



USER GUIDE

MULTI-COMPONENTS IN PHAST AND SAFETI

DATE: December 2023





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

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ABSTRACT

Phast supports multi-component consequence modelling, which delivers improved consequence and risk results for mixtures compared with the traditional “pseudo-component” approach.

MC modelling for discharge and dispersion can be performed for the following Scenarios: Catastrophic rupture, Leaks, Fixed duration releases, and Short pipe releases. The MC modelling of dispersion does not cover time-varying discharge or rainout and pool formation, and liquid will never rain out when MC modelling is being used for a Scenario, even if the cloud contains a high fraction of liquid. Time-varying releases and a more complete treatment of dispersion are planned for future releases.

Table of contents

ABSTRACT.....	I
1 INTRODUCTION.....	3
2 SCOPE OF MULTI-COMPONENT MODELLING IN PHAST.....	4
MULTI-COMPONENT MODELLING AND CONSEQUENCE ANALYSIS.....	6
2.1 Justification	6
2.2 A typical scenario	7
2.3 Multi-component phase equilibrium	8
2.4 Implementing MC in consequence models	9
2.5 Single and multiple aerosol methods	9
3 THE PROPERTY SYSTEM AND MATERIALS TAB.....	10
3.1 An example: creating a Mixture	11
4 DISCHARGE AND DISPERSION MODELLING: AN EXAMPLE.....	14
APPENDICES.....	16
Appendix A Basic principles for phase equilibrium	16
Appendix B Property calculation methods and ‘templates’	19

1 INTRODUCTION

Phast includes an add-on that makes significant improvements in modelling releases of mixtures. This “multi-component” (MC) modelling is founded on the more rigorous calculation of mixture properties and phase equilibria. Along with most other consequence and risk analysis packages, Phast and Phast Risk have used a “pseudo-component” (PC) approach for mixtures, where the thermodynamic behaviour and properties of a mixture resemble that of a pure component, whose properties are averaged from the constituent components.

The functionality covered by the multi-component add-on will be available to you if you have a Phast MC license.

While the impact of using MC rather than PC modelling will vary from case to case, risk and consequence analyses are frequently used as the basis for decisions resulting in significant investment, and it is important that users have confidence that their results are as accurate as current technology allows. In this respect MC modelling is widely recognised as a key enhancement, and Phast users are among the first to be given this capability for risk and consequence analysis.

A technical overview of the multi-component modelling in Phast, including a brief summary of the theory and examples, is provided by Witlox, H.W.M., Harper M., Topalis, P., and Wilkinson, S., “Modelling the consequence of hazardous multi-component two-phase releases to the atmosphere”, pp. 135-143, ASSE-MEC 7th Professional Development Conference, Bahrain, 18-22 March 2006. This paper is included in the technical reference documentation.

The objective of the current document is to provide a brief overview and tutorial on how to use MC modelling in Phast:

- Section 2 describes the range of release scenarios covered by the current release, and the method for choosing between PC and MC modelling for a particular set of scenarios.
- Section 2.3 summarises the underlying theory of phase equilibrium calculations for all MC modelling in Phast, and discusses why it is important for consequence analysis.
- Section 3 guides you through using the physical property system.
- Section 3.1 presents an example case illustrating the effect if using MC logic within Phast.

You should consult the technical reference documentation for details on how it is implemented in each of the models. The DISC discharge theory manual covers the multi-component discharge scenarios, while the THRM thermodynamics theory manual includes multi-component dispersion modelling. More general information on how the property system in Phast supports property and phase equilibrium calculations is given in the XPRP Theory document.

Full help documentation is included for the features related to MC modelling, including for the screens relating to material and mixture properties.

For technical support on MC, please use the normal channels.

2 SCOPE OF MULTI-COMPONENT MODELLING IN PHAST

MC Scenarios

The calculations for the following storage Scenarios in the current version of Phast can be performed with MC modelling:

- Catastrophic ruptures
- Leaks
- Short pipe releases (i.e. for modelling line ruptures, disc ruptures, or relief valve lifting)
- Fixed duration leaks

There is also a standalone Scenario that can be performed with MC modelling:

- Standalone Pool vaporisation

Other Scenarios cannot currently use MC modelling. These include:

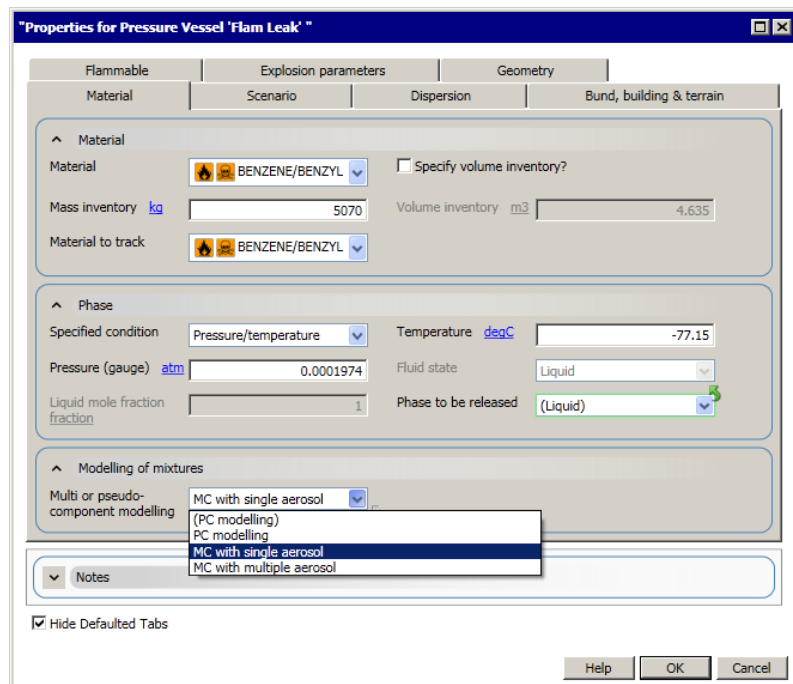
- Time-varying leaks
- Time-varying short pipe releases
- Spill
- User-defined release
- Standalone fire or explosion

Selecting MC Modelling for a Storage Equipment Item

For storage Scenarios, the choice between using pseudo-component and multi-component modelling is made at the level of the Equipment item level to which the Scenario belongs, using the **Multi or pseudo-component modelling** field in the Material tab as shown.

Note: if you do not have a Phast MC license, this field will be disabled and set to "PC modelling".

If a given storage Equipment item has one of the MC options selected, then you will not be able to insert a Time-varying, Spill or User-defined release Scenario underneath the item. Any such Scenarios that are already present under the Equipment item will be shown as deselected if you change to multi-component modelling, and the option to run them will be disabled.





Selecting MC Modelling for a standalone Pool vaporisation Scenario

For the standalone Pool vaporisation Scenario, the choice between using pseudo-component and multi-component modelling is made in the input dialog for the Scenario itself, and not in the dialog for the standalone Equipment item to which the Scenario belongs.

Note: if you do not have a Phast MC license, this field will be disabled and set to “PC modelling”.

A default value for the modelling of mixtures can be set in the Study dialog

The **Multi or pseudo-component modelling** field is also present in the Study dialog, which is the level above the Equipment item. The value that you set in the Study dialog will be used as the default for all storage Equipment items under the Study and for all standalone Pools.

Note: if you do not have a Phast MC license, this field will be disabled and set to “PC modelling”.

Limitations in the modelling for a storage Scenario

Currently the dispersion following on from a MC discharge calculation for a storage Scenario will not allow rainout to occur. Effectively the calculations force the dispersion parameter “Droplet evaporation thermodynamics model” to be “equilibrium, no-rainout”. This means that rainout will never occur when MC modelling is being used for a storage Scenario, you will get no pool results or pool fires, and downwind results may be inaccurate if the case is likely to have rained out. See Section 0 for further discussion on this and other limitations.

In practice this means that cases which are likely to have significant rainout – typically heavier or non-volatile materials and mixtures – will give less accurate results after the point of rainout using MC modelling.

MC functionality will be extended over subsequent releases to address these limitations.

MULTI-COMPONENT MODELLING AND CONSEQUENCE ANALYSIS

2.1 Justification

A typical hazard analysis of a chemical process installation involves several hazardous materials/streams and often these streams are a mixture of two or more chemical substances. Modelling of the behaviour of the mixture requires calculation of mixture thermodynamic properties such as densities, enthalpies, entropies, fugacities and phase equilibrium conditions.

Rigorous thermodynamics is a standard feature of models used in process plant design and process simulation. However, models used in hazard and risk assessment frequently make simplistic assumptions in order to avoid the use of rigorous multi-component (MC) thermodynamics. The “pseudo component” (PC) approach is often used and the mixture is assumed to have a constant composition throughout the calculations and to behave like a single component. The properties of the mixture are calculated from the component properties with a simple averaging equation.

The error from a pseudo-component approach is difficult to predict but, generally, it varies according to:

- the component volatility range
- the non-ideality of the mixture
- the consequence model itself

Two-phase discharge is an example of a calculation which can be strongly affected by inaccurate thermodynamics. The actual compositions and properties of the two phases can be very different from the ones predicted from the simple pseudo-component approach, affecting the accuracy of the release flow rate calculation.

A common justification of the use of simplified thermodynamics is that hazard and risk assessment do not require the same accuracy as process design. In addition to that, the integration of rigorous thermodynamics might affect the speed and robustness of the consequence. However, the industry often makes important decisions based on the results of consequence models and we believe MC technology will be an invaluable tool to those who wish to maximise the accuracy of the risk assessments.

2.2 A typical scenario

Figure 1 illustrates a typical release scenario from a 2-phase vessel (an example is given below in Section 3.1). Some of the key differences in using an MC approach to modelling such a scenario are given in red text.

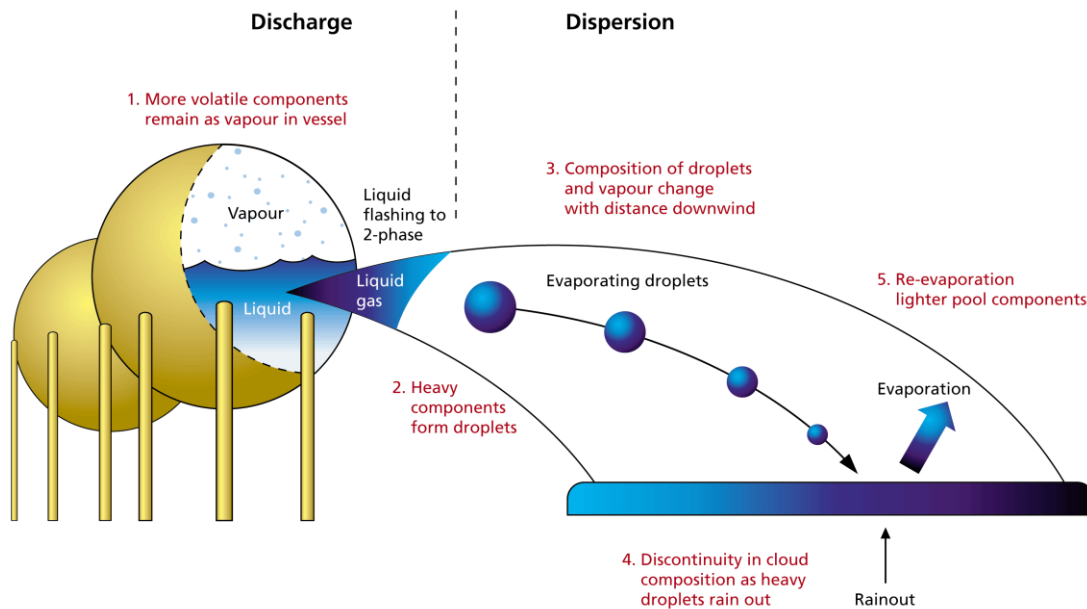


Figure 1. The influence of multi-component calculations on a typical release scenario

You can see from the figure that the composition of the material and its constituent phases can change from the bulk composition stored in the vessel. Heavier components are preferentially concentrated in the liquid phase, and lighter components in the vapour phase. In fact after rainout the cloud composition will change continuously due to the time-dependent evaporation off the pool (lighter components preferentially evaporated first, and heavy ones later).

In Phast this scenario can be modelled using MC logic but rainout and therefore pool formation and re-evaporation are switched off. This clearly limits the functionality of the models, but allows us for now to ignore time-dependent compositional changes in the cloud and pool. For the same reason time varying sources are also disallowed as for these too the composition of the cloud would change continuously with time.

It is planned to include the modelling of rainout and pools for storage Scenarios and time-dependent releases in future releases of Phast.

The current Phast does include a standalone Pool vaporisation Scenario that can perform calculations with MC modelling. This Scenario does not link to the rainout or dispersion modelling, but does allow more realistic modelling of the pools resulting from spills of mixtures, including the compositional changes over time in evaporated vapour. More details of this model can be found in the PVAP Theory manual which is part of the technical reference.

2.3 Multi-component phase equilibrium

Underpinning the MC models is the ability to calculate more rigorously the equilibrium state of mixtures using ‘flash’ calculations. The details of these calculations are complex, and are described in detail in the XPRP Theory manual in the Technical Reference documentations. 0 in this report includes a summary.

PC predictions do not match the actual behaviour of mixtures in key respects, especially for a wide range of component volatilities. For example, as illustrated in the figure below, at a given pressure a mixture might be 2-phase across a range of temperatures, but under PC logic the bubble point and dew point temperatures for a mixture are identical. This is in fact the essence of the “pseudo-component” approach, as this is exactly how a pure component behaves.

Thus a 2-phase or 100% liquid mixture may, according to PC logic, be a vapour. The use of MC modelling will mean that an analyst no longer has to adjust the starting conditions to ensure the correct phase (for example by reducing storage temperature) with the inevitable loss of accuracy.

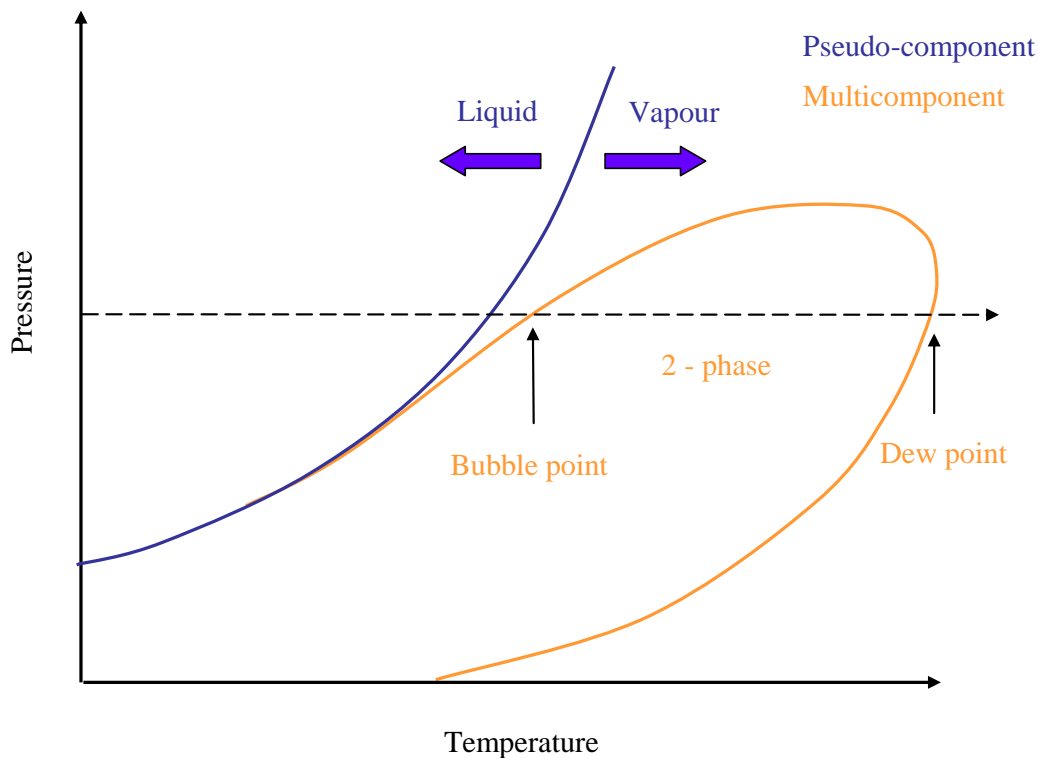


Figure 2. Multi-component phase equilibrium.

Moreover, the liquid phase of the 2-phase mixture will preferentially contain the heavier components, but under PC logic the composition of both phases are identical. So a release of vapour from a 2-phase vessel near its bubble point is likely to be of very different composition to that predicted using PC methods.

2.4 Implementing MC in consequence models

Essentially, the theory and assumptions for the MC modelling is the same as for the PC models, and indeed Phast uses the same models for both calculations. The major difference is that equilibrium calculations performed by the models use MC rather than PC methods.

The models calculate a series of equilibrium states. For the discharge models, these are at the bulk vessel conditions, the orifice or pipe exit, and post expansion to atmospheric pressure (Figure 3). For the dispersion modelling, an equilibrium state is recalculated at each downwind step (reported in the dispersion report) taken by the model.

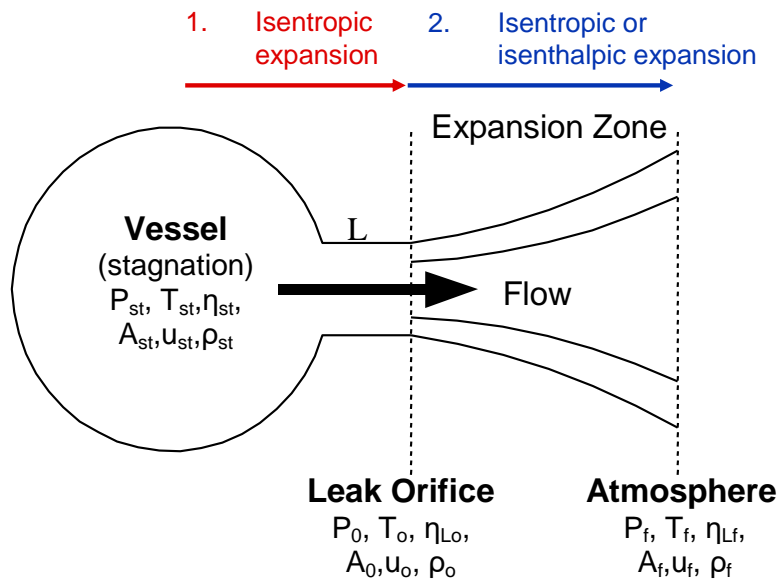


Figure 3. Discharge modelling through a vessel orifice (leak scenario).

Often these equilibrium states are defined by isentropic (fixed pressure and entropy), isoenergetic (fixed pressure and energy) or isenthalpic (fixed pressure and enthalpy) expansions. Typically In such cases temperature is varied until a fixed pressure and temperature flash results in (say) an entropy equal to the required value.



2.5 Single and multiple aerosol methods

The dispersion modelling includes two methods of calculating phase equilibrium: single aerosol and multiple aerosol. The single aerosol is the method described in Section 2.3, where all the liquid components form a single liquid aerosol. The multiple aerosol method is used only in the dispersion modelling, and has components forming in separate aerosols (for example water and propane form two separate liquid aerosols). A fuller description of these methods is included in the MC paper referred to previously (Witlox et al., 1996)

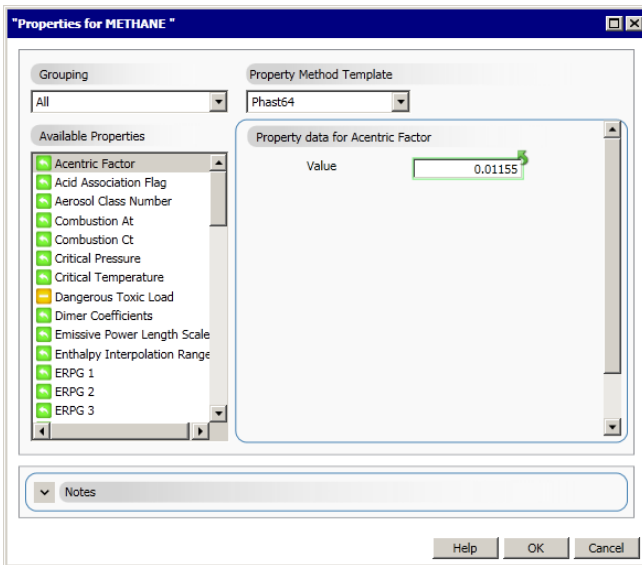
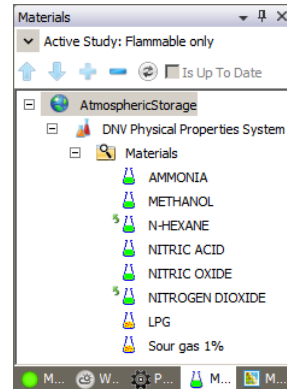
The SA method will be the appropriate method for most Scenarios, as currently there are a number of restrictions on using the MA method. For further details of these restrictions see the Help documentation. However for single components the MA method is frequently the most accurate (e.g. for a hydrocarbon release into humid air, where condensed water vapour will form a separate aerosol).

3 THE PROPERTY SYSTEM AND MATERIALS TAB

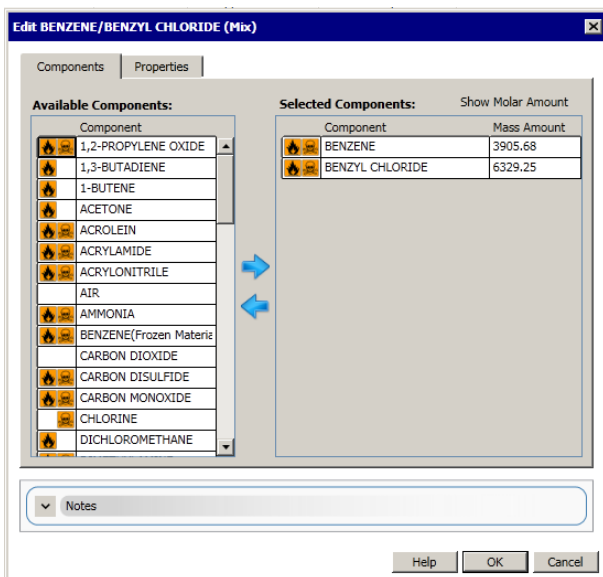
The structure and input data for materials data are the same for pseudo-component and multi-component modelling, i.e. the features are the same, whether or not you have a Phast MC license.

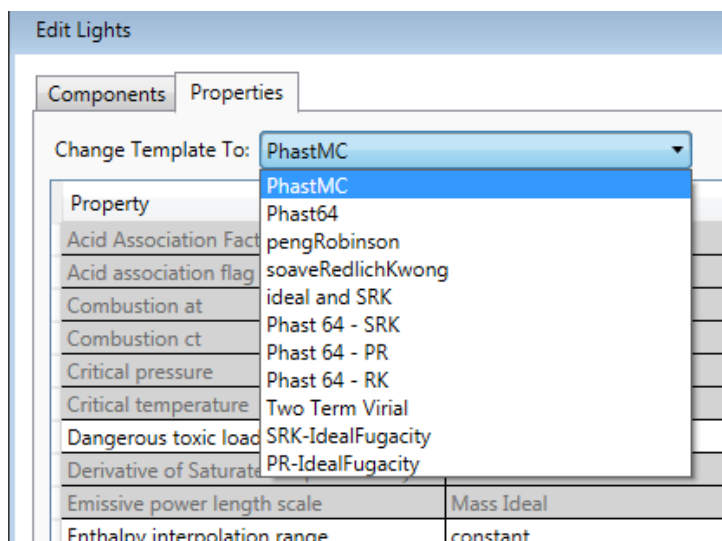
You define both pure Components  and Mixtures  by inserting them under the Materials folder in the Materials tab of the Study Tree.

There is a single dialog for editing the property settings for a pure Component, as shown below:



There is also a single dialog for defining a Mixture, with a tab section for defining the composition of the Mixture, and a tab section for changing the selection of methods to use for calculating properties, and for setting values for properties that are set to use a constant value. You can select up to 18 Components for a given Mixture.





Both dialogs include fields for choosing a **Property Method Template** from a list, and this is how you choose the equation of state (and other types of method) to be used in the calculations for the Component or Mixture.

The default template is called “PhastMC”, as shown in the illustration. This template has a selection of methods that is particularly suitable for the multi-component modelling of mixtures, but the template is also applicable to pseudo-component modelling.

A short glossary of terms associated with the materials system is given in Table 1.

Name	Description
Component	A pure chemical (such as methane) and its associated data. You can calculate some simple temperature dependent (e.g. DIPPR) properties for a component by right clicking and choosing the “Calculate...” option.
Property Method Template	A pre-defined set of methods for calculating properties. Several are installed with Phast, and you can set any of your stream types so it uses a particular template of property calculation methods. A list of available templates is included in 0. There is a ‘default’ template, which is PhastMC. The default template will be selected for any new Components and Mixtures that you insert into the workspace, although any Components and Mixtures that are upgraded from earlier versions of the program will keep their original selection of a template.
Method	The method used to calculate a property (such as enthalpy, molecular weight, vapour pressure, etc.). Typically this will be a mixing rule, or equation of state.

Table 1. Glossary of terms used in the property system and materials tab.

3.1 An example: creating a Mixture

To show how these concepts work in Phast, try creating a light hydrocarbon mixture consisting of equal mole amounts of: methane, ethane, propane, butane, and pentane (0.2 moles of each). This Mixture is added in the Materials tab of the Study Tree.

Step 1. Inserting a Mixture

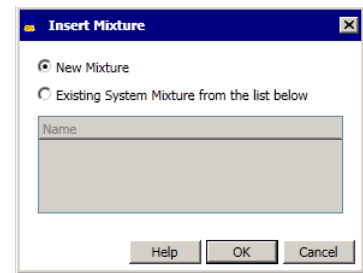
Right click on the Materials folder and choose Insert > Mixture.



A dialog will appear as shown after you have chosen the Insert option. You can insert a New Mixture, which will be completely blank, or if any Mixtures have been defined in the System Materials, you can insert a copy of a selected Existing System Mixture.

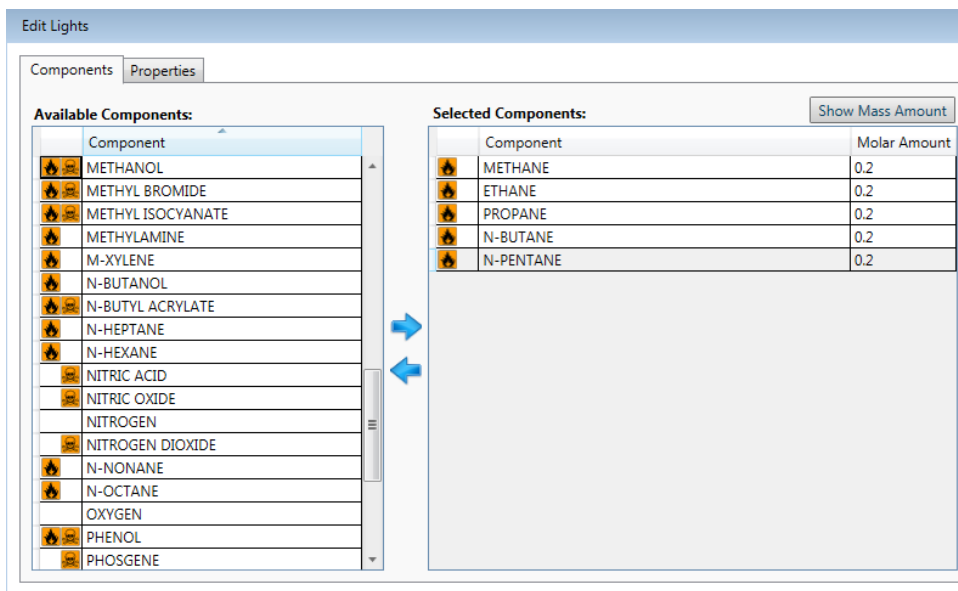
After you have select the appropriate option and clicked on OK, an icon for the Mixture will be added to the Materials tree.

Rename the Mixture node, giving it the name "Lights".



Step 2. Selecting the Components for the Mixture

Double click on the icon for the Mixture to open the dialog. In the Components tab, select the five Components from the list of those available, and use the Add button to add them to the list of selected Components.



Step 3. Specifying the Composition for the Mixture

When you have selected all of the Components, make sure that the table of Selected Components is displaying a **Molar Amount** column rather than a **Mass Amount** column. If the Mass Amount column is displayed, click on Show Molar Amount at the top right of the table to change the basis used in the table.

In the table, enter a value of 0.2 for each Component to set the composition.

Step 4: Selecting the Property Method Template to use

In the dialog, move to the Properties tab. The list of templates at the top of the tab will be set to the default template of PhastMC, and for this example you should leave the field with this default setting.

Step 5: Calculating the values for constant properties

The tab lists all of the material properties, and shows the method that is specified for calculating them with the selected Property Method Template.

Most of the properties will be disabled in the table, but those with the method set to “constant” will be enabled. These properties are not recalculated during model runs, but must be specified initially. Any constant properties required by the program will have red edges to the input field, while others are optional and can be left blank

You can either set the values for constant properties directly yourself, or click on the Calculate button at the top right of the tab to have the program calculate the values based on the composition specified for the Mixture. For this example, use the Calculate option to set the values. Some properties might be left unset after the calculations have been performed; these are properties for which no mixture-calculation method has been defined.

Once the Mixture has values set for all required constant properties, you can click on OK to close the dialog, and you will then be able to select the Mixture in the Materials tab for any Equipment item, and use it in the calculations.

4 DISCHARGE AND DISPERSION MODELLING: AN EXAMPLE

Discharge and dispersion modelling usually involves a succession of equilibrium calculations (typically isentropic, isoenergetic or isenthalpic expansions) at different stages (within the vessel, at the orifice or pipe exit, at atmospheric conditions). For mixtures therefore an MC approach will give very different answers to a PC one.

The release includes an MC example ("Multi component example.psux", in the Examples folder of your installation) which includes a number of MC vessels and sample mixtures. The current section includes a worked-out example on the differences between MC and modelling which you can try in Phast.

The problem considered is the pressurised release of a multi-component hydrocarbon mixture from the leak of a vessel. Below details are given in the subsequent steps of the consequence analysis, i.e. creation of the mixture, release scenario definition, discharge and dispersion modelling.

Step 1. Creation of Mixture in the Materials tab

For the purposes of this exercise, we will use the mixture of five light hydrocarbons that you created in Section 3.1.

Step 2. Definition of Pressure Vessel Equipment item with the Mixture and with multi-component modelling selected

In the Models tab, insert a Pressure Vessel Equipment item under a Study node, name it "Multi-component" and then set the values given below. All of these input fields are in the Materials tab section, and the other fields in the dialog can be left with default values.

Input field	Value
Multi or pseudo-component modelling	MC with single aerosol
Material	Lights
Mass inventory	10 ⁵ kg
Temperature	290 degK
Pressure (gauge)	10 bar
Storage temperature	290 K
Phase to be released	Liquid

Step 3. Definition of a Leak Scenario under the Pressure Vessel

Under the Pressure Vessel Equipment item, insert a Leak Scenario and then set the values given below. All of these input fields are in the Scenario tab section, and the other fields in the dialog can be left with default values.

Release condition	Value
Orifice diameter	0.05 m
Elevation	0.2 m

Step 4: Creating a version of the Equipment item with pseudo-component modelling selected

In the tree, select the Pressure Vessel, and then use Copy and Paste to create a copy of it. You have to create a separate Pressure Vessel Equipment item in order to set up a version with PC modeling selected, as the selection of method is made at the Equipment item level rather than at the Scenario level, which means that all Scenario under a given Equipment item will be using either PC modeling or MC modeling.

Name the copy of the Pressure Vessel Pseudo-component, then edit it, and change the selection for **Multi or pseudo-component modelling** to PC modelling.

When you do this, you will find that the **Phase to be released** field changes from Liquid to Vapour. With MC modeling, the initial state of the mixture is correctly determined to be 2-phase, and therefore you can select a leak from the liquid or vapour side. With PC modelling, the specified temperature and pressure suggest a pure vapour and you will not be able to model a liquid leak (Figure 2 shows how this can happen).

An experienced analyst would know this, and might therefore specify a saturated liquid vessel when using PC modelling. To do this, change the setting for **Specified condition** to Pressure/bubble point. With the pressure set as the actual operating pressure of 10 bar, the temperature field will display the saturation temperature with PC modelling, which is 195K, almost 100K less than the correct value.

You will now be able to select Liquid for the **Phase to be released**, giving a Scenario definition that is the closest possible equivalent of the MC definition, so that the results for the two Scenarios can be compared.

Step 5. Discharge modelling

If you run the calculations for the Scenarios and compare the results in the Discharge Report for the PC and MC modelling you will see that most of the discharge results are similar (within about 10%), with the exception of final temperature which is 235K for MC, and 135K for PC. However in MC the Release Condition composition (as given on page 3 of the report) is very different to that of the bulk mixture (

Table 2). The released liquid contains more of the heavier components and less of the lighter ones:

Component	Mole fraction (PC)	Mole fraction (MC)
Methane	0.2	0.02
Ethane	0.2	0.10
Propane	0.2	0.23
Butane	0.2	0.31
Pentane	0.2	0.34

Table 2. MC example – composition of released liquid.

Therefore all the calculations ‘downstream’ of the discharge calculation will use very different compositions for the PC and MC cases. Many physical properties will therefore be different – including LFL, UFL and heat of combustion, and this will affect models such as the jet fire.

Step 6. Dispersion modelling

For weather 1.5F the distance to the various concentrations of interest as given in the Summary Report of Phast 8.0 are as follows:

Concentration of interest	Distance (PC)	Distance (MC)
UFL	65 m	55 m
LFL	414 m	435 m
½ LFL	535 m	576 m

Table 3. MC Example – distance to concentrations

You can see here the significant differences in MC and PC results – differences that are not consistent throughout the dispersion. In this particular case there are competing influences on centreline concentration: initially the PC cloud is much colder and smaller (due to higher density) and therefore entrains less air. Eventually though the heavier composition of the released material in the MC case combined with a higher discharge rate results in higher concentrations.

The point is not to highlight different results and mechanisms for a particular case, but rather to indicate that a variety of often coupled and non-intuitive factors influence the results if using MC logic – factors that cannot easily be allowed for using PC methods.

The example does illustrate one danger using MC modelling in Phast. The PC case rains out, though with a small fraction which does not greatly affect the distance to concentