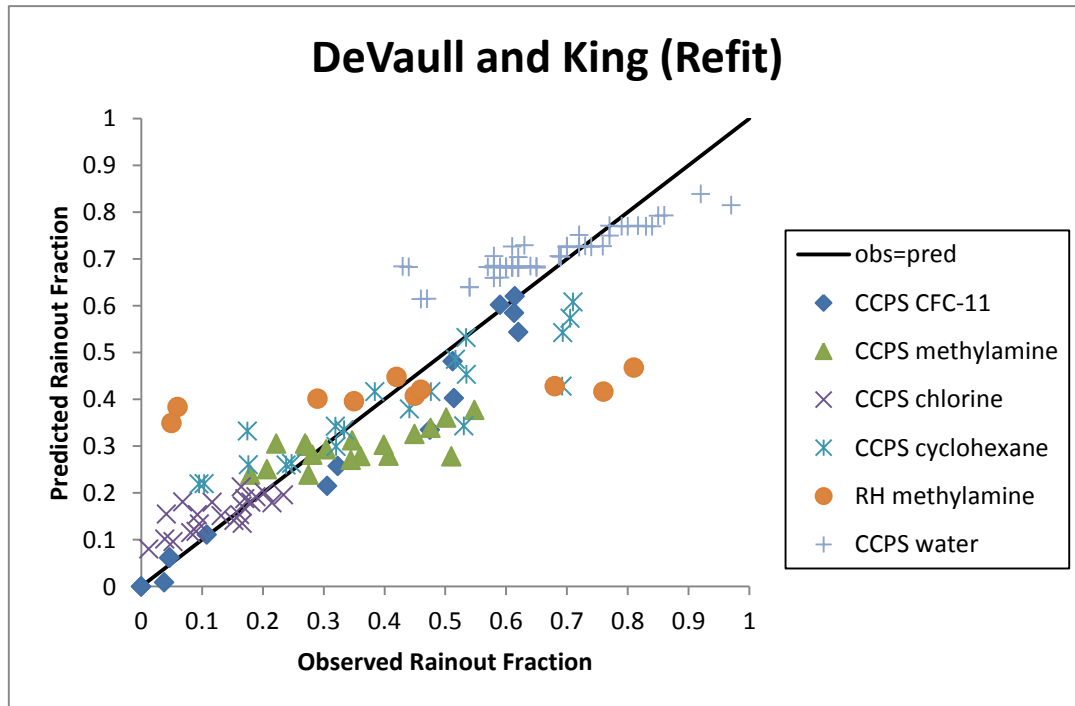


Figure 3-7 DeVaul and King refit correlation plotted against uncorrected CCPS rainout measurements

3.3 Lautkaski

18. In addition to refitting the DeVaul and King correlation, Lautkaski [15] devised new correlations based on CCPS corrected rainout data. When the results from water are discarded, on the basis that rainout for these is artificially enhanced due to the saturated atmosphere in the experiments, then the measured rainout corrected for evaporation losses is broadly consistent with a rainout fraction of 0.6 at low superheats (as pointed out also in [16]). Since the corrected rainout data is independent of T_{as} , Lautkaski did not need to divide fluids into non-volatile and volatile categories to fit the data. Plotting corrected rainout against isenthalpic flash fraction the following linear function is fitted

$$\frac{x_R}{0.6} = 1 - 3 x_H \quad (3-7)$$

19. This fit, equation (8) in [15], is shown compared with the CCPS corrected rainout fractions in Figure 3-8 and Figure 3-9.

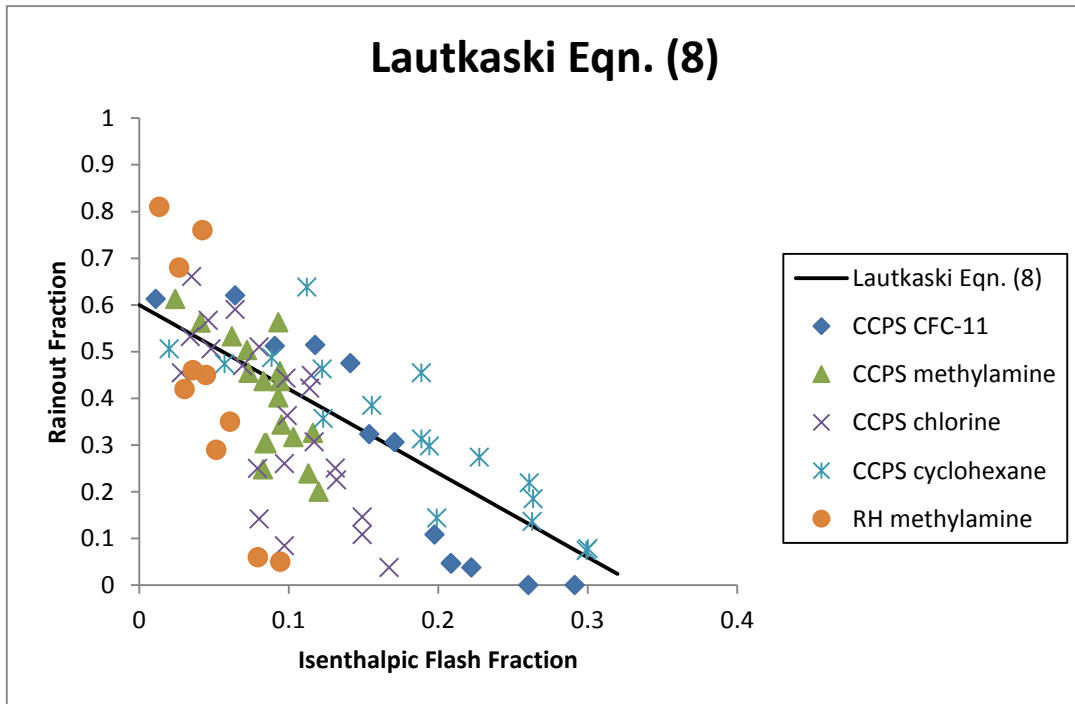


Figure 3-8 Lautkaski linear fit for rainout as a function of isenthalpic flash fraction compared with CCPS corrected rainout measurements

