UDM THERMODYNAMICS: CHAPTER 2

DATE: December 2023

Non-Reactive Equilibrium Model;

Heat/Water Transfer From Substrate

No.	Date	Reason for Issue	Prepared by	Verified by	Approved by
1	1999	PHAST 6.0	Witlox and Holt		
2	Oct 2005	SAFETI 6.5	Witlox and Harper		
3	Dec 2020	Generalised multiple aerosol algorithm	Witlox	Harper	
4	May 2021	Apply new template	D. Vatier		

Date: December 2023

Prepared by: Digital Solutions at DNV

Verification

ABSTRACT

A large number of errors were corrected in the UDM thermodynamics model as part of the quality-improvement and verification work for version 6.0 of PHAST. The UDM thermodynamics model has been further extended to allow the mixing of air with a multi-component pollutant. Two different methods are included, i.e. either a 'single-aerosol algorithm ('SA' method based on the XPRP property system) or a 'multiple-aerosol' aerosol algorithm ('MA' method based on the thermodynamics model included in the HEGADAS dispersion model in HGSYSTEM).

The following verification has been carried out:

1. In the absence of liquid component, the equilibrium and non-equilibrium model lead to identical results.

2. The equilibrium model is tested for mixing of propane with moist air at 20C. Ambient humidity, propane liquid fraction, propane temperature have been varied. The cooling effect because of component evaporation and the heating effect because of water condensation is shown.

3. In the case of the presence of single-component aerosols only, the UDM thermodynamics predictions using the MA method are shown to be in agreement with HEGADAS (e.g. mixing of propane pollutant or ammonia/butane pollutant with dry or moist air).

4. The MA and SA methods are shown to produce very close results in the case of a presence of a single aerosol (e.g. mixing of multi-component hydrocarbon pollutant with dry air), and are also in agreement with HEGADAS predictions.

5. The effect of heat and water-vapour transfer has been studied by variation of ground temperature.

6. Dry air properties (vapour enthalpy) and water properties (vapour/liquid/ice enthalpy, saturated vapour pressure for solid/vapour and liquid/vapour equilibrium) are now determined in the UDM thermodynamics module using DIPPR. This resulted in virtual identical results for the former non-DIPPR option (except for reduced liquid water enthalpies). Moreover the moist air density is set using the new property system.

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2 NON-REACTIVE EQUILIBRIUM MODEL; HEAT/WATER TRANSFER FROM SUBSTRATE

2.1 Introduction

This chapter describes the verification of the non-reactive equilibrium module in the UDM thermodynamics model for the mixing of a pollutant with moist air. It also includes testing of the logic for heat and water-vapour transfer from the substrate in the UDM.

The non-reactive equilibrium module in the UDM thermodynamics model does not account for reactions and assumes thermal equilibrium at the atmospheric pressure. Thus the same temperature T_{vap} is adopted for all components in the cloud (vapour and liquid). The equilibrium model determines the phase distribution [pollutant (liquid, vapour), water (liquid, vapour, ice)] and the mixture temperature, by imposing phase equilibrium calculations for given cloud enthalpy H_{cld} and given pressure P_a.

A new multi-compound thermodynamics has been introduced to the UDM. This allows for improved handling of mixture thermodynamics by means of two new equilibrium thermodynamic models (so-called multi-compound or MC approach):

- Single aerosol (SA – XPRP method). A single aerosol is presumed for all liquid components (including both pollutant and ambient water). This is based on standard 2-phase vapour liquid equilibrium calculations using the new multi-component property system XPRP.

- Multiple aerosols (MA – HGSYSTEM method). There are potentially several aerosols for different liquid components. Each component has an aerosol class, with components that share the same class forming a single aerosol.

The old UDM method treated pollutant mixtures as pure components (so-called pseudo-component or PC approach). This option is retained in the new UDM as a specific case of the 'multiple aerosol' thermodynamics.

See the theory manual for the UDM thermodynamics model for further full details of the theory.

This chapter verifies the above thermodynamics model of mixing of a released pollutant with dry or moist air, including a comparison between the MA and SA results and a comparison of the MA results with the HEGADAS model in HGSYSTEM.

- Section 2.2 considers the example of a one-component pollutant (propane), including effects of heat and water vapour.
- Section 2.3 considers the example of a multi-component pollutant (propane/butane) with the presence of a single aerosol.
- Section 2.4 considers the example of a multi-component pollutant (ammonia/butane) with the presence of multiple aerosols.
- Section 2.5 includes the results of a further sensitivity analysis for the case of mixing of propane with air.

2.2 Mixing of one-component pollutant (propane) with air

This section describes the application of the thermodynamics model to illustrate the effect of component aerosol evaporation and water condensation/evaporation. The equilibrium model is tested for mixing of propane with moist air at 20C. The following parameter variations are carried out:

- Liquid mole fraction η_{cL}^o of released propane

  * $\eta_{cL}^o = 0$ (100% propane vapour), with the release temperature T_c^o of the propane just above the boiling temperature $T_{boil}^c = -42.1$: $T_c^o = -42$C. No liquid propane aerosol forms, since the mixture temperature T remains above the boiling temperature of the propane.

  * $\eta_{cL}^o = 1$ (100% propane liquid), with the release temperature T_c^o of the propane just below the boiling temperature: $T_c^o = -43$C. Upon mixing of the propane with the air, the propane aerosol evaporates.

- Humidity r_h of air

  * $r_h = 0$ (dry air). No water aerosol forms

* r_h = 0.7 (70% humid air). Upon mixing of the moist air with the cold propane, the water condenses and a water aerosol forms.

2.2.1 UDM thermodynamics model predictions (MA method)

Figure 2.1 includes the thermodynamic predictions of the mixture temperature against the propane mole fraction in the mixture. This figure demonstrates the initial mixture-cooling effect of the evaporating propane (η_{cL}^o = 1) and the initial mixing-heating effect of the condensing water (r_h = 0.7). Note the discontinuous temperature slopes at the point where the propane aerosol disappears. Note that Figure 2.1 compares well with an identical exercise carried out by Witlox[i] for the two-phase multi-compound thermodynamics model implemented in HEGADAS in the HGSYSTEM 3.0 version.

Figure 2.2 includes the mass fractions of the several mixture compounds against the propane mole fraction:

a.   Figure 2.2a illustrates the dilution of the propane vapour during mixing with dry air.

b.   Figure 2.2b illustrates the initial condensation of water vapour into ice during mixing of the cold propane vapour with air of 70% humidity, the subsequent melting of ice into liquid water (at 0°C), and final disappearance of the liquid water fog with further dilution with the air

c.   Figure 2.2c illustrates the evaporation of the propane liquid into propane vapour during mixing with dry air. After the propane liquid has entirely evaporated, the propane vapour fraction reduces with further dilution with the air.

d.   Figure 2.2d illustrates the evaporation of propane liquid and simultaneous condensation of water into ice, for mixing of propane liquid with air of 70% humidity.

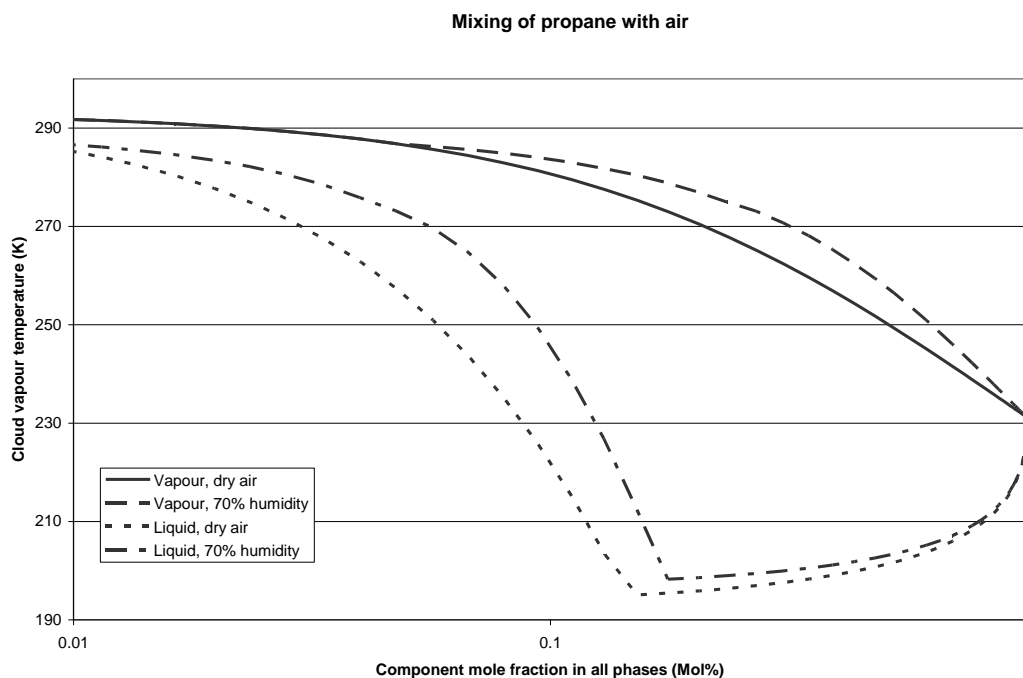**Mixing of propane with air**

Figure 2.1.   Temperature predictions by UDM thermodynamics equilibrium model for mixing of propane with air; propane release temperature = -42C (propane vapour) or –43C (propane liquid); ambient humidity is 0% (dry air) or 70%
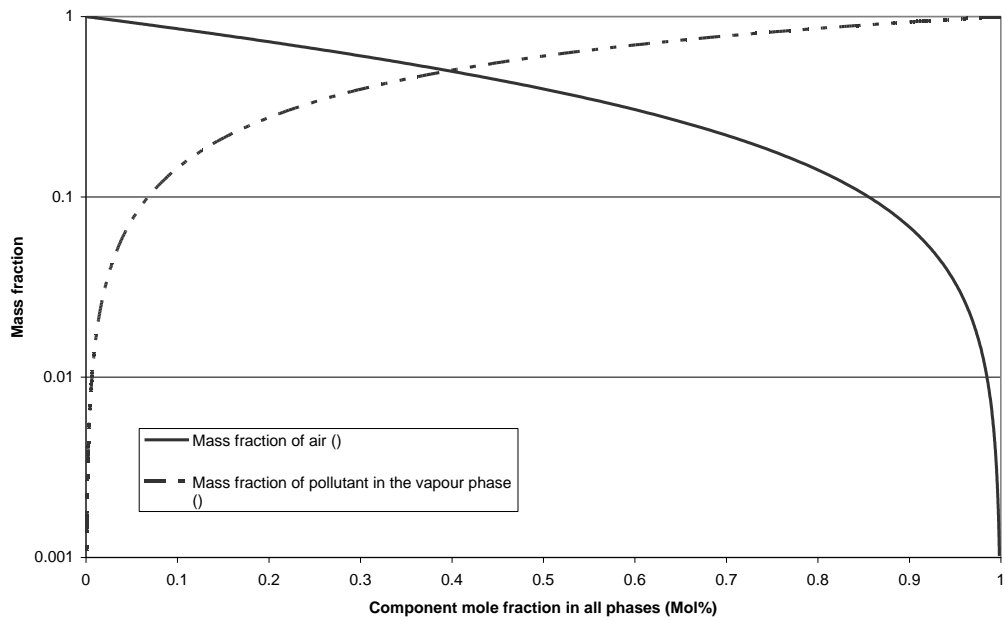
Mixing of propane vapour with dry air

