

Phast Online model considerations

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

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INTRODUCTION

At the time of writing DNV offers three Phast Online applications: Vessel leak, Hydrogen leak and User defined source. These are web-based applications with a simple and intuitive user-interface where consequence calculations are carried out in the cloud. These applications offer a simplified approach compared to the traditional desktop version of Phast where a far more extensive range of consequence scenarios are available. Importantly though, the underlying models for the estimation of consequences in Phast Online are the same as in Phast, and as such their validation and theory documentation is the same as the <u>Technical Documentation</u>¹ provided for Phast.

Generally, any pre-populated inputs in the Phast Online apps have the same values as their counterparts in Phast. To keep the user-experience of the Phast Online apps simple and intuitive, a significantly reduced number of inputs and parameters are available to users compared to Phast. Those model inputs that are not exposed in Phast Online are set "behind the scenes", normally with values matching Phast default.

The intention is that the Phast Online apps generally produce the same consequence results as their counterpart Phast scenarios where applicable. Results do however differ to an extent, and this is due to slightly different scenario set up or certain modelling decisions. The purpose of this document is to shed light on areas where the Phast Online apps and the latest version of Phast diverge and result differences may occur. It is not intended as a standalone document for the purposes of understanding the theory and validation behind the consequence models used in Phast Online.

The rest of this document is organized into sections for each of the three Phast Online apps. The focus is on comparison with Phast, and the discussion follows the order of a typical linked run: first discussing the differences in the source term definition and discharge results, followed by dispersion, jet fire, pool fire, and explosion.

¹ The Phast Technical documentation relevant to Phast Online can be found in the sections for Explosions, Fire, Dispersion, Pool vaporization, Discharge and Material properties PHAST MODEL CONSIDERATIONS



1. VESSEL LEAK

1.1 Vessel definition and leak scenario

The Vessel leak app allows for the following input data when specifying a pressurised vessel:

Material				
NAPHTHA		✓ ≑		
Mass inventory				
220462	/	lb 🛛		
Pressure (gauge)				
72.5189	/	psi 🛛		
Temperature				
50	/	degF 🛛		

Users are only able to specify a mass inventory and no options of bubble point or liquid fraction are available.

The phase of the pollutant inside the vessel is calculated and feedback to the user and for two-phase storage conditions, the release can be vapour or liquid depending on the user- selection:

Fluid state					
Two-phase		✓ ÷			
Phase to be released					
Phase to be released					
Phase to be released Vapour	ß	√ ≑			
	6	√ ≑			

When comparing results between Phast and Phast Online for conditions close to saturation, we should make sure that the vessel conditions (i.e., gas, liquid or two-phase) are the same in both environments to expect comparable results – this could mean nudging the temperature or pressure by a small amount to release in the appropriate phase.

Liquid head is fixed to zero, so low gauge pressure tanks will have very low liquid flow rates.

The Vessel leak app is also limited to pressurised vessels, so atmospheric storage vessels are not modelled. It also only considers outdoor releases.

The source term used in the Vessel leak app is a time varying leak which returns the initial rate as opposed to a leak calculation as in Phast. In most cases the predicted initial rate by both methods is the same, but it could be different for edge cases.

In the Vessel leak it is possible to vary the elevation of the release as in the Phast and the user can select the release angle, but no impingement options are modelled.



Droplet size

There is a minor dependency on the weather when carrying out discharge calculations. For simplicity, an assumption has been made in the Vessel leak app that has fixed the weather to wind speed of 5 m/s and stability class D for the discharge calculations, with the remaining weather inputs matching Phast defaults. The droplet size correlation used for subcooled liquid releases involves the atmospheric density, which does depend on the atmospheric temperature. For droplet size calculations in the Vessel leak app, the atmospheric temperature is always fixed to 9.85 °C, while in Phast the atmospheric temperature used for the droplet size calculations is as specified by the user (default value 9.85 °C). So, in case the atmospheric temperature in Phast significantly differs from 9.85 °C, then the predicted droplet size for subcooled liquid releases may differ from the one predicted in the Vessel leak app.

The assumption about fixed weather for discharge calculations in the Vessel leak app does not cause differences in any other discharge results; only the droplet size may be impacted.

1.2 Dispersion

Phast Online includes the Unified Dispersion Model (UDM) that also is present in Phast. There are not many differences in the dispersion modelling in the Vessel leak app as compared to the implementation in Phast. Yet, the dispersion is still the area of modelling with potential for the most significant differences between Phast Online and Phast, and this will be discussed in the following.

1.2.1. Mixture modelling and rainout

Phast

Users of Phast may be familiar with two different user options to handle materials: the default pseudocomponent (PC) approach, and the multi-component (MC) approach, where the latter is available as a separate licence for Phast. For details on the modelling of these two approaches please refer to the Multicomponents technical documentation, but in short, the MC approach includes more rigorous thermodynamic modelling for mixtures (i.e. multiple components present in the fluid). However, there is a notable limitation in Phast when using multi-component modelling: rainout cannot occur.

Phast Online apps

In the Phast Online apps, the situation around handling materials has been simplified. Unlike Phast, there is no option available to users to choose pseudo-component (PC) or multi-component (MC with single or multiple aerosol) modelling in Phast Online. Instead, the Vessel leak app automatically sets the mixture modelling flag to either pseudo-component (PC) or multi-component (MC) modelling based on the following rule set:

For a mixture:

- If the phase at storage conditions (user specified Temperature and Pressure) is vapour or liquid the PC logic will be applied,
- If it is two-phase the MC multiple aerosol logic will be applied.

For a single component PC logic will always be applied.



This rule set is designed to ensure that the user gets the most accurate modelling available without having to make this choice themselves; in Phast Online multi-component modelling is therefore automatically available when applicable.

Furthermore, the Phast Online apps do allow for rainout even when MC-multiple aerosol modelling is applied by the rule set. Result differences between Phast Online apps and Phast with MC modelling will therefore occur in cases where rainout is relevant.

The following is an example of a mixture of N-Butane, N-Pentane and N-Hexane in the Vessel leak app where the capability of multi-component rainout can be evidenced:

Input data				Connect Lines A.C.
		 Graphs 		
Material		Flammable dispersio	on Jet fire radiation Pool fire radiation Overpressure	
LIGHT HYDROCARBON MIX 🗸	⊽ ⊼			
Mass inventory		Footprint Side view	w	
1000 🗸	kg 🛛		Height of interest = 1 m	
Pressure (gauge)			Flame shape	
2 🗸	bar 🛛	60		
Temperature				
80 🗸	degC 🛛	40		
Hole size				
120 🗸	mm 🛛	- 20		
Fluid state		d distance [m]		
Two-phase	✓ ○	er sp		
Phase to be released				
Liquid	✓ ÷	Crosswi		
Release elevation		Ŭ -20		
1 🗸	m 🛛			
Release angle (from horizontal)		-40		
0 🗸	deg 🛛			
Weather category		-60	-20 0 20 40 60 80 100	
Day	√ ÷		Downwind distance [m]	

Other implications of the PC/MC automatic selection in Phast Online apps

As part of the rule set for setting the PC/MC flag in Phast Online apps, pseudo-component modelling is always applied if the material is single component, while in Phast multi-component modelling will still be applied if selected for a pure component. In specific instances this could cause result differences between the Phast Online apps and Phast.

When the fluid state is 100% liquid, the Phast Online apps will automatically run all calculations based on pseudo-component logic.

1.2.2. Toxic dispersion

In the Vessel leak app, the toxic calculations are limited to contours to concentration levels of interest. Unlike in Phast, there are no dose, probit or lethality contours. There are no indoor calculations, either.

The averaging time used for toxic dispersion is the toxic averaging time of 600 seconds. In Phast to obtain dispersion results with toxic averaging time we run the dispersion at the core averaging time (default value 18.75 s) and then apply a correction to the concentration and cloud width. In Phast Online we run the dispersion model twice with different core averaging times, once at 18.75 s to generate the flammable dispersion results and the second time at 600 s to generate toxic dispersion results. Therefore, in Phast Online there is no further correction applied to toxic dispersion results as in Phast. This can result in differences between Phast and Phast Online in the far field for distances to concentration of interest.



1.2.3. Other notable points

There is a vastly reduced number of parameters available for user input, including some atmospheric data such as the substrate temperature which is set to be identical to the atmospheric temperature in the Vessel Leak app.