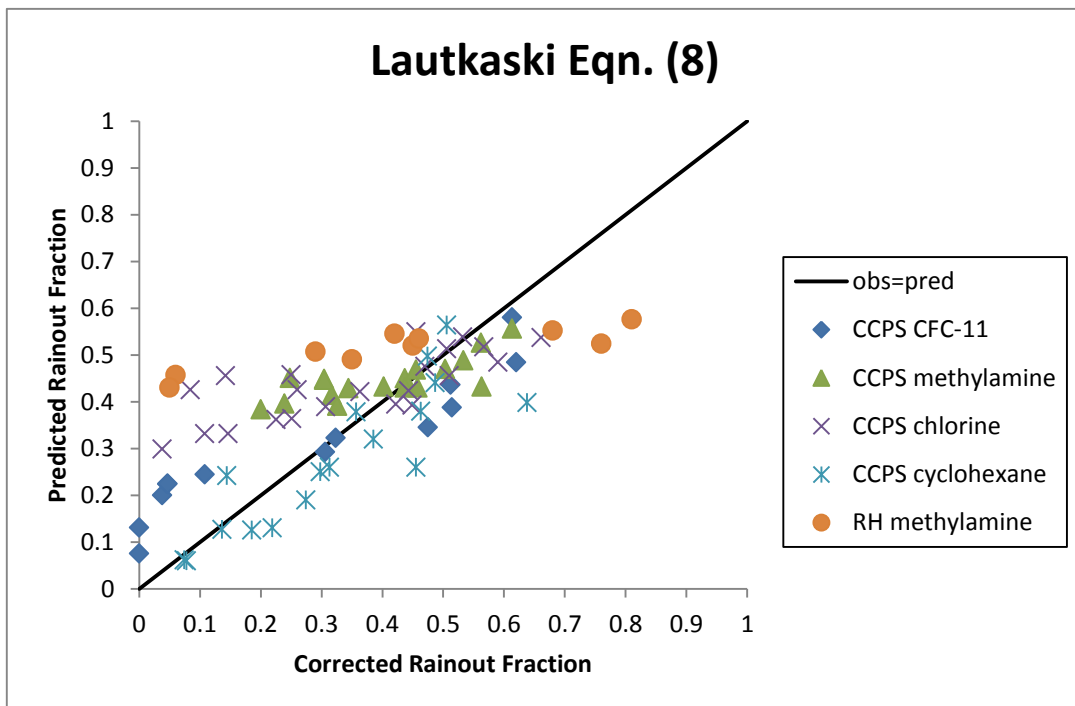


Figure 3-9 Lautkaski linear fit for rainout as a function of isenthalpic flash fraction plotted against CCPS corrected rainout measurements

20. An improved fit in [15] was found by correlating the rainout with Jakob number, Ja :

$$\frac{x_R}{0.6} = 1 - \left(\frac{Ja}{93}\right)^{1.36} \quad (3-8)$$

where

$$Ja = \frac{C_{pL}(T_0 - T_b) \rho_L}{\Delta H_{vap} \rho_v} \quad (3-9)$$

is a dimensionless ratio of the liquid superheat to enthalpy of vaporisation with an adjustment for the ratio of liquid density ρ_L to vapour density ρ_v .

21. This correlation, equation (10) in [15], is shown compared with CCPS corrected rainout fractions in Figure 3-10 and Figure 3-11.

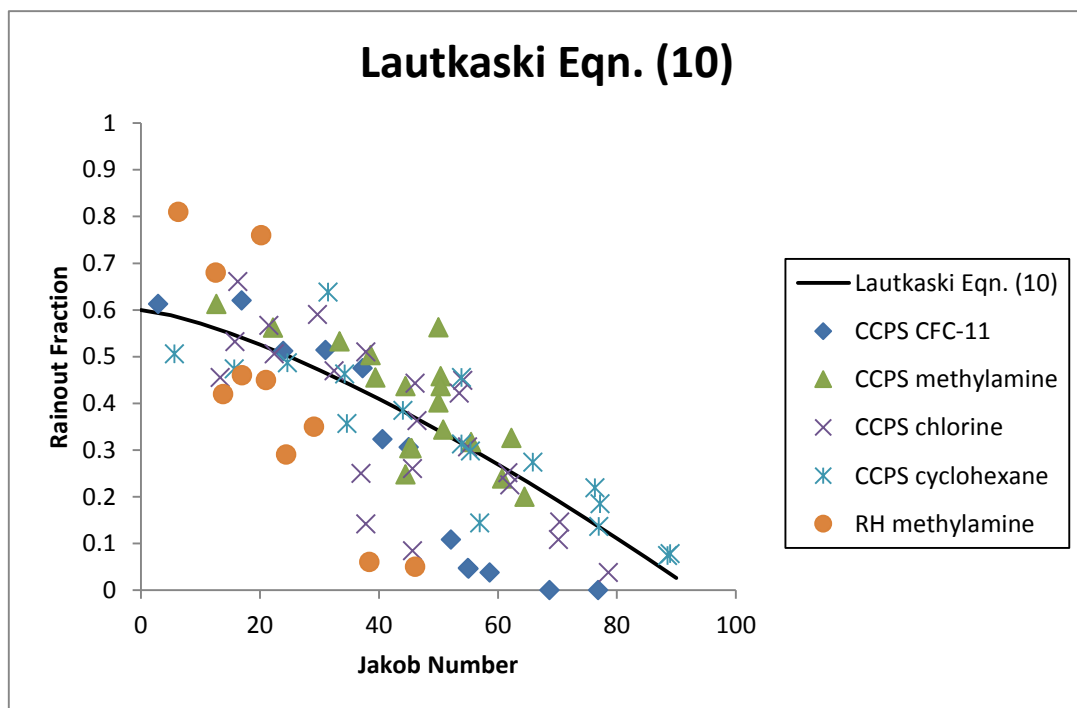


Figure 3-10 Lautkaski fit for rainout as a function of Jakob number compared with CCPS corrected rainout measurements

