



SUMMARY

PROPERTY DATABASE

DATE: December 2023

This document summarises the properties included in the property database, including properties from both the DIPPR and the DNV property databases. It also includes (where known) a discussion of or reference to the source on non-DIPPR data.

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





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ABSTRACT

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Table of contents

ABSTRACT.....	I
1 INTRODUCTION.....	1
2 DIPPR PROPERTIES.....	1
2.1 Compound descriptors	1
2.2 Property constants	1
2.3 Temperature-dependent properties	2
3 DNV PROPERTIES.....	2
4 SOURCE OF DNV DATA	4
4.1 Aerosol Class	4
4.2 PVAP material properties for pools on water	7
4.3 Pool fire flammable material properties	31
4.4 Laminar Burning Velocity	38
4.5 Dangerous Dose and Toxic Probit A, B and N	39
4.6 Materials Added for 8.4	43
4.7 Materials added for Safeti-NL 8.5	43
REFERENCES.....	46

1 INTRODUCTION

This document summarises the properties currently included (and to be added) in the property database, including properties from both the DIPPR and the DNV property databases.

For further information and more details please refer to the XPRP theory manual¹, the PHAST HELP information and the information included in the DIPPR and DNV property databases (DIPPR_2018.MDB, DNV.MDB). These properties are combined in the property master database PROPERTY.MDB.

2 DIPPR PROPERTIES

This section lists all DIPPR properties in the DIPPR property database DIPPR_2018.MDB, which are taken directly from the DIPPR 2018 database². These data are listed below.

2.1 Compound descriptors

The compound descriptors are as followsⁱ:

1. Names for compound: CAS name, Compound name, iupac name, synonyms
2. CAS number, DIPPR id
3. Empirical chemical formula, structure (one dimensional representation of the molecule)

2.2 Property constants

See Sections 2.2 and 2.5 in Reference 2 for further details. See also the DIPPR section in the PROP theory manual.

1. Molecular weight (kg/kmol)
2. Phase diagram data (fusion and vaporisation line in pressure/temperature curve): critical temperature (K), critical pressure (Pa), triple point temperature (K), triple point pressure (Pa), melting point at 1atm (K), normal boiling point (K)
3. Related data: critical volume (m³/kmol), critical compressibility factor (-), enthalpy of fusion at melting point (J/kmol)
4. Liquid molar volume at 25C (m³/kmol)
5. Enthalpy of formation for ideal gas at 25C, gibbs energy of formation for ideal gas at 25C and 1atm
6. Absolute entropy of ideal gas at 25C and 1 atm (J/kmol/K)
7. Standard state data at 25C and 1atm: enthalpy of formation (J/kmol), Gibbs energy of formation (J/kmol), absolute entropy (J/kmol/K)
8. Net standard state enthalpy of combustion at 25C (J/kmol)
9. Acentric factor (-)
10. radius of gyration (m)
11. solubility parameter at 25C (J/m²)^{1/2}
12. dipole moment (c m)
13. van der Waals reduced volume (m³/kmol) and area (m²/kmol)
14. refractive index (-)
15. flammable data: flash point (K), lower and upper flammable limit (volume % in air), lower and upper flammable limit temperature (K), auto ignition temperature (K)

Note that in DNV's DIPPR database there are also added data in the database derived from the above data. These are the combustion coefficients A_t , C_t defined byⁱⁱ

$$A_t = \frac{\text{moles of fuel} + \text{moles of air}}{\text{moles of combustion products}}, \quad C_t = \frac{\text{moles of fuel}}{\text{moles of fuel} + \text{moles of air}} \quad (1)$$

ⁱ ADD. Except for CASID, these are at present not made available via DNV's DIPPR database DIPPR.MDB. For future POLF/WHFIRE applications the chemical formula/structure will be required. Note that the latter is now already used in our tools to derive A_t, C_t

ⁱⁱ DOC. See the XPRP theory manual on details on how these are derived. Note that further combustion reaction data may be required for the future POLF and WHFIRE models. In the future A_t, C_t logic should ideally be moved to XPRP.

2.3 Temperature-dependent properties

See Sections 2.3 and 2.5 in Reference 2 for further details. See also the DIPPR section in the PROP theory manual. Temperature-dependent properties are actually stored as a DIPPR equation number and coefficients. For each property are also stored minimum and maximum temperatures for evaluation, and property values at these temperatures. These properties are as follows:

1. Densities: solid, liquid (kmol/m^3) [liquid density is at 1 atm for temperatures below normal boiling point, and at saturation pressure for temperatures above the NBP]
2. Vapour pressures: solid for solid-vapour equilibrium, liquid for liquid-vapour equilibrium (Pa)
3. Heat of vaporisation (J/kmol)
4. Heat capacities: solid, liquid, ideal gas (J/kmol/K) [up to NBP saturated heat capacity (C_s) and heat capacity at constant pressure (C_p) liquid heat capacity]
5. Second virial coefficient (m^3/kmol)
6. Viscosities: liquid, vapour (Pa s)
7. Thermal conductivities: solid, liquid, vapour (W/m/K)
8. Surface tension (N/m)

3 DNV PROPERTIES

1. Flammable/toxic flag: -2 = neither (inert), -1 = toxic, 0 = both, 1 = flammable
2. Flammable data (see e.g. POLF theory manual for details)
 - 2.1. Flame type: 0 = luminous, 1 = smoky, 2 = general
 - 2.2. Maximum Surface Emissive Power (kW/m^2).
 - 2.3. Emissive power scale length (m)
 - 2.4. Pool fire burn rate length (m)
 - 2.5. Pool fire maximum burn rate ($\text{kg/m}^2/\text{s}$)
3. Explosion data
 - 3.1. TNT explosion efficiency (%)
4. Toxic data:
 - 4.1. ERPG levels (mole fraction, ppm; Emergency Response Planning Guideline):
 - 4.1.1. ERPG1: Health effects more severe than mild odour perception or irritation, if relevant
 - 4.1.2. ERPG2: Irreversible adverse health effects or symptoms which could impair an individual's ability to take protective action
 - 4.1.3. ERPG3: Life-threatening health effects.
 - 4.2. IDLH concentration (mole fraction, ppm): immediately Dangerous to Life and Health, and the concentration is defined with an exposure time of 30 minutes
 - 4.3. STEL concentration (mole fraction, ppm): Short Term Exposure Limit, and the concentration is defined with an exposure time of 15 minutes.
 - 4.4. Probit equation constants: A,B,N. There are used in the probit function $\text{Pr} = A + B \ln(C^N t)$, which is used to obtain the probability of death; c is the concentration in ppm, and t is the duration of the exposure in minutes.
 - 4.5. Dangerous toxic load, up to 6 values³
5. Thermodynamic data
 - 5.1. Equation of state (see XPRP theory manual for further details)
 - 5.1.1. flag for type of equation of state: two term virial, Soave Redlich Kwong, Redlich Kwong, Peng Robinson. Note: this flag is no longer used in the new property system. It has effectively been replaced by the new property system 'templates', which define methods (including EOS) for individual properties.

5.1.2. for Soave cubic equation of state, (integer) method flag for treatment of super-critical components (calculation of α). Values are as follows:

- 1 - Mathias correlation: N₂, CO, CO₂, H₂S
- 2 - Penn State Equation suggested by Graboski and Daubert: H₂
- 0 - Binary parameter used for binary pair involving the component: other chemicals

5.2. Reaction/association data:

- 5.2.1. Reactivity with atmosphere: 0 = not strongly reactive (no reactions modelled), 1 = reactive (model reactions using (association reaction otherwise; however not recommended for non-HF), 2 = HF only. This flag is used by the UDM only, to identify HF specific modelling. ⁱⁱⁱ
- 5.2.2. Material produced by reaction^{iv}
- 5.2.3. Association flag^v: 1 = modelled, 0 = not modelled (not recommended to be modelled for non-HF)
- 5.2.4. Association coefficients A_p, B_p (dimer, trimer, hexamer, octamer) required for setting the association factor etc.
- 5.2.5. Enthalpy interpolation range (K)

5.3. Aerosol class number (integer): Using multi-component logic, separate immiscible aerosols can form, and this will capture the separation between water and hydrocarbons. The aerosol classes are included below in **Error! Reference source not found.** these are listed in the following tables

6. Water data [used in PVAP model; see PVAP theory manual]:

- 6.1. Liquid-water surface tension (N/m)
- 6.2. Solubility in water f_s (kg/kg)
- 6.3. Heat of solution ΔH_{sol} (J/kg) [used in PVAP model; see PVAP theory manual]
- 6.4. Reaction with water model: 0 = none, 1 = Raj and Reid
- 6.5. In case of reaction with water: liquid-water enthalpy coefficients A_{L,w}, B_{L,w}, C_{L,w}, D_{L,w}
- 6.6. Water heat-transfer coefficient (W/m²/K). Used for the transfer of heat to boiling pools on water.

ⁱⁱⁱ JUSTIFY. Note that the intermediate option seem never to be used

^{iv} JUSTIFY. This seems to be never used in MDE. Why is this present?

^v IMPROVE. This was designed for organic acids (such as acetic acid) as well as for HF, however users will need to specify their own coefficients. Only HF amongst the default materials uses association modelling. It is used in DISC/TVDI discharge models only in the case of HF. Note that hardwired values are used in the HGS HF dispersion modelling. This needs retesting for DISC as part of multi-compound work. See XPRP theory manual for details. Overall association modelling between DISC/TVDI and UDM should be more rationalised.

4 SOURCE OF DNV DATA

This section describes in more detail the origin and derivation (where known) of the values stored in the DNV database.

4.1 Aerosol Class

Aerosol class is used during dispersion of 2-phase releases, where multiple and immiscible liquid phases can occur. The reader is referred to the THRM Theory manual for further details on the calculations. The following aerosol classes have been adopted in the current version (8.4+) of Phast and Safeti.

CAS	Name	Aerosol class (v8.2)	DIPPR Solubility parameter	DIPPR Dielectric constant	Non Polar?	Aerosol class (v8.4)	Notes
75569	1,2-PROPYLENE OXIDE		18930	10.881	FALSE	1	
106990	1,3-BUTADIENE		14420	2.05	TRUE	2	
106989	1-BUTENE		13630	2.2195	TRUE	2	
107051	3-CHLOROPROPENE		18360	8.2	FALSE	1	
67641	ACETONE	8	19730	20.7	FALSE	11	Soluble in polar and non-polar
75058	ACETONITRILE		24130	36.02	FALSE	11	Soluble in polar and non-polar
74862	ACETYLENE		8057	2.484	TRUE	2	
107028	ACROLEIN		20100	18.947	FALSE	1	
79061	ACRYLAMIDE		106087	44.95	FALSE	1	
107131	ACRYLONITRILE		21970	31.8	FALSE	1	
132259100	AIR	5	12580	1.463	TRUE	2	
107186	ALLYL ALCOHOL		25090	19.7	FALSE	1	
7664417	AMMONIA	4	24790	16.61	FALSE	1	
71432	BENZENE		18730	2.2825	TRUE	2	
100447	BENZYL CHLORIDE		20040	6.854	FALSE	1	
7726956	BROMINE		23650	3.1484	TRUE	2	
124389	CARBON DIOXIDE	3	14560	1.6	TRUE	3	Solid phase
75150	CARBON DISULFIDE		20310	2.58	TRUE	2	
630080	CARBON MONOXIDE	9	12250	1.501	TRUE	2	
7782505	CHLORINE	2	17360	2.047	TRUE	2	
75092	DICHLOROMETHANE		20300	8.93	FALSE	1	
124403	DIMETHYLAMINE		18050	5.26	FALSE	1	
74840	ETHANE	8	5263.3	1.325	TRUE	2	
64175	ETHANOL		26150	25.3	FALSE	11	Soluble in polar and non-polar
74851	ETHYLENE		15650	1.483	TRUE	2	
75218	ETHYLENE OXIDE		20970	12.42	FALSE	1	
151564	ETHYLENEIMINE		24650	18.3	FALSE	1	
7782414	FLUORINE		15250	1.54	TRUE	2	
50000	FORMALDEHYDE		21390	32.89	FALSE	1	
302012	HYDRAZINE		36220	51.7	FALSE	1	
1333740	HYDROGEN	10	5045	1.228	TRUE	2	
7647010	HYDROGEN CHLORIDE		12170	4.6	TRUE	2	
74908	HYDROGEN CYANIDE		24820	105.7	FALSE	1	
7664393	HYDROGEN FLUORIDE	1	15880	83.6	FALSE	1	
7722841	HYDROGEN PEROXIDE		106194	74.6	FALSE	1	
7783064	HYDROGEN SULFIDE	11	16320	9.05	FALSE	1	
78831	ISOBUTANOL (2-METHYL-1-PROPANOL)		23090	17.93	FALSE	1	
67630	ISOPROPANOL (Isopropyl alcohol)		23820	18.3	FALSE	11	Soluble in polar and non-polar
74828	METHANE	8	13810	1.6	TRUE	2	
67561	METHANOL		29360	33	FALSE	11	Soluble in polar and non-polar
74839	METHYL BROMIDE		19000	9.82	FALSE	1	

CAS	Name	Aerosol class (v8.2)	DIPPR Solubility parameter	DIPPR Dielectric constant	Non Polar?	Aerosol class (v8.4)	Notes
624839	METHYL ISOCYANATE		21320	21.75	FALSE	1	
74895	METHYLAMINE		21310	10	FALSE	1	
74931	METHYL MERCAPTAN		19370	8.55	FALSE	1	
108383	M-XYLENE		18040	2.359	TRUE	2	
106978	N-BUTANE	8	13510	1.7697	TRUE	2	
71363	N-BUTANOL		23530	17.84	FALSE	2	being polar
141322	N-BUTYL ACRYLATE		17950	5.25	FALSE	1	
142825	N-HEPTANE	8	15240	1.9209	TRUE	2	
110543	N-HEXANE	8	14880	1.8865	TRUE	2	
7697372	NITRIC ACID		106109	19.079	FALSE	1	
10102439	NITRIC OXIDE		23150	16.75	FALSE	1	
7727379	NITROGEN	5	11919	1.454	TRUE	2	
10102440	NITROGEN DIOXIDE		33390	2.44	TRUE	2	
111842	N-NONANE	8	15690	1.9722	TRUE	2	
111659	N-OCTANE	8	15490	1.948	TRUE	2	
109660	N-PENTANE	8	14380	1.8371	TRUE	2	
7782447	OXYGEN	6	14676	1.507	TRUE	2	
108952	PHENOL		24900	12.4	FALSE	1	
75445	PHOSGENE		17030	4.3	TRUE	2	
74986	PROPANE	8	11716	1.6678	TRUE	2	
115071	PROPYLENE		11890	2.671	TRUE	2	
100425	STYRENE		19120	2.4737	TRUE	2	
7446095	SULFUR DIOXIDE	7	21050	16.3	FALSE	1	
78002	TETRAETHYL LEAD		16530	2.222	TRUE	2	
108883	TOLUENE		18230	2.379	TRUE	2	
121448	TRIETHYLAMINE		15190	2.418	TRUE	2	
75503	TRIMETHYLAMINE		14260	2.44	TRUE	2	
108054	VINYL ACETATE		18650	6.315	FALSE	1	
75014	VINYL CHLORIDE		15840	6.26	FALSE	1	
7732185	WATER	1	47860	80.1	FALSE	1	

CAS	Name	Aerosol class (v8.2)	DIPPR Solubility parameter	DIPPR Dielectric constant	Non Polar?	Aerosol class (v8.4)	Notes
Additional Materials for v8.4							
463821	NEOPENTANE					2	
589811	3-METHYLHEPTANE					2	
112403	n-Dodecane					2	
75285	ISOBUTANE					2	
78784	ISOPENTANE					2	
630024	N-OCTACOSANE					2	
124185	n-Decane					2	
1120214	n-Undecane					2	
629505	n-Tridecane					2	
629594	n-Tetradecan					2	
629629	n-Pentadecane					2	
629787	n-Heptadecane					2	
1081772	N-NONYLBENZENE					2	
1459092	N-HEXADECYLBENZENE					2	
544854	N-DOTRIACONTANE					2	
630068	N-HEXATRIACONTANE					2	
630035	N-NONACOSANE					2	
638686	N-TRIACONTANE					2	
872059	1-DECENE					2	
111875	1-OCTANOL					2	
108112	4-METHYL-2-PENTANOL					2	
7637072	BORON TRIFLUORIDE					2	Reacts violently with water
115117	ISOBUTENE					2	
7446119	SULFUR TRIOXIDE					2	Reacts violently with water
78922	2-BUTANOL					2	
60297	Diethyl Ether					2	many oils
64186	Formic Acid					1	xylenes
74873	Chloromethane					2	chloroform
75070	Acetaldehyde					11	slightly soluble in chloroform
75081	Ethanethiol					2	dilute alkali and ether
96333	Methylacrylate					11	most organic solvents
106898	1-CHLORO-2,3-EPOXYPROPANE					4	with petroleum hydrocarbons
107153	1,2-DIAMINOETHANE					1	aromatic solvents
107313	METHYLFORMATE					2	other HC liquids
109795	1-BUTANETHIOL					2	n-hexane
109897	ETHYLETHANAMINE					11	acids.
109944	ETHYLFORMATE					2	ORGANIC SOLVENTS
110010	TETRAHYDROTHIOPHENE					2	Water immiscible.
110827	CYCLO-HEXANE					2	tetrachloride
7784421	ARSINE					2	chloroform and benzene
7803512	PHOSPHINE					2	Water immiscible.
544763	n-HEXADECANE					2	Water immiscible.
593453	n-OCTADECANE					2	Water immiscible.
629925	n-NONADECANE					2	Water immiscible.
112958	n-EICOSANE					2	Water immiscible.

Table 1. Aerosol classes for materials in the standard set

In general, aerosol class has been determined on the basis of polarity, adjusted according to actual solubility in water data. For example if a polar substance is insoluble in water, then we re-classify it as AC = 2. Some adjustment has also been made however for substances miscible with both water and organic solvents^{vi,vii,viii}. These include the lighter alcohols. A separate aerosol class (AC = 11) is used to indicate such materials, and these are replaced at run-time by either non-polar (if the release stream contains any non-polar solvents) or polar (otherwise) values. In addition a special case is made of n-butanol, which despite being polar is not miscible in water^{ix} and is therefore assigned to the non-polar class (AC = 2). Note that CO₂

^{vi} e.g. https://en.wikipedia.org/wiki/List_of_water-miscible_solvents

^{vii} https://www.organicdivision.org/wp-content/uploads/2016/12/organic_solvents.html

^{viii} <https://www.solubilityofthings.com/water/alcohols>

^{ix} https://erowid.org/archive/rhodium/pdf/solvent_miscibility.pdf
[https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Supplemental_Modules_\(Organic_Chemistry\)/Fundamentals/Intermolecular_Forces/Polar_Protic_and_Aprotic_Solvents](https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Supplemental_Modules_(Organic_Chemistry)/Fundamentals/Intermolecular_Forces/Polar_Protic_and_Aprotic_Solvents)

is assigned its own aerosol class (AC = 3) due to its occurrence at atmospheric pressure as a solid rather than liquid.

Real miscibility is complex, and there is some flexibility available to users. Altogether 11 aerosol classes can be used, of which we currently use only 4. Therefore, any materials can be assigned to one of the remaining 7 aerosol classes if it is desired to model different behaviour.

4.2 PVAP material properties for pools on water

4.2.1 Introduction

Table 2 lists the material properties used in Phast (Risk) and SAFETI-NL for pools on water, including the PVAP module where they are used. These are all non-DIPPR properties. The last two properties in Table 2 concern ammonia only, and for this case the properties are obtained from Raj and Reid as described in the PVAP theory manual. For the remaining first four properties limited justification for the original values in Phast 6.54 has been found.

Property	PVAP Module
Material-water interfacial tension, $\sigma_{L,w}$ (N/m)	Spreading of instantaneous releases on water
Heat of solution, ΔH_{sol} (J/kg)	Dissolution in water
Solubility in water, f_s (kg/kg)	Dissolution in water
Heat transfer coefficient, h_s (W/m ² K)	Boiling on water
Reaction with water (0, none, 1=Raj and Reid)	Reaction with water (=1, for ammonia only)
Liquid-water enthalpy coefficients $A_{L,w}$, $B_{L,w}$, $C_{L,w}$, $D_{L,w}$	Reaction with water (ammonia only)

Table 2. Material properties for pools on water and corresponding PVAP module

The effect of each of the above first four material properties on the prediction of the evaporation rate by PVAP was briefly tested in this task to obtain a preliminary indication of the sensitivity of the model predictions to the material property. Following a limited literature review regarding selection of appropriate values for the above properties, new values for these material properties have been proposed and implemented in Phast 6.7.