Figure 2.2a
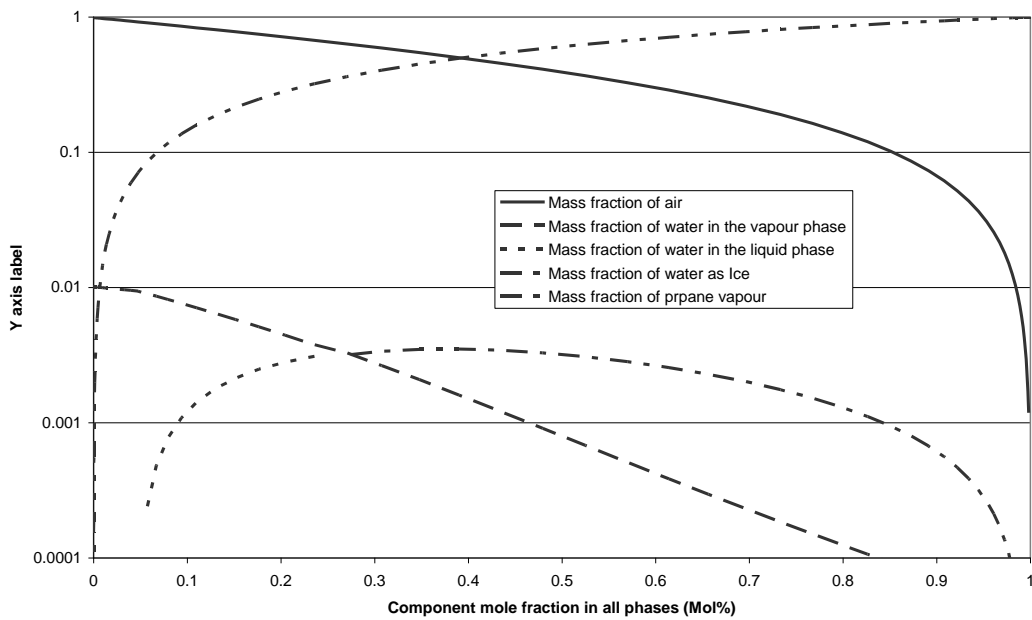

Mixing of propane vapour with 70% humid air

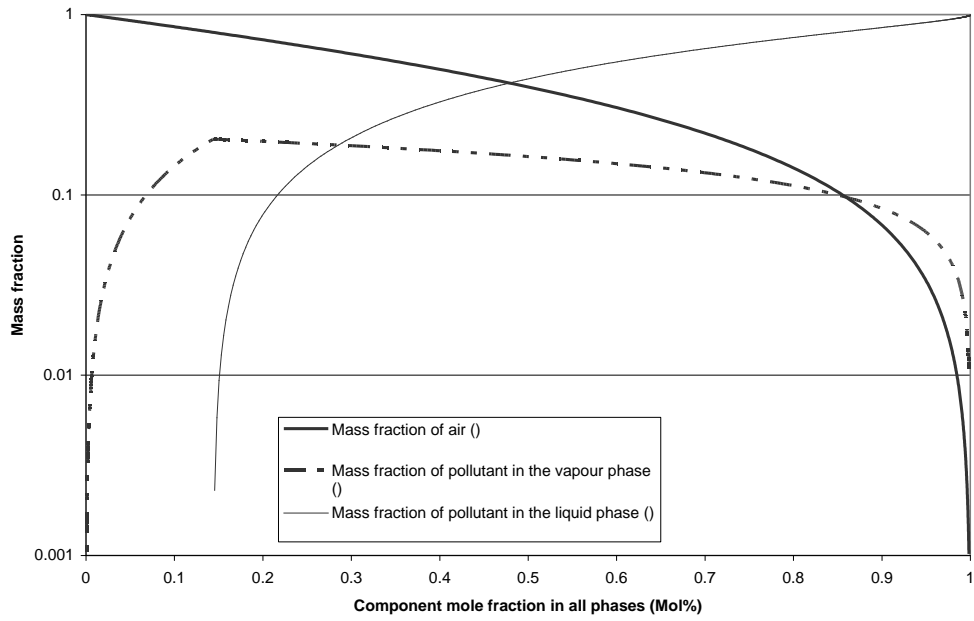Figure 2.2b

Mixing of propane liquid with dry air

Figure 2.2c

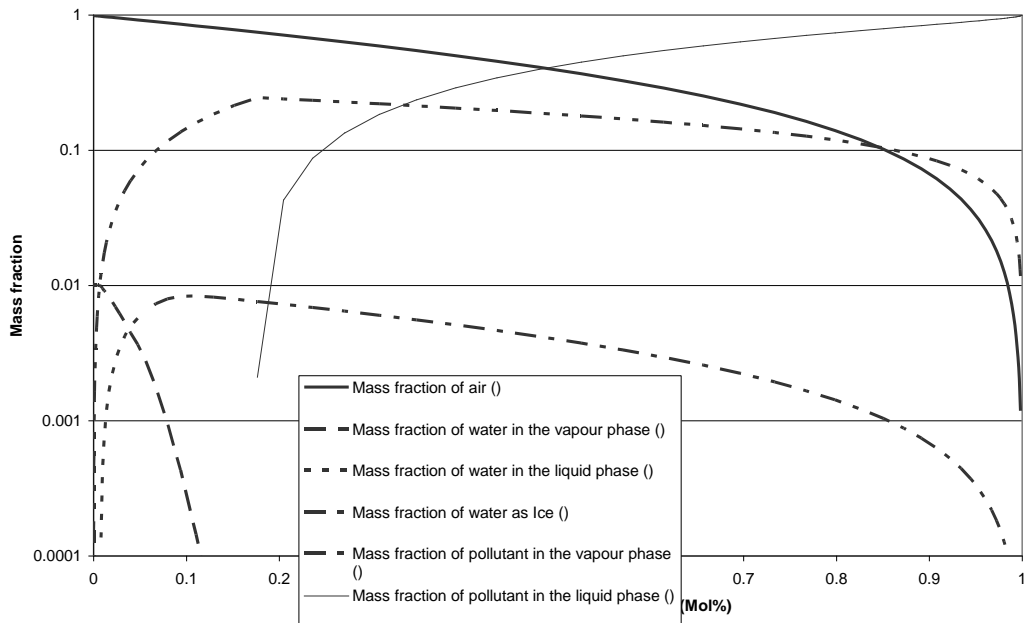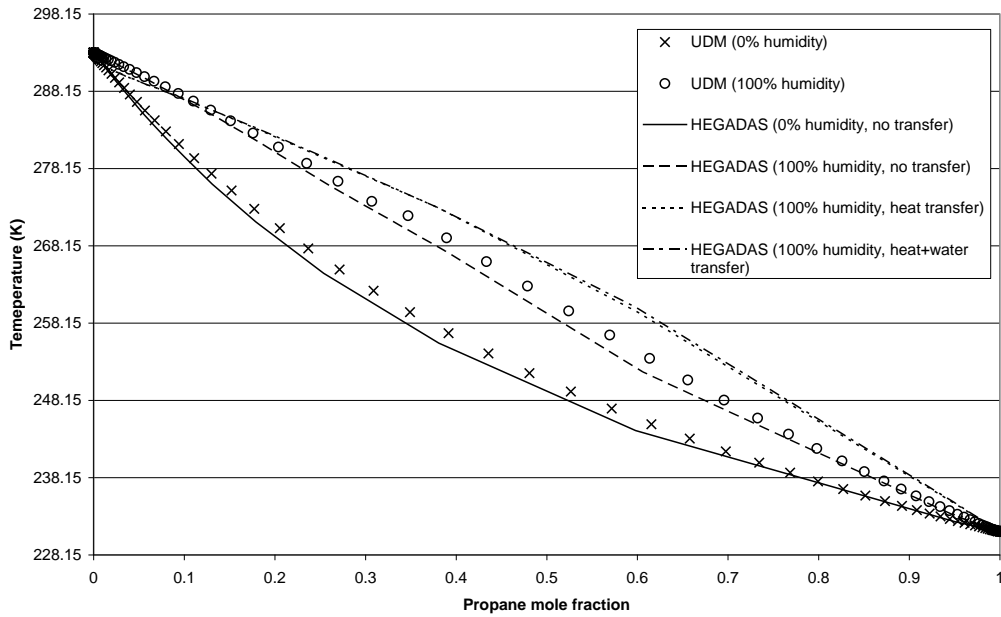**Mixing of propane liquid with 70% humid air**

Figure 2.2d

Figure 2.2.   **Predictions of mass fractions by UDM thermodynamics model for mixing of propane (vapour of liquid) with air (dry or 70% humidity)**

2.2.2 Comparison of MA method (UDM) with HEGADAS and SA method (UDM)

Figure 2.3 compares UDM results against HEGADAS predictions. UDM predictions are shown to be in very close with HEGADAS predictions for the case of mixing of propane vapour/liquid (at –43/42C) with 0%/100% humid air. The minor differences can be explained because the HEGADAS thermodynamics model assumes the specific heats of the vapour and the liquid to be constant as function of temperature, while the UDM thermodynamics derives them directly from the temperature-dependent vapour and liquid enthalpies (from DIPPR database). The approximate constant values of the HEGADAS specific heats (taken at 20C) are larger than the variable specific heat. As a result, the following applies:
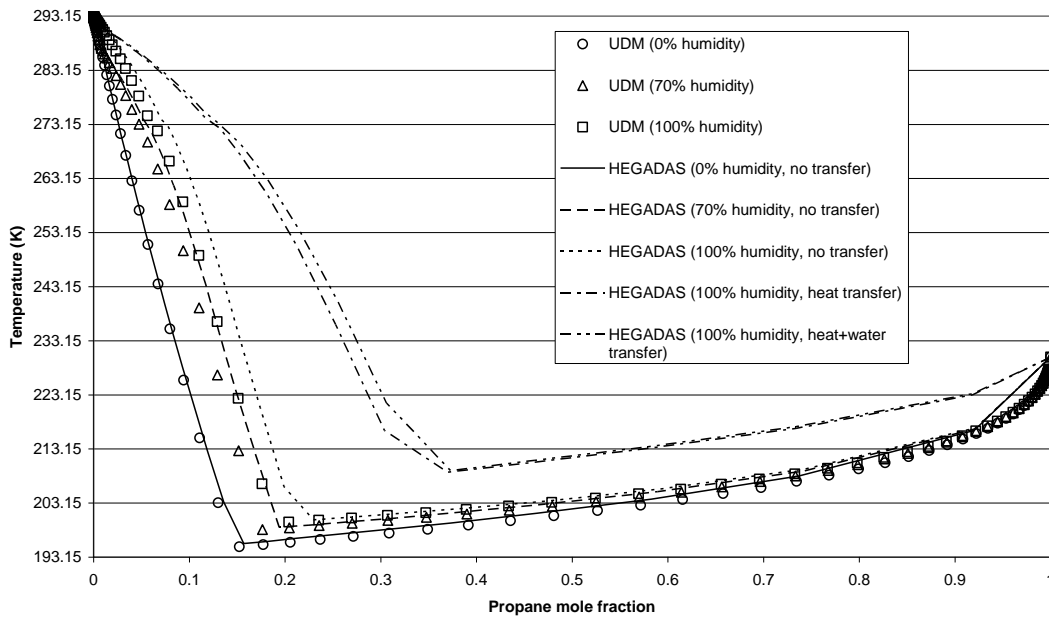
- For mixing of pure propane vapour with air (Figure 2.3a) , the HEGADAS plume heats up slightly less quick than the UDM plume because of the lower HEGADAS vapour specific heat.

- For mixing of pure propane liquid with humid air (Figure 2.3b), the HEGADAS plume cools down slightly less quick than the UDM plume and as a result the liquid component aerosol disappears somewhat earlier. This may be caused by slight differences in specific heats and/or water vapour pressure.

Mixing of propane vapour (-42C) with air (20C)

(a)

Mixing of propane liquid (-43C) with air (20C)

(b)

Figure 2.3. **Temperature predictions by HEGADAS and UDM thermodynamics equilibrium models for mixing of propane (vapour or liquid) with air (dry or humid). The plots also include results of HEGADAS runs including heat and/or water transfer.**

Figure 2.4 shows the mixing of pure propane liquid with dry and wet (100% humidity) air. Results are shown for both the MA method (separate propane and water aerosols) and the SA method (single propane/water aerosol). For dry air, both methods give almost identical results, since no water is present. For wet air the MA and SA methods give different results. This is due to the water forming part of the same aerosol as propane under the flash model. The MA method exhibits more cooling.
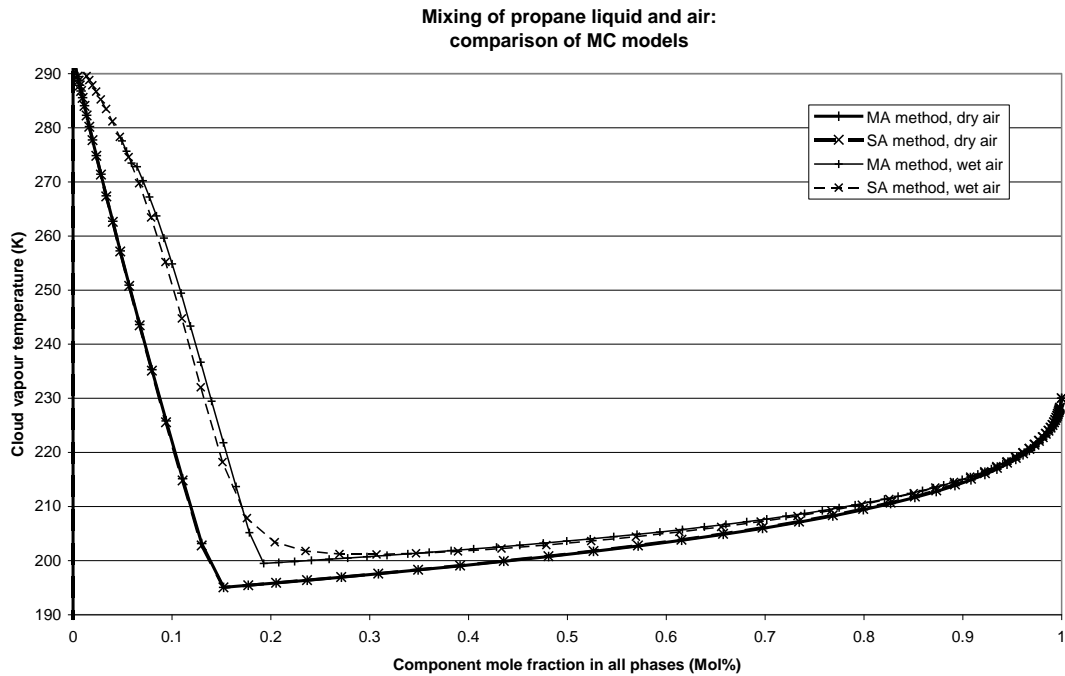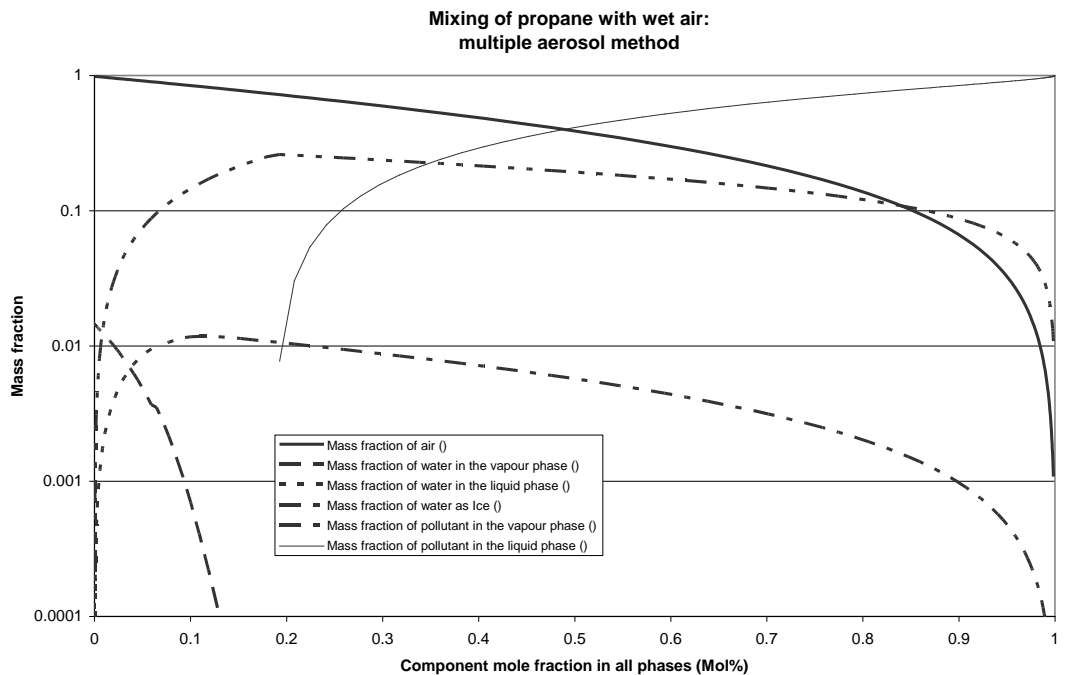

Figure 2.4. Mixing of propane with dry and wet (100% humidity) air.

Figure 2.5 shows a more detailed plot of mass fractions for the wet air case above. The principal difference is the occurrence of ice in the multiple-aerosol case, which is not present in the flash. Currently, the flash method has no solid phase equilibrium calculations.
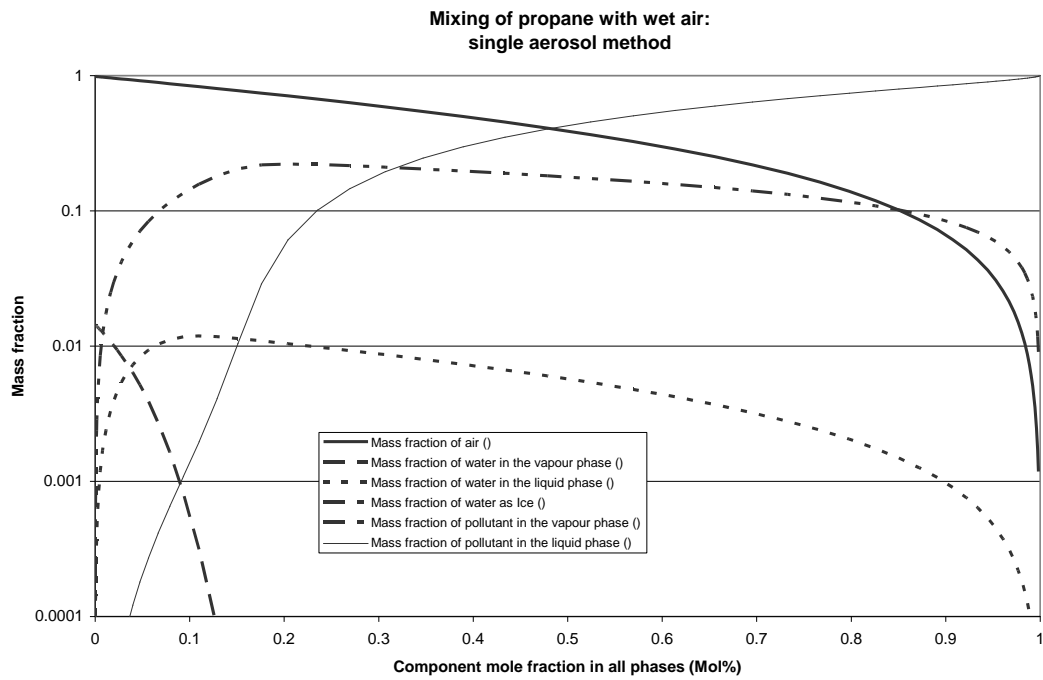

(a) MA method

**Mixing of propane with wet air:
single aerosol method**

(b) SA method

Figure 2.5. Mass fractions for mixing of propane with wet (100% humidity) air.