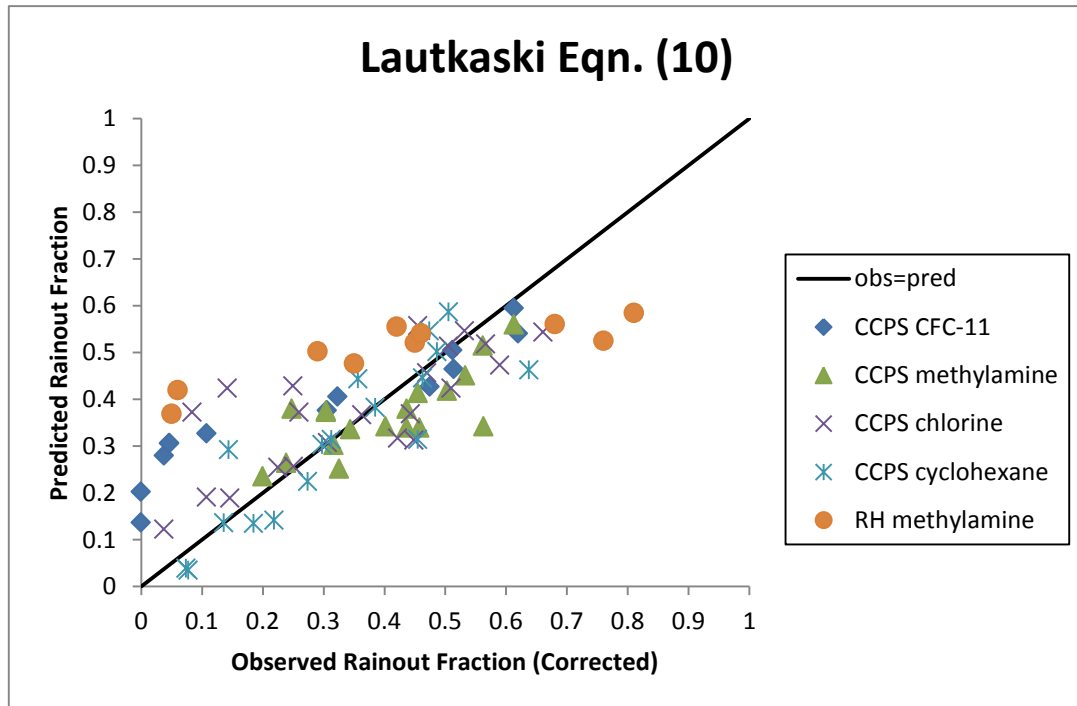


Figure 3-11 Lautkaski fit for rainout as a function of Jakob number plotted against CCPS corrected rainout measurements

4 Rainout Models

4.1 RELEASE

22. The RELEASE rainout model [5] takes a different approach from the correlations presented in the preceding sections. RELEASE estimates rainout based on a predicted mean droplet size and assumed droplet size distribution. RELEASE does not model droplet evaporation or full droplet trajectories, but estimates rainout on the basis of an estimated initial droplet trajectory angle compared to the spread angle of the jet. In the original version of RELEASE there was an error in the integration over droplet size distribution. This was corrected in [5] resulting in improved agreement with CCPS data, although the corrected RELEASE still predicts rainout fractions approaching 1 at low superheat. Johnson corrects for this by including an empirical 0.6 multiplying factor which he attributes to the effects of droplet evaporation [16].
23. Figure 4-1 shows the results from the corrected RELEASE model compared with CCPS corrected rainout fractions.

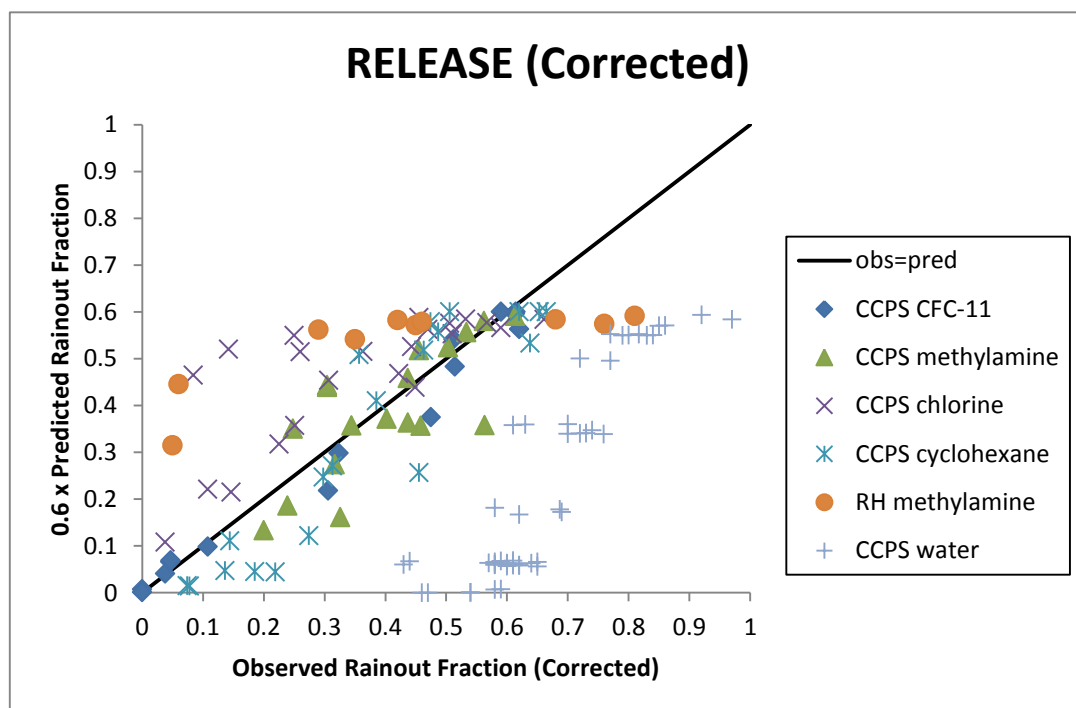


Figure 4-1 0.6 x RELEASE predictions for rainout plotted against CCPS corrected rainout.