A more detailed literature review can be considered and/or persuading DIPPR to include added properties (including investigation) to their database. Further analysis of the sensitivity of PVAP results with respect to the material properties may be considered to obtain a more complete overall understanding.

The plan of the current section is as follows. In Section 4.2.2 the main findings from the brief sensitivity analysis of PVAP results with respect to variations on the material properties are shown and discussed. Section 4.2.3 lists the main sources consulted on this task which contain databases of material properties. Section 4.2.5 presents the proposed changes in the values of the material properties stored in the property database for Phast Risk and SAFETI-NL.

4.2.2 Limited sensitivity analysis

The impact of the above material properties for pools on water on the evaporation rate predicted by PVAP was briefly investigated and the results of this are presented in this section.

Figure 1 shows the effect on the maximum evaporation rate predicted by PVAP of a 50% increase on the material properties.

In

Figure 1 the effect of the interfacial tension on the evaporation rate was analysed for a release of 1 ton of n-octane at 298 K and a wind speed of 5 m/s. To analyse the impact of the heat of solution and the solubility factor, an instantaneous release of 1 ton of methanol at 298 K and a wind speed of 5 m/s was simulated. The sensitivity of the evaporation rate with respect to the heat transfer coefficient was investigated for an instantaneous release of 1 ton of n-pentane at 298 K and a wind speed of 5 m/s.

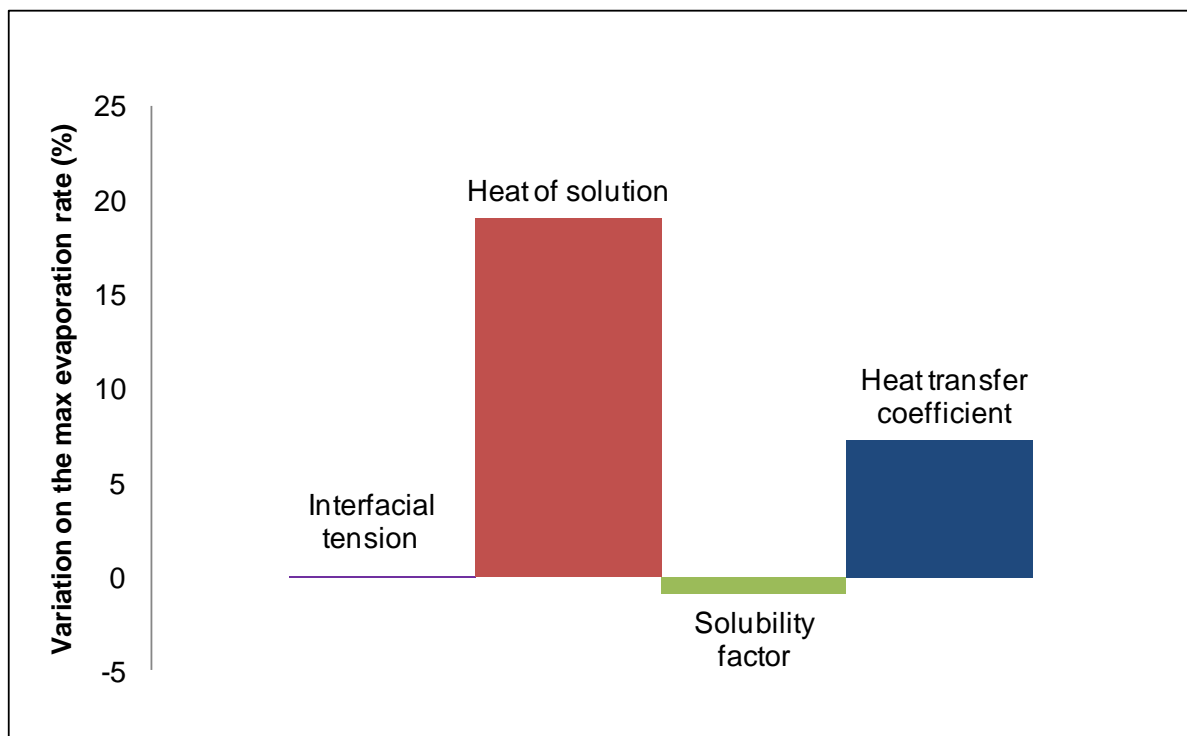


Figure 1. Comparison of the effect on the maximum evaporation rate predicted by PVAP of a 50% increase on the material properties.

The effect of the material properties on the variation of the evaporation rate with time was also investigated. These results are shown in the figures below.

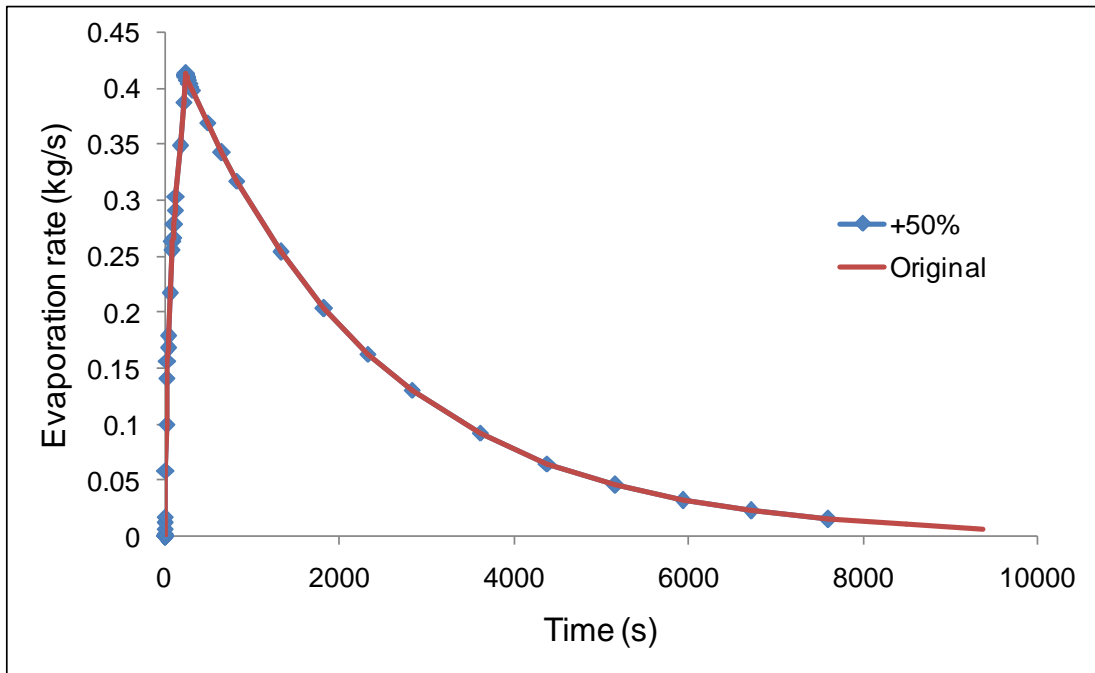


Figure 2. Comparison of the effect of a 50% increase of the interfacial surface tension on the variation of the evaporation rate with time, for an instantaneous release of 1 ton of n-octane at 298 K and a 5 m/s wind speed.

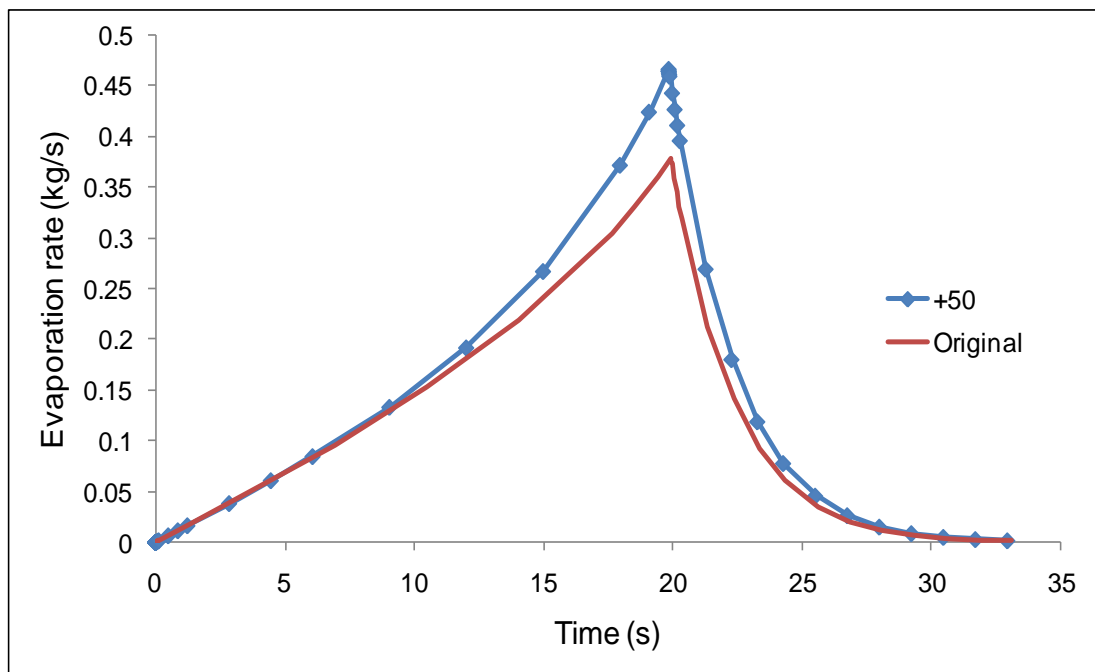


Figure 3. Comparison of the effect of a 50% increase of the heat of solution on the variation of the evaporation rate with time, for an instantaneous release of 1 ton of methanol at 298 K and a 5 m/s wind speed.

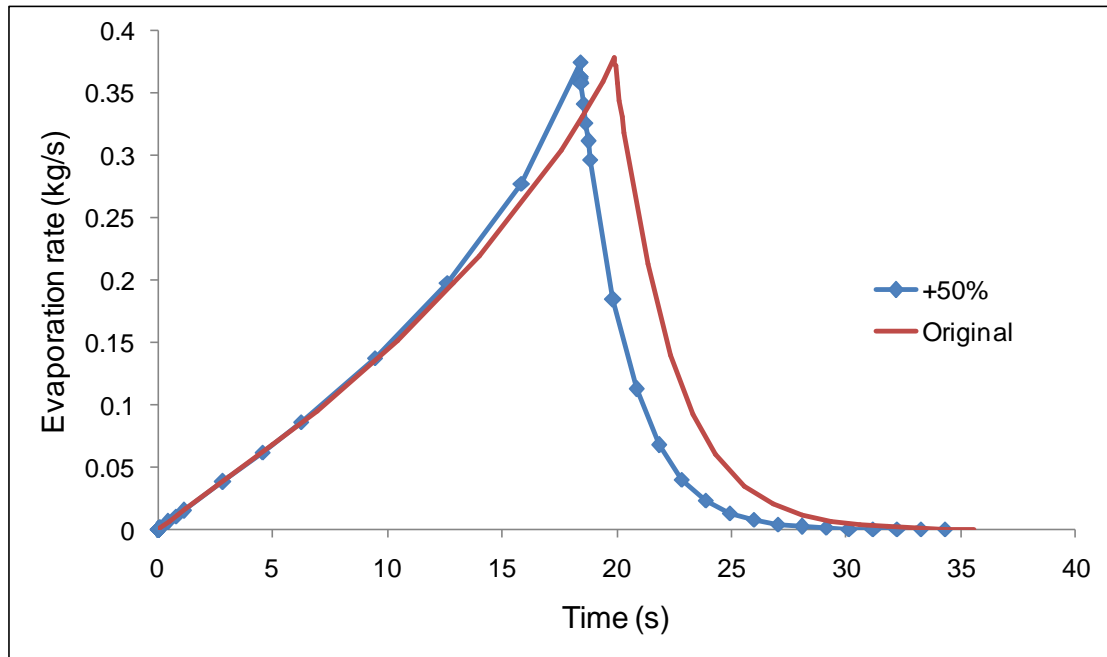


Figure 4. Comparison of the effect of a 50% increase of the solubility factor on the variation of the evaporation rate with time, for an instantaneous release of 1 ton of methanol at 298 K and a 5 m/s wind speed.

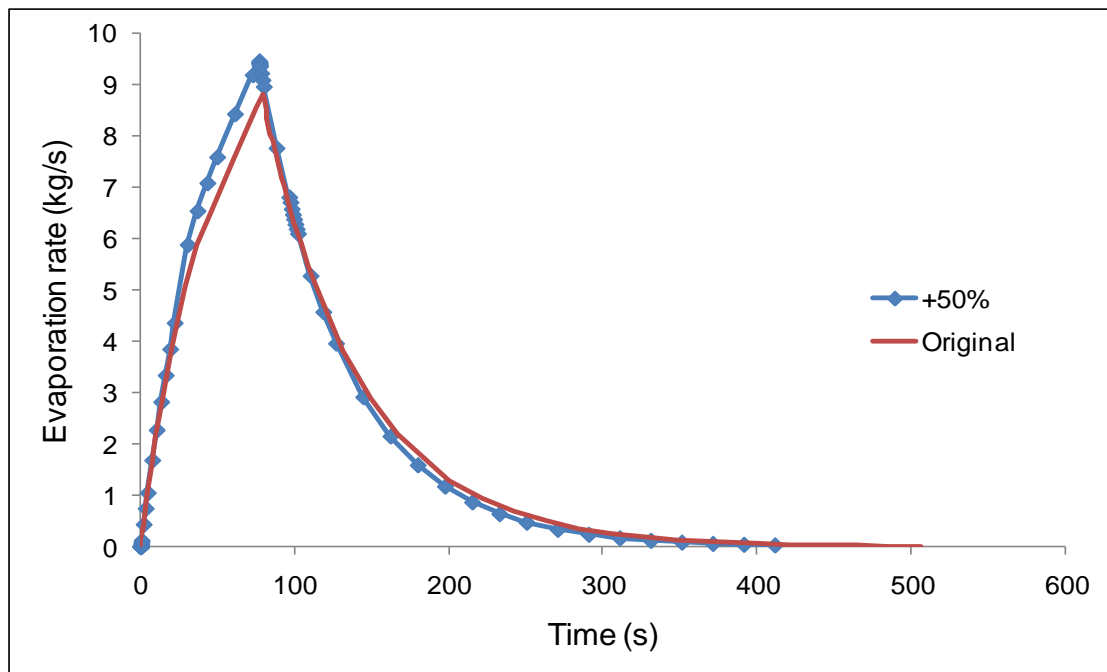


Figure 5. Comparison of the effect of a 50% increase of the heat transfer coefficient on the variation of the evaporation rate with time, for an instantaneous release of 1 ton of methanol at 298 K and a 5 m/s wind speed.

INTERFACIAL TENSION

The liquid-water interfacial surface tension σ_{LW} (N/m) is used in the last viscous surface-tension regime for instantaneous spills on water. The start time of this regime is

$$t_2 = (K_{20})^2 \left(\frac{M_{pool}^2(0)g\mu_w\Delta}{\rho_w\rho_L^2} \right)^{1/3} \left(\frac{\rho_w}{2\sigma} \right) \quad (2)$$

and the pool radius $r(t)$ versus time t during this regime is given by

$$r(t) = \left(\frac{4\sigma^2}{\rho_w\mu_w} \right)^{1/4} t^{3/4} \quad (3)$$

Here $\sigma = \sigma_{wa} - \sigma_{La} - \sigma_{LW}$ is the net surface tension (N/m), with σ_{wa} , σ_{La} , σ_{LW} being the surface tension of water-air, liquid-air, liquid, water, respectively

See PVAP theory manual for details including notation, etc. It is seen that with increasing values of σ_{LW} , σ decreases, the viscous surface-time regime start later and the pool radius increases less.

The interfacial tension was found to have very little impact on the predicted evaporation rate, as in practice with the minimum thickness criterion implemented in this model the viscous surface tension regime is not encountered (see PVAP theory manual for details). For the example of an instantaneous release of 1 ton of n-octane (shown in figure 1) the transition to the viscous-surface tension regime would take place at 800 s and the pool dimensions at that time would be 27.6 m radius and $6 \cdot 10^{-4}$ m height. For water surfaces the minimum thickness is $1 \cdot 10^{-3}$ m, which indicates that the pool stops spreading before the viscous-surface tension regime is reached.

HEAT OF SOLUTION

The heat of solution of the material in water, ΔH_{sol} (J/kg) is used in evaluation of the heat flow rate from dissolution, Q_{sol} (W)

$$Q_{sol} = \Delta H_{sol} E_{sol}(t) \quad (4)$$

Returning to

Figure 1 it can be seen that the property which has the major effect on PVAP results for the evaporation rate is the heat of solution. An increase on the heat of solution causes an increase on the net heat flux entering the pool, consequently rising the pool temperature and the evaporation rate.

Figure 6 to Figure 9 show the variation of the maximum evaporation rate with the heat of solution for continuous and instantaneous releases of different masses of methanol at 293 K and a wind speed of 0.1 m/s. These figures also highlights two different values for the heat of solution, i.e. $2E4$ J/kg (adopted in 6.54 and 6.7; corresponding to value from Cameo database) and $2.62E5$ J/kg (corresponding to value from Critical Tables). For small values of the heat of solution, Q_{sol} is relatively smaller compared to the other heat terms and therefore the change in evaporation rate is very small. For large values Q_{sol} will become dominant, and therefore the evaporation rate will increase rapidly. This is confirmed by

Figure 6,

Figure 7,

Figure 8 and

Figure 9, where it is seen that the maximum evaporation rate hardly changes for values less than 10^5 J/kg, and increases rapidly for values larger than 10^5 J/kg.

Therefore, from this sensitivity analysis it is not possible to establish a default conservative value for the heat of solution of soluble chemicals and accurate values for the heat of solution are required.

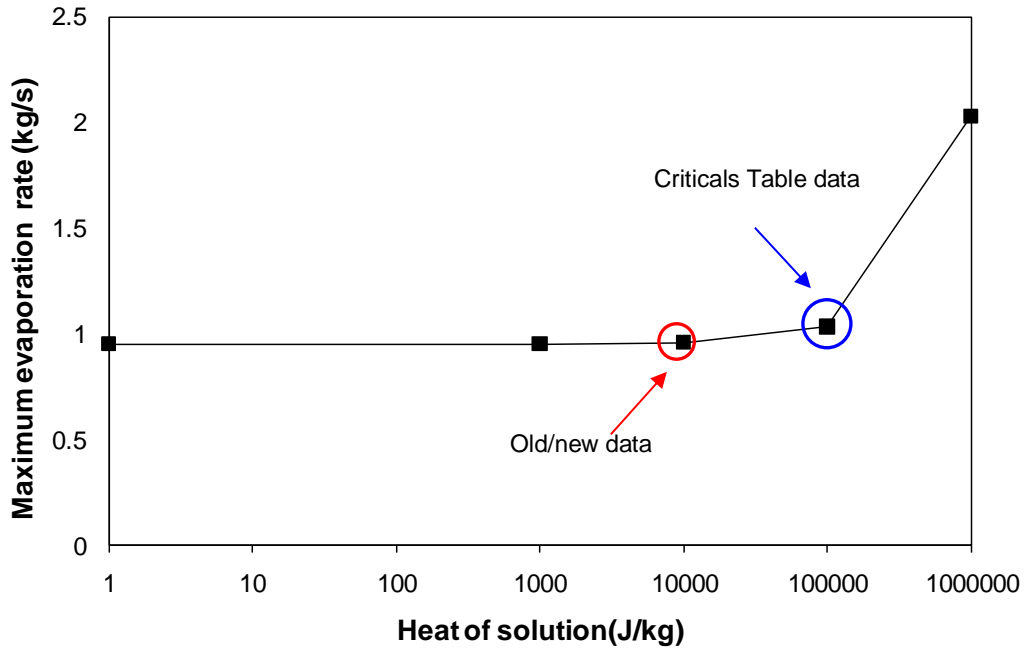


Figure 6. Variation of the maximum evaporation rate against the heat of solution for an instantaneous spill of 100,000 kg of methanol at 298 K and a wind speed of 0.1 m/s at 10 m height.