The maximum distances to concentration levels are predicted based on the maximum concentration footprint and will therefore be closer to the distances seen in the graphs in Phast rather than the distances in the summary report.

By default, the height of interest for dispersion results is 1 m in Phast Online and 0 m in Phast. The height of interest can be changed in the General Parameters in Phast Online.

1.3 Jet fire

The jet fire model implemented in the Vessel leak app is the Phast Cone model, and there is no option for the user to change it. The Vessel leak app will therefore produce different results for a pure vapour hydrogen jet fire than Phast as the latter by default will apply the Miller jet fire model. Otherwise, the jet fire parameters in the Vessel leak app are hard-coded to their Phast default values.

Various results from the jet fire calculations in the Vessel leak app are produced, including radiation contours to certain radiation levels. This differs from Phast where the linked jet fire results are simplistically shown as radiation ellipses.

1.4 Pool fire

In the Vessel leak application pool fires are modelled in the same manner as Phast Late Pool fires. Various results from the pool fire calculations in the Vessel leak app are produced, including radiation contours to certain radiation levels. This differs from Phast where the linked pool fire results are simplistically shown as radiation ellipses.

1.5 Explosion

In the Vessel leak app, the explosion calculation results show the worst-case scenario radii, centred at the point where the worst-case explosion would take place. As by default in Phast, the Vessel Leak app uses the Multi-Energy method for uniform confined explosion with a user input explosion strength which can be modified in the Explosion Parameters. The explosion strength has a default value of 7 in the Vessel Leak app, while Phast has a default value of 10.

The height of the calculations is at the centreline, which is also the default approach in Phast. The explosion results are sensitive to the grid step size in the x-direction which is set to be 10 m. This parameter can be modified in Phast, but it is hard coded in the Vessel leak app.

Note that any differences observed in explosion results between Phast Online and Phast may be caused by differences in the dispersion modelling rather than differences in the actual explosion modelling.



2. HYDROGEN LEAK

The Hydrogen leak app is the same as the Vessel leak app with three exceptions:

- 1) The material cannot be changed it is always set to pure hydrogen
- 2) Jet fire: pure vapour hydrogen jet fires are handled by the Miller jet fire model; otherwise the Cone model is applied. This logic is consistent with Phast default modelling of hydrogen
- 3) Explosion: The default value for the Multi-energy explosion strength is 10 (can be modified by the user)

Therefore, any further differences between the Hydrogen leak app and a hydrogen leak in Phast is as described in Section 1 on the Vessel Leak.

3. USER DEFINED SOURCE

In Phast Online, the User defined source term modelling is limited to leaks and there is no capability to generate a User defined source from a Vessel or Hydrogen leak result as can be done in Phast. The user will have to provide the following input data:

Material				
AMMONIA (7664417)	~	▽	A	
Mass flow rate				
10000	~	k	cg∕s Ø	
Release duration				
600	~	s 🕑		
Velocity				
100	~		m/s 📀	
Phase to be released				
Two-phase (liquid mole fraction spe	ecified	l) •	✓ ÷	
Temperature				
-33,4024	~	de	egC 🛛	
Liquid mole fraction				
0.6	~	fract	tion 🗿	
Droplet diameter				
700	~		um 📀	
Release elevation				
1	~		m 📀	
Release angle (from horizontal)				
0	~	C	deg 🛛	
Weather category				
Day		,	✓ ÷	

The selection of multi-component or pseudo-component modelling is based on the same rule set presented in section 1.3.1 now applied to post-expansion conditions. This differs from Phast where user-defined sources are strictly limited to PC modelling.



The modelling of Jet and Pool fires, Flammable and Toxic dispersion and Explosions is the same as explained in the Vessel Leak section.

4. SUMMARY

The Phast Online applications make use of the same underlying mathematical models to predict consequences as the Phast applications. The theory and validation published for Phast therefore also apply to Phast Online. In Phast Online the use of the models is aligned with Phast defaults, and Phast Online model parameters typically set equal to Phast default values. As a result, Phast Online generally predicts similar consequences to the corresponding Phast scenarios with default settings. However, there are instances where the Phast Online modelling and parameter choices differ from Phast, and consequence results may differ on those occasions. The most significant difference is perhaps in the automated use of pseudo- and multi-component modelling and the impact this can have on the dispersion. Further details about these differences have been described in this document.



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