4.2 DNV Rainout Model

24. The rainout modelling approach in the DNV Unified Dispersion Model (UDM) is based upon modelling the size, vaporisation and trajectory of droplets [17]. The rainout model has been tuned to match the corrected rainout from the CCPS experiments – in fact the rainout correction is, in part, based on modelling in the UDM. Validation of the UDM rainout model is presented by Witlox and Harper in [12]. They found that the drop size correlations derived in Phase III of the JIP produced inferior rainout predictions compared with the CCPS drop size correlations. The CCPS drop size correlations were modified to use only mechanical break-up droplet sizes for sub-cooled jets and only flashing break-up droplet sizes for superheated releases, rather than taking

the minimum of these as specified in the original CCPS droplet size correlation. Witlox and Harper [12] attribute the poor performance of the JIP Phase III droplet size correlation for predicting rainout as being due to this correlation being based on measurements closer to the release point and neglecting secondary droplet break-up. The modified CCPS droplet size correlation is used as the new default for rainout in Phast 6.7.

25. Figure 4-2 shows the UDM rainout predictions using the Phast 6.7 default (modified CCPS correlation) plotted against the CCPS corrected rainout data for the selected cases reported in [12]. The Phast 6.7 data points in Figure 4-2 have been estimated from Figure 8 in [12].

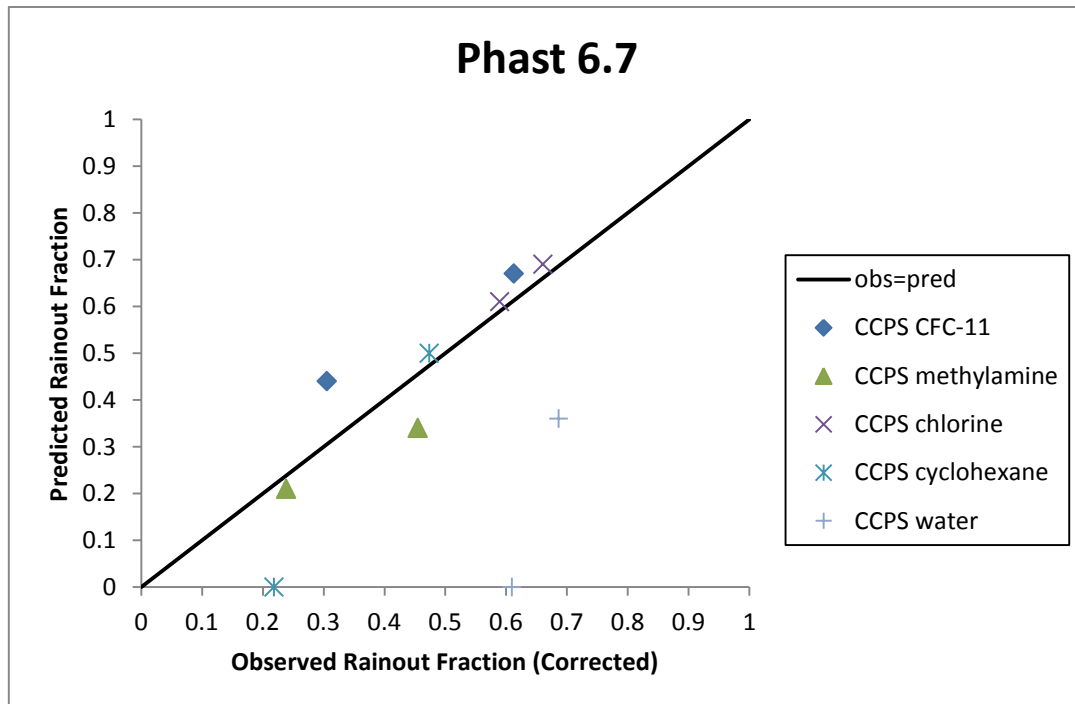


Figure 4-2 DNV Phast 6.7 rainout predictions plotted against CCPS corrected rainout measurements for the selected cases given in [12]

5 New Rainout Correlation

26. Here we present a new correlation for the CCPS uncorrected rainout fractions. Uncorrected rainout fractions retain more material in the airborne release, implicitly including material vaporised from raining out droplets and/or the resulting pool. Allowing for such vapour sources directly as part of the rainout correlation may be advantageous when used in dispersion models that do not directly include these effects.

27. To preserve the DeVaul and King agreement for low-volatility $(T_a - T_{as})/T_a < 0.14$ fluids we retain the x_R scaling:

$$x_R = 1 - \frac{C_{pL}(T_0 - T_{as})}{\Delta H_{vap}} \quad (5-1)$$

28. For volatile $(T_a - T_{as})/T_a \geq 0.14$ superheated releases we assume a Jakob number dependence with the new correlation given by:

$$\frac{x_R}{x_*} = 1 - \left(\frac{Ja}{75}\right)^3 \quad (5-2)$$

29. Comparisons of the new correlation with CCPS uncorrected rainout data for volatile liquids are shown in Figure 5-1 and Figure 5-2.

30. For low-volatility liquids, the correlation is the same as that of DeVaul and King. For superheated releases the new correlation can be thought of as a Jakob number alternative to the DeVaul and King correlation.