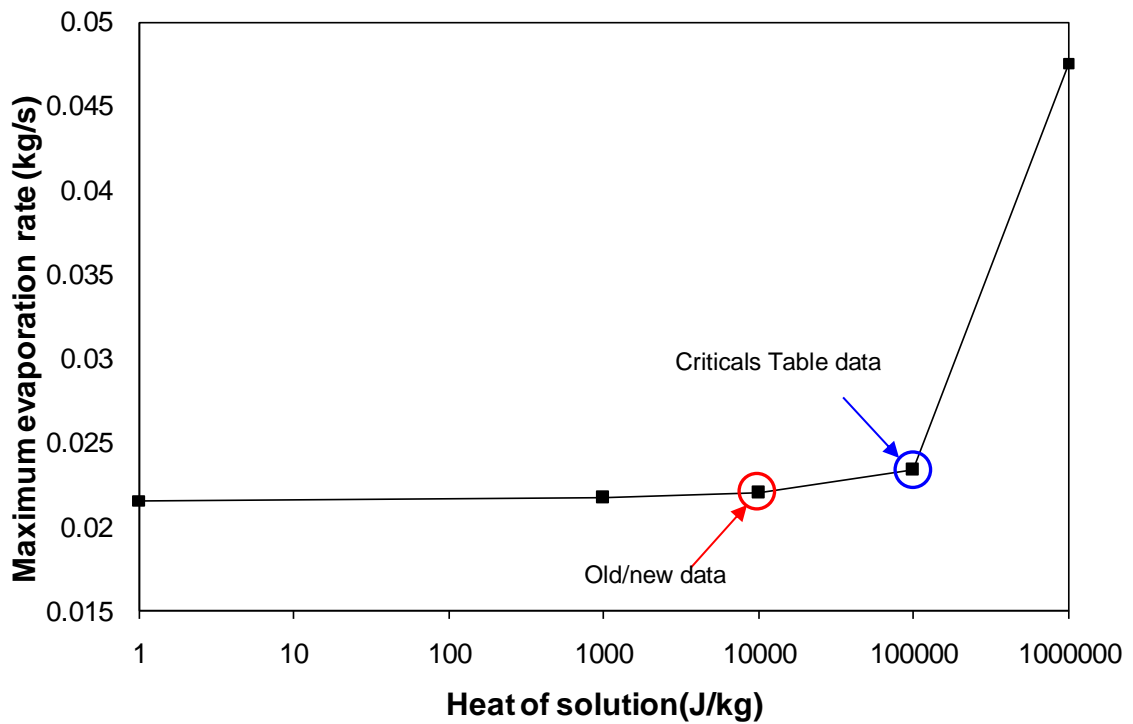


Figure 7. Variation of the maximum evaporation rate against the heat of solution for an instantaneous spill of 10,000 kg of methanol at 298 K and a wind speed of 0.1 m/s at 10 m height.

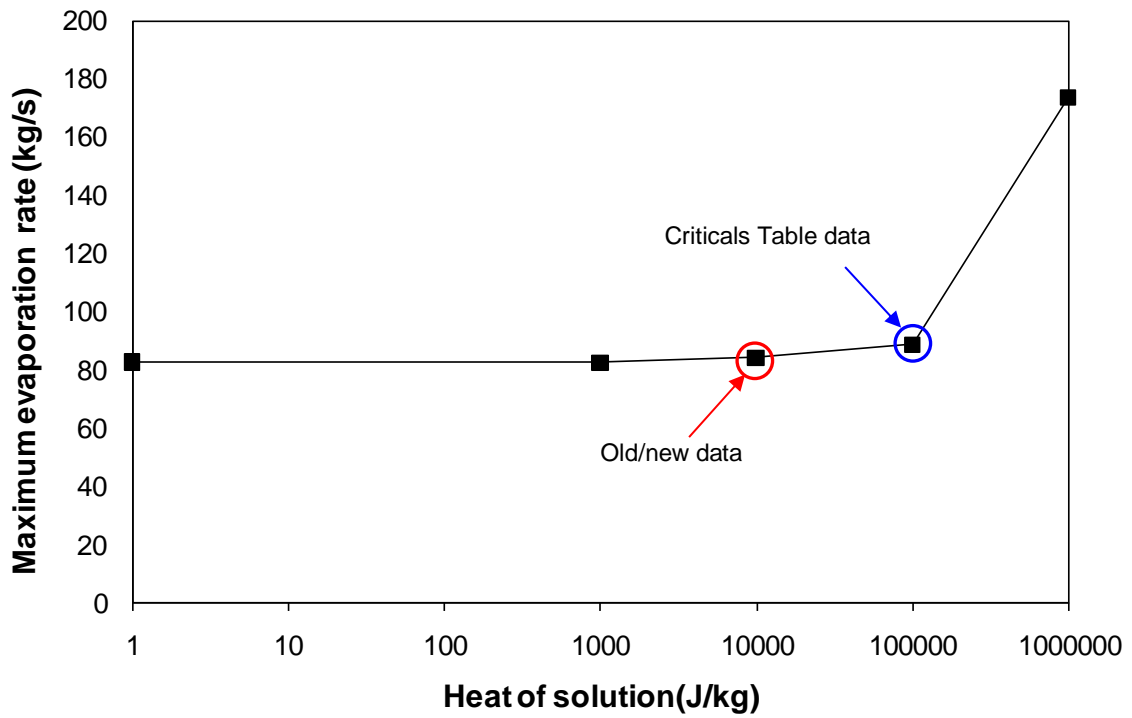


Figure 8. Variation of the maximum evaporation rate against the heat of solution for a continuous spill of 10,000 kg/s of methanol at 298 K and a wind speed of 0.1 m/s at 10 m height.

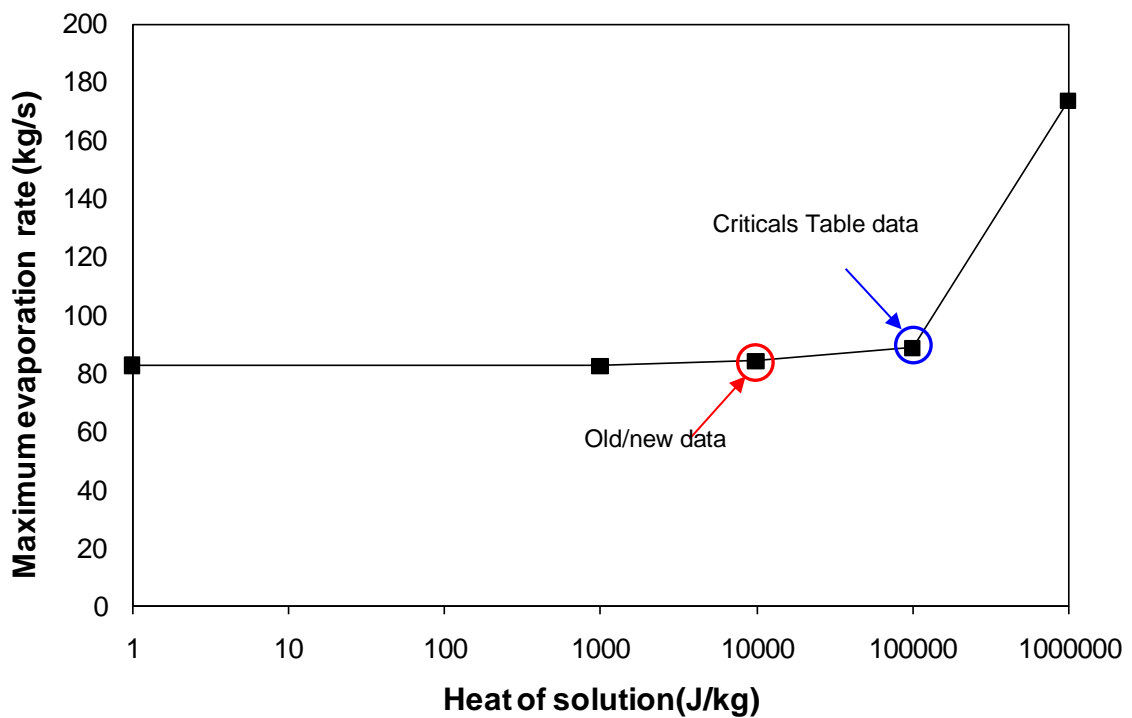


Figure 9. Variation of the maximum evaporation rate against the heat of solution for a continuous spill of 1,000 kg/s of methanol at 298 K and a wind speed of 0.1 m/s at 10 m height.

SOLUBILITY FACTOR

The mass solubility in water, f_s (kg/kg) is used in PVAP to evaluate the molar solubility w_s , which is used to calculate the rate of dissolution of material of liquid pool into water, E_{sol} [kg/s]. Relevant PVAP theory equations are as follows:

$$E_{sol}(t) = 10\pi r^2 U_w^* \rho_w Da^* \ln\left(\frac{1 - w_{infinity}}{1 - w_s}\right) \quad (5)$$

$$w_s = \frac{f_s}{1 + f_s} \quad (6)$$

It is seen from the above equations that $E_{sol}(t)$ increases with increasing molar solubility w_s , and therefore it increases with increasing mass solubility f_s .

According to Equation (4) increased solubility leads to increased heat of solution and therefore increased pool temperature and therefore increased pool evaporation rate. Thus on the one hand increased solubility reduces the pool evaporation rate (because of solution in water), while on the other hand it increases the evaporation rate (because of increased heat of solution).

Figure 1 confirms that the maximum evaporation rate showed a slight decrease when the solubility factor increases. The higher the solubility factor is, the higher the rate at which the pool loses mass from dissolution; this reduces the spreading rate of the pool and consequently its evaporation rate.

Figure 10 to Figure 13 show the variation of the maximum evaporation rate with the solubility factor for continuous and instantaneous releases of different masses of ethanol at 293 K and a wind speed of 0.1 m/s. The old and proposed new values for the solubility factor of ethanol are also highlighted in the figures.

From Figure 10 to Figure 13 it is also observed that for solubility values less than 10^{-3} the maximum evaporation rate is not visibly impacted by variations on the solubility factor. At solubility values between 10^{-3} and 1 the maximum evaporation rate decreases rapidly with respect to the solubility factor. This behaviour is more pronounced for continuous spills (

Figure 12 and Figure 13) than for instantaneous releases (Figure 10 and Figure 11). For both continuous and instantaneous releases the maximum evaporation rate decreases at a slower rate for solubility factors greater than 1 or 3, and eventually will converge to a lower limit as may be observed in figure 2. A value of the solubility factor of 1 is currently selected in cases when the literature flags a material as very soluble without giving a specific value. For highly soluble chemicals, the actual value may be higher.

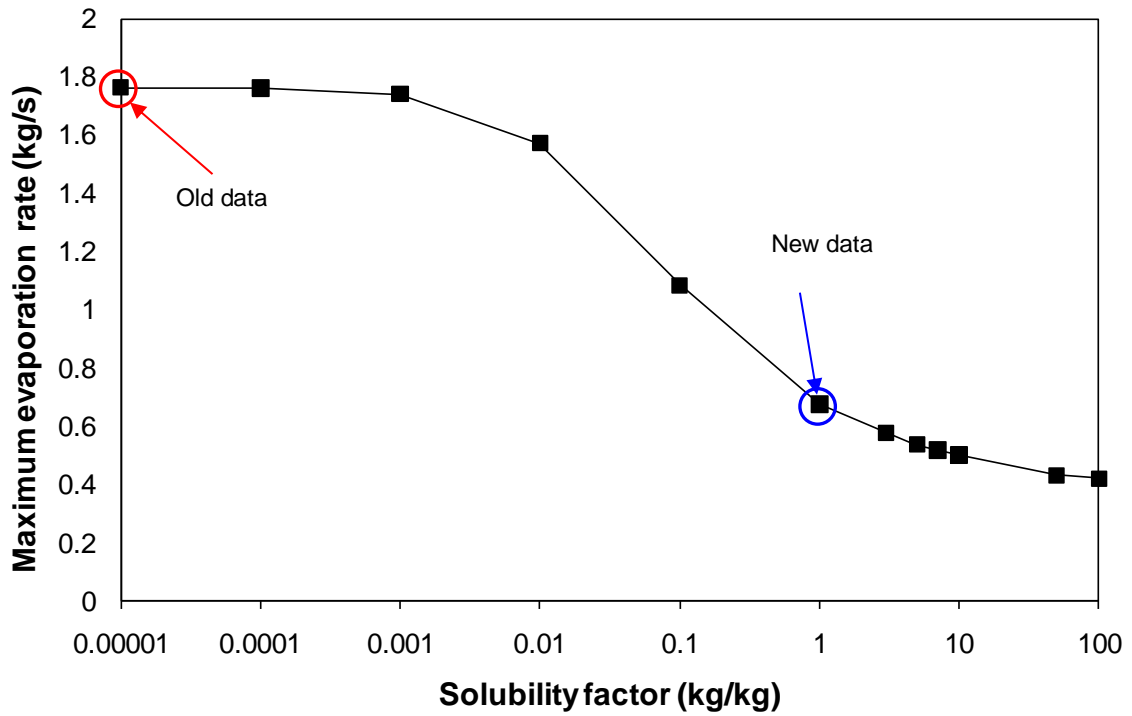


Figure 10. Variation of the maximum evaporation rate against the solubility factor for an instantaneous spill of 100,000 kg of ethanol at 298 K and a wind speed of 0.1 m/s at 10 m height.

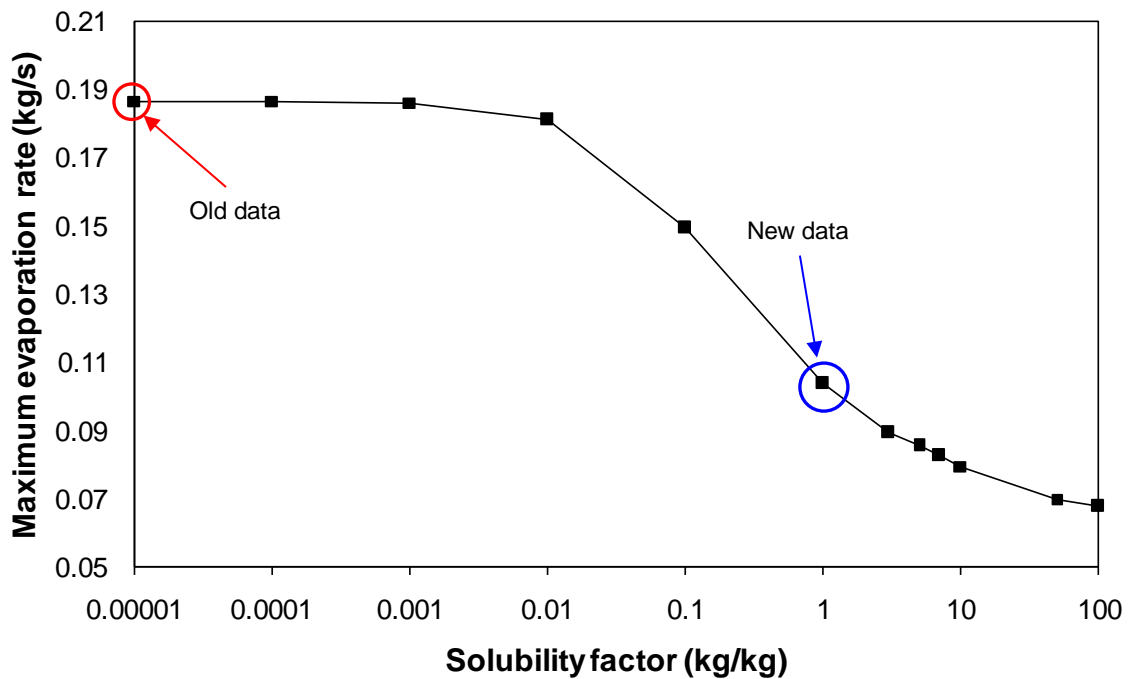


Figure 11. Variation of the maximum evaporation rate against the solubility factor for an instantaneous spill of 10,000 kg of ethanol at 298 K and a wind speed of 0.1 m/s at 10 m height.

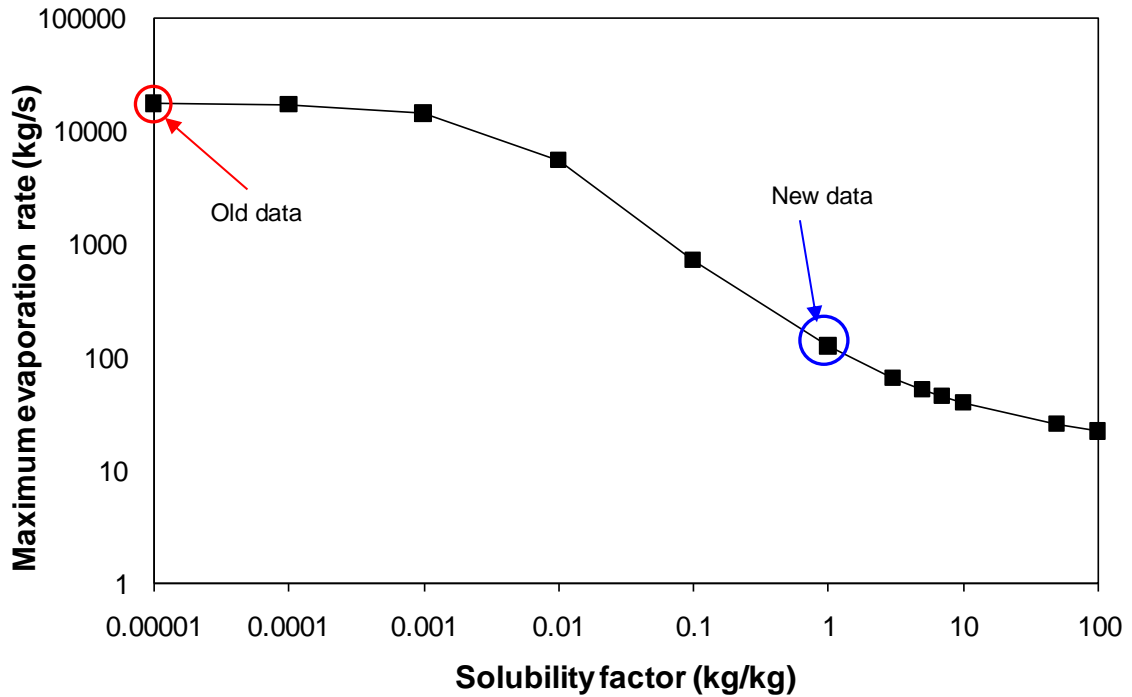


Figure 12. Variation of the maximum evaporation rate against the solubility factor for a continuous spill of 10,000 kg/s of ethanol at 298 K and a wind speed of 0.1 m/s at 10 m height.

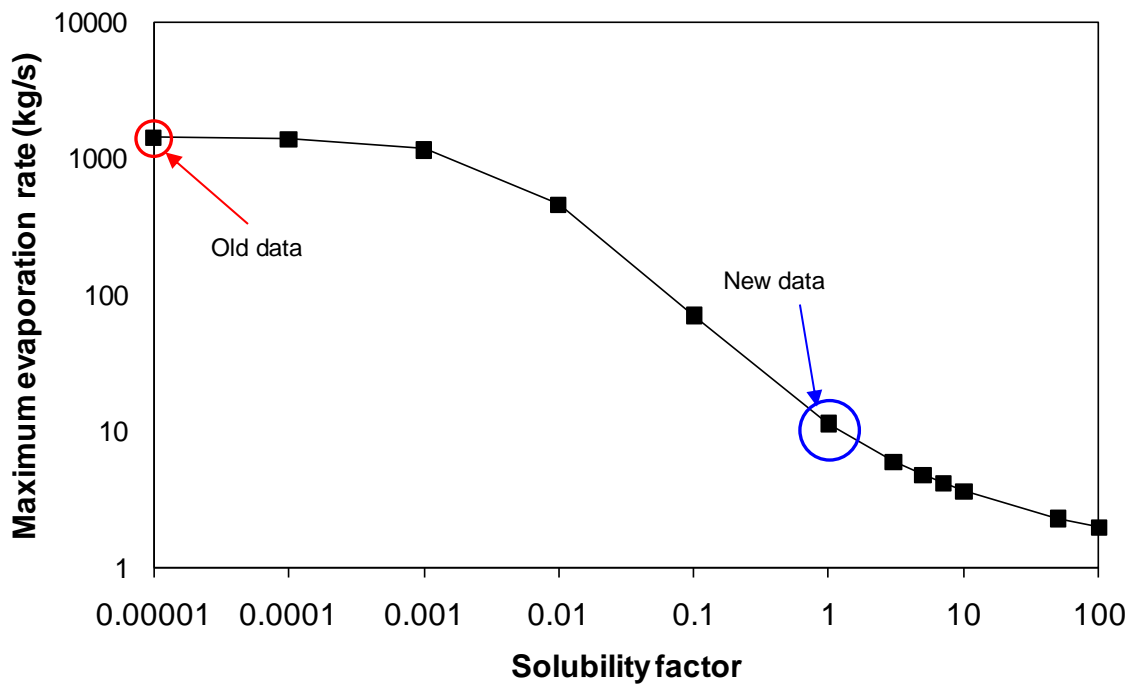


Figure 13. Variation of the maximum evaporation rate against the solubility factor for a continuous spill of 1,000 kg/s of ethanol at 298 K and a wind speed of 0.1 m/s at 10 m height.