2.2.3 UDM dispersion model predictions (no heat and water transfer; MA method)

Above results are included by the UDM thermodynamics model, and the model has been compared against the HGSYSTEM model. Below results are presented for UDM concentration predictions using the new UDM thermodynamics model. In line with the assumptions adopted by Witlox[i] for HEGADAS, the following input data were selected:

- Release rate = 32 kg/s
- Release velocity = 0.08 m/s (vapour), 0.0003m/s (liquid)
- Surface roughness z_o = 0.01 m
- Stability class D
- Constant temp and wind profile
- atmospheric temperature = 293 K
- Wind speed = 6 m/s
- Drop size = 1E-05 m (liquid)
- Ground temperature = 20C

Release velocities were chosen to give an initial effective half width of 10 m. The transition to passive dispersion was disabled. For the liquid releases the UDM was modified to exclude liquid rainout.

Figure 2.1 and Figure 2.2 presented thermodynamic results for the mixing of cold propane vapour (at –42C) or liquid (at –43C) with 0% or 70% humidity air (at 20C). Figure 2.6 includes UDM dispersion predictions for these cases. It illustrates that qualitatively, the trend in centre-line concentration and effective half-width are the same as those presented for HEGADAS[i] for this case:

- Effects of humidity are small on both cloud half-width and centre-line concentration.
- The concentration for the liquid releases is higher in the near field than for vapour releases. This is caused by the suppressed entrainment resulting from the larger Richardson number due to the larger density.
- The larger density also causes a larger spread rate (larger cloud half-widths).
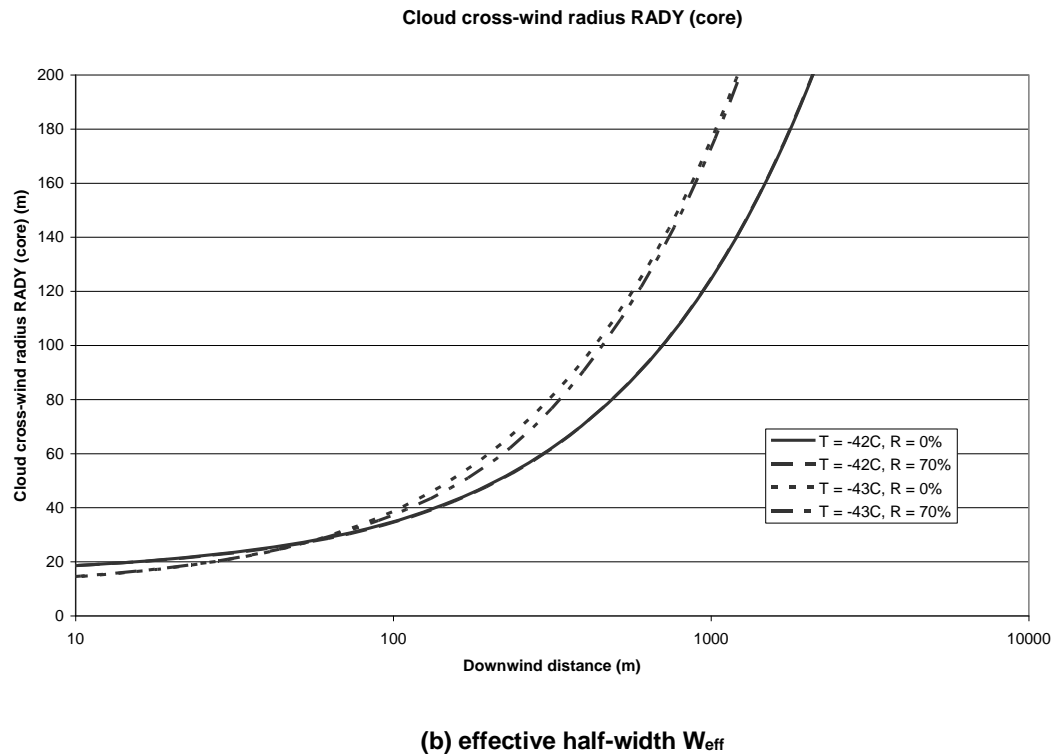
Centre-line concentration (core)

(a) centre-line concentration

Cloud cross-wind radius RADY (core)

(b) effective half-width W_{eff}
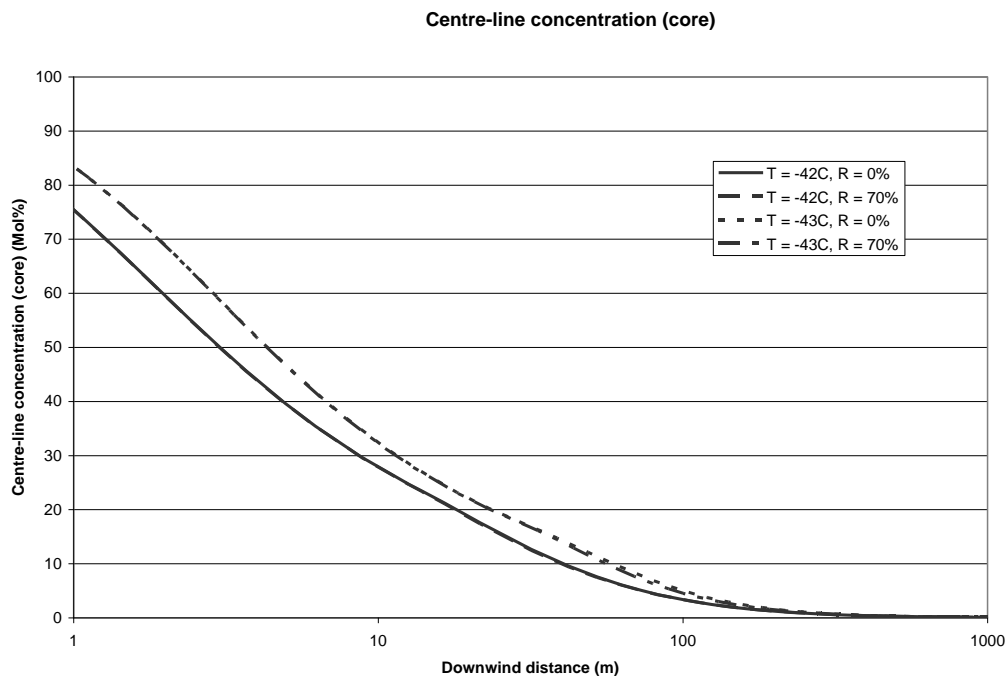
Figure 2.6. **UDM dispersion predictions using thermodynamics equilibrium model for mixing of propane with air (no heat and water substrate transfer); propane release temperature = -42C (propane vapour) or –43C (propane liquid); ambient humidity is 0% (dry air) or 70%**

2.2.4 UDM dispersion model predictions (heat and water transfer; MA method)

Figure 2.7 illustrates the effect of substrate heat and water-vapour transfer in case of mixing of propane vapour (at –42C) with dry or 100% humidity air. The ground temperature was chosen equal to the ambient temperature. The effect of heat and water-vapour transfer is different to that for the HEGADAS runs in Figure 2.3a, because the ground temperature was chosen to be 20C instead of 1C[1].

In Figure 2.7 the black lines/markers correspond with 0% ambient humidity, while the red lines/markers correspond with 100% humidity. The markers correspond with THRM predictions, where no substrate heat and substrate water-vapour transfer is included.

In case of 100% humidity, the mixing of cold propane with the air results in condensation of the water from the air which generates added heat. Therefore the mixture temperature increases with ambient humidity.

As should be the case, it is confirmed that the THRM prediction match the UDM predictions (solid lines - RH0, RH100) where no heat and water-vapour transfer is included. Inclusion of heat transfer (dashed lines - RHOH, RH100H) from the hotter substrate results in added heating from the cloud, while also including water-vapour transfer generates further cloud heating (dotted lines - RHOHW, RH100HW).

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[1] TO CHECK. Further analysis should be carried out. Particularly heat transfer would be expected for UDM to be larger than that for HEGADAS. Suggest to do HTAG case (for which exact agreement of widths, concentrations has been demonstrated) with ground temperature different to ambient temperature (30 degrees below, and 10 degrees above) and to do runs with heat transfer and with heat+water transfer. If results don't match, UDM would need to adopt identical assumptions!
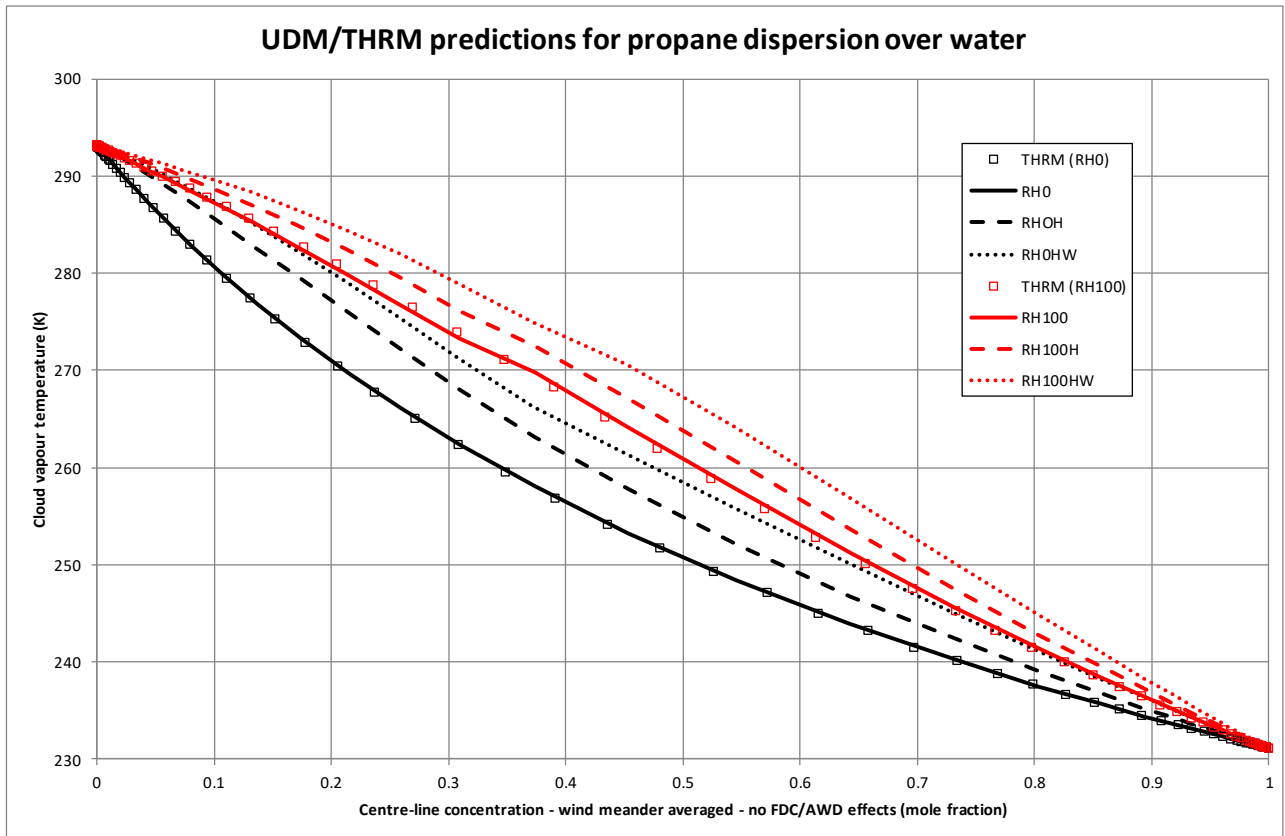
Figure 2.7. **UDM or THRM predictions using thermodynamics equilibrium model for mixing of propane with air**

## 2.3 Mixing of multi-component pollutant with air – single aerosol

A mixture of materials which have the same aerosol class (for example any hydrocarbons, with aerosol class = 8) should form a single aerosol according to the MA method. Under these circumstances, and for dry air, the results from both SA and MA methods will be very similar.

Figure 2.8 illustrates this, with a 0.5 / 0.5 mole fraction mixture of propane and n-butane mixed in dry air for different starting temperatures using the MA method. For the -20 Celsius case, the results from the SA and from an independent HEGADAS simulation are plotted as well. There is good agreement between all three.

A reduction of the temperature of the initial pollutant (propane/butane) from its dew point temperature (-13.1C) to its bubble point temperature (-27.7C) results in an increase of the initial pollutant liquid fraction from 0 to 1. Therefore, with reducing initial pollutant temperature, more mixture cooling occurs and more air needs to be mixed in to evaporate all liquid.