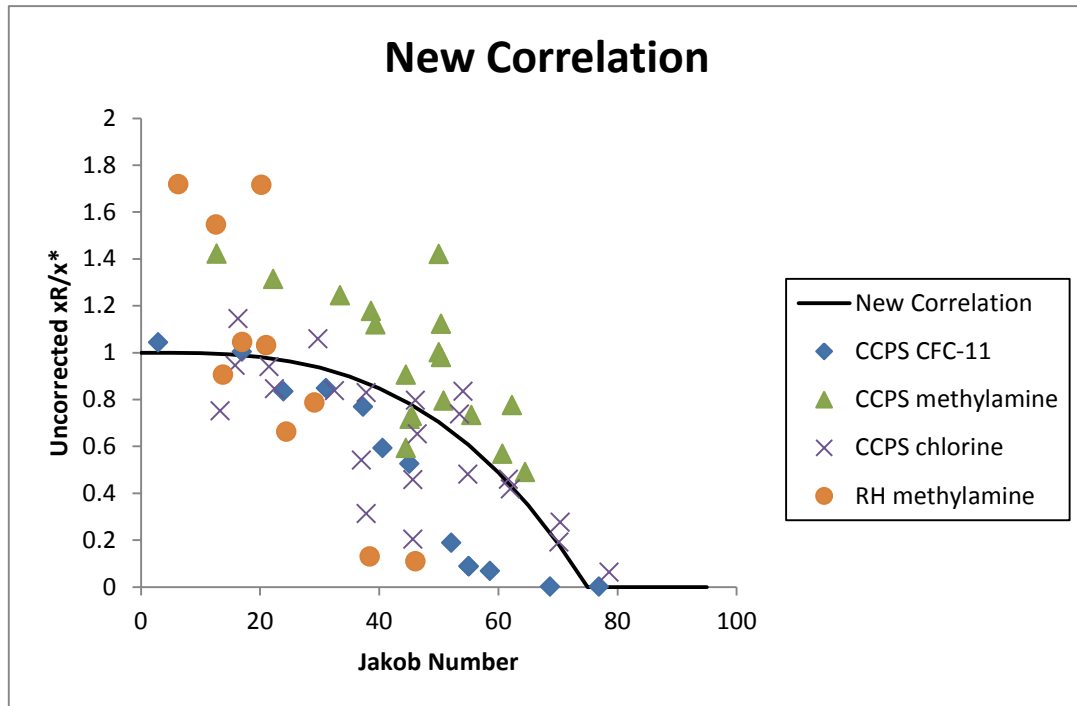


Figure 5-1 New correlation for rainout of volatile liquids compared with CCPS uncorrected rainout measurements. x^* is defined as in the DeVaul and King correlation.

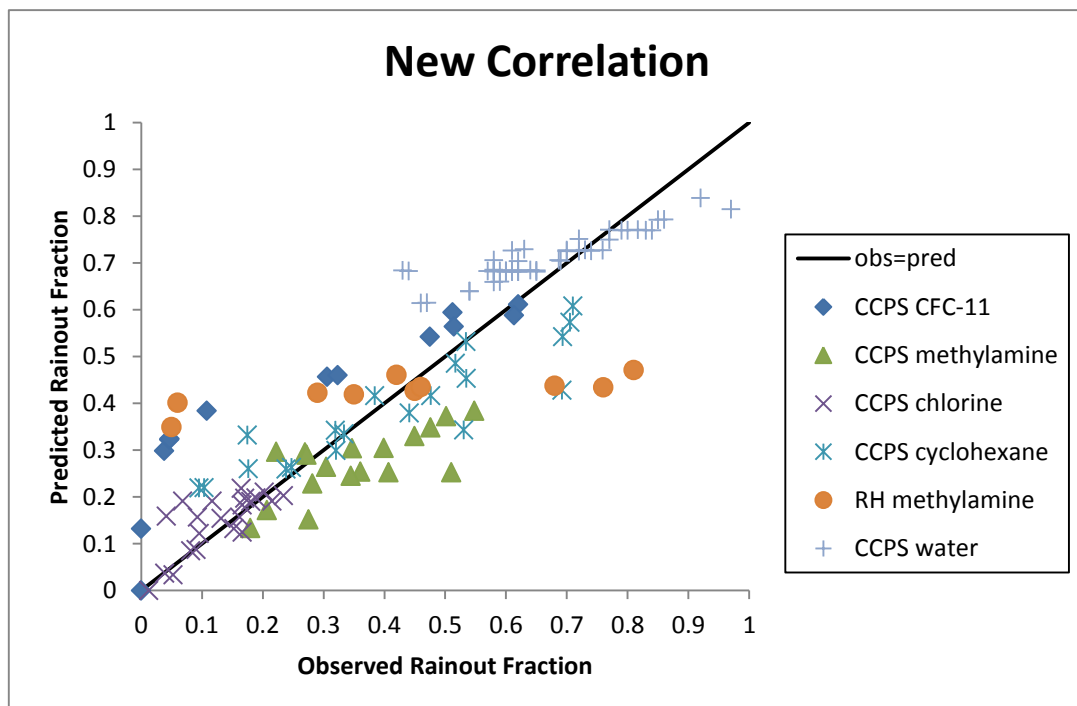


Figure 5-2 New correlation for rainout plotted against CCPS uncorrected rainout measurements

6 Comparisons with Observations from Large Scale Two-Phase Field Trials

31. Witlox and Harper [12] present a comparison of rainout model predictions with observations from large scale two-phase field experiments. Although the field experiments report no rainout, this provides a useful consistency check of rainout models. We repeat this comparison for the rainout models considered in this report, the results of which are given in Table 6-1.