Figure 14 to Figure 17 show the variation of the maximum evaporation rate with the solubility factor for continuous and instantaneous releases of different masses of ammonia at 239K (just below boiling point) and a wind speed of 0.1 m/s. The old and proposed new values for the solubility factor of ammonia are also highlighted in the figures. For the instantaneous cases the new values of maximum evaporation rate are about 15% larger than the old values, while for the continuous cases they are around 60% larger.

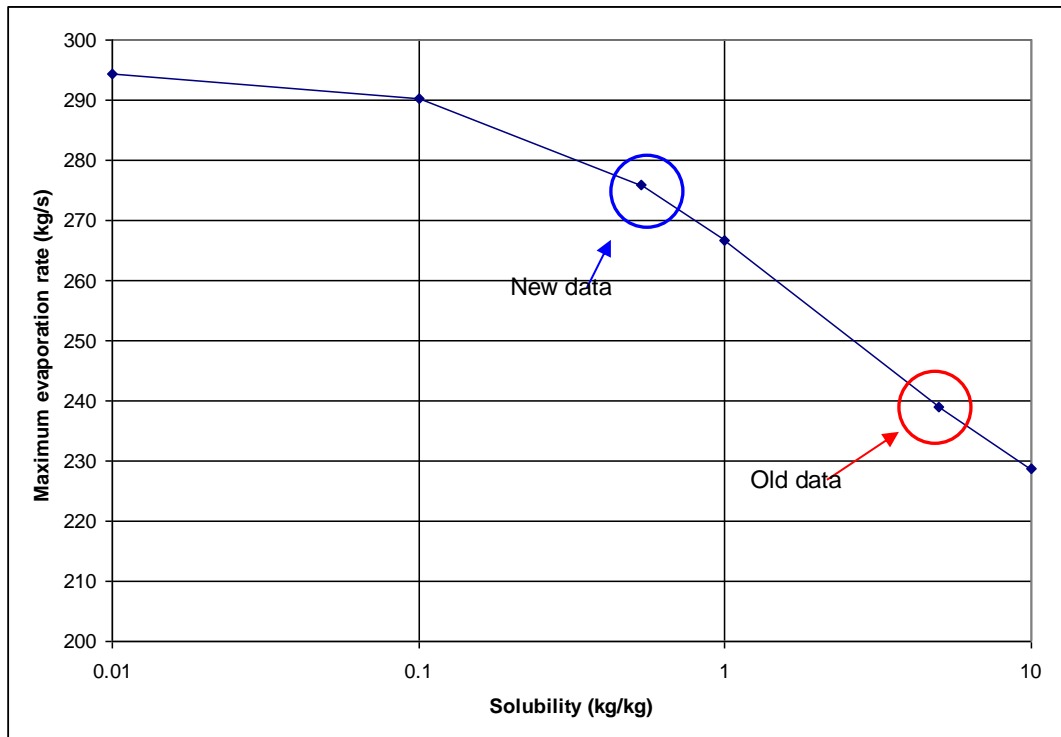


Figure 14. Variation of the maximum evaporation rate against the solubility factor for an instantaneous spill of 100,000 kg of ammonia at 239 K and a wind speed of 0.1 m/s at 10 m height.

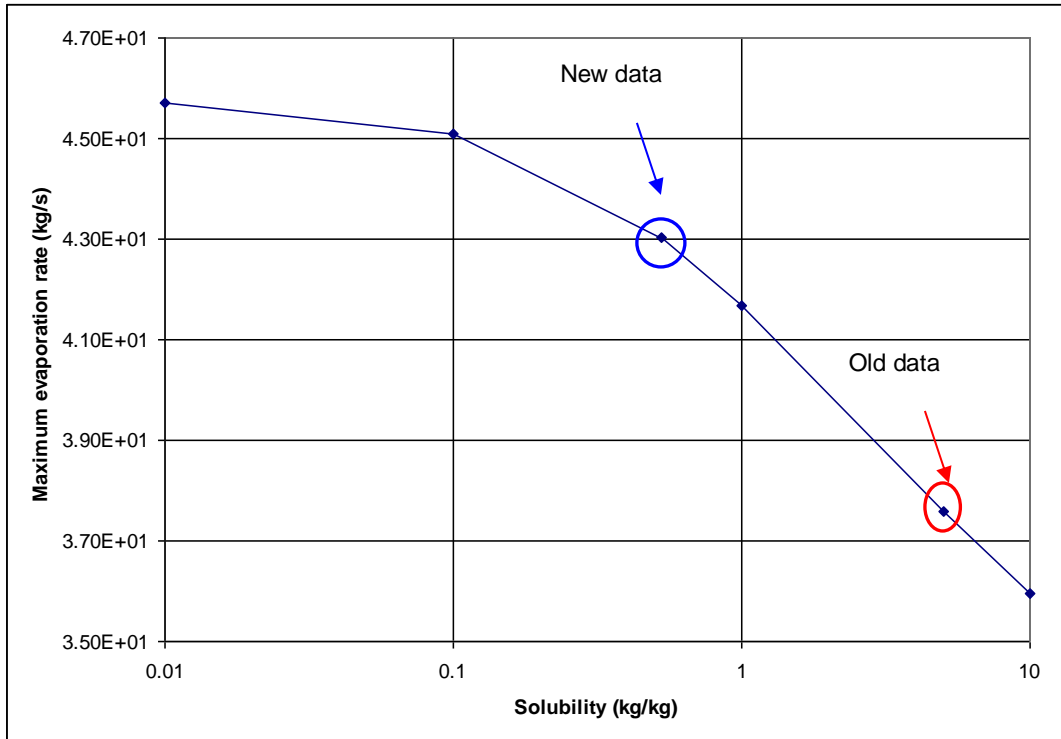


Figure 15. Variation of the maximum evaporation rate against the solubility factor for an instantaneous spill of 10,000 kg of ammonia at 239 K and a wind speed of 0.1 m/s at 10 m height.

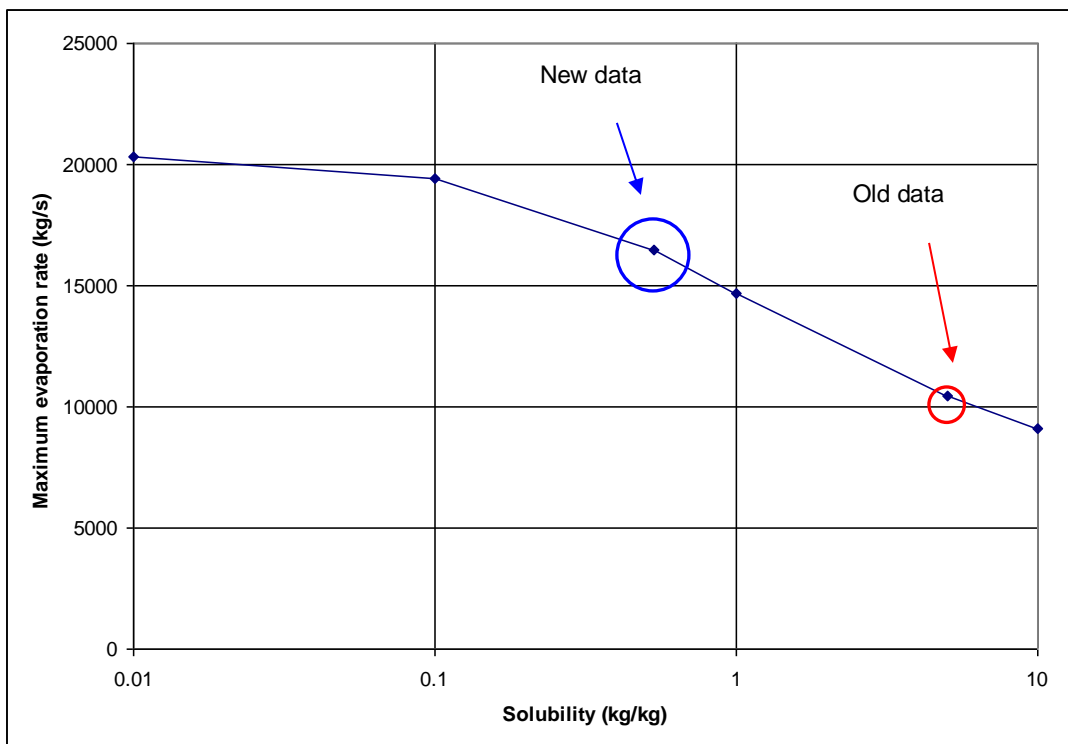


Figure 16. Variation of the maximum evaporation rate against the solubility factor for a continuous spill of 10,000 kg/s of ammonia at 239 K and a wind speed of 0.1 m/s at 10 m height.

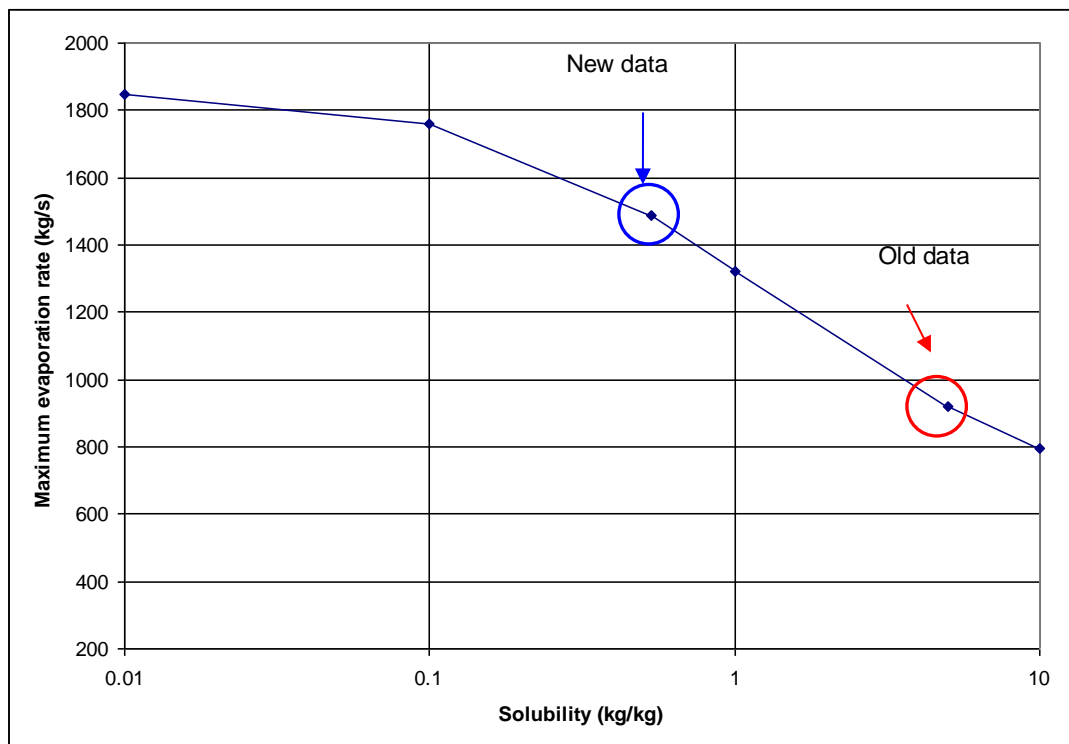


Figure 17. Variation of the maximum evaporation rate against the solubility factor for a continuous spill of 1,000 kg/s of ammonia at 239 K and a wind speed of 0.1 m/s at 10 m height.

HEAT TRANSFER COEFFICIENT

The heat transfer coefficient h_s W/m²K, is used to calculate the heat conduction Q_{cond} (W) from water to the pool, in case of no ice formation. The relevant PVAP theory equation is as follows:

$$Q_{cond} = h_s \pi r^2 (T_{surf} - T_{pool}) \quad (7)$$

Returning to

Figure 1, when the heat transfer coefficient is increased the maximum evaporation rate also increases. Higher heat transfer coefficients increase the net heat flux into the pool, causing the pool temperature and consequently the evaporation rate to rise.

Figure 18 to Figure 21 show the variation of the maximum evaporation rate with the heat transfer coefficient for continuous and instantaneous releases of different masses of propane at 231 K with a wind speed of 0.1 m/s and a surface temperature of 293 K. The old and proposed new values for the heat transfer coefficient of propane are also highlighted in the figures.

For the case of instantaneous propane spills (Figure 18 and Figure 19) it is observed that the maximum evaporation rate continuously increases with the heat transfer coefficient. On the other hand, for continuous propane spills (Figure 20 and Figure 21) it is observed that values for the heat transfer coefficient greater than 500 W/m²K have little effect on the maximum predicted evaporation rate. Thus, in case of missing data from the literature, a default value of 500 W/m²K for the heat transfer coefficient is suggested, bearing in mind this is a mostly conservative estimate for continuous spills, but it may not be conservative for instantaneous cases.

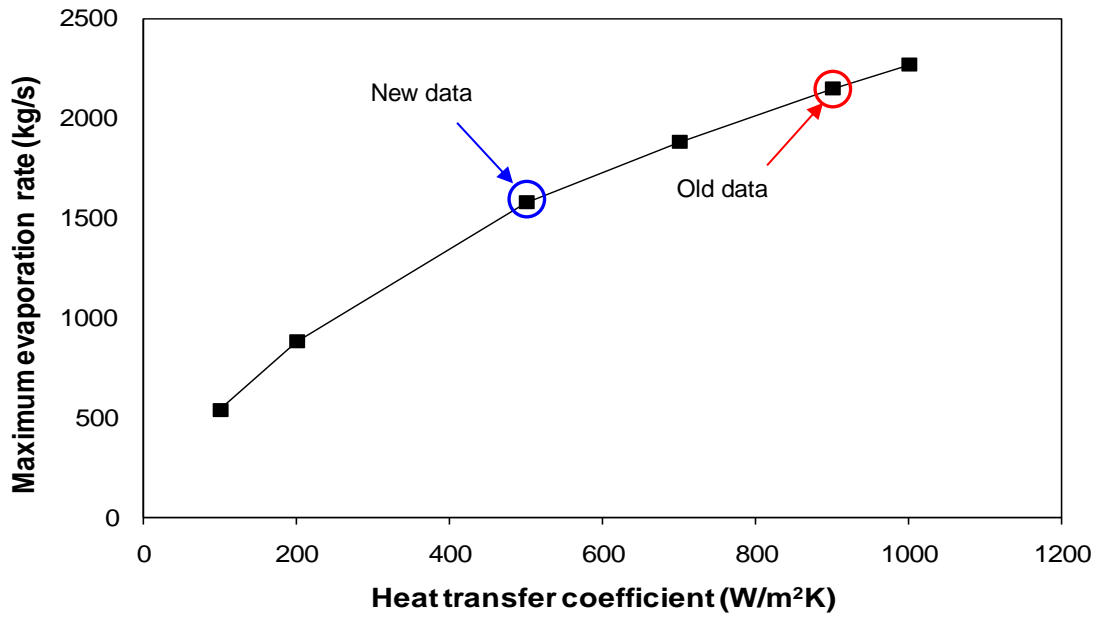


Figure 18. Variation of the maximum evaporation rate against the heat transfer coefficient for an instantaneous spill of 100,000 kg of propane at 231 K with a surface temperature of 293 K and a wind speed of 0.1 m/s at 10 m height.

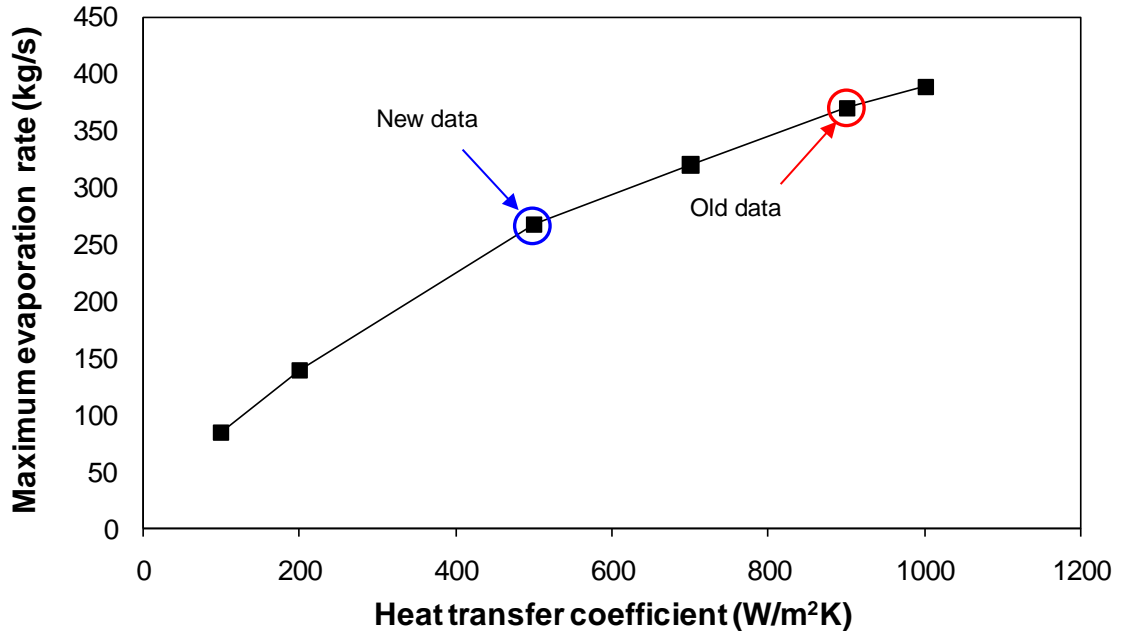


Figure 19. Variation of the maximum evaporation rate against the heat transfer coefficient for an instantaneous spill of 10,000 kg of propane at 231 K with a surface temperature of 293 K and a wind speed of 0.1 m/s at 10 m height

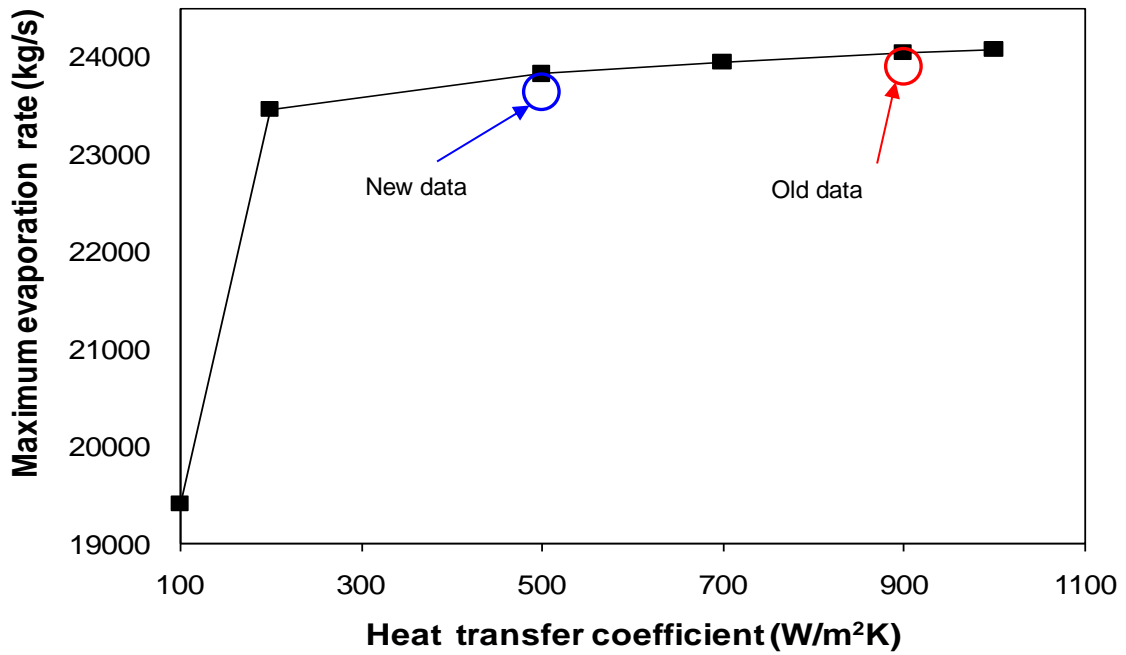


Figure 20. Variation of the maximum evaporation rate against the heat transfer coefficient for a continuous spill of 10,000 kg/s of propane at 231 K with a surface temperature of 293 K and a wind speed of 0.1 m/s at 10 m height

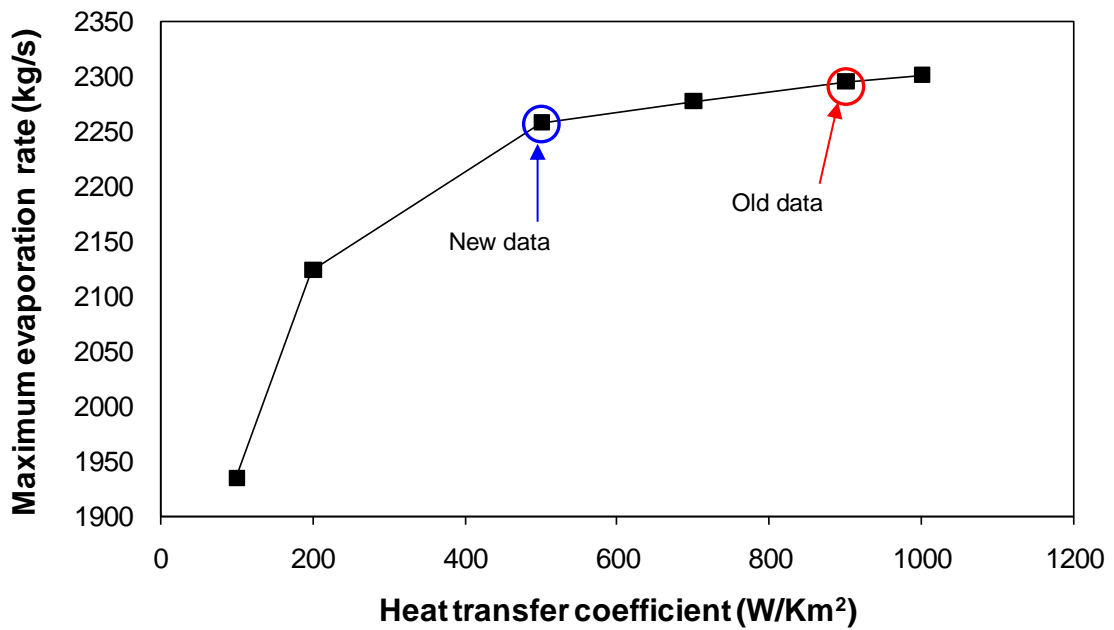


Figure 21. Variation of the maximum evaporation rate against the heat transfer coefficient for a continuous spill of 1,000 kg/s of propane at 231 K, with a surface temperature of 293 K and a wind speed of 0.1 m/s at 10 m height.

4.2.4 List of literature sources

A list of the sources referred to in the literature review for improved material properties for pools on water is presented next. Some material properties currently in version 6.54 of SAFETI-NL and version 6.6 of Phast (Risk) use data from some of these references. This is indicated in the list below:

INTERFACIAL TENSION (N/m):

- Demond and Lindner (1993)⁴. Provides a database for interfacial tension measurements of 67 organic chemicals at temperatures ranging from 20 to 25 °C.
- International Critical Tables (1928)⁵. Provides a large database of interfacial tension measurements for organic chemicals.
- Dodge et al. (1983)⁶. Includes data for the interfacial tension of relevant chemicals at 20 – 25 °C. Phast 6.6 is using this as the reference for the material property of some chemicals.
- Cameo (2011)⁷. This appears to be the most up-to-date and trustworthy database with the most comprehensive set of values.

HEAT OF SOLUTION (J/kg or J/kmol):

- International Critical Tables (1928)⁵. Provides a large database of values for the heat of solution of organic chemicals
- Cameo (2011)⁷. This appears to be the most up-to-date and trustworthy database with the most comprehensive set of values.

SOLUBILITY FACTOR (kg/kg or kmol/kmol):

- Dodge et al. (1983)⁸. Provides a database for solubility factor of 20 chemicals in water. Phast 6.6 is using Dodge et al. (1983) as the reference for the material property of some chemicals.
- Demond and Lindner (1993)⁴. Provides a comprehensive database of molar solubility (kmol/kmol) of 67 organic chemicals in water at temperatures between 20 °C and 25°C.
- IUPAC-NIST Solubility Database⁹. Is an online database which contains solubility measurements of about 1800 chemical substances with literature references. Typical solvents and solutes include water, sea water, heavy water, inorganic and organic chemicals.
- Cameo (2011)⁷. For most chemicals in this database the solubility is given at 20C (68F). For those chemicals for which the solubility was given as a function of the temperature (e.g. diethylether), the value of solubility was selected at 20C. Note that for some chemicals the solubility may be significantly dependent on the temperature.
- Serida (1998)¹⁰. This RIVM database is no longer kept up to date, and contains some values of solubilities largely based on 'Chemiekaarten'. However some values were not found to be trustworthy and therefore Cameo values have been selected if present.

HEAT TRANSFER COEFFICIENT WITH WATER (W/m²K):

- Webber (1990)¹¹. Proposes a value of 500 W/m²K taken from Reid and Smith (1978)¹² n-butane experiments.
- Woodward (1990)¹³. Proposes a rule of thumb $h_s = 0.001\Delta H_v$ based on cryogenic liquid tests; where, h_s is the heat transfer coefficient with water and, ΔH_v is the latent heat of vaporisation. According to Woodward (private communication) this rule of thumb has now been superseded by the reference below.
- Woodward and Pitblado (2010)¹⁴ Provides a limited list of heat transfer coefficients of pure chemicals (nitrogen, methane, ethylene, ethane, propane and n-butane) and LNG mixtures. The heat transfer coefficient is quoted to be obtained as the heat flux divided by the temperature difference between water (assumed at 10C) and the normal boiling point. The quoted value in this book for n-butane based on Reid and Smith (1978)¹² was found to be incorrect while the above value quoted by Webber appears to be correct.

4.2.5 Proposed changes in values

In Table 3 the old and proposed new values for the material properties for pools on water are shown. New values are shown only when they differ from the old values and/or when a value has been found from the

literature. An 'undefined' value of -9.95E36 refers to a material property for which no value is included in the DNV database, and for which the user himself needs to define a value.

The chemicals listed in the table are classified as standard and non-standard compounds. All chemicals indicated by an "x" in the "NL" column in Table 3 are included in the 6.54/6.7 SAFETI-NL material property database. The other chemicals, indicated by blanks in the "NL" column, are less frequently consulted and users are often prompted to supply missing material properties for these compounds.

The data in the table have been colour-coded according to the following legend:

- *Orange values*: are set in DNV database and no reference was found for them; no change will be applied.
- *Red values*: are new values found with expected significant differences; here, approximately more than 1% variation is considered significant but the actual variation has not been checked (to follow from sensitivity analysis)
- *White values* in the new data column: are new values for which no significant difference in the results is expected.
- *Bold values*: are the best choices amongst different new values, chosen because they are either the conservative assumption or come from a more trustworthy reference. Where multiple references are found, Dodge et al. (1983)⁶ has been perceived as a less trustworthy reference since it does not include a justification/reference for the values of the material properties. Since the IUPAC-NIST Solubility Database⁹ is a more recent source (2006) than Demond and Lindner (1993)⁴, values of the IUPAC-NIST Solubility Database have been adopted when values are found in both references. Furthermore whenever interfacial tension or solubility data (heat of solution or solubility) are given by the Cameo database⁷ they are selected. Finally in case no solubility is provided by the Cameo database, the SERIDA¹⁰ value has been selected if available.

Interfacial tension (N/m):

From the sensitivity analysis it was found that the viscous-surface tension spreading regime is rarely encountered in pools on water. The new data found for the interfacial tension of several chemicals is shown as "white values" in **Table 3**, as no significant impact on the results is expected.

Values indicated in the Cameo database as 'Not pertinent' are interpreted with zero values, and this was found not to lead to inconsistent values with the other literature. Moreover applying zero values is conservative.

Heat of solution (J/kg):

This property is used in the calculation of heat losses due to dissolution of the material in water. Values for this property are only present in chemicals with positive values for the solubility factor f_s (kg/kg).

Values indicated in the Cameo database as 'Not pertinent' are interpreted with zero values, and this was found not to lead to inconsistent values with the other literature.

For a limited number of chemicals (n-butanol, methylamine, 3-chloro1-propene, nitric acid, arsine, phosphine) the Cameo database indicates that the material is soluble but a value of the heat of solution is listed as not being available. It has therefore been decided not to change the heat of solution and solubility for these chemicals, and to wait until we have complete values and therefore justification for the change. Thus this applies a zero solubility for all chemicals except methylamine, n-butanol, methylamine, 3-chloro1-propene, nitric acid, arsine, phosphine.

Solubility factor (kg/kg):

Default zero values for the solubility factor are the conservative assumption as the sensitivity analysis showed that lower solubility factors produce higher evaporation rates..

The Cameo database indicates 'insoluble', which has also been interpreted as not soluble (zero solubility factor).

Except acrylamide, Cameo lists no values of solubility larger than 0.4 kg/kg, and thus it appears to be that in Cameo chemicals are set as 'very soluble (miscible)' if the solubility is larger than this value. Serida marks a chemical as 'very soluble' in case the solubility is larger than 0.1 kg/kg. A value of the solubility factor of 1 kg/kg is currently selected in case the material is known to be very soluble but a specific value of solubility is not given in the Cameo or Serida database. In Phast 6.6 a less conservative value of 5 kg/kg instead of 1 kg/kg was adopted in this case. Ideally a further reliable reference would be found with more precise values of solubilities for 'very soluble' materials. Quite a large number of chemicals have become fully soluble in 6.7.



For a limited number of chemicals (phosgene, methyl isocyanate, fluorine, nitric oxide) the Cameo database indicates that the chemical reacts with water. Note that this reaction is not modelled currently by the PVAP model. For all these cases the Serida value has been selected as the solubility factor.

Heat transfer coefficient (W/m²K):

Default values of 500 W/m²K are close to the new data found for various chemicals, with the exception of the new data for liquid hydrogen.

Additionally, the sensitivity analysis showed that for continuous releases increasing values beyond 500 W/m²K for the heat transfer coefficient have little effect on the prediction of the maximum evaporation rate. However, this is not the case for instantaneous releases for which a heat transfer coefficient of 500 W/m²/K may be an un-conservative estimate.

CAS	Material name	NL	Interfacial tension (N/m)		Heat of solution (J/kg)		Solubility in water (kg/kg)		Heat transfer coefficient (W/m ² K)		Comments
			Old Data	New Data	Old Data	New Data	Old Data	New Data	Old Data	New Data	
50000	Formaldehyde	x	0	0 ^f	0	2E+04 ^f	0	1 ^f	500		Expected lower E _{vap}
60297	Diethyl ether		-9.95E+36	0 ^f 0.0107 ^a 0.0107 ^c	-9.95E+36	0 ^f -3.33E+05 ^a	-9.95E+36	7.5E-02 ^f 7.28E-02 ^b 7.50E-02 ^c 6.9E-02 ^g	500		Cameo includes solubility versus temperature. Data at 20C selected.
64175	Ethanol	x	0	0 ^f	0	2.3E+05 ^f 2.25E+05 ^a	0	1 ^f	500		Expected lower E _{vap} ; additional reference for high solubility of ethanol: CRC Handbook of Chemistry and Physics 91 st Ed. ¹⁵
64186	Formic acid		-9.95E+36	0 ^f	-9.95E+36	6E+04 ^f 7.17E+03 ^a	-9.95E+36	1 ^f	500		
67561	Methanol	x	0.05	0 ^f	2.00E+04	2E+04 ^f 2.61E+05 ^a	5	1 ^f	500		
67630	Isopropanol	x	0	0 ^f	0	2E+04 ^f 2.62E+05 ^a	0	1 ^f	500		Expected lower E _{vap}
67641	Acetone	x	0	0 ^f	0	0 ^f	0	1 ^f	500		Expected lower E _{vap}
71363	N-butanol	x	0	0.056 ^f 0.0021 ^a 0.0016 ^c	0	N/Avail ^f	0	0 7.8E-02 ^f 7.90E-02 ^b 7.70E-02 ^c 8E-02 ^g	500		- Much larger tension value by Cameo! Lower E _{vap} . Soluble chemical, uncertainty on pool temperature estimation; original solubility value maintained. - Interfacial tension given at 27C
71432	Benzene	x	0.035	0.035 ^f 0.0350 ^b	0	0 ^f	1.80E-03	1.8E-03 ^f 1.73E-03 ^b 1.75E-03 ^c 1.8E-03 ^g	500		Solubility given at 25C.
74828	Methane	x	0.05	0.05 ^f	0	0 ^f	0	0 ^f 2.4E-06 ^g	500	500 683 ^e 535 ^e	Wide range of values reported ^e for heat transfer coefficient, with value of 500 in middle of this range. Also better validation results for 500 than 683. Therefore value not changed.
74839	Methyl bromide	x	0.05	0 ^f	0	0 ^f	9.00E-04	9E-04 ^f 1.7E-02 ^g	500		Solubility given at 20C
74840	Ethane	x	0.045	0.045 ^f	0	0 ^f	0	0 ^f	500	555 ^e	Slightly higher E _{vap} . Interface tension at -88C
74851	Ethylene	x	0.05	0.05 ^f	0	0 ^f	0	0 ^f	500	545 ^e	Slightly higher E _{vap} Interface tens. at -104C
74862	Acetylene	x	0	0 ^f	0	0 ^f	0	0 ^f	500		
74873	Chloromethane		-9.95E+36	0.05 ^f	-9.95E+36	0 ^f	-9.95E+36	6.0E-03 ^f	500		Interfacial tension estimated at -24C
CAS	Material name	NL	Interfacial tension (N/m)		Heat of solution (J/kg)		Solubility in water (kg/kg)		Heat transfer coefficient (W/m ² K)		Comments
			Old Data	New Data	Old Data	New Data	Old Data	New Data	Old Data	New Data	

74895	Methylamine	x	0.05	0 ^f	0	N/Avail ^f	1.08	1.08 ^f	500	Soluble chemical, uncertainty on pool temperature estimation	
74908	Hydrogen cyanide	x	0.05	0 ^f	0	0 ^f	5	1 ^f	500	Lower E _{vap}	
74931	Methylmercaptan	x	0	0 ^f	0	0 ^f	0	2.4E-02 ^f 2.3E-02 ^g	500	Lower E _{vap} . Solubility at 15C	
74986	Propane	x	0.05	0.05 ^f	0	0 ^f	0	0 ^f	900	586 ^g	
75014	Vinyl chloride	x	0.03	0.03 ^f	0	0 ^f	6.00E-03	6.00E-03 ^f	500	Interface tension and solubility at 20C	
75058	Acetonitrile		-9.95E+36	0 ^f	-9.95E+36	0 ^f	-9.95E+36	1 ^f	500		
75070	Acetaldehyde		-9.95E+36	0 ^f	-9.95E+36	0 ^f 3.43E+05 ^a	-9.95E+36	1 ^f 0 ^g	500		
75081	Ethanthiol		-9.95E+36	0.025 ^f 0.0261 ^b 0.0250 ^c	-9.95E+36	0 ^f	-9.95E+36	1.50E-02 ^f 1.03E-03 ^b 1.50E-02 ^c 7E-03 ^g	500	Interface tension and solubility at 20C	
75092	Dichloromethane	x	0	0 ^f 0.0283 ^b	0	0 ^f	0	1.38E-02 ^f 1.99E-02 ^b 2.00E-02 ^d 2E-02 ^g	500	Lower E _{vap} Solubility at 20C.	
75150	Carbon disulfide	x	0	0.0484 ^f 0.0484 ^a 0.0481 ^b	0	0 ^f	0	0 (insol.) ^f 1.88E-03 ^b 2.2E-03 ^g	500	Interfacial tension at 20C.	
75218	Ethylene oxide	x	0.05	0 ^f	1.40E+05	1.4E+05 ^f	5	1 ^f	500		
75445	Phosgene	x	0.05	0 ^f	0	0 ^f	0	6.83E-03 ^g Reacts ^f	500	Slightly lower E _{vap} . use Serida solubility (Cameo - Reacts in water)	
75503	Trimethylamine	x	0	0 ^f	0	8.96E+05 ^f 6.20E+05 ^a	0	4.8E-01 ^g 1 ^f	500	Different E _{vap}	
75569	1,2-propylene oxide	x	0	0 ^f	0	4.5E+04 ^f	0	4.05E-01 ^f 4.1E-01 ^g	500	Different E _{vap} . Solubility at 20C	
78002	Tetraethyl lead	x	0	0.04 ^f	0	0 ^f	0	0 ^f	500		
78831	Isobutanol	x	0	0 ^f	0	2E+04 ^f 1.63E+05 ^a	0	8.5E-02 ^f 9.18E-02 ^b	500	Different E _{vap} . Solubility at 20C.	
79061	Acrylamide		0	0 ^f	0	0 ^f	0	2.16 ^f 2.15 ^g	500	Lower E _{vap} . Solubility at 20C.	
96333	Methylacrylate		-9.95E+36	0.03 ^f	-9.95E+36	0 ^f	-9.95E+36	5.5E-02 ^f 6E-02 ^g	500	Interface tension and solubility at 20C	
100425	Styrene	x	0	0.03548 ^f 0.0355 ^b	0	0 ^f	0	3.00E-03 ^f 3.02E-04 ^b 3.06E-04 ^d 3E-04 ^g	500	Slightly lower E _{vap} ; inconsistency of Cameo with all other listed data, but higher value confirmed against our databases on website. Interface tension at 19C and solubility at 20C	
CAS	Material name	NL	Interfacial tension (N/m)		Heat of solution (J/kg)		Solubility in water (kg/kg)		Heat transfer coefficient (W/m²K)		Comments
			Old Data	New Data	Old Data	New Data	Old Data	New Data	Old Data	New Data	
100447	Benzyl chloride	x	0	0.030 ^f	0	0 ^f	0	3E-05 ^f	500		Interface tension at 20C and solubility at 25C

106898	1-chloro-2,3-epoxypropane		-9.95E+36	0 ^f	-9.95E+36	0 ^f	-9.95E+36	5E-04 ^g 6.00E-02 ^f 6.00E-02 ^g	500		Solubility at 25C
106978	N-butane	x	0.065	0.065 ^f	0	0 ^f	0	0 (insol.) ^f	500	500	Value based on Reid and Smith ¹² as quoted by Webber ¹¹ . Int.tension at 22C.
106989	1-butene	x	0	N/Avail ^f	0	N/Avail ^f	0	0 ^f	500		CAMEO: Missing CHRIS Code
106990	1,3-butadiene		0	0.067 ^f	0	0 ^f	0	0 (insol.) ^f	500		Interface tension at 22C
107028	Acrolein	x	0	0.035 ^f	0	0 ^f	0	2.1E-01 ^f 2.06E-01 ^g	500		Lower E _{vap} ; Cameo includes solubility versus temperature. Data at 20C selected.
107051	3-chloro1-propene	x	0	N/Avail ^f 0.0571 ^c	0	N/Avail ^f	0	0 3.30E-03 ^f 3.30E-03 ^c 3.98E-03 ^d	500		Soluble chemical, uncertainty on pool temperature estimation; original solubility value maintained
107131	Acrylonitrile	x	0.05	0 ^f	0	0 ^f	8.00E-02	8.00E-02 ^f 7.3E-02 ^g	500		Solubility at 21.1C.
107153	1,2-diaminoethane		-9.95E+36	0 ^f	-9.95E+36	2E+04 ^f 5.29E+05 ^a	-9.95E+36	1 ^f	500		
107186	Allyl alcohol	x	0	0 ^f	0	0 ^f (est.) ^f 1.44E+05 ^a	0	1 ^f 0 ^g	500		Lower E _{vap}
107313	Methylformate		-9.95E+36	0 ^f	-9.95E+36	0 ^f 7.88E+04 ^a	-9.95E+36	3.0E-01 ^f	500		Solubility at 20C
108054	Vinyl acetate	x	0	0.03 ^f	0	0 ^f	0	2.30E-02 ^f 2.5E-02 ^g	500		Lower E _{vap} . Interfacial tension and solubility at 20C.
108383	m-xylene	x	0	0.0364 ^f 0.0379 ^b 0.0364 ^c	0	0 ^f	0	0 (insol.) ^f 1.73E-04 ^d 1.67E-04 ^b 1.96E-04 ^c	500		Interfacial tension at 30C.
108883	Toluene	x	0.0361	0.0361 ^f 0.0361 ^b	0	0 ^f	5.00E-04	5.0E-4 ^f 4.92E-04 ^d 5.42E-04 ^b 4.50E-04 ^c 5E-04 ^g	500		Interfacial tension at 25C and solubility at 20C.
108952	Phenol		0	0 ^f	0	0 ^f	0	8.4E-02 ^f 8E-02 ^g	500		Lower E _{vap}
CAS	Material name	NL	Interfacial tension (N/m)		Heat of solution (J/kg)		Solubility in water (kg/kg)		Heat transfer coefficient (W/m²K)		Comments
			Old Data	New Data	Old Data	New Data	Old Data	New Data	Old Data	New Data	
109660	N-pentane	x	0.0502	0.0502 ^f 0.0490 ^b	0	0 ^f	0	0 ^f 4.77E-05 ^d	500		Interfacial tension at 20C