Propane / Butane Mixture:
Multiple aerosol method

(a) Cloud temperature
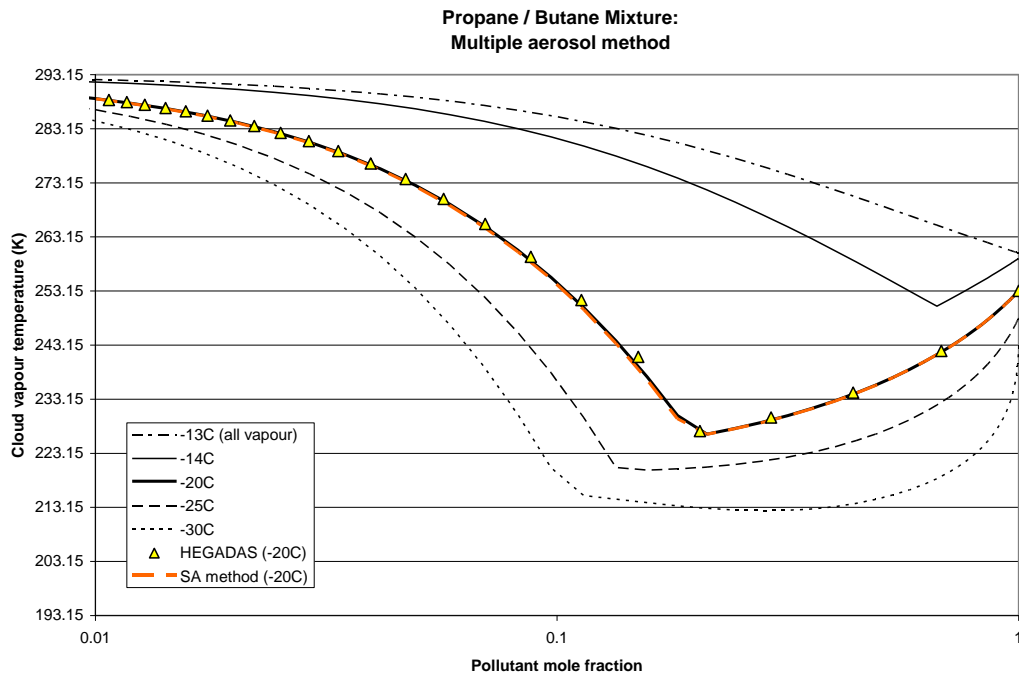
Propane / Butane Mixture:
-20C, dry air
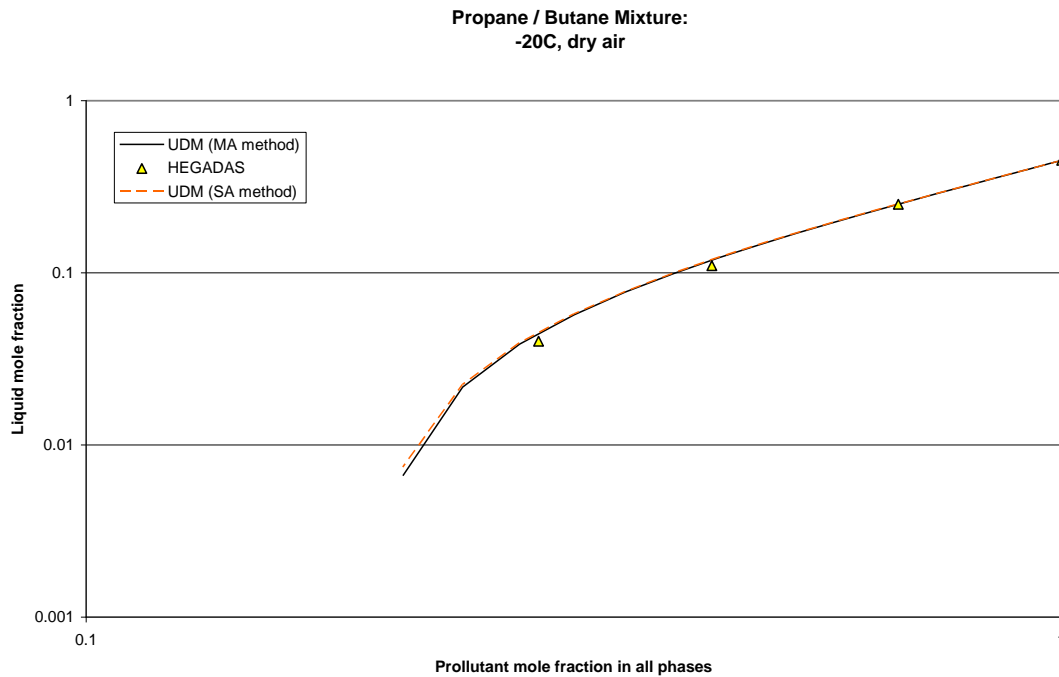
(b) Aerosol mole fraction, -20ºC

Figure 2.8. Mixing of propane/butane mixture in dry air using MA method

The figure includes UDM MA results for initial pollutant temperatures of -14C, -20C, -25C and -30C corresponding with increasing initial liquid pollutant fraction. Also HEGADAS MA results are shown, as well as UDM SA results.

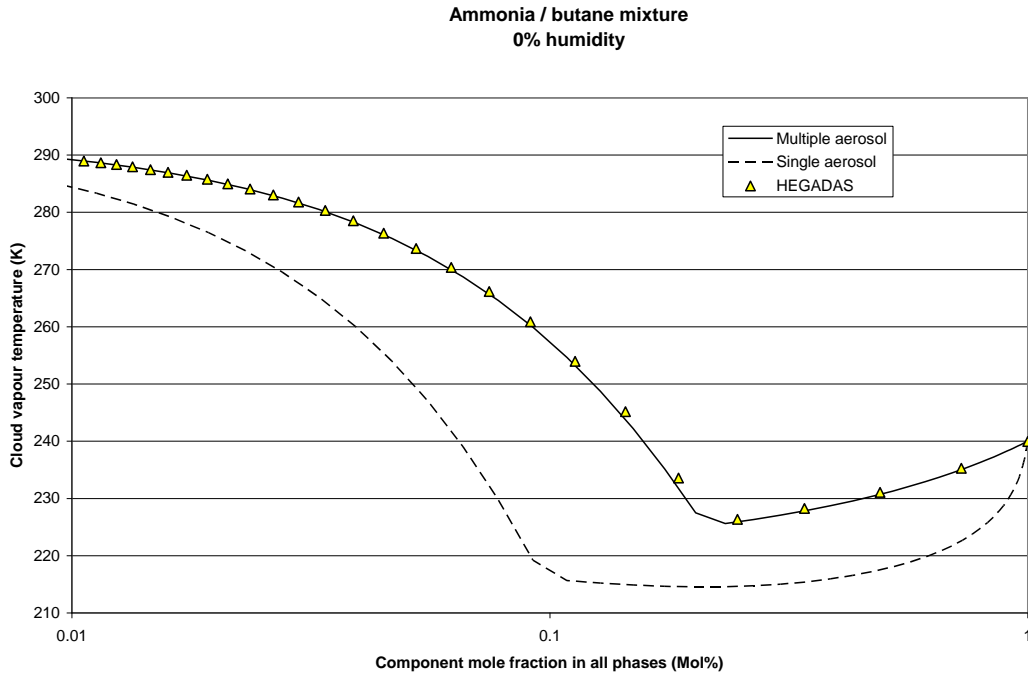## 2.4 Mixing of multi-component pollutant with air – multiple aerosols

2.4.1 Mixing of ammonia/butane pollutant with air

Difference in results will occur between the MA and SA methods, for mixtures that tend to form more than one aerosol. To illustrate this we use an ammonia / n-butane mixture (0.5 / 0.5 mole fraction) in dry and wet air. Again we compare the results with HEGADAS, which should in theory be close to the multiple aerosol results.
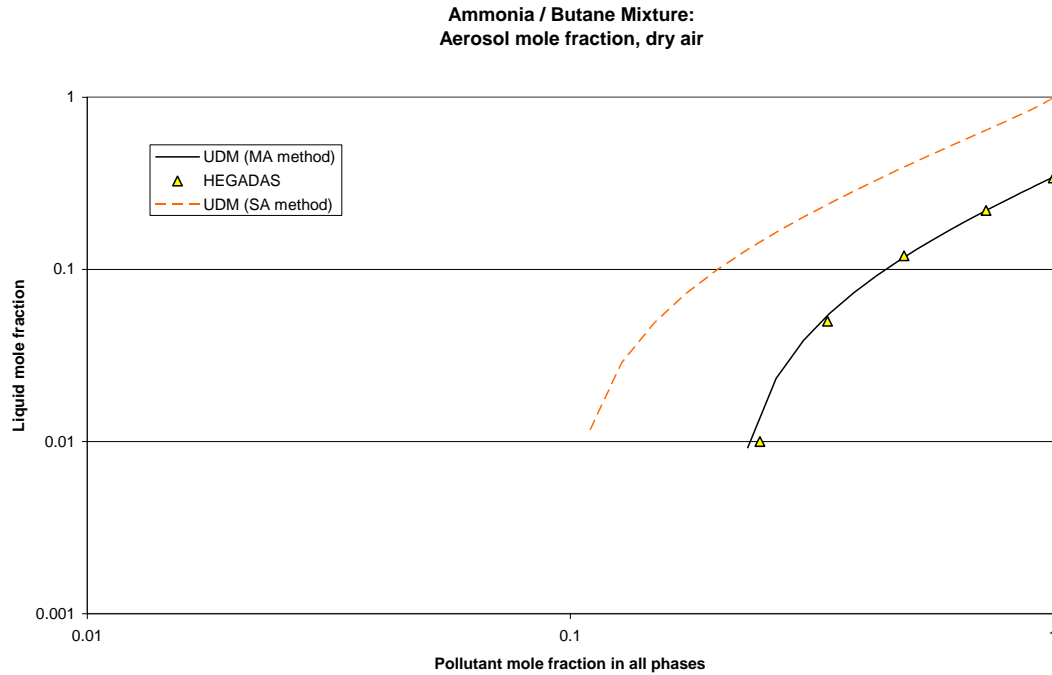
Figure 2.9 and Figure 2.10 indicate good agreement between HEGADAS and the MA method for dry air, but less so for wet air[2]. The results between the MA and SA methods are very different, with temperatures up to 40+ K cooler for the SA method.   In these instances, it is expected that the MA method will provide a more accurate description of the thermodynamics.   The wet air case has in fact up to three separate aerosols as water, ammonia, and n-butane all have different aerosol classes.

Further detail on the dry-air case is given in Figure 2.11 with mass fractions plotted for the air, water and component (here component is the aggregate of ammonia and butane). This illustrates the different starting conditions, with the SA method predicting initially all liquid and the MA method some vapour.

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[2] This is despite the starting conditions being different. We should rerun these cases at a low enough temperature to ensure all liquid at the initial temperature for all methods. This is a persistent difficulty when comparing methods (especially PC with MC)

Ammonia / butane mixture
0% humidity

(a) temperature

Ammonia / Butane Mixture:
Aerosol mole fraction, dry air

(b) aerosol mole fraction

Figure 2.9. **Comparison of SA and MA methods for ammonia / butane pollutant released at 240K into dry air**

Ammonia / butane mixture
100% humidity

(a) temperature

Ammonia / Butane
Aerosol mole fraction, 100% wet air
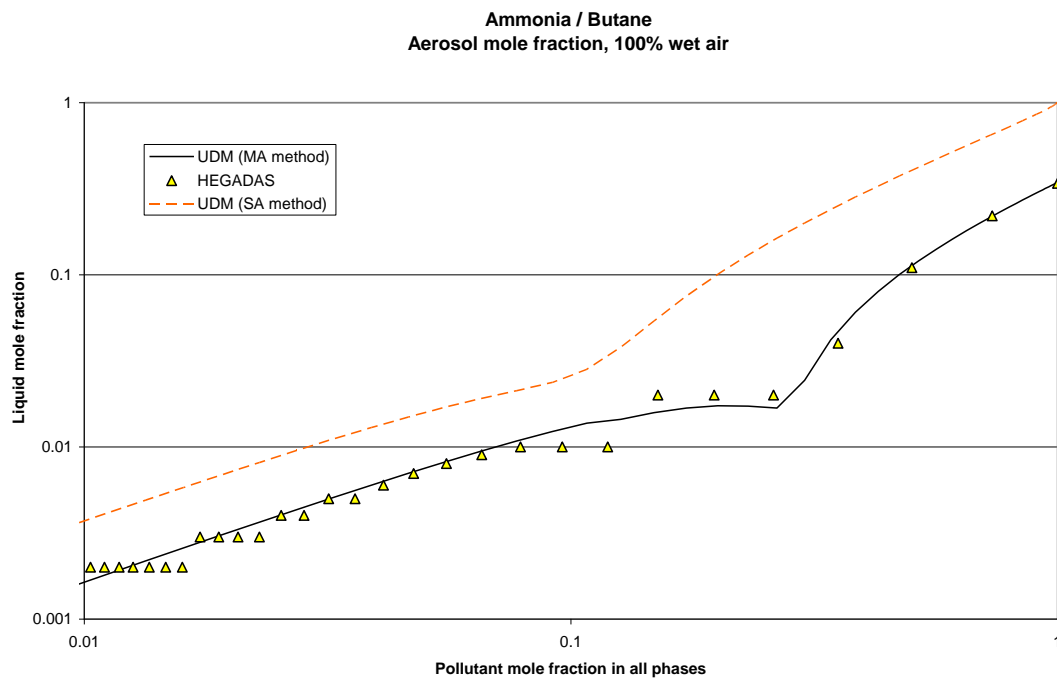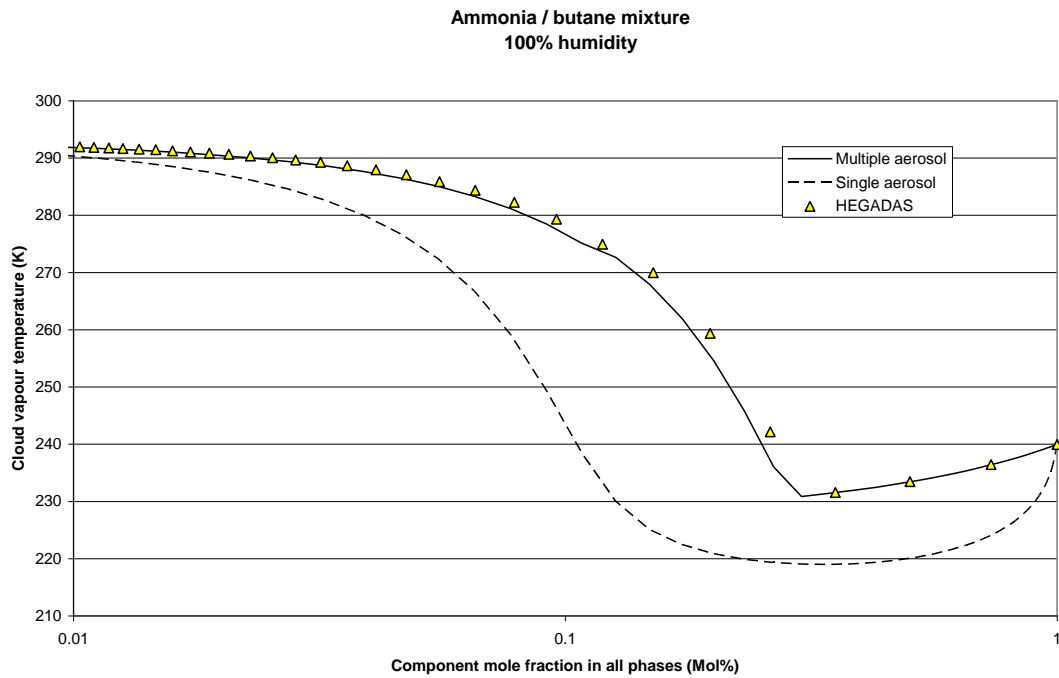
(b) aerosol mole fraction[3]

Figure 2.10. **Comparison of SA and MA methods for ammonia / butane pollutant released at 240K into 100% wet air**

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[3] For low aerosol mole fractions, the HEGADAS results demonstrate poor precision of reporting (sometimes only 1 or 2 significant figures).

Ammonia/butane mixture:
multiple aerosol method

(a) MA method

Ammonia/butane mixture:
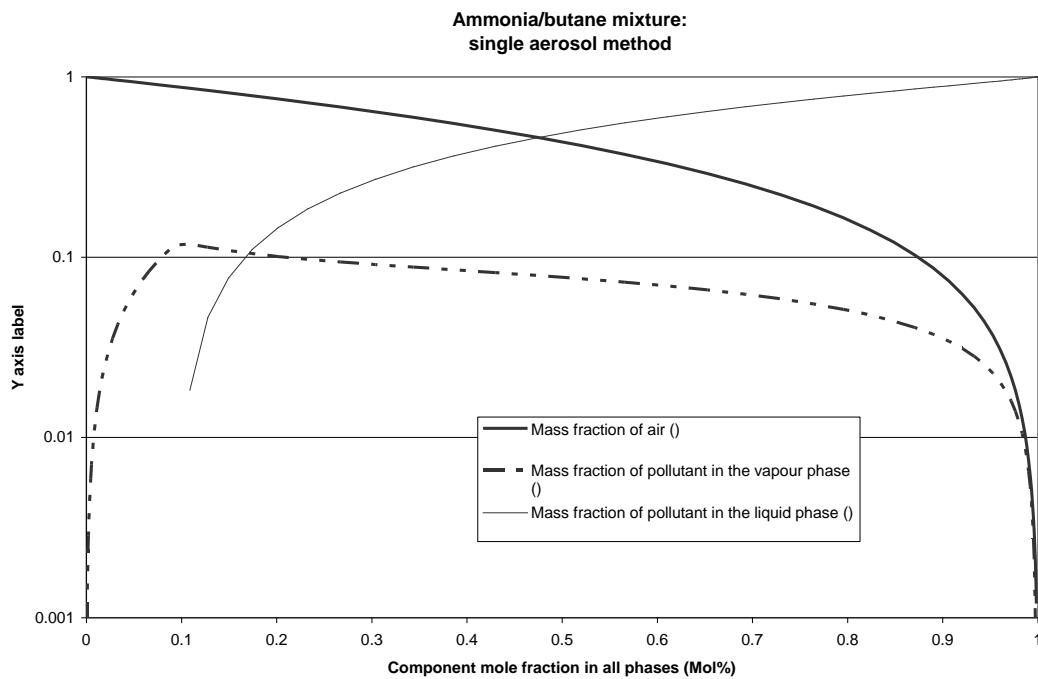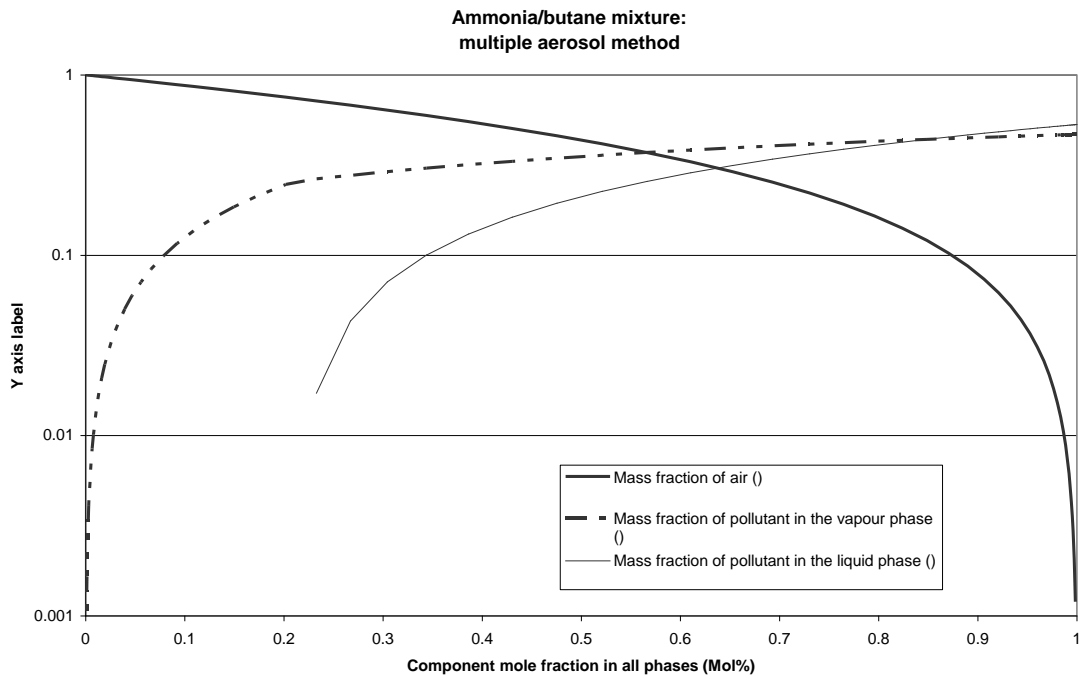single aerosol method

(b) SA method

Figure 2.11. Mass fractions for mixing of propane/butane pollutant with dry air

2.4.2 Mixing of propane/butane/pentane/chlorine/ammonia pollutant with wet air

The pollutant mixture is chosen to consist of 5 components with equal 20% mass fractions. The 5 components are propane (boiling point 231.1K), butane (boiling point 272.6K), pentane (boiling point 309.2K), chlorine (boiling point 239.1K) and ammonia (boiling point 239.7K). The pollutant is mixed with moist air. Thus there are 4 potential aerosols: one three-component hydrocarbon aerosol (propane/butane/pentane) and three one-component aerosols (chlorine, ammonia, water).

The bubble point of the mixture was found to be 219.5K. Please note that this is below the minimum atmospheric boiling point of each individual components (231.1K – boiling point of propane). The reason of this is the presence of other vapour components in the mixture. Likewise the dew point of the pollutant mixture (about 268.15K) is considerable below the maximum boiling point (309.2K – boiling point of pentane).

Figure 2.12 shows results of mass fraction and the cloud temperature of mixture components, while mixing the pollutant at the bubble point of 219.5C with moist air at 293.15K (70% humidity). Figure 2.12c shows component mass fractions of overall pollutant (black lines), propane within pollutant (orange line) and ambient water (green lines). The solid lines refer to the liquid phase, dashed lines to the vapour phase, and dotted line to the water ice phase.

Figure 2.12a and Figure 2.12c show that initially all pollutant components are liquid, and that the aerosols disappear in the following order while mixing with air: chlorine (at about 50% pollutant concentration), ammonia (at 17%), propane/butane/pentane (at 10%) and finally the water aerosol (at 0.6%). From Figure 2.12d it is seen that the mixture temperature initially drops during mixing (because of liquid evaporation), and subsequently rises to the ambient temperature (293.15K).
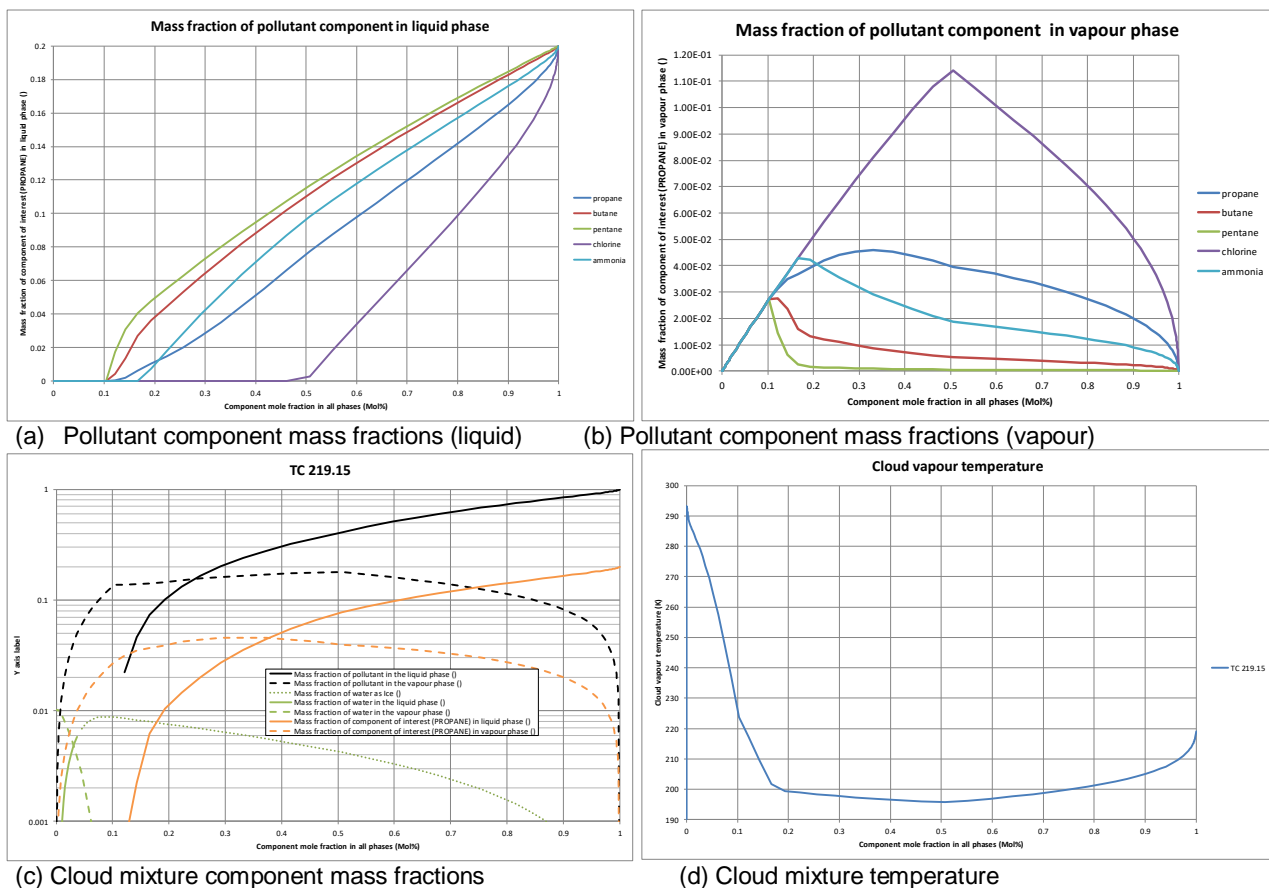

(a) Pollutant component mass fractions (liquid)

(b) Pollutant component mass fractions (vapour)

(c) Cloud mixture component mass fractions

(d) Cloud mixture temperature

Figure 2.12. Mixing of propane/butane/pentane/chlorine/ammonia pollutant (219.5C) with wet air

In Figure 2.13 the initial pollutant temperature is varied between the bubble point of 219.5K and the dew point of 268.15K. It is seen that with increasing initial pollutant temperature there is a reducing amount of initial liquid present in the pollutant, and hence less cooling effect resulting from the evaporating liquid.
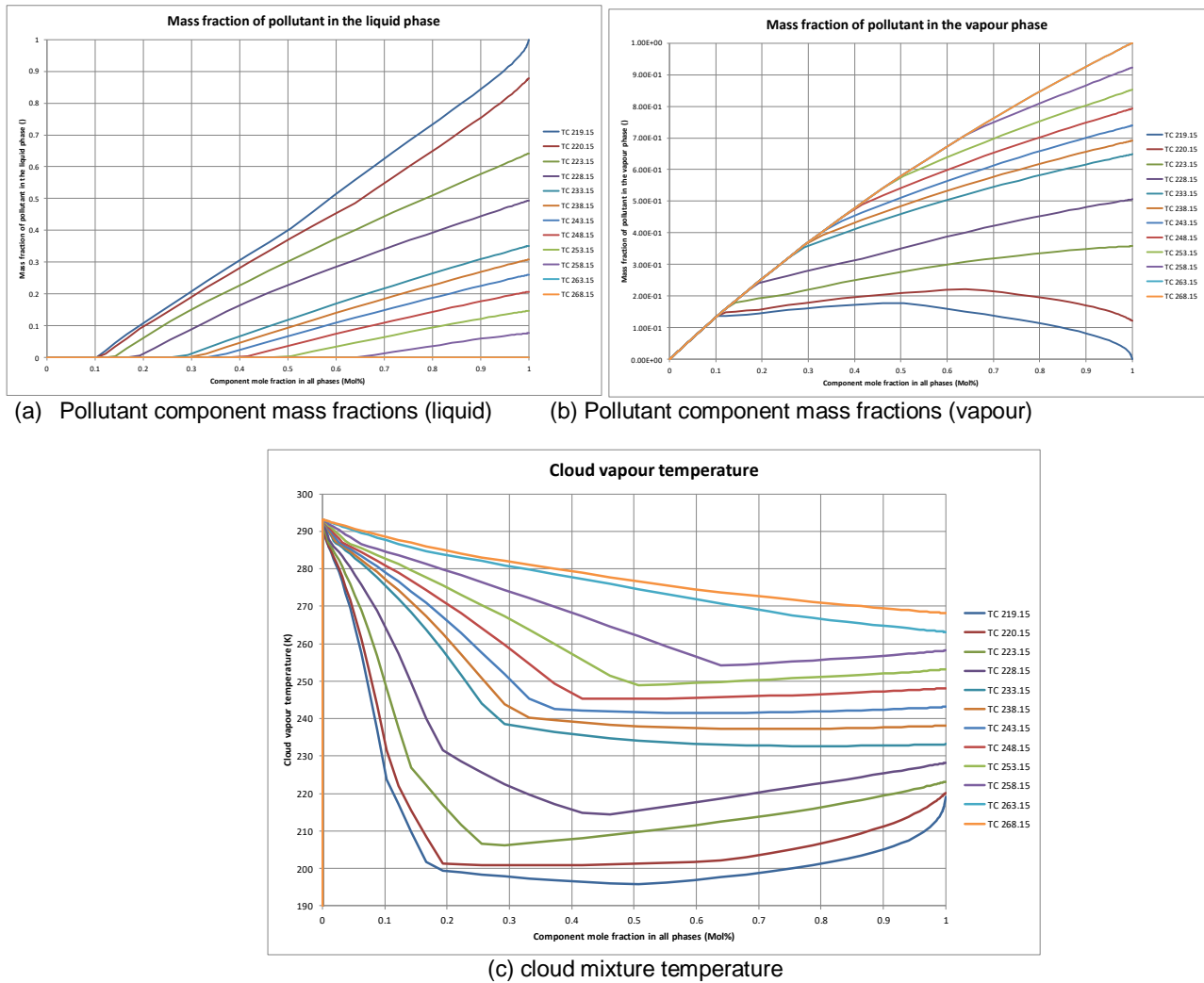
(a) Pollutant component mass fractions (liquid)

(b) Pollutant component mass fractions (vapour)

(c) cloud mixture temperature

Figure 2.13. Mixing of propane/butane/pentane/chlorine/ammonia pollutant (vary temperature) with wet air

Effect of substrate heat and water-vapour transfer (UDM dispersion model predictions)

Figure 2.15 illustrates the effect of substrate heat and water-vapour transfer in case of mixing of propane/butane/pentane/chlorine/ammonia pollutant (at the bubble point of 219.5C) with dry, 70% or 100% humidity air (at 20C). The black lines/markers correspond with 0% ambient humidity, the green lines/markers with 70% humidity, and the red lines/markers correspond with 100% humidity. The markers correspond with THRM predictions, where no substrate heat and substrate water-vapour transfer is included.

In case of increasing humidity, mixing of the pollutant with the air results in added condensation of the water from the air which generates added heat. Thus the mixture temperature increases with ambient humidity.

As should be the case, it is confirmed that the THRM prediction match the UDM predictions (solid lines - RH0, RH70, RH100) where no heat and water-vapour transfer is included. Inclusion of heat transfer (dashed lines - RH0H, RH70H, RH100H) from the hotter substrate results in added heating from the cloud, while also including water-vapour transfer generates further cloud heating (dotted lines - RH0HW, RH70HW, RH100HW).
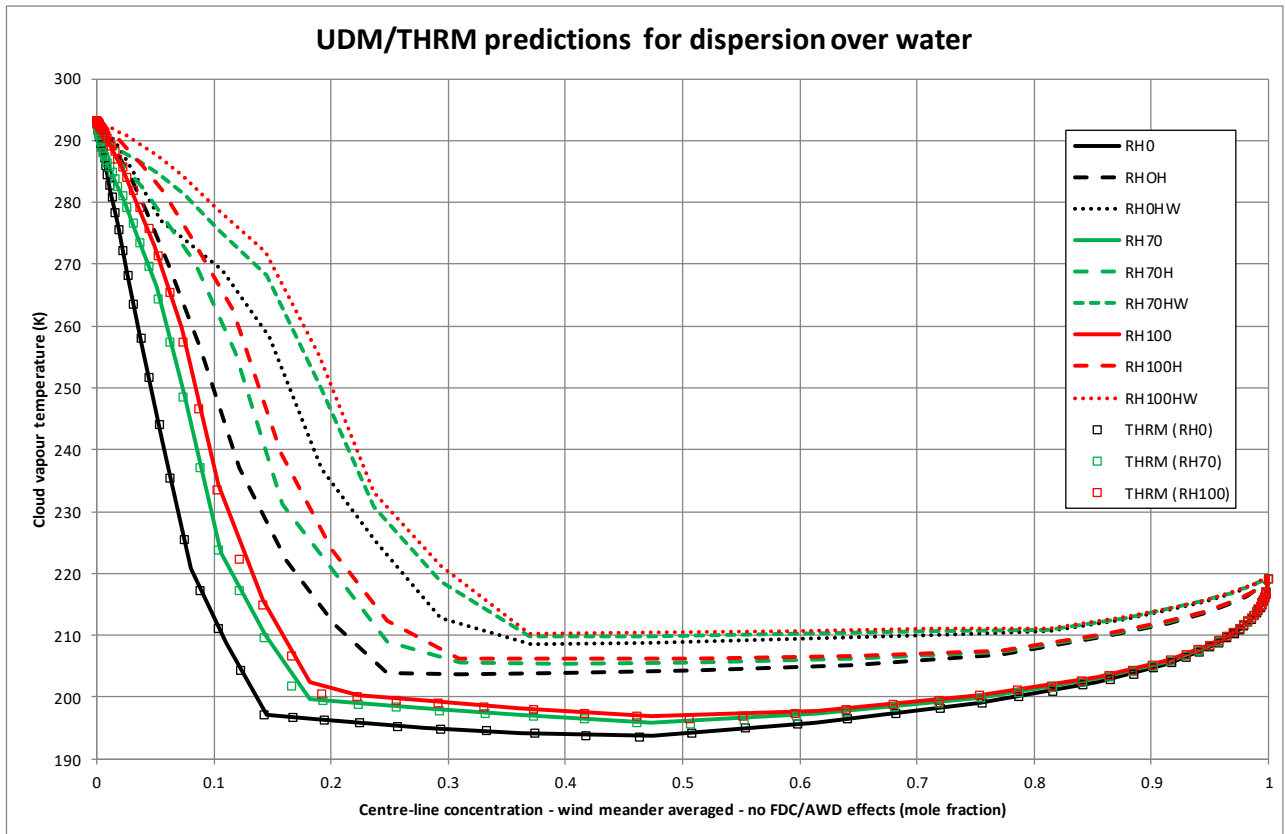
Figure 2.14. **UDM or THRM predictions using thermodynamics equilibrium model for mixing of propane with air**

2.4.3 Mixing of methane/propane/pentane/heptane/nonane pollutant with wet air

The pollutant mixture is chosen to consist of 5 hydrocarbon components with equal 20% mass fractions and a wide range of volatility. The 5 components are methane (boiling point 111.7K), propane (boiling point 231.1K), pentane (boiling point 309.2K), heptane (boiling point 371.6K) and nonane (boiling point 424K). The pollutant is mixed with moist air. Thus there are 2 potential aerosols: one 5-component hydrocarbon aerosol (methane/propane/ /pentane/heptane/nonane) and one one-component aerosol (water).

Figure 2.15 shows results for mixing of the pollutant at the bubble point of 119.5K with moist air at 293.15K (70% humidity). Due to the mixing with the much hotter air, the cooling effect of liquid evaporation is less pronounced (but still visible). It is seen that during mixing more volatile pollutant components evaporate more quickly (most volatile component methane fastest, least volatile component nonane slowest).
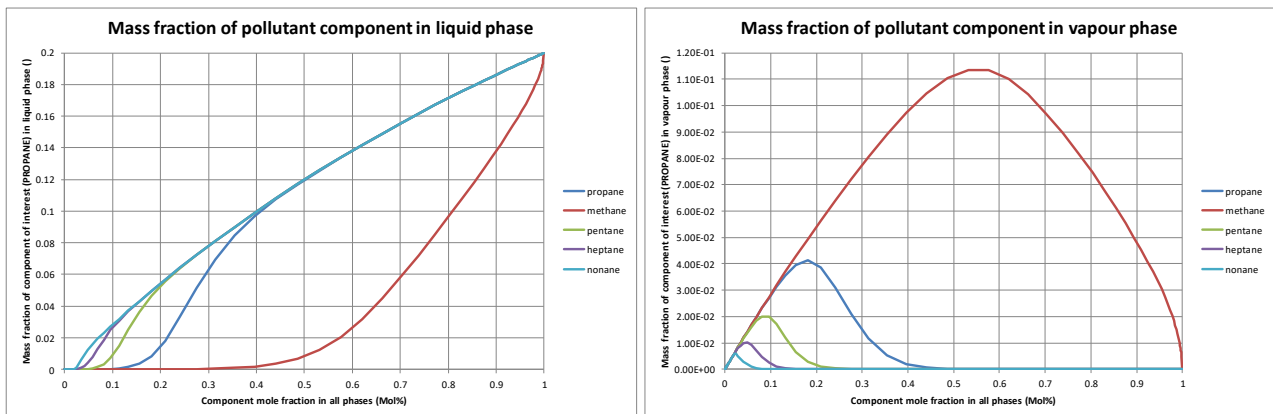
(a) Pollutant component mass fractions (liquid)

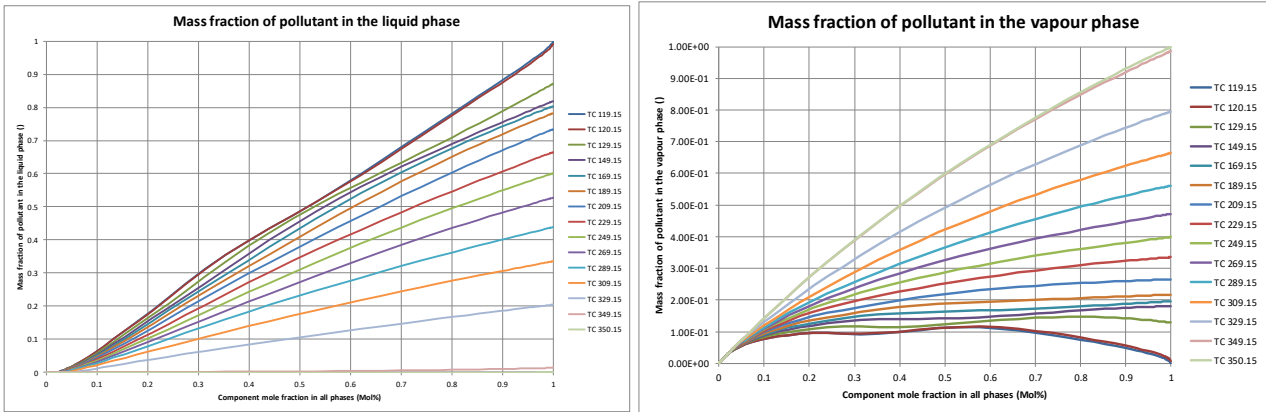(b) Pollutant component mass fractions (vapour)
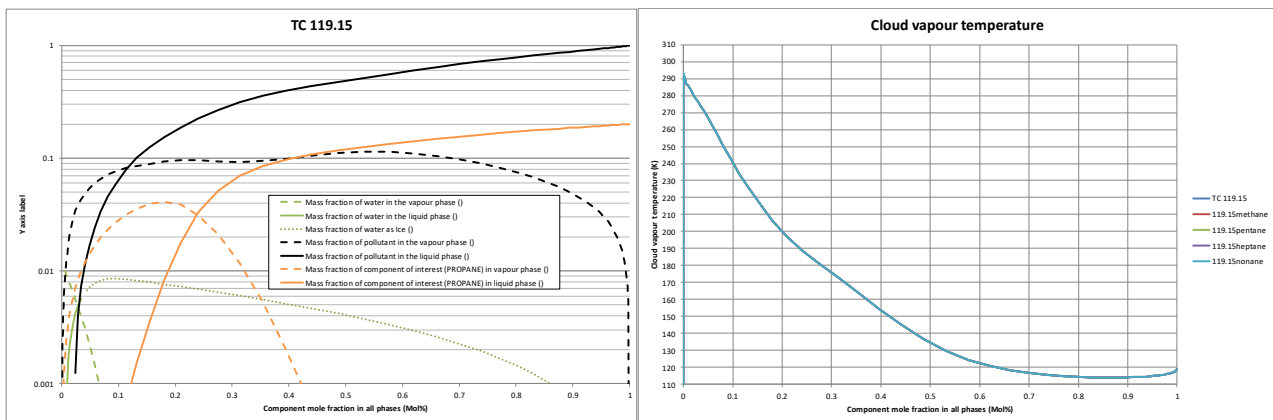
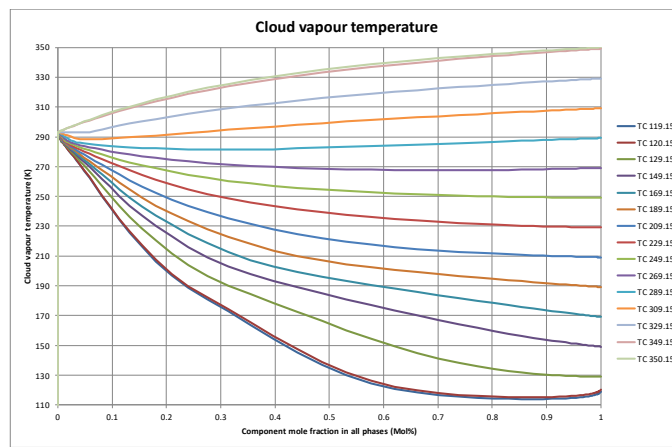(c) Cloud mixture component mass fractions

(d) Cloud mixture temperature

Figure 2.15. Mixing of methane/propane/pentane/heptane/nonane pollutant (119.5K) with wet air

Figure 2.16 shows results while increasing the initial pollutant temperature from the bubble point 119.15K to dew point of 350.15K.

(a) Pollutant component mass fractions (liquid)

(b) Pollutant component mass fractions (vapour)

(c) cloud mixture temperature

Figure 2.16. Mixing of methane/propane/pentane/heptane/nonane pollutant (vary temperature) with wet air

2.5 Sensitivity analysis (mixing of propane with air; MA method)

This section reports the results of parameter variations for the thermodynamics model. The base case of mixing propane with air (at 20C) is considered. Parameter variations have been carried out to the propane release temperature, the ambient humidity, and the propane liquid fraction. In addition effects of heat and/or water-vapour transfer is considered. See Chapter 3 for analyses for chemicals different to propane.

2.5.1 No heat and water-vapour transfer from substrate

Figure 2.17 demonstrates the effect of variation of the propane temperature, for mixing of propane vapour with dry or 100% humid air. Note that for the release of propane vapour below the boiling point $T_{boil}{}^c$, the propane immediately condenses until the temperature reaches $T_{boil}{}^c$. Afterwards the thus formed aerosol evaporates and the mixture cools.

Figure 2.18 demonstrates the effect of variation of the ambient humidity for mixing of propane vapour or propane liquid. For increasing humidity, more water aerosol will form and the amount of heating therefore increases.

Figure 2.19 demonstrates the effect of variation of the liquid propane fraction for mixing of propane (at –43C) with dry or 100% humid air. For increasing liquid propane fraction, more propane aerosol will evaporate and the amount of cooling therefore increases.

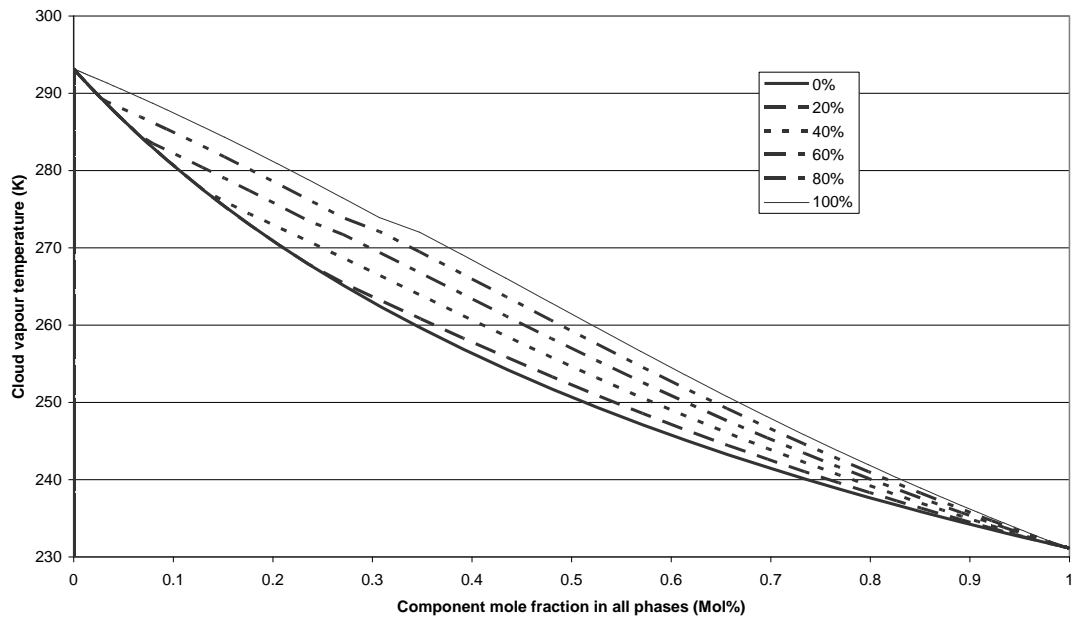**Mixing of propane vapour with dry air, vary propane temeprature**

(a)
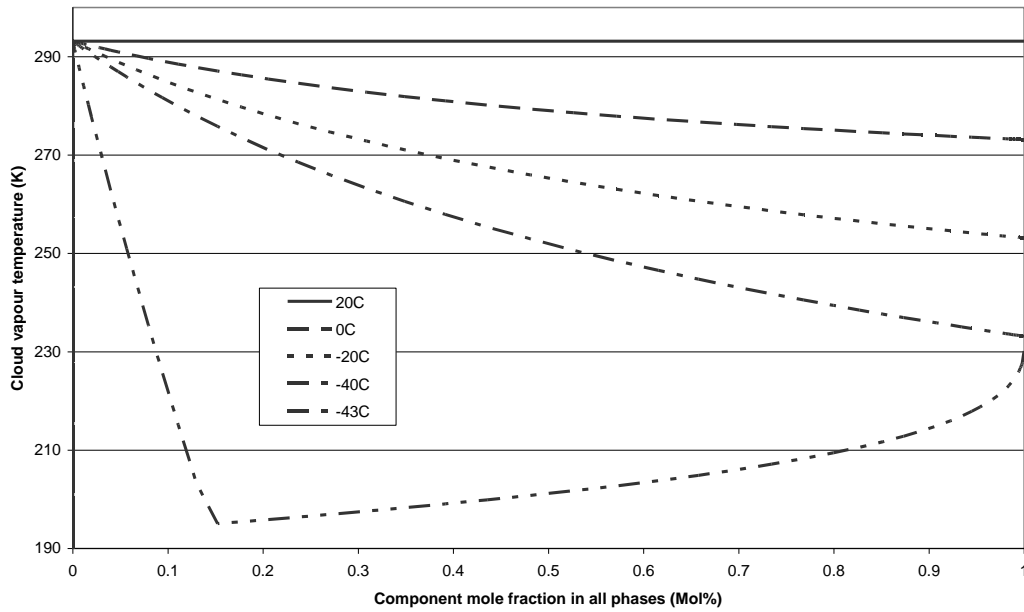
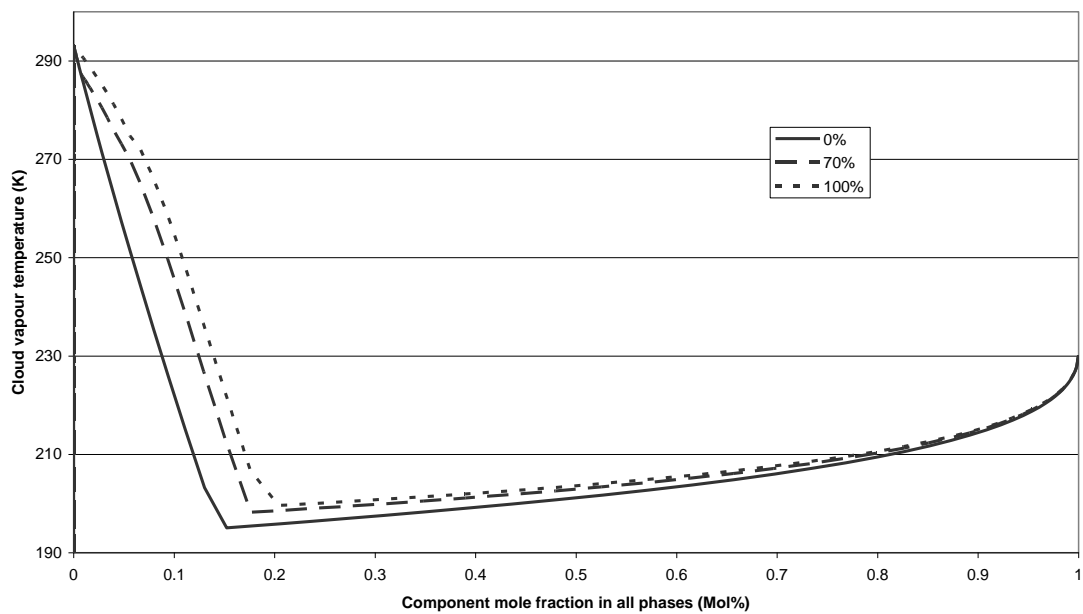**Mixing of propane vapour with 100% wet air, vary propane temperature**
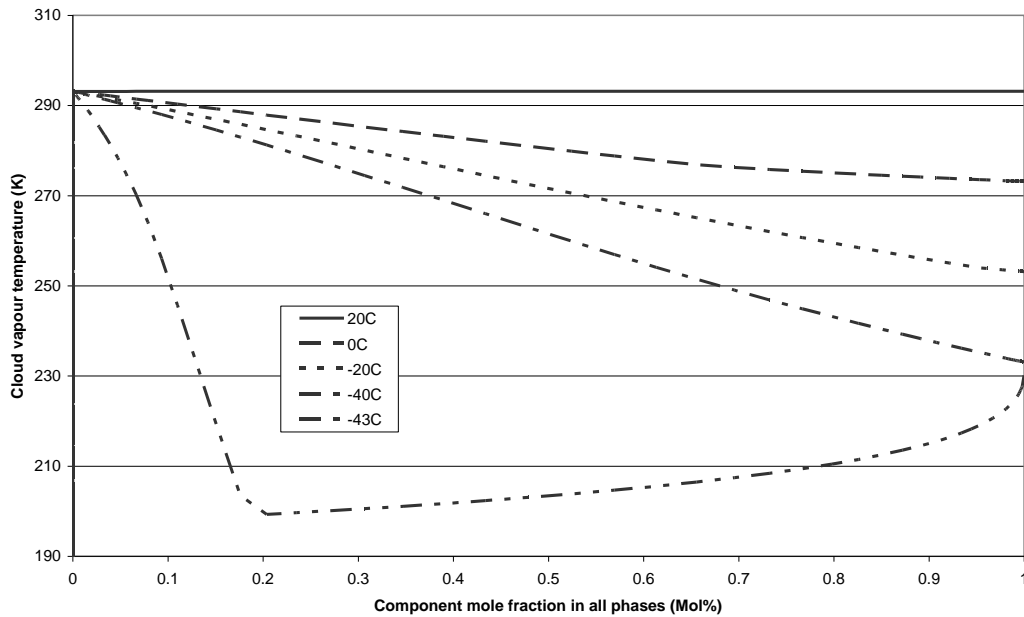
(b)

Figure 2.17.   Variation of propane release temperature for mixing of propane vapour with air; (a) dry air, (b) 100% humid air. Temperature variations are –43C (below boiling temperature), -40C (just above boiling temperature), -20C, 0C, and 20C (ambient temperature).
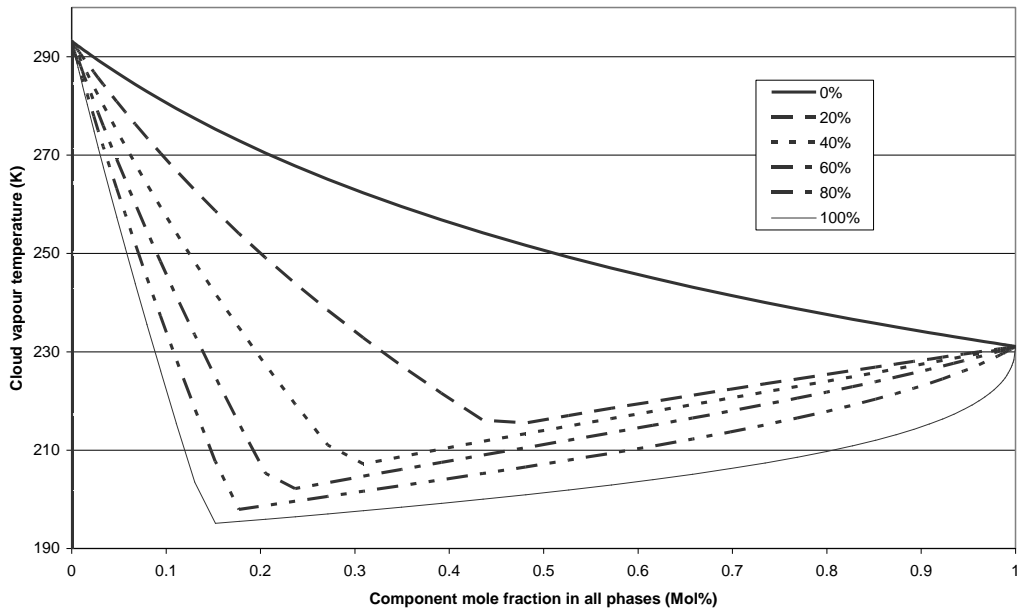
Mixing of propane vapour with air, vary humidity

(a)

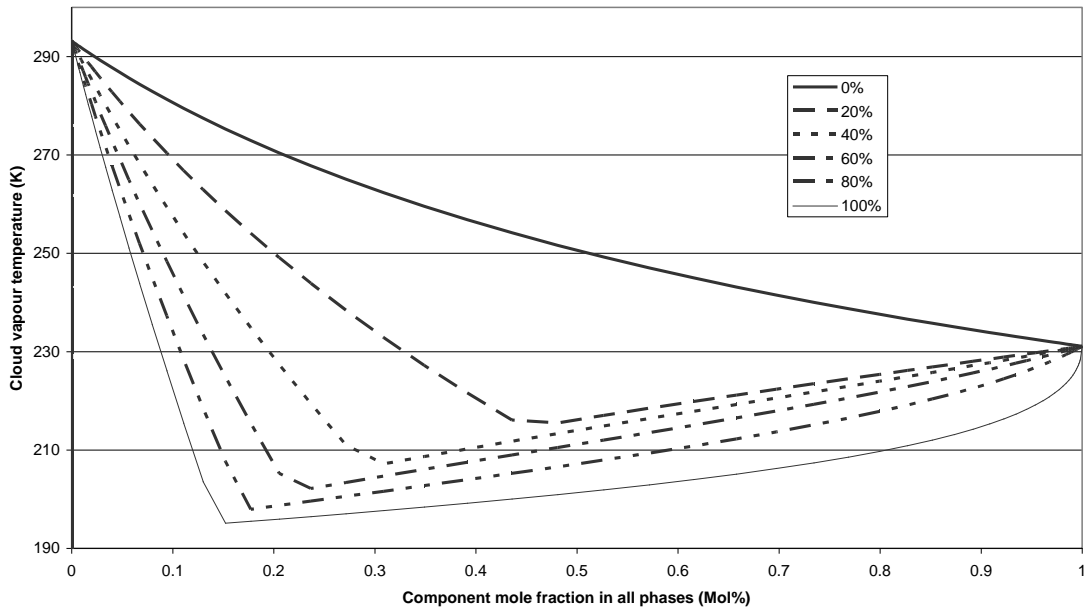**Mixing of propane liquid with air, vary humidity**

(b)

Figure 2.18.   Variation of ambient humidity for mixing of propane with air; (a) propane vapour (-42C), (b) propane liquid (-43C)

Mixing of dry air (20C) with propane, vary liquid fraction

(a)

Mixing of wet air with propane, vary liquid fraction

(b)

Figure 2.19.   **Variation of propane liquid fraction for mixing of propane (-43C) with air (20C); (a) dry air, (b) 100% humid air**

2.5.2 Inclusion of heat and water-vapour transfer from substrate

The above figures exclude the effect of heat and water-vapour transfer from the substrate.

Figure 2.20 includes results of UDM runs taking into account the effect of substrate heat transfer for mixing of propane vapour (at 20C) with 100% humid air (at 20C). The ground temperature T_{gnd} has been varied between –10C (263K) and 30C (303K). Notice that the cloud naturally cools down for ground temperature below 20C, and heats up for ground temperature above 20C.

Figure 2.21 studies the effect of substrate water-vapour transfer for both cold water-substrate (ground temperature of 10C) and a warm water-substrate (ground temperature of 30C). Note that water transfer only takes place from a warm water substrate. No water transfer (or water deposit) takes place from a cold-water substrate.
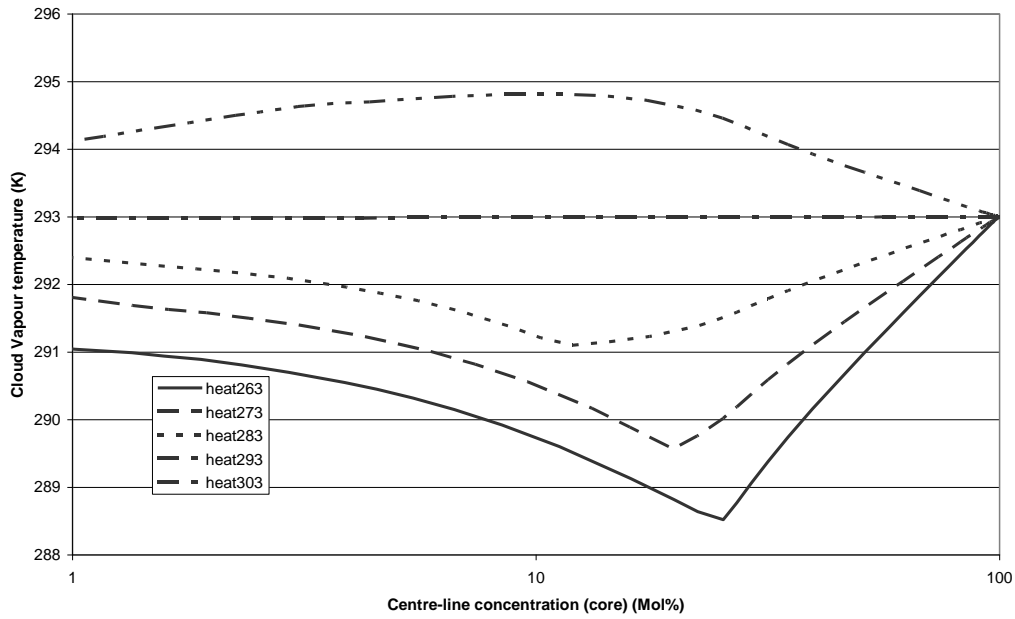
Figure 2.20. **Variation of ground temperature for mixing of propane vapour (20C) with air (20C); inclusion of substrate heat transfer only**
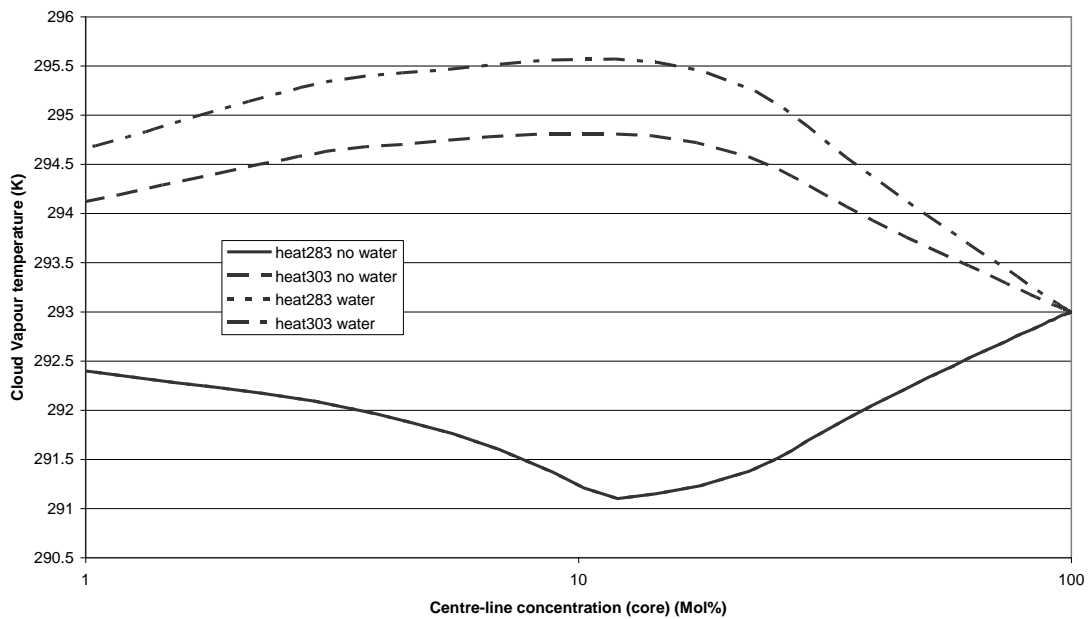

Figure 2.21. **Variation of ground temperature for mixing of propane vapour (20C) with air (20C); inclusion of either substrate heat transfer only, or both heat and water substrate transfer**

Appendix A.   DIPPR versus non-DIPPR data for ambient air and water

As part of the MC implementation for PHAST 6.5, the ambient air and water properties were extended to allow use of DIPPR.[4] After detailed testing it was concluded that:

(a) The default option should be to use DIPPR based properties
(b) The only significant difference between the two formulations was in liquid water enthalpy
(c) Use of DIPPR resulted in closer agreement with HEGADAS
(d) Use of DIPPR will yield more accurate air and water properties than HEGADAS since HEGADAS assumes a constant specific heat C_{pi} for ice, and no separate formulation for solid vapour pressure.

The following sections compare the different properties of interest: air enthalpy, water (soild and liquid) enthalpy, and water (solid and liquid) vapour pressure

A.1   Vapour pressure

Figure 2.1 below shows almost perfect agreement between DIPPR, non-DIPPR and HEGADAS formulations for vapour pressure.
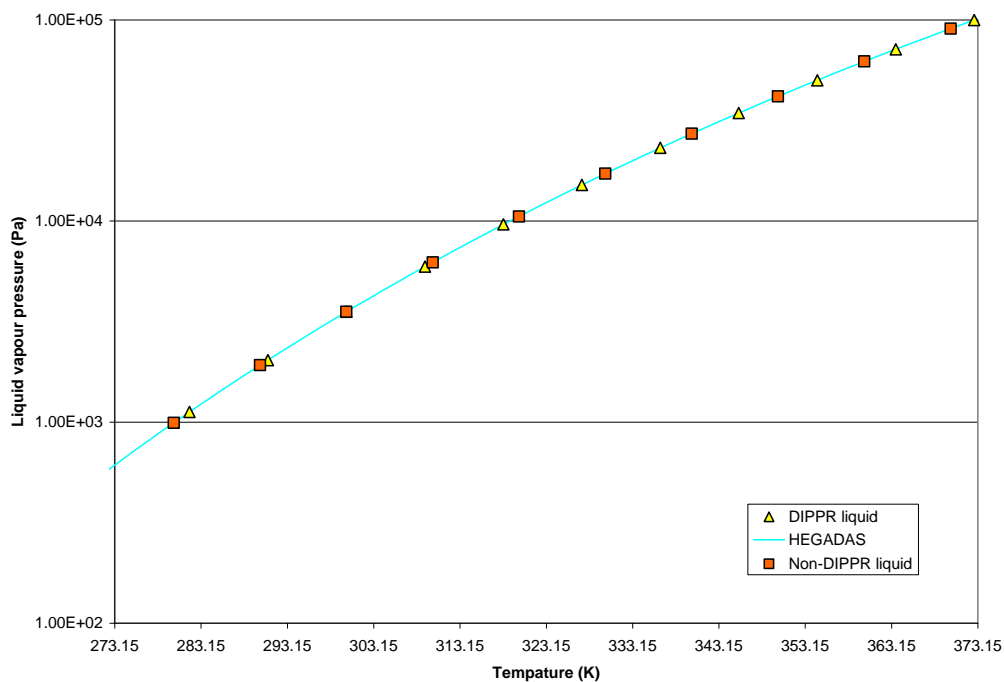

Figure 2.1. Comparison of DIPPR (Phast 6.5), non-DIPPR (Phast 6.42) and HEGADAS liquid water vapour pressures.

Figure 2.2 shows a similar plot but for solid vapour pressures. Note that HEGADAS models no separate solid vapour pressure, but uses the liquid vapour pressure below freezing point, and that is what is plotted here. Otherwise there is good agreement between the non-DIPPR and DIPPR formulations.

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[4] The non DIPPR is retained as an option in THRM spreadsheet, but not in the UDM and it should eventually (soon after 6.5 release) be removed and in the process the AMBI model considerably simplified.
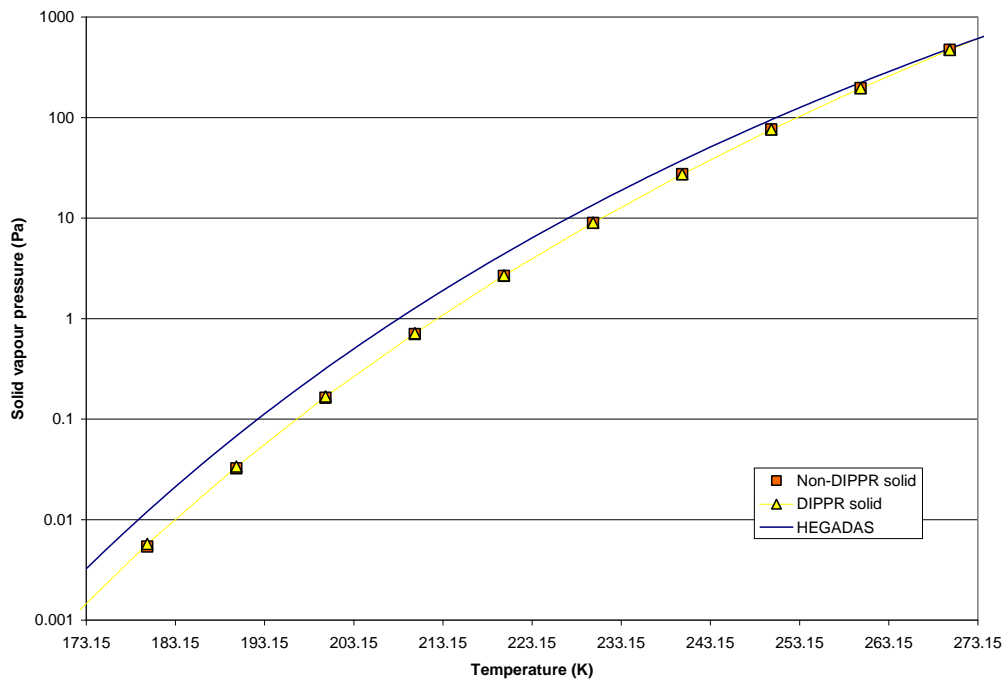
Figure 2.2. Comparison of DIPPR (Phast 6.5), non-DIPPR (Phast 6.42) and HEGADAS solid water vapour pressures.

A.2 Enthalpy

The DIPPR derived air enthalpy is in close agreement with the non DIPPR values (Figure 2.3)
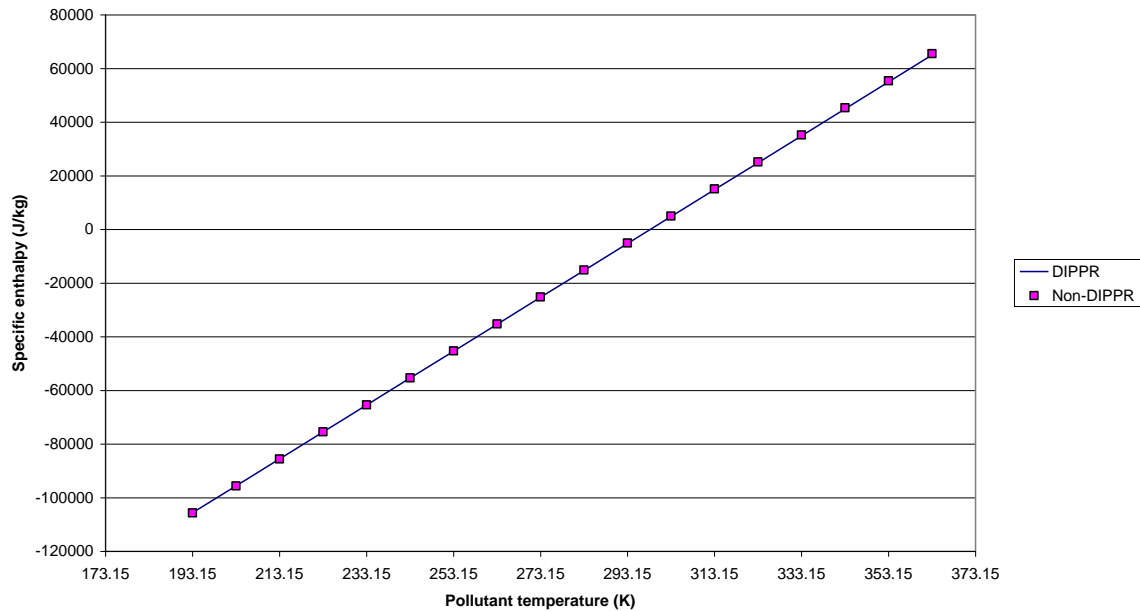
Air enthalpy

Figure 2.3. Comparison of DIPPR and non-DIPPR air enthalpies

For water enthalpy, the picture is more complex as illustrated in Figure 2.4. Below zero Celsius the model uses ice enthalpy, and above it liquid water enthalpy. At the transition there is a discontinuity (corresponding to the enthalpy of fusion) where water turns to ice. In addition the absolute values of enthalpy are different.
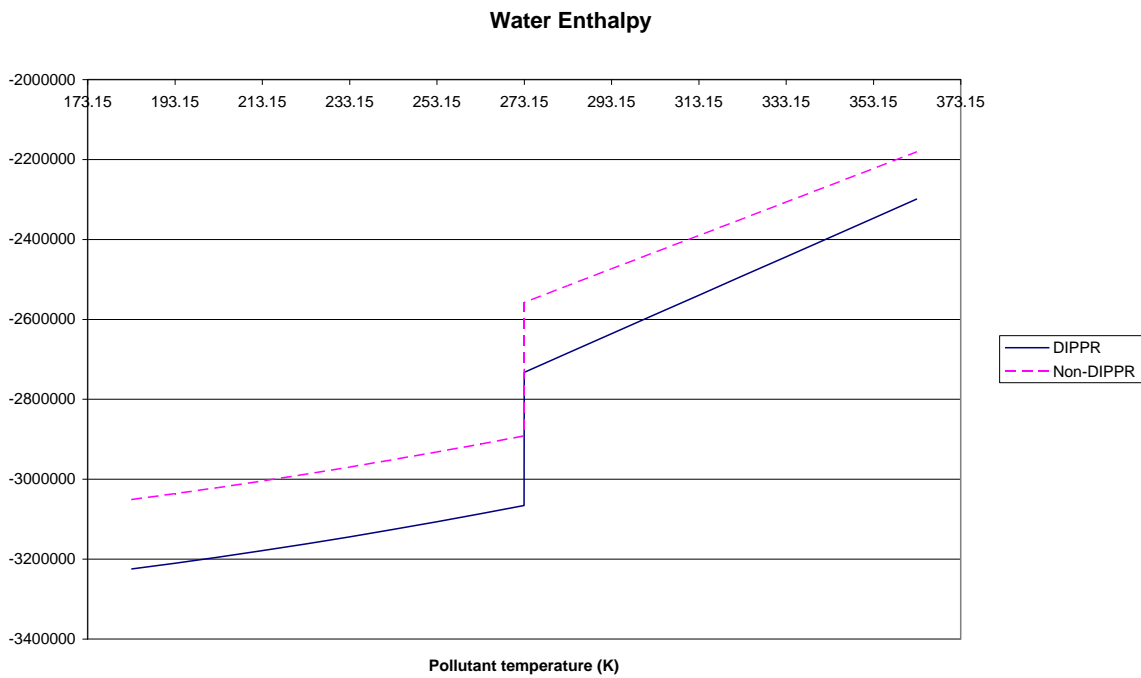
Water Enthalpy

Figure 2.4. Comparison of DIPPR and non-DIPPR water enthalpies

A more useful comparison is given in Figure 2.5. It is Δh rather than absolute values that are relevant to THRM calculations, and therefore here enthalpies are normalized such that h = 0 at T = 273.15 K.
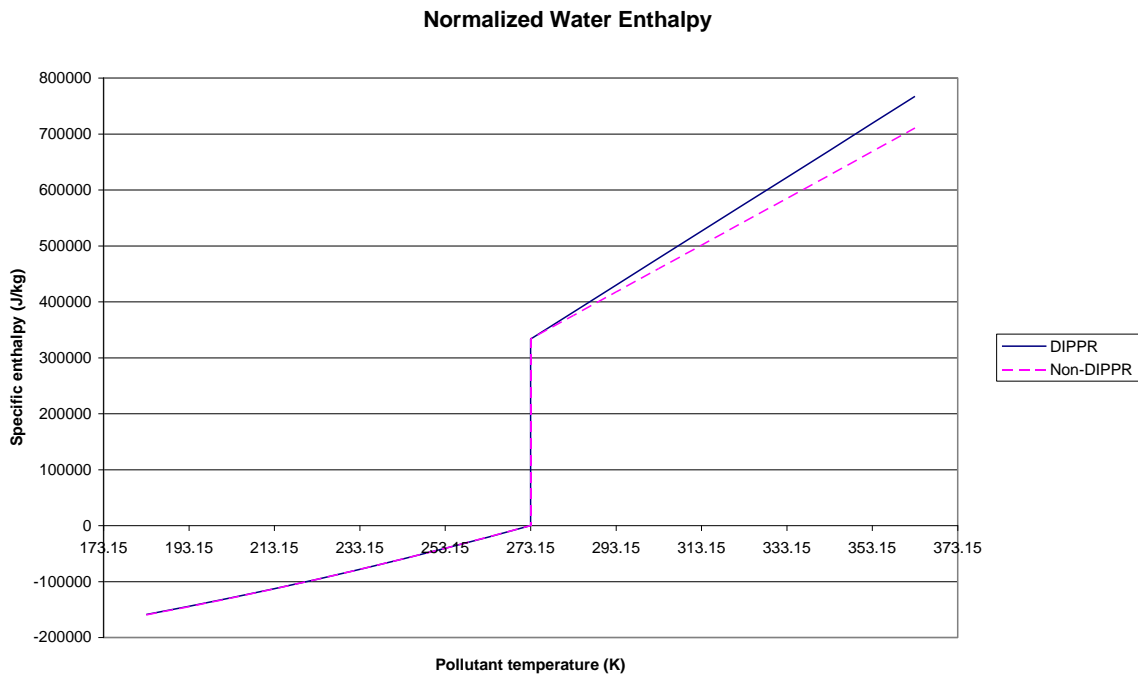
Normalized Water Enthalpy

Figure 2.5. Water enthalpy comparison normalized such that h = 0 at 273.15K.

This demonstrates that for ice and enthalpy of fusion there is good agreement between the two methods, but significant differences exist in liquid water enthalpies.

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[i] Witlox, H.W.M, Two-phase thermodynamics model for mixing of a non-reactive multi-compound pollutant with moist air, Report TNER.93.022 (non-confidential), Thornton Research Centre, Shell Research, Chester, England (1993)