Table 6-1 Predicted rainout for selected large scale two-phase field trials

Trial	Substance	Exit pressure (bar)	Super-heat (K)	Nozzle diameter (m)	Ambient Temp. (K)	Prediction Rainout Fraction						Phast 6.7	Rainout reported	
						Kletz	Lautkaski (xH)	Lautkaski (Jakob)	DeVaull & King (Orig) ¹	DeVaull & King (Refit)	New Correl.			RELEASE corrected x0.6
Fladis 9	ammonia	6.93	47	0.0063	289	0.68	0.30	0.00	0.00	0.13	0.00	0.00	0.00	none
Fladis 16	ammonia	7.98	50.4	0.0063	289	0.65	0.28	0.00	0.00	0.11	0.00	0.00	0.00	none
Fladis 24	ammonia	5.7	42.9	0.0063	291	0.70	0.33	0.00	0.00	0.15	0.00	0.01	0.00	none
EEC36	propane	7.7	55.9	0.004	289	0.31	0.02	0.06	0.00	0.00	0.00	N/A ²	0.00	none
EEC55	propane	10.13	55.4	0.0155	283	0.32	0.02	0.06	0.00	0.00	0.00	N/A	0.00	none
EEC56	propane	10.23	42.4	0.0155	285	0.48	0.14	0.23	0.00	0.00	0.09	N/A	0.00	none
DT 1	ammonia	10.12	57.1	0.081	302	0.61	0.25	0.00	0.00	0.05	0.00	0.00	0.27	<0.2 ³
DT 2	ammonia	11.16	55.7	0.0945	304	0.62	0.26	0.00	0.00	0.06	0.00	0.00	0.41	<0.36
DT 3	ammonia	11.374	57.8	0.0945	307	0.60	0.24	0.00	0.00	0.04	0.00	0.00	0.42	<0.39
DT4	ammonia	11.798	59.8	0.0945	307	0.59	0.23	0.00	0.00	0.03	0.00	0.00	0.38	<0.3
Goldfish 1	HF	6.89	20.4	0.0419	310	0.73	0.34	0.00	0.06	0.35	0.00	0.14	0.00	none
Goldfish 2	HF	7.45	18.4	0.0242	309	0.75	0.37	0.00	0.15	0.39	0.00	0.25	0.00	none
Goldfish 3	HF	7.58	19.4	0.0242	307	0.74	0.36	0.00	0.11	0.38	0.00	0.19	0.00	none

Note

1. HSE’s RAIN v1.2 spreadsheet is an implementation of the original DeVaull and King correlation and produces very similar predictions (allowing for small differences due to use of slightly different substance property values)
2. N/A in the table indicates predictions which are not available (due to no substance properties file being available for this substance within the RELEASE model)
3. The rainout values reported for Desert Tortoise Trials (DT1-DT4) are estimated ‘missing mass’ from the cloud, some of which may be due to rainout, but could also be due to difficulties in calculating the mass balance of the cloud from the field trial measurements [12]

7 Rainout from Sub-Cooled Releases

32. The correlations in the previous sections are derived from fits to CCPS experiments which are predominantly superheated liquid releases.
33. Sub-cooled liquid releases are expected to produce larger rainout fractions due to the reduced volatility (lower vapour pressure) and the lack of flashing break-up mechanism with only mechanical liquid break-up occurring.
34. Although the liquid break-up mechanism at low superheats in the CCPS experimental data is believed to be mainly mechanical, the majority of the data³ are for superheated releases and therefore provide limited information on the sensitivity of rainout to substance volatility for sub-cooled releases.
35. Of the simple correlations considered, only the DeVaul and King correlation has the desired behaviour of smoothly increasing rainout for sub-cooled releases from the CCPS observed values to complete rainout when the release temperature T_0 equals the adiabatic saturation temperature T_{as} .
36. Johnson [16] suggests an empirical correction to the RELEASE predictions for sub-cooled liquids. This correction is based upon introducing a multiplying factor on rainout fraction of

$$F_2 = \left[\frac{P_{vap}(T_0)}{P_a} \right]^m \quad F_2 \leq 1.0 \quad (7-1)$$

where

$P_{vap}(T_0)$ is the vapour pressure of the release liquid at the release temperature T_0

P_a is the ambient pressure

37. Johnson [16] suggests m in the range 0.2 to 0.5. There are problems with this approach:
1. The sign of m should be negative so as to enhance rainout for less volatile substances.
 2. The factor is not well defined in the limit $P_{vap}(T_0) \rightarrow 0$, one interpretation being that a rainout fraction of 1.0 occurs at a finite $P_{vap}(T_0)$.
 3. The above form is not validated.
38. Figure 7-1 shows a comparison of the DeVaul and King correlation with the CCPS low volatility and sub-cooled liquid rainout data together with the rainout data from sub-cooled releases of xylene and water in the JIP Phase IV tests [11].

³ Three experiments involving cyclohexane were sub-cooled by up to 13 K

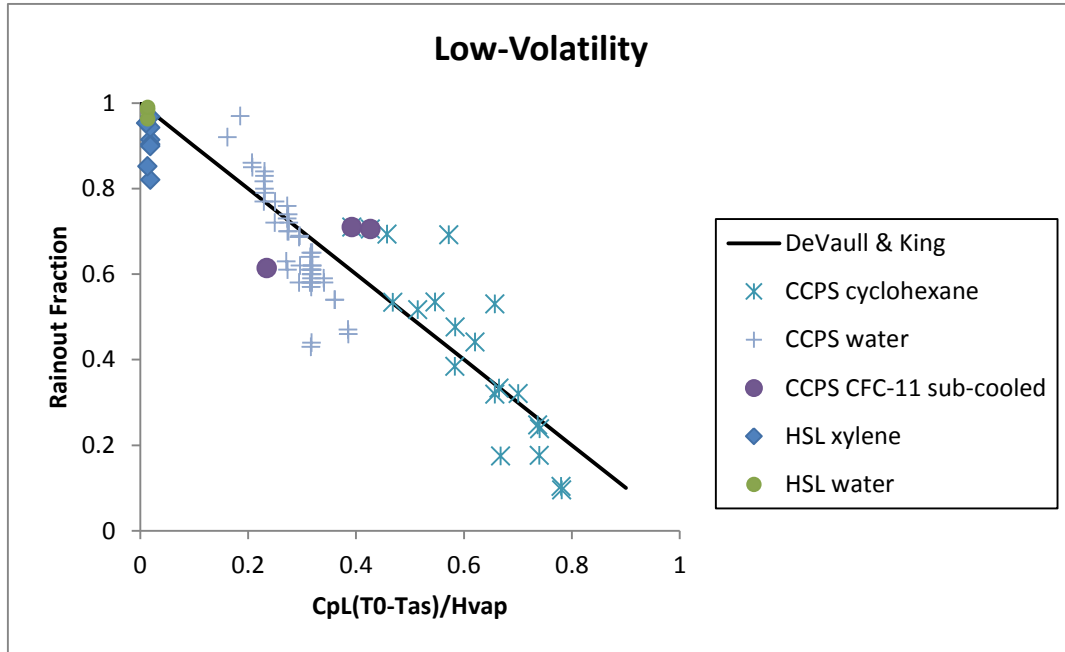


Figure 7-1 DeVaul and King correlation for low-volatility liquids compared with CCPS measured rainout and HSL measured rainout from JIP Phase IV

39. Table 7-1 shows a comparison of the observed rainout in the HSL JIP Phase IV experiments with the rainout predictions from the DeVaul and King correlation. The DeVaul and King values are based on adiabatic saturation temperatures calculated using the same method as in HSE’s RAIN v1.2 spreadsheet. The DeVaul and King rainout fractions calculated here are significantly higher than those given in Table 1 of [12] and are in better agreement with the experimental data. Predictions from the RELEASE model (substance properties for xylene from the AIChE DIPPR 801 database 2012 version) are shown with no multiplication by the factor of 0.6. Rainout predictions from UDM using the Phast 6.7 default rainout model [12] are also shown for comparison.

Table 7-1 Measured and predicted rainout for HSL experiments

Subst	Nozzle diameter (mm)	Stag. Pressure (barg)	Release Temp. (K)	Ambient Temp. (K)	Measured Rainout	DeVaul & King	RELEASE model (Corrected)	Phast 6.7 Default
water	2.5	5	280	280	0.984	0.986	1.0000	0.995
water	2.5	9.5	280	280	0.963	0.986	0.9998	0.987
water	2.5	4.8	280	280	0.990	0.986	1.0000	0.995
xylene	2.5	4.2	284	284	0.968	0.981	0.9904	0.967
xylene	2.5	8	284	284	0.914	0.981	0.7125	0.908
xylene	2.5	10.3	284	284	0.904	0.981	0.4389	0.867
xylene	2.5	15.8	284	284	0.821	0.981	0.0834	0.751
xylene	5	4	284	284	0.943 ¹	0.981	0.9933	0.972
xylene	5	7.7	284	284	0.899	0.981	0.7479	0.931
xylene	5	8.5	275	284	0.953	0.989	0.6819	0.952
xylene	5	13.1	278	284	0.852 ¹	0.987	0.2176	0.888

¹ indicates cases where [12] suggests that significant liquid was missed by the rainout capture system.

8 Summary of Comparison Results

8.1 Comparisons against CCPS Rainout Data

40. When comparing against CCPS rainout data one should remember that the correlations are derived directly from these data, so this is not the same as an independent validation. The ability of the correlations to collapse rainout across the range of the data is, however, a useful indicator of the performance, at least under the experimental conditions.
41. The comparisons against CCPS data show:
1. Apart from water, the Kletz rule-of-thumb performs poorly - it over-predicts rainout compared to most experiments.
 2. As pointed out in [15], the good agreement of the original DeVaul and King correlation with CCPS uncorrected rainout data deteriorates once errors in some substance properties are corrected. Lautkaski's refit of the the DeVaul and King correlation improves on this - resulting in better collapse of the data.
 3. Lautkaski's correlations to CCPS corrected rainout data are simpler than the DeVaul and King correlations in that the corrected data doesn't require partitioning into 'volatile' and 'low-volatile' subsets. Lautkaski's correlation based on Jakob number yields better collapse of the corrected rainout data than the one based on isenthalpic flash x_H . However, these correlations do not give a good prediction of the measured water rainout.
 4. The Jakob number dependence of the new correlation to CCPS uncorrected rainout data provides little, if any, improvement in collapse of the data compared with the DeVaul and King isenthalpic flash dependence.
 5. Apart from water, 0.6 times the RELEASE model predictions provide a reasonably good collapse of the CCPS corrected rainout data. RELEASE shows a tendency to over-predict rainout for the lower corrected chlorine rainout fractions.
 6. The selected Phast 6.7 default model rainout results available from [12] show generally good agreement with the CCPS corrected rainout, except for water and one of the cyclohexane tests.

8.2 Comparisons with Observations from Large Scale Field Trials

42. These are essentially a repeat of the comparisons given in [12]:
1. The Kletz rule of thumb predicts significant rainout for all trials, even though none was observed.
 2. The Lautkaski correlation based on the Jakob number is in better accord with observations (of no rainout) compared with the Lautkaski correlation based on isenthalpic flash (x_H).
 3. The original DeVaul and King correlation is in better accord with observations compared with the refit DeVaul and King correlation.

4. The new correlation for uncorrected rainout is in accord with observations of no rainout.
5. For the field trials simulated using the RELEASE model, non-negligible rainout is predicted by RELEASE only for the Goldfish HF trials.
6. The Phast 6.7 default rainout predictions are in accord with observations of no rainout, apart from some uncertainty regarding rainout for the Desert Tortoise (DT) ammonia trials.

8.3 Rainout from Sub-Cooled Releases

43. For sub-cooled releases:

1. Most of the simple correlations are only appropriate for superheated releases.
2. Comparison with the low-volatility case from the DeVaul and King correlation (used also in the new correlation for uncorrected rainout data) shows, that for these particular sub-cooled releases, the DeVaul and King correlation provides a reasonable estimate of the maximum observed rainout. However, this correlation cannot properly account for the reduction in rainout associated with higher pressure releases through small holes.
3. The DeVaul and King correlation results from this study (Table 7-1) are in much better accord with the experimental data than those in Table 1 of [12]. We are unsure of the reason for this disparity.
4. The RELEASE rainout model shows too strong a dependency of rainout on release pressure for the xylene releases.
5. The Phast 6.7 default rainout model best captures the variation of rainout for the sub-cooled releases.

9 Recommendations

44. Based on our findings, we recommend adopting the new correlation based on the Jakob dependent fit to CCPS uncorrected rainout data. Despite this not being the best fit in each case, this correlation is recommended for its overall behaviour. In particular this correlation:

- a. Results in reasonable overall agreement with uncorrected CCPS data, including water.
- b. Is in accord with the lack of rainout observed in large scale field trials.
- c. Is based on uncorrected rainout data, hence it will retain more material in the direct release, including that vaporised from raining out droplets and/or the resulting pool. In many cases this will be cautious, and will result in fewer cases which will require combining with separate dispersion runs from pool vaporisation.
- d. Provides a reasonable extrapolation for rainout in sub-cooled conditions.
- e. Performs reasonably well compared with the other simple correlations.

45. Over a longer time-scale, alternative rainout methods should be sought that more completely reflect the factors believed important in controlling rainout. In particular, the following modelling approaches merit further investigation:

1. Seeking alternative correlating parameters which better describe the important physics (e.g. comparing characteristic droplet evaporation timescales with characteristic droplet flight times).
2. Inclusion of coupled droplet and pool modelling within DRIFT and tuning to experimental data in a similar way to DNV's UDM rainout modelling.

10 Addendum

46. The recommended correlation has now been implemented in HSE's RAIN v2.0 spreadsheet.

11 References

- [1] G. A. Tickle and J. E. Carlisle, "DRIFT Version 3.6.7: Mathematical Model Description," ESR Technology Report ESR/UC000417/001/Draft B, 2013.
- [2] G. A. Tickle and J. E. Carlisle, "Extension of the dense gas dispersion model DRIFT to include buoyant lift-off and buoyant rise," HSE Books, HSE Research Report RR629, 2008.
- [3] A. H. Shepherd and D. H. Deaves, "Source Term Calculation for Flashing Releases - Background to the Development of ACE," WS Atkins, WSA Report No. AM5233-R1, 2000.
- [4] G. A. Tickle, "Toxic spray releases - A proposed screening tool and source term estimate," GT Science & Software Report, GTS/HSE/R004, In preparation, 2015.
- [5] D. W. Johnson and J. L. Woodward, "RELEASE: A model with data to predict aerosol rainout in accidental releases," AIChE CCPS, 1999.
- [6] S. A. Ramsdale and G. A. Tickle, "Review of RELEASE rainout model and CCPS," HSE Books, HSE Contract Research Report 277, 2000.
- [7] H. W. Witlox and P. J. Bowen, "Flashing liquid jets and two-phase dispersion - A review," HSE Books, HSE Contract Research Report 403, 2002.
- [8] H. W. M. Witlox, M. Harper, P. J. Bowen and V. M. Cleary, "Flashing liquid jets and two-phase dispersion – II. Comparison and validation of droplet size and rainout formulations," *J. Haz. Mat.*, vol. 142, pp. 797-809, 2007.
- [9] H. W. M. Witlox, M. Harper, A. Oke, P. Kay and P. J. Bowen, "Sub-cooled and flashing liquid jets and droplet dispersion, I. Overview and model implementation/validation," *J. Loss Prev. Proc. Ind.*, vol. 23, pp. 831-842, 2010.
- [10] P. Kay, P. J. Bowen and H. W. M. Witlox, "Sub-cooled and flashing liquid jets and droplet dispersion, II. Scaled Experiments and derivation of droplet atomisation correlations," *J. Loss Prev. Proc. Ind.*, vol. 23, pp. 849-856, 2010.
- [11] R. J. Bettis, S. J. Jagger, H. W. M. Witlox and M. Harper, "Two-phase jet releases, droplet dispersion and rainout, II. Rainout experiments," *J. Loss Prev. Proc. Ind.*, vol. 26, no. 3, pp. 462-467, May 2013.
- [12] H. W. M. Witlox and M. Harper, "Two-phase jet releases, droplet dispersion and rainout, I. Overview and model validation," *J. Loss Prev. Proc. Ind.*, vol. 26, no. 3, pp. 453-461, May 2013.
- [13] T. A. Kletz, "Unconfined vapor cloud explosions," *AIChE Loss Prevention*, vol. 11, p. 50, 1977.

- [14] G. E. DeVaul and J. A. King, "Similarity scaling of droplet evaporation and liquid rain-out following a release of superheated flashing liquid to the environment," in *85th Annual Meeting, Air and Waste Management Association, Kansas City, MO, June 21-26, 1992. Paper 92-155.08*, 1992.
- [15] R. Lautkaski, "Experimental correlations for the estimation of the rainout of flashing liquid releases - Revisited," *J. Loss Prev. Proc. Ind.*, vol. 21, pp. 506-511, 2008.
- [16] D. W. Johnson, "RELEASE: An aerosol model with potential," in *1999 International Conference and Workshop on Modeling Consequences of Accidental Releases of Hazardous Materials, San Francisco, California, Sept 28-Oct 1, 1999*.
- [17] H. W. Witlox and A. Holt, "A unified model for jet, heavy and passive dispersion including droplet rainout and re-evaporation.," in *International Conference and Workshop on Modeling the Consequences of Accidental Releases of Hazardous Materials, CCPS, San Francisco, California, Sept 28- Oct 1, 1999*.