								4.04E-05 ^b 4.10E-05 ^c			
109795	1-butanethiol		-9.95E+36	0.030^f 0.0300 ^c	-9.95E+36	0 ^f	-9.95E+36	0 (insol.)^f 6.00E-04 ^c	500		Interfacial tension at 20C
109897	Ethylethanamine		-9.95E+36	0 ^f	-9.95E+36	4.69E+05^f 4.70E+05 ^a	-9.95E+36	1 ^f	500		
109944	Ethylformate		-9.95E+36	0.028 ^f	-9.95E+36	1.2E+05^f 1.19E+05 ^a	-9.95E+36	9.10E-02 ^f	500		Interfacial tension at 20C and solubility at 21.7C
110010	Tetrahydrothiophene		-9.95E+36		-9.95E+36		-9.95E+36	0 ^f	500		CAMEO: Missing CHRIS Code
110543	N-hexane	x	0.0511	0.0511^f 0.0511 ^b	0	0 ^f	0	0^f 1.24E-05 ^d 1.39E-05 ^b 1.25E-05 ^c	500		Interfacial tension at 20C
110827	Cyclo-hexane		-9.95E+36	0.050^f 0.0500 ^c	-9.95E+36	0 ^f	-9.95E+36	1.5E-04^f 5.61E-05 ^b 1.50E-04 ^c	500		Interfacial tension at 25C and solubility at 28.3C
111659	N-octane	x	0.035	0.035^f 0.0508 ^b	0	0 ^f	2.00E-05	2E-05^f 8.50E-07 ^d 7.16E-07 ^b 6.60E-07 ^c	500		Interfacial tension at 20C and solubility at 15.6C
111842	N-nonane	x	0	0.035^f 0.0350 ^c	0	0 ^f	0	0^f 2.71E-07 ^d 1.50E-07 ^c	500		Interfacial tension at 20C
115071	Propylene	x	0.05	0 ^f	0	0 ^f	0	0 ^f	500		
121448	Triethylamine	x	0	0 ^f	0	4.1E+05^f 4.15E+05 ^a	0	5.50E-02^f 1.7E-01 ^g	500		Different E _{vap} . Solubility at 20C
124389	Carbon dioxide	x	0.05	0 ^f	0	0 ^f	0	1.86E-03^f 1.6E-03 ^g	500		Lower E _{vap} but note CO2 solid at atmospheric pressure (no liquid pool)
124403	Dimethylamine	x	0	0 ^f	0	1.2E+06^f	0	1 ^f	500		Different E _{vap}
141322	N-butyl acrylate	x	0	0.060 ^f	0	0 ^f	0	2.00E-03^f 1E-03 ^g	500		Lower E _{vap} . Interface tension at 27C and solubility at 20C
142825	N-heptane	x	0.051	0.051^f 0.0502 ^b 0.0510 ^c	0	0 ^f	0	0^f 2.57E-06 ^d 2.78E-06 ^b 2.70E-06 ^c	500		Interfacial tension at 20C
CAS	Material name	NL	Interfacial tension (N/m)		Heat of solution (J/kg)		Solubility in water (kg/kg)		Heat transfer coefficient (W/m ² K)		Comments
			Old Data	New Data	Old Data	New Data	Old Data	New Data	Old Data	New Data	
151564	Ethyleneimine	x	0	0 ^f	0	6E+04^f	0	1 ^f	500		Different E _{vap}
302012	Hydrazine	x	0	0 ^f	0	5.07E+05^f	0	1 ^f	500		Different E _{vap}
624839	Methyl isocyanate	x	0.05	N/Avail ^f	0	0 ^f	0	0^g	500		Use Serida solubility

630080	Carbon monoxide	x	0.05	0 ^f	0	0 ^f	0	Reacts ^f	4E-05 ^f	500		(Cameo - Reacts in water)
1333740	Hydrogen	x	0.05	0 ^f	0	0 ^f	0	0 ^f	0 ^f	500	194 ^e 159 ^e 123 ^e	Highest value chosen for the heat transfer coefficient as the most conservative. Lower E _{vap} .
7446095	Sulfur dioxide	x	0.05	0 ^f	0	2.19E+05 ^f	1.00E-01	1.00E-01 ^f 1.05E-01 ^g	500			Different E _{vap} . Solubility at 20C.
7647010	Hydrogen chloride	x	0.05	0 ^f	2.06E+06	2.06E+06 ^f	5	7.2E-01 ^g 1 ^f	500			Lower E _{vap}
7664393	Hydrogen fluoride	x	0.05	0 ^f	3.076E+06	3.076E+06 ^f	5	1 ^f	500			Lower E _{vap}
7664417	Ammonia	x	0.05	0 ^f	5.40E+05	5.40E+05 ^f	5	0.53 ^g 1 ^f	200			Lower E _{vap}
7697372	Nitric acid		0		0		0	0 1 ^g	500			CAMEO: Missing CHRIS Code, soluble chemical, uncertainty on pool temperature estimation; original solubility value maintained
7722841	Hydrogen peroxide		0	0 ^f	0	4.69E+04 ^f	0	1 ^f	500			Different E _{vap}
7726956	Bromine	x	0	N/Avail ^f	0	0 ^f	0	3.50E-02 ^f 3.58E-02 ^g	500			Lower E _{vap} . Solubility at 25C.
7727379	Nitrogen	x	0.05	0 ^f	0	0 ^f	0	0 ^f	500			Liquid nitrogen
7732185	Water ^x	x	0.05		0		0		500			Old interface tension water in water?? CAMEO: Missing CHRIS Code
7782414	Fluorine	x	0	0 ^f	0	0 ^f	0	0 ^g Reacts ^f	500			Use Serida solubility (Cameo - Reacts in water)
7782447	Oxygen	x	0.05	0 ^f	0	0 ^f	0	0 ^f 1E-05 ^g	500			
7782505	Chlorine	x	0.05	0 ^f	0	0 ^f	6.50E-03	6.50E-03 ^f 7E-03 ^g	500			Solubility at 25C.
CAS	Material name	NL	Interfacial tension (N/m)	Heat of solution (J/kg)	Solubility in water (kg/kg)	Heat transfer coefficient (W/m²K)	Comments					
7783064	Hydrogen sulfide	x	0.05	N/Avail ^f	0	0 ^f	0	0 ^f 6E-03 ^g	500			
7784421	Arsine		0		0		0	0 7E-04 ^g	500			CAMEO: Missing CHRIS Code; ; soluble chemical, uncertainty on pool temperature estimation; original solubility value maintained

^x For water, usage of the current properties for pools on water may make little sense. We have however not modified these data, but we would normally not expect that the user would attempt to model a 'water' pool on water. However it may become relevant for rainout of mixtures on water, which contain a fraction of water. This may be considered as part of future work.

7803512	Phosphine		0		0		0	0 2.6E-01 ^g	500		CAMEO: Missing CHRIS Code; ; soluble chemical, uncertainty on pool temperature estimation; original solubility value maintained
10102439	Nitric oxide	x	0	0 ^f	0	5.98E+05 ^f	0	6E-05 ^g Reacts ^f	500		Use Serida solubility (Cameo - Reacts in water)
10102440	Nitrogen dioxide	x	0		0		0		500		CAMEO: Missing CHRIS Code
132259100	Air	x	0.05		0		0		500		CAMEO: Missing CHRIS Code

Table 3. Material properties for pools on water

^a Values taken from International Critical Tables (1928)⁵

^b Values taken from Demond and Lindner (1993)⁴

^c Values taken from Dodge et al. (1983)⁸

^d Values taken from IUPAC-NIST Solubility database (2006)⁹

^e Values taken from Woodward and Pitblado (2010)¹⁴

^f Values taken from Cameo (2011)⁷

^g Values taken from SERIDA (1998)¹⁰

4.3 Pool fire flammable material properties

The pool fire data are as follows (see POLF theory manual for details):

- Flame type: 0 =luminous, 1 = smoky, 2 = general
- Maximum Surface Emissive Power (kW/m²), E_{max}.
- Emissive power scale length (m), L_s
- Pool fire burn rate length (m), L_b
- Pool fire maximum burn rate (kg/m²/s), M_{max} (if defined)

The correctness of the above data was reviewed against available data from the literature (Lees^{xvi}, the TNO Yellow Book^{xvii}, Rew et al.^{xviii}, and the SFPE Handbook of fire Protection Engineering^{xix, xxi}).

4.3.1 Burn rate

For a pool fire on land the maximum burn rate (kg/m²/s) is taken from the material database if defined. Otherwise it is calculated as:

$$m_{\max} = 1.27 * 10^{-6} \rho_L \frac{\Delta H_c}{\Delta H_v^*}, \text{ general (flame type = 2)} \quad (8)$$

$$m_{\max} = 10^{-3} \frac{\Delta H_c}{\Delta H_v^*}, \quad \text{hydrocarbon (flame type = 0 or 1)}$$

With the modified heat of evaporation given by

$$\Delta H_v^* = \Delta H_v + C_{pL}(T_b) \max\{0, T_b - T_a\} \quad (9)$$

The general formula in Equation (2) is derived by multiplying the burning velocity y_{\max} (m/s) given by Equation (3) in Mudan with the liquid density ρ_L (kg/m³). The second formula in Equation (2) follows from the general formula by using the typical density $\rho_L = 787$ kg/m³. It is quoted by Mudan^{xxi} that the latter formula covers a wide range of hydrocarbon fuels, including liquefied gases (LNG and LPG).

For a pool fire on water the burn rate is multiplied with a factor of 2.5, if the normal boiling temperature is less than the ambient temperature. This is because considerable heat transfer takes places between the large body of water and the pool of liquefied gas. The factor of 2.5 is in line with Mudan and Croce^{xxi}, who quote a factor of nearly three for LNG and two for LPG.

Fuel	Rew et al. ^{xviii}		Babrouskas ^{xix}	
	m_{\max} [kg/m ² s]	L_b^{-1} [m ⁻¹]	m_{\max} [kg/m ² s]	L_b^{-1} [m ⁻¹]
Acetone	0.038	2.238	0.041	1.9
Benzene	0.085	2.700	0.085	2.7
Benzine			0.048	3.6
Butane	0.110	0.852	0.078	2.7
Crude Oil	0.051	1.301	0.0022 - 0.045	2.8
Diesel	0.054	1.301		
Diethyl ether			0.085	0.7
Dioxane (C ₄ H ₈ O ₂)			0.018	5.4
Ethane	0.141	0.136		
Ethanol	0.020			
Fuel Oil, heavy	0.034	1.670	0.035	1.7
Gasoline/Petrol	0.067	1.480	0.055	2.1
Heptane	0.081	1.394	0.101	1.1
Hexane	0.075	1.394	0.074	1.9
Hydrogen (Liquefied)	0.161	6.741	0.017	6.1

<i>JP4</i>	0.056	1.962	0.051	3.6
<i>JP5</i>	0.063	1.296	0.054	1.6
<i>Kerosene</i>	0.063	1.296	0.039	3.5
<i>LEG</i>	0.140			
<i>LNG/methane</i>	0.141	0.136	0.078	1.1
<i>LNG/methane (water)</i>	0.282			
<i>LPG/propane</i>	0.118	0.5	0.099	1.4
<i>LPG/propane (water)</i>	0.256			
<i>Methanol</i>	0.020			
<i>Naptha/pentane</i>	0.095			
<i>Octane</i>	0.081	1.394		
<i>Polymethylmethacrylate</i>			0.020	3.3
<i>Toluene</i>	0.066	3.370		
<i>Transformer oil</i>			0.039	0.7
<i>Xylene</i>	0.090	1.400	0.09	1.4

Table 4. Fuel data for maximum burn rate and inverse of characteristic burn length

The actual burn rate is set as

$$m = m_{\max} \left[1 - e^{-\frac{D}{L_b}} \right] \quad (10)$$

Table 4 contains a list of published data for pool fire maximum burn rate (i.e. m_{\max}) and the inverse of the pool fire characteristic burn length (i.e. L_b^{-1}) for a number of flammable compounds. These data are taken from Babrouskas (SFPE Handbook)^{xx} and Rew et al.^{xviii}.

The maximum burn rate length L_b for methane, ethane, propane equals 7.25m, 6.41m, 2m and these are in line with the above data for Rew et al.

For the following materials modified values are proposed for 6.6 in line with most conservative estimates from the literature:

- butane: change LB from 0.1 m to 0.35 m (Rew quotes 1.17m, SFPE handbook 0.37 m)
- pentane: change LB from 5.0m to 0.1m (conservative value, since no data found from the literature)
- hexane: change LB from 5.0m to 0.5m (Rew quotes 0.72m, SFPE handbook 0.53m)
- heptane: change LB from 10.0m to 0.7m (Rew quotes 0.72m, SFPE handbook 0.9m)
- octane: change LB from 10.0m to 0.7m (Rew quotes 0.72m, no value in SFPE handbook)
- xylene: change LB from 0.1m to 0.7 m (both Rew and SFPE quote 0.7m)

For all other chemicals the value is either 0.1m (luminous or smoke fires) or 0 (general fires), which is confirmed to be a conservative value from Table 4.

Pritchard and Binding^{xx} refer to validation for hydrocarbon pool fires. Their proposed values together with ours are included in the table below. Note that our values are virtually identical for both m_{\max} and L_b .

Fuel	m_{\max} (PB) (kg/m ² /s)	L_b (PB) (m)	E_{\max} (PB) (kW/m ²)	L_s (PB) (m)	m_{\max} (6.51) (kg/m ² /s)	L_b (6.51) (m)	E_{\max} (6.51) (kW/m ²)	L_s (6.51) (m)
LNG	0.14	6.41	265	6.71	0.141	7.25	220	6.75
Ethane	0.14	6.41	250	0	0.14	6.41	170	2.75
Propane	0.12	2	250	0	0.12	2	160	2.75
Butane	0.12	0	225	0	0.12	0.1	170	2.75

Table 5. Comparison of pool fire data by PHAST6.51 and Pritchard and Binding (PB)

The maximum burn rate calculation is shown in Table 6 for all flammable materials available in the DNV database, along with data from the literature. It is seen that the maximum burn rate is currently specified for methane, ethane, propane and butane only, and, these data are in line with the above data from the SFPE handbook (Babrouskas). For all other chemicals the maximum burn rate is calculated according to Equation (8). Overall the data are in line with the literature and/or they are conservative.

For hydrogen the general formula produces a maximum burn rate of 0.024 kg/m²/s, which is considerably smaller than the values of 0.161-0.169 kg/m²/s from Lees/YB and Rew, but larger than 0.017 kg/m²/s from the SFPE Handbook.

BURN RATE CALCULATION												
NAME OF CHEMICAL	SAFETI maximum burn rate calculation						Burn rate (literature)					
	heat of combustion (kJ/kmol)	molecular weight (kg/kmol)	heat of evaporation (kJ/kmol)	6.51 LB (m)	6.6 LB (m)	Proposed 6.6 maximum burn rate (kg/m2/s)	Lees/ Yellow Bk handbook			SFPE		
							maximum burn rate (kg/m2/s)	Rew max. burn rate (kg/m2/s)	max. burn rate (kg/m2/s)	Rew LB (m)	SFPE LB (m)	
METHANE	802620	16.0428	na	7.25	7.25	0.141	0.078	0.141	0.078	7.35	0.91	
ETHANE	1428640	30.0696	na	6.41	6.41	0.14		0.141		7.35		
PROPANE	2043110	44.0965	na	2.00	2.00	0.12	0.099	0.118	0.099	2.00	0.71	
N-BUTANE	2657320	58.1234	na	0.10	0.35	0.12	0.078	0.11	0.078	1.17	0.37	
METHANOL	638200	32.0422	36574	0.10	0.00	0.017	0.017 / 0.015	0.02				
ETHANOL	1235000	46.069	38935	0.10	0.00	0.030	0.015	0.02				
ISOPROPANOL	1830000	60.0959	39384	0.10	0.00	0.043						
ETHYLENE	1323000	28.0538	13489	0.10	0.00	0.071						
PROPYLENE	1925700	42.0806	18433	0.10	0.00	0.081						
1-BUTENE	2540800	56.1075	22131	0.10	0.00	0.091						
1,3-BUTADIENE	2409000	54.0916	22533	0.10	0.00	0.088						
ETHYLENE OXIDE	1218000	44.0532	25793	0.10	0.00	0.053						
1,2-PROPYLENE OXIDE	1785500	58.08	27532	0.10	0.00	0.067						
ACETONE	1659000	58.08	29557	0.10	0.00	0.053	0.041	0.038	0.041	0.45	0.53	
METHYLAMINE	975080	31.0574	26085	0.10	0.00	0.033						
DIMETHYLAMINE	1614600	45.0843	26613	0.10	0.00	0.052						
TRIMETHYLAMINE	2244900	59.1112	23086	0.10	0.00	0.081						
DICHLOROMETHANE	513880	84.9323	28369	0.10	0.00	0.030						
ACRYLAMIDE	1573100	71.0788	53731	0.10	0.00	0.030						
ACRYLONITRILE	1690000	53.0636	31061	0.10	0.00	0.051						
ACROLEIN	1546800	56.0642	28612	0.10	0.00	0.055						
METHYL ISOCYANATE	1060000	57.052	29186	0.10	0.00	0.042						
VINYL CHLORIDE	1178000	62.4985	22564	0.10	0.00	0.064						
HYDROGEN	241820	2.01588	897	0.10	0.00	0.024	0.169	0.161	0.017	0.15	0.16	
HYDROGEN SULFIDE	518000	34.0819	18738	0.10	0.00	0.033						
HYDROGEN CYANIDE	623290	27.0257	26926	0.10	0.00	0.020						
HYDRAZINE	534200	32.0452	40837	0.10	0.00	0.015						
AMMONIA	316830	17.0306	23328	0.10	0.00	0.012						
CARBON MONOXIDE	283000	28.0104	5998	0.10	0.00	0.047						
CARBON DISULFIDE	1076900	76.143	27009	0.10	0.00	0.062						
ETHANETHIOL	1736600	62.1356	26803	0.10	0.00	0.068						
ACETALDEHYDE	1104500	44.0532	25731	0.10	0.00	0.043						
ACETONITRILE	1190430	41.0526	30196	0.10	0.00	0.036						
FORMIC ACID	211500	46.0257	22062	0.10	0.00	0.014						
CHLOROMETHANE	675380	50.4875	21562	0.10	0.00	0.040						
1-CHLORO-2,3-EPOXYPR	1635000	92.5248	35669	0.10	0.00	0.061						
CYCLO-HEXANE	3656000	84.1613	29909	0.10	0.00	0.112						
METHYLACRYLATE	1930300	86.0904	32142	0.10	0.00	0.067						
METHYLFORMATE	892400	60.0526	28171	0.10	0.00	0.039						
1-BUTANETHIOL	2955400	90.1894	32181	0.10	0.00	0.089						
ETHYLFORMATE	1506960	74.0794	29985	0.10	0.00	0.056						
DIETHYL ETHER	2503500	74.1228	26777	0.10	0.00	0.083	0.085		0.085		1.43	
TETRAHYDROTHIOPHEN	2765490	88.1735	34617	0.10	0.00	0.092						
1,2-DIAMINOETHANE	1691000	60.099	39705	0.10	0.00	0.044						
ETHYLETHANAMINE	2800300	73.1381	29064	0.10	0.00	0.082						
ALLYL ALCOHOL	1731900	58.08	39950	0.10	0.00	0.043						
FORMALDEHYDE	526800	30.0263	23065	0.00	0.00	0.024						
TETRAETHYL LEAD	5899500	323.447	41489	0.00	0.00	0.251						
ETHYLENEIMINE	1481000	43.0684	31752	0.00	0.00	0.047						
3-CHLORO-1-PROPENE	1750000	76.5254	29073	0.00	0.00	0.069						
ACETYLENE	1257000	26.0379	16503	0.00	0.00	0.060						
METHYLMERCAPTAN	1151700	48.1088	24586	0.00	0.00	0.053						
PHOSPHINE	1260000	33.9976	14581	0.00	0.00	0.082						
VINYL ACETATE	1950000	86.0904	31571	0.10	0.00	0.062						
N-PENTANE	3244940	72.1503	25815	5.00	1.0	0.126						
N-HEXANE	3855100	86.1772	28786	5.00	0.50	0.134	0.074	0.075	0.074	0.72	0.53	
N-HEPTANE	4464730	100.204	31837	10.0	0.7	0.140	0.101	0.081	0.101	0.72	0.9	
N-OCTANE	5074150	114.231	34667	10.0	0.7	0.146		0.081		0.72		
N-BUTANOL	2456010	74.1228	43083	0.10	0.00	0.057						
ISOBUTANOL	2449000	74.1228	41857	0.10	0.00	0.059						
TRIETHYLAMINE	4040500	101.192	30855	0.10	0.10	0.131						
METHYL BROMIDE	705420	94.9388	24175	0.10	0.00	0.029						
N-BUTYL ACRYLATE	3770000	128.171	39106	0.10	0.10	0.096						
PHENOL	2921000	94.113	46477	0.10	0.10	0.063						
BENZENE	3136000	78.1136	30804	0.10	0.10	0.102	0.085	0.085	0.085		0.07	
TOLUENE	3734000	92.1405	33363	0.10	0.10	0.112		0.066		0.30		
M-XYLENE	4331800	106.167	36203	0.10	0.70	0.120	0.09	0.09	0.09	0.71	0.71	
STYRENE	4219000	104.152	37072	0.10	0.10	0.114						
BENZYL CHLORIDE	3570430	126.585	40578	0.10	0.10	0.088						

Meaning of colours:
 data directly from SAFETI-NL property database
 data derived in SAFETI-NL by "calculate" material property
 calculated data by spreadsheet

Table 6. Comparison of literature against SAFETI maximum burn rate calculation

4.3.2 Surface emissive power

The surface emissive power of the flame (W/m^2) is set as

$$\begin{aligned}
 E_f &= E_m \left[1 - e^{-\frac{D}{L_s}} \right], && \text{luminous fires (flame type = 0)} \\
 &= E_m \left[e^{-\frac{D}{L_s}} \right] + E_s \left[1 - e^{-\frac{D}{L_s}} \right] && \text{sooty fires (flame type = 1)} \\
 &= \frac{\chi_R m \Delta H_c}{\left[1 + 4 \frac{H}{D} \right]}, && \text{'general' fire (flame type = 2)}
 \end{aligned} \tag{11}$$

where E_m is the maximum emissive power for luminous fires, E_s the smoke emissive power, and L_s a characteristic length for decay of E_f . If experimental data are not available, the above equation for a 'general fire' is used. This equation is derived from the definition of the radiative fraction χ_R ; χ_R is the ratio of the total energy radiated (from the fire surface) to the total energy released (from the pool area):

$$\begin{aligned}
 \chi_R &= \frac{\text{radiated energy}}{\text{released energy}} = \frac{(\text{flame surface}) * (\text{surface emissive power})}{(\text{burn rate}) * (\text{pool area}) * (\text{heat of combustion})} \\
 &= \frac{\left[\frac{1}{4} \pi D^2 + \pi D H \right] E_f}{m \left[\frac{1}{4} \pi D^2 \right] \Delta H_c} = \frac{\left[1 + 4 \frac{H}{D} \right] E_f}{m \Delta H_c}
 \end{aligned} \tag{12}$$

Table 7 includes results for SAFETI calculations of the surface emissive power, including a comparison against data from the Yellow Book. Results are included using both the former 6.51 properties, as well as the new proposed 6.6 SAFETI properties. Note that the Yellow Book data appear to be based on the above "general formula" (flame type = 2).

SAFETI 6.51 applies $L_s = 6.75$ m for methane [which is in line with the experimental value quoted by Pritchard and Binding; see Table 5] and $L_s = 2.75$ m for all other luminous flammable chemicals. It applies $E_m = 220$ kW/m² for methane, 160 kW/m² for propane, and the value of 170 kW/m² for all other chemicals. According to the Yellow Book the radiative fraction is typically in the range 0.15-0.4. It is seen that the calculated SEP is typically conservative except for perhaps hydrogen (always) and methane/ethane/propane/butane (for small diameters). Moreover for several chemicals the radiative fraction is larger than one, which is unrealistic. Therefore for several chemicals the predicted SEP values appear to be larger than most of those in the Yellow Book.

To overcome the above problem, all chemicals modelled 'luminous' in SAFETI 6.51 (except for methane, ethane, propane, butane), are now proposed to be modelled in the new SAFETI as general with $L_b=0$ (i.e. always apply maximum burn rate). Furthermore the radiation fraction of $\chi_R=0.4$ is now applied instead of the former values of $\chi_R=0.35$. It is seen from Table 7 that this leads to considerably more realistic predictions.

For methane, ethane, propane, butane, the SEP at diameter $D=1$ appears to be rather small. However in the POLF validation, the radiation predictions for methane appeared to be accurate (e.g. for experiments by Johnson where small pool fire diameters were included). As a result at this stage no changes are proposed. However, following further data and investigation these data may be considered to be updated.

Smoky fires

The adopted formula in equation (11) for smoky fires agrees with formula (6.19) in the Yellow Book^{xvii} and Mudan and Croce^{xxi}, and in line with these references it applies the maximum emissive power $E_m = 140$ kW/m², the smoke emissive power $E_s = 20$ kW/m², and the emissive power scale length $L_s=8.33$ m (corresponding to $L_s^{-1}=0.12m^{-1}$)¹¹. Mudan derived

¹¹ For 6.6 it is proposed to set $L_s=8.33$ also for Xylene to be in line with all other chemicals (6.51 value =2.75m).

this correlation using data from gasoline, kerosene and JP-5. This formula corresponds to a reduced SEP for larger pool fire diameters. This is in conflict with Table 6.8 in the Yellow Book, where the SEP increases with large pool fire diameters for hexane, benzene, vinyl acetate and methyl bromide. However the latter Table is derived using the general formula for SEP (with 0.35 as radiative fraction), and this seems not to be correct for smoky fires.

Mudan quotes that for large hydrocarbon fires with a carbon-to-hydrogen ratio greater than about 0.3, a substantial part of the fire is obscured by a thick black smoke on the outer periphery. Using this criterion e.g. butane should be modelled as a smoky fire. It is however proposed for 6.6 to maintain modelling butane as a luminous fire, since quoted maximum value of SEP by Pritchard and Binding is 225 kW/m² while the smoky fire criterion would give a maximum of 140 kW/m² only.

For 6.6 it is proposed to model a fire as a smoky fire only if they have five or more hydrocarbon atoms. Thus vinylacetate, n-butanol, isobutanol and methylbromide are proposed to be modelled as a “general” fire instead of a “smoky” fire. Note that this also avoids unrealistic high radiative fraction for these chemicals.

Finally it is noted that the maximum surface emissive power of $E_m = 140 \text{ kW/m}^2$ and the smoke emissive power $E_s = 20 \text{ kW/m}^2$ may only be applicable to smoky hydrocarbon fires without an additional functional group. For other chemicals (such as e.g. benzylchloride) other values may be appropriate.

SURFACE EMISSIVE POWER (SEP) CALCULATION													
NAME OF CHEMICAL	6.51 SEP Calculation			Proposed 6.6 SEP calculation				SEP data (literature)					
	Thomas flame height at D=30 (m)	type of fire	max. SEP (kW/m ²)	radiative fraction at D=30 (-)	type of fire	6.6 LS (m)	SEP at D=1 (kW/m ²)	SEP at D=10 (kW/m ²)	SEP at D=1,10 YB Table 6.7-6.8(6.9) (kW/m ²)	Pritch.& Binding max. SEP (kW/m ²)	Mudan SEP (kW/m ²)	radiative fraction (Yellow Book) (-)	radiative fraction (Lees) (-)
METHANE	59.4	luminous	220	0.278	luminous	6.75	30.3	170.0	100-193	265	150-220 (D=20)	0.15-0.34	0.16-0.23
ETHANE	59.1	luminous	170	0.227	luminous	2.75	51.8	165.5	96-185	250			
PROPANE	53.8	luminous	160	0.235	luminous	2.75	48.8	155.8	98-188	250			0.26
N-BUTANE	53.8	luminous	170	0.253	luminous	2.75	51.8	165.5	86-165	225		0.199-0.269	0.27-0.30
METHANOL	16.6	luminous	170	1.572	general	unset	18.7	33.1	19-34 (70)			0.162-0.177	0.17-0.20
ETHANOL	23.9	luminous	170	0.837	general	unset	33.0	60.2					0.2
ISOPROPANOL	30.2	luminous	170	0.603	general	unset	44.1	82.0					
ETHYLENE	47.6	luminous	170	0.270	general	unset	85.2	161.5	90-173		130 (D=2.5)		
PROPYLENE	49.4	luminous	170	0.270	general	unset	87.6	166.7	92-178				
1-BUTENE	52.4	luminous	170	0.261	general	unset	91.2	174.2					
1,3-BUTADIENE	50.1	luminous	170	0.274	general	unset	88.5	168.9	87-168				
ETHYLENE OXIDE	30.5	luminous	170	0.659	general	unset	44.1	82.8	37-68				
1,2-PROPYLENE OXIDE	37.0	luminous	170	0.506	general	unset	54.2	102.5					
ACETONE	33.8	luminous	170	0.585	general	unset	45.7	85.7	42-79				
METHYLAMINE	26.4	luminous	170	0.655	general	unset	40.6	74.5					
DIMETHYLAMINE	35.5	luminous	170	0.449	general	unset	56.5	105.7	59-112				
TRIMETHYLAMINE	47.3	luminous	170	0.337	general	unset	72.6	138.3					
DICHLOROMETHANE	17.0	luminous	170	5.063	general	unset	7.5	13.6					
ACRYLAMIDE	22.8	luminous	170	1.058	general	unset	27.3	49.8					
ACRYLONITRILE	33.2	luminous	170	0.533	general	unset	49.9	93.5	36-67				
ACROLEIN	33.1	luminous	170	0.617	general	unset	44.8	84.1					
METHYL ISOCYANATE	26.0	luminous	170	1.124	general	unset	26.8	49.8					
VINYL CHLORIDE	32.4	luminous	170	0.919	general	unset	32.6	61.6	26-46				
HYDROGEN	88.2	luminous	170	0.067	general	unset	134.6	242.9					
HYDROGEN SULFIDE	22.0	luminous	170	1.590	general	unset	19.7	36.3	18-32				
HYDROGEN CYANIDE	19.7	luminous	170	1.156	general	unset	23.7	42.2					
HYDRAZINE	13.9	luminous	170	2.227	general	unset	15.1	26.5					
AMMONIA	14.2	luminous	170	1.951	general	unset	14.8	25.5	17-30				
CARBON MONOXIDE	30.4	luminous	170	1.804	general	unset	15.3	28.6	13-24				
CARBON DISULFIDE	27.5	luminous	170	1.406	general	unset	24.1	45.5					
ETHANETHIOL	36.9	luminous	na	na	general	unset	49.5	93.6					
ACETALDEHYDE	28.7	luminous	na	na	general	unset	36.3	67.4	35-64				
ACETONITRILE	27.3	luminous	na	na	general	unset	38.8	71.6	34-62				
FORMIC ACID	11.5	luminous	na	na	general	unset	3.9	6.8					
CHLOROMETHANE	23.7	luminous	na	na	general	unset	18.9	34.9					
1-CHLORO-2,3-EPOXYPR	29.9	luminous	na	na	general	unset	30.0	56.6					
CYCLO-HEXANE	54.4	luminous	na	na	general	unset	95.3	183.2					
METHYLACRYLATE	35.3	luminous	na	na	general	unset	39.7	75.1					
METHYLFORMATE	23.9	luminous	na	na	general	unset	20.6	38.1	18-33				
1-BUTANETHIOL	45.7	luminous	na	na	general	unset	65.3	124.8					
ETHYLFORMATE	31.6	luminous	na	na	general	unset	33.2	62.4	29-54				
DIETHYL ETHER	46.2	luminous	na	na	general	unset	65.2	124.3					
TETRAHYDROTHIOPHEN	42.0	luminous	na	na	general	unset	63.3	120.9					
1,2-DIAMINOETHANE	28.6	luminous	na	na	general	unset	41.2	76.7					
ETHYLETHANAMINE	47.1	luminous	na	na	general	unset	73.7	140.4	71-135				
ALLYL ALCOHOL	28.9	luminous	na	na	general	unset	43.2	80.2	37-68				
FORMALDEHYDE	20.0	general	na	0.35	general	unset	19.5	35.1					
TETRAETHYL LEAD	84.4	general	na	0.35	general	unset	55.9	109.4					
ETHYLENEIMINE	30.5	general	na	0.35	general	unset	52.2	97.4					
3-CHLORO-1-PROPENE	38.4	general	na	0.35	general	unset	40.9	77.4					
ACETYLENE	35.3	general	na	0.35	general	unset	81.3	153.2					
METHYLMERCAPTAN	32.6	general	na	0.35	general	unset	38.1	71.4					
PHOSPHINE	42.5	general	na	0.35	general	unset	71.1	135.5					
VINYL ACETATE	35.9	smoky	140	0.579	general	unset	38.6	72.8	32-59				
N-PENTANE	55.4	smoky	140	0.208	smoky	8.33	126.4	56.1	61		61 (D=1)		
N-HEXANE	57.5	smoky	140	0.203	smoky	8.33	126.4	56.1	87-166				0.2-0.4
N-HEPTANE	59.2	smoky	140	0.199	smoky	8.33	126.4	56.1					
N-OCTANE	60.7	smoky	140	0.196	smoky	8.33	126.4	56.1					
N-BUTANOL	34.2	smoky	140	0.412	general	unset	54.5	102.5					
ISOBUTANOL	34.7	smoky	140	0.408	general	unset	55.0	103.5					
TRIETHYLAMINE	56.8	smoky	140	0.229	smoky	8.33	126.4	56.1					
METHYL BROMIDE	22.7	smoky	140	2.601	general	unset	9.1	16.6	9-16				
N-BUTYL ACRYLATE	47.1	smoky	140	0.359	smoky	8.33	126.4	56.1					
PHENOL	36.3	smoky	140	0.419	smoky	8.33	126.4	56.1					
BENZENE	48.7	smoky	140	0.257	smoky	8.33	126.4	56.1	71-135		0.345-0.360	0.14-0.38	
TOLUENE	51.6	smoky	140	0.243	smoky	8.33	126.4	56.1					
M-XYLENE	53.7	smoky	140	0.234	smoky	8.33	126.4	56.1					
STYRENE	52.1	smoky	140	0.241	smoky	8.33	126.4	56.1					
BENZYL CHLORIDE	44.5	smoky	140	0.391	smoky	8.33	126.4	56.1					

Meaning of colours:
 data directly from SAFETI-NL property database
 data derived in SAFETI-NL by "calculate" material property
 calculated data by spreadsheet

Table 7. Comparison of literature against SAFETI surface emissive power calculation¹²

¹² Cyclohexane has been modified in Phast 3D to be smoky (D-4184)

4.3.3 Summary of changes between 6.51 and 6.6

1. Change all existing “luminous” fires to “general” (using $L_b=0$), except for methane, ethane, propane and butane.
2. Modify values in line with the literature for the maximum burn rate length L_b adopted in SAFETI for the following chemicals:
 - a. reduce values for the “smoky” chemicals pentane, heptane, octane and hexane
 - b. slight increase of values for butane and xylene
3. Use a radiative fraction χ_R of 0.40 instead of 0.35 for all general fires. Consider making this input parameter available to the user (rather than hard coded, with default value of 0.4).
4. Set $L_s=8.33$ also for xylene to be in line with all other smoky chemicals
5. Model vinylacetate, n-butanol, isobutanol and methylbromide as a “general” fire instead of a “smoky” fire, in order to avoid unrealistic high radiative fraction and also to satisfy the criterion that chemicals are only modelled as smoky if they have five or more carbon atoms).
6. Possibly further investigate the literature for additional references, e.g. on
 - a. SEP’s for smoky fires (with increasing diameter), including the validity of the usage of the maximum surface emissive power of 140 kW/m^2 and the smoke emissive power $E_s = 20 \text{ kW/m}^2$ for hydrocarbons containing an additional functional group (such as e.g. benzylchloride).
 - b. SEP for methane/ethane/propane/ethane. Particularly for smaller pool diameter we have currently poor agreement against reviewed literature. Further data may assist in a final recommendation for these chemicals.
 - c. Burn rate for hydrogen. There is inconsistency of data in the literature.

4.4 Laminar Burning Velocity

Lees^{xvi} and CCPS^{xxii} give experimental values of laminar burning velocity for a range of fuels. These are:

<u>Material</u>	<u>Laminar Burning Velocity (m/s) (CCPS)</u>	<u>Laminar Burning Velocity (m/s) (Lees)</u>
Methane	0.448	0.45
Ethane	0.476	-
Propane	0.464	0.52
Ethylene	0.735	0.83
Propylene	0.512	-
Hydrogen	3.25	-
Acetone	0.444	-
Diethyl ether	0.486	-
Acetylene	1.55	-
Cyclo-hexane	-	0.52

Table 8. Experimental laminar burning velocities

A ‘default’ value of 0.45 m/s was suggested by Mercx et al. (1998)^{xxiii}. However Baker et al. (1996)^{xxiv} observed the laminar burning velocity of a fuel is closely related to its reactivity. Based on the three reactivity levels the following has been adopted in Phast:

- **High reactivities.** There are only five fuels in this category: Hydrogen, Acetylene, Ethylene, Ethylene oxide, and Propylene oxide. The last two have no available experimental data and have been set at the value suggested by Lees for ethylene (0.83 m/s)¹³.
- **Low reactivity.** Methane and carbon dioxide. Set as the same as the reactivity for methane from Lees (0.45 m/s)

¹³ JUSTIFY. Ethylene and propane in Phast 7.2 have values of 0.735 and 0.464 respectively, corresponding to the older CCPS data.
Summary | Property Database|

- **Medium reactivities.** All other fuels fall into this category, including propane and cyclohexane which are assigned an LBV of 0.52 m/s by Lees. Based on this, all other medium reactivity fuels in Phast without specific experimental data will be given a value of 0.52.

4.5 Dangerous Dose and Toxic Probit A, B and N

Toxic probit coefficients have been reviewed for PHAST 6.4 by Phil Crossthwaite and Mike Harper, with a view to bringing the PHAST values up-to-date. The Purple Book values are used if available, after first being modified for units conversion (see below). For materials where these are not given, the coefficients are derived from the HSE SLOT (Significant Level of Toxicity) and SLOD (Significant Likelihood of Death)³.

4.5.1 Conversion of Purple Book Probit Coefficients

The Purple Book probit coefficients (A,B,N) are derived assuming concentration C in mg/m³ and exposure time t_{exp} in minutes:

$$P = A + B \ln [t_{\text{exp}} C^N] \quad (13)$$

In PHAST / SAFETI coefficients are used assuming concentration C' in ppm and time in minutes. Thus a conversion is necessary:

$$C' = C \times f \quad (14)$$

Where f is 1 mg/m³ air expressed in ppm of a substance X in air:

$$\begin{aligned} f &= 1 \times 10^6 \times \frac{\text{moles of } X \text{ in } 1\text{mg}}{\text{moles of air in } 1\text{m}^3} \\ &= 1 \times 10^6 \times \frac{1 \times 10^{-6} \text{ kg} / M_w(X)}{\rho_a / M_w(\text{air})} \end{aligned} \quad (15)$$

M_w = molecular weight (kg/kmol)
ρ_a = density of air

The density of air, ρ_a, is calculated to be 1.25375 kg/m³ at 282 K, 101510 Pa¹⁴. We can thus write:

$$P = A + B \ln \left[t_{\text{exp}} \left(\frac{C'}{f} \right)^N \right] \quad (16)$$

Rearranging gives:

$$P = A + BN \ln \left(\frac{1}{f} \right) + B \ln [t_{\text{exp}} C'^N] \quad (17)$$

Thus to convert the Purple Book probit coefficients for use in PHAST / SAFETI we must replace A by A' where:

$$A' = A + BN \ln \left(\frac{1}{f} \right) \quad (18)$$

4.5.2 Derivation of Probit Coefficients from DTLs

The HSE provides data on the dangerous toxic load (DTL) associated with specified levels of toxicity corresponding to ~ 1% (SLOT) and 50% (SLOD) mortality. It also provides the N coefficient. These are based on concentrations in ppm and exposure time in minutes, so no units conversion is required for their use in PHAST. They can be used to derive probit coefficients. We know by definition of SLOT and SLOD that:

¹⁴ These are the conditions appropriate for Holland from the TNO books. Note that N, A and B expressed using ppm will therefore be very weakly dependent on T and P. However, this is unlikely to significantly affect consequence or risk results.

$$\begin{aligned}P(p_d = 0.01) &= A + B \ln[SLOT] \\P(p_d = 0.5) &= A + B \ln[SLOD]\end{aligned}\tag{19}$$

where $P(p_d = 0.01)$ is the probit number corresponding to 1% lethality (= 2.674) and $P(p_d = 0.5)$ is the probit number corresponding to 50% lethality (= 5.0).

The A and B coefficients can easily be determined by solving these equations simultaneously.

4.5.3 Data and Source for Specific Materials

The toxic data for the materials in the material database are given by Table 9.

Substance	Purple book or HSE data	A	B	N	HSE		B	A
					SLOT	SLOD		
1,2-Propylene oxide	HSE	-15.688	1.692	1.000	5.16E+04	2.04E+05	1.692	-15.688
Acrolein	PB	-3.21	1	1	420	1680		
Acrylamide	HSE	-17.084	1.678	1.000	1.30E+05	5.20E+05	1.678	-17.084
Acrylonitrile	PB	-7.52	1	1.3	9600	2.52E+04	2.410	-19.427
Ammonia	PB	-16.21	1	2	3.78E+08	1.03E+09	2.320	-43.156
Benzene		-109.8	5.3	2				
Benzyl chloride	HSE	-10.277	1.678	1.000	2250	9000	1.678	-10.277
Boron trifluoride	HSE	-10.018	1.638	1.000	2.32E+03	9.60E+03	1.638	-10.018
Carbon disulfide	HSE	-16.575	1.678	1.000	9.60E+04	3.84E+05	1.678	-16.575
Carbon dioxide	HSE				1.50E+40	1.50E+41	1.010	-90.778
Carbon monoxide	PB	-7.21	1	1	40125	5.70E+04	6.626	-67.560
Chlorine	PB	-4.81	0.5	2.75	1.08E+05	4.84E+05	1.551	-15.299
Ethylene oxide	PB	-6.15	1	1	4.68E+04	1.87E+05	1.678	-15.370
Hydrazine	HSE	-13.452	1.676	1.000	1.51E+04	6.05E+04	1.676	-13.452
Hydrogen chloride	PB	-15.69	1.69	1.18	2.37E+04	7.65E+04	1.985	-17.321
Hydrogen cyanide	PB	-5.80	1.08	1.85	1.92E+05	4.32E+05	2.868	-32.221
Hydrogen fluoride	PB	-8.62	1	1.5	1.20E+04	2.10E+04	4.157	-36.367
Hydrogen peroxide	HSE	-16.390	1.678	1.000	8.60E+04	3.44E+05	1.678	-16.390
Hydrogen sulfide	PB	-8.53	0.44	4.55	2.00E+12	1.50E+13	1.154	-30.024
Methanol	HSE	-23.618	1.934	1.000	8.02E+05	2.67E+06	1.934	-23.618
Methyl bromide	PB	-5.74	1	1.1	3.00E+04	4.80E+04	4.949	-48.345
Methyl isocyanate	PB	-0.57	1	0.7	750	1680	2.884	-16.420
Nitric oxide	HSE	-150.838	15.43	1.000	2.09E+04	2.43E+04	15.432	-150.838
Nitrogen dioxide	PB	-16.05	1	3.7	9.60E+04	6.24E+05	1.243	-11.582
Phenol	HSE	-13.460	1.678	1.000	1.50E+04	6.00E+04	1.678	-13.460
Phosgene	PB	-7.69	2	1	108	348	1.988	-6.634
Sulphur dioxide	PB	-16.75	1	2.4	4.66E+06	7.45E+07	0.839	-10.207
Sulphur trioxide	HSE	-5.27	0.839	2	1.30E+04	2.08E+05	0.839	-5.273
Toluene		-6.794	0.408	2.5				
Vinyl chloride	HSE	-22.502	1.674	1.000	3.39E+06	1.36E+07	1.674	-22.502
Additional SafetiNL								
Allyl alcohol	PB	-9.86	1	2	6.30E+03	2.52E+04	1.678	-12.005
Arsine	PB	-8.77	1.61	1.24	3.71E+03	5.90E+04	0.840	-4.233
Bromine	PB	-8.53	1	2	2.50E+05	8.67E+05	1.870	-20.574
Ethyleneimine	PB	-10.35	1.77	1.13	1.16E+03	8.25E+03	1.183	-5.669
Fluorine	HSE	-19.091	1.694	2.000	3.80E+05	1.50E+06	1.694	-19.091
Formaldehyde	HSE	-54.572	6.619	1.000	5.70E+03	8.10E+03	6.619	-54.572
Phosphine	PB	-6.03	1	2	6.90E+03	1.08E+04	5.192	-43.218
Tetraethyl lead	PB	-4.52	1	2	1.52E+03	3.79E+03	2.546	-15.978
Methylmercaptan	PB	-16.33	2.05	0.98				

Table 9. Toxic probit data for PHAST system materials and their source

The toxic data a,b,N are based on units ppm for concentration and time t for minutes. These data are derived from either the Purple Book (PB) or the HSE. All SLOT and SLOD values are from the HSE. Unlike PHAST/SAFETI, SAFETI-NL does not apply the HSE data. These values have been updated for Phast 3D, with values taken from the HSE website as of June 2013. For benzene and toluene the values are taken from Lees (2005)^{xv}.

Values for nitrogen and carbon dioxide

The A, B & N values for nitrogen (N₂) and carbon dioxide (CO₂) have been updated as shown in the table below.

Component	A	B	N
Nitrogen (N ₂)	-65.7	1	5.2
Carbon Dioxide (CO ₂)	-90.778	1.01	8

The above values for nitrogen correspond to the probit function recommended in the "Reference Manual BEVI Risk Assessments" (New Purple Book) for inert gases such as nitrogen.

Using the method described in Section 4.5.2, the above values of A,B,N for carbon dioxide are derived from values recommended by the HSE for SLOT (1% probability of death), SLOD (50% probability of death) and N. The HSE SLOT DTL and SLOD DTL values for Carbon Dioxide are 1.5×10^{40} and 1.5×10^{41} respectively (units ppm for concentration c and minutes for time t), where the dangerous toxic load DTL is defined by

$$DTL = \int c^N dt$$

Please note that the above values are not used currently by default, since both nitrogen and carbon dioxide are flagged as inert materials. The material needs to be changed into a toxic material to enable toxicity calculations (and associated risk).

4.6 Materials Added for 8.4

A number of materials have been added to the standard set for convenience. These are materials that many customers have chosen to add themselves in the past. The non-DIPPR flammable properties are not researched for each individual material. Instead, the properties are set according to a 'similar' material already in the set. These are listed below in the Reference column.

Material name	Formula	CAS ID	Reference
NEOPENTANE	C5H12	463821	n-Pentane
3-METHYLHEPTANE	C8H18	589811	n-Nonane
n-DODECANE	C12H26	112403	n-Nonane
ISOBUTANE	C4H10	75285	n-Butane
ISOPENTANE	C5H12	78784	n-Pentane
n-DECANE	C10H22	124185	n-Nonane
n-HEPTADECANE	C17H36	629787	n-Nonane
n-UNDECANE	C11H24	1120214	n-Nonane
n-PENTADECANE	C15H32	629629	n-Nonane
n-NONYLBENZENE	C15H24	1081772	n-Nonane
n-HEXADECYLBENZENE	C22H38	1459092	n-Nonane
n-HEXATRIACONTANE	C36H74	630068	n-Nonane
n-TETRADECANE	C14H30	629594	n-Nonane
n-TRIDECANE	C13H28	629505	n-Nonane
1-Decene	C10H20	872059	n-Nonane
1-Octanol	C8H18O	111875	n-Nonane
4-Methyl-2-Pentanol	C6H14O	108112	Isobutanol
Boron Triflouride	BF3	7637072	Not applicable
Isobutene	C4H8	115117	1-Butene
n-Butanol	C4H10O	71363	Isobutanol
Sulphur Trioxide	SO3	7446119	Not applicable
2-Butanol	C4H10O	78922	Isobutanol

Table 10. Materials Added for Version 8.4

4.7 Materials added for Safeti-NL 8.5

This version of Safeti-NL includes an additional 33 standard materials in the main application, largely identifiable due to the suffix (TG) have been added. The properties for these materials have had various modifications to the flammable/toxic flag, probit values and NLIV values.

**In Safeti-NL 8.5 carbon dioxide has been renamed CARBON DIOXIDE (HSE_RR749 PROBITS) and set as 'toxic'. As suggested by the name, A B and N values are taken from the HSE report RR749.

These new materials are:



DNV

8.3										
8.5										
New material added to 8.5, not in 8.3										
Property difference in 8.5										

Version	Material	Flammable	Toxic fl _{CL}	WRW (ppm)	AGW (ppm)	LBW (ppm)	Toxic property A (ppm. min.)	Toxic property B	Toxic property N
8.5	ACETONITRILE (TG)	Both		19	676	1015	-16.65328413	1	2
8.3	ACROLEIN	Both		0.029	0.17	2.4	-3.21	1	1
8.5	ACROLEIN	Both		0.029	0.17	2.4	-3.21	1	1
8.5	ACROLEIN (TG)	Both		0.029	0.17	2.4	-8.021767546	1.85	1.08
8.3	ACRYLONITRILE	Both		14	105	192	-7.52	1	1.3
8.5	ACRYLONITRILE	Both		14	105	192	-7.52	1	1.3
8.5	ACRYLONITRILE (TG)	Both		14	105	192	-15.6307974	1.69	1.19
8.3	ALLYL ALCOHOL	Both		2	4	24	-9.855	1	2
8.5	ALLYL ALCOHOL	Both		2	4	24	-9.855	1	2
8.5	ALLYL ALCOHOL (TG)	Both		2	4	24	-15.26229477	2.56	0.78
8.3	AMMONIA	Toxic		29	272	1495	-16.21	1	2
8.5	AMMONIA	Toxic		29	272	1495	-16.21	1	2
8.5	AMMONIA (TG)	Toxic		29	272	1495	-17.11290772	0.99	2.02
8.3	BENZYL CHLORIDE	Toxic		13	5.5	26	0	0	0
8.5	BENZYL CHLORIDE	Toxic		13	5.5	26	0	0	0
8.5	BENZYL CHLORIDE (TG)	Toxic		13	5.5	26	-10.00116443	1	2
8.3	BROMINE	Toxic		0.48	2.8	36	-8.531	1	2
8.5	BROMINE	Toxic		0.48	2.8	36	-8.531	1	2
8.5	BROMINE (TG)	Toxic		0.48	2.8	36	-8.316494502	1.57	1.28
8.3	1,3-BUTADIENE	Flammable		642	6417	26524	0	0	0
8.5	1,3-BUTADIENE	Flammable		642	6417	26523	0	0	0
8.3	N-BUTANE	Flammable		6768	15926	51758	0	0	0
8.5	N-BUTANE	Flammable		6768	15925	51755	0	0	0
8.3	N-BUTYL ACRYLATE	Flammable		7.9	451	848	0	0	0
8.5	N-BUTYL ACRYLATE	Flammable		7.9	451	849	0	0	0
8.3	CARBON DISULFIDE	Flammable		16	192	578	0	0	0
8.5	CARBON DISULFIDE	Flammable		16	191	577	0	0	0
8.3	CARBON DIOXIDE	Inert		0	0	0	-90.778	1.01	8
8.5	CARBON DIOXIDE (HSE_RR749 probits)	Toxic		0	26290	52579	-90.778	1.01	8
8.3	CARBON MONOXIDE	Toxic		0	149	578	-7.21	1	1
8.5	CARBON MONOXIDE	Toxic		0	149	578	-7.21	1	1
8.5	CARBON MONOXIDE (TG)	Toxic		0	149	578	-15.5161019	1.11	1.81
8.3	CHLORINE	Toxic		0.49	2.7	36	-4.81	0.5	2.75
8.5	CHLORINE	Toxic		0.49	2.7	36	-4.81	0.5	2.75
8.5	CHLORINE (TG)	Toxic		0.49	2.7	36	-11.45223636	1.93	1.04
8.3	3-CHLORO-1-PROPENE	Flammable		2.7	333	968	0	0	0
8.5	3-CHLORO-1-PROPENE	Flammable		2.7	333	968	0	0	0
8.5	3-CHLORO-1-PROPENE (TG)	Both		2.7	333	968	-23.50533087	3.66	0.547
8.3	DIMETHYLAMINE	Flammable		10	82	313	0	0	0
8.5	DIMETHYLAMINE	Flammable		10	82	313	0	0	0
8.5	DIMETHYLAMINE (TG)	Both		10	82	313	-13.96645796	1.02	1.96
8.3	ETHYLENE OXIDE	Both		0	79	1156	-6.15	1	1
8.5	ETHYLENE OXIDE	Both		0	79	1156	-6.15	1	1
8.5	ETHYLENE OXIDE (TG)	Both		0	79	1156	-16.21219648	1	2
8.3	ETHYLENEIMINE	Both		0	5.4	14	-10.35	1.77	1.13
8.5	ETHYLENEIMINE	Both		0	5.4	15	-10.35	1.77	1.13
8.5	ETHYLENEIMINE (TG)	Both		0	5.4	15	-11.75530097	1.89	1.06
8.3	FLUORINE	Toxic		1.6	21	35	0	0	0
8.5	FLUORINE	Toxic		1.6	21	35	0	0	0
8.5	FLUORINE (TG)	Toxic		1.6	21	35	-6.936996566	1.1	1.82
8.3	FORMALDEHYDE	Toxic		1	13	68	0	0	0
8.5	FORMALDEHYDE	Toxic		1	13	68	0	0	0
8.5	FORMALDEHYDE (TG)	Toxic		1	13	68	-7.699366296	0.54	3.7
8.5	FORMIC ACID (TG)	Both		14	55	654	-13.4245926	1	2
8.3	HYDRAZINE	Both		0.09	22	65	0	0	0
8.5	HYDRAZINE	Both		0.09	22	65	0	0	0
8.5	HYDRAZINE (TG)	Both		0.09	22	65	-12.64869766	1	2
8.3	HYDROGEN CHLORIDE	Toxic		1.7	51	152	-35.6145	3.69	1
8.5	HYDROGEN CHLORIDE	Toxic		1.7	51	152	-35.6145	3.69	1
8.5	HYDROGEN CHLORIDE (TG)	Toxic		1.7	51	152	-16.19043707	1.46	1.37
8.3	HYDROGEN CYANIDE	Both		7.4	9	44	-9.42238	1	2.4
8.5	HYDROGEN CYANIDE	Both		7.4	9	44	-9.42238	1	2.4
8.5	HYDROGEN CYANIDE (TG)	Both		7.4	9	44	-9.059307235	1.17	1.71
8.3	HYDROGEN FLUORIDE	Toxic		1	34	59	-8.62	1	1.5
8.5	HYDROGEN FLUORIDE	Toxic		1	34	59	-8.62	1	1.5
8.5	HYDROGEN FLUORIDE (TG)	Toxic		1	34	59	-13.49012714	1.83	1.09
8.3	HYDROGEN SULFIDE	Both		1.9	31	57	-10.7603	1	1.9
8.5	HYDROGEN SULFIDE	Both		1.9	31	57	-10.7603	1	1.9
8.5	HYDROGEN SULFIDE (TG)	Both		1.9	31	57	-7.087249437	0.31	6.52
8.3	METHANOL	Both		644	13016	20248	0	0	0
8.5	METHANOL	Both		643	12999	20221	0	0	0
8.3	METHYL BROMIDE	Toxic		0	365	1267	-5.74	1	1.1
8.5	METHYL BROMIDE	Toxic		0	366	1267	-5.74	1	1.1
8.5	METHYL BROMIDE (TG)	Toxic		0	366	1267	-16.27539813	1.64	1.22
8.3	METHYL ISOCYANATE	Both		0	0.39	2.7	-0.57	1	0.7
8.5	METHYL ISOCYANATE	Both		0	0.39	2.7	-0.57	1	0.7
8.5	METHYL ISOCYANATE (TG)	Both		0	0.39	2.7	-8.495246697	1.98	1.01
8.3	METHYLAMINE	Flammable		14	89	491	0	0	0
8.5	METHYLAMINE	Flammable		14	89	492	0	0	0
8.5	METHYLAMINE (TG)	Both		14	89	492	-14.41105335	1.07	1.87
8.3	METHYL MERCAPTAN	Both		1.9	27	82	-16.33	2.05	0.98
8.5	METHYL MERCAPTAN	Both		1.9	27	82	-16.33	2.05	0.98
8.5	METHYL MERCAPTAN (TG)	Both		1.9	27	82	-9.836062244	1	2
8.3	NITROGEN DIOXIDE	Toxic		0.48	15	75	-16.05	1	3.7
8.5	NITROGEN DIOXIDE	Toxic		0.48	15	75	-16.05	1	3.7
8.5	NITROGEN DIOXIDE (TG)	Toxic		0.48	15	75	-6.388906894	0.5	3.99
8.3	PHOSGENE	Toxic		0	0.58	2.2	-7.69	2	1
8.5	PHOSGENE	Toxic		0	0.58	2.2	-7.69	2	1
8.5	PHOSGENE (TG)	Toxic		0	0.58	2.2	-7.782832321	2.51	0.9
8.5	PHOSPHINE (TG)	Both		0	3.8	6.8	-7.900412601	1	2
8.3	PROPANE	Flammable		6837	16303	32080	0	0	0
8.5	PROPANE	Flammable		6822	16268	32010	0	0	0
8.3	1,2-PROPYLENE OXIDE	Both		72	558	1275	0	0	0
8.5	1,2-PROPYLENE OXIDE	Both		72	558	1275	0	0	0
8.3	STYRENE	Flammable		19	151	1843	0	0	0
8.5	STYRENE	Flammable		19	151	1844	0	0	0
8.3	SULFUR DIOXIDE	Toxic		0.72	7.2	112	-16.75	1	2.4
8.5	SULFUR DIOXIDE	Toxic		0.72	7.2	112	-16.75	1	2.4
8.5	SULFUR DIOXIDE (TG)	Toxic		0.72	7.2	112	-10.56320233	1	2
8.5	SULFUR TRIOXIDE (TG)	Toxic		0.06	5.2	58	-8.394682048	0.94	2.14
8.3	TETRAETHYL LEAD	Toxic		0	0	0	-4.521	1	2
8.5	TETRAETHYL LEAD	Toxic		0	0	0	-4.521	1	2
8.5	TETRAETHYL LEAD (TG)	Toxic		0	0	0	-3.364921934	1	2
8.3	TOLUENE	Flammable		65	729	5025	0	0	0
8.5	TOLUENE	Flammable		65	728	5023	0	0	0
8.5	TRIMETHYLAMINE (TG)	Both		7.8	149	470	-14.527153	0.96	2.08



About DNV

We are the independent expert in risk management and quality assurance. Driven by our purpose, to safeguard life, property and the environment, we empower our customers and their stakeholders with facts and reliable insights so that critical decisions can be made with confidence. As a trusted voice for many of the world's most successful organizations, we use our knowledge to advance safety and performance, set industry benchmarks, and inspire and invent solutions to tackle global transformations.

Digital Solutions

DNV is a world-leading provider of digital solutions and software applications with focus on the energy, maritime and healthcare markets. Our solutions are used worldwide to manage risk and performance for wind turbines, electric grids, pipelines, processing plants, offshore structures, ships, and more. Supported by our domain knowledge and Veracity assurance platform, we enable companies to digitize and manage business critical activities in a sustainable, cost-efficient, safe and secure way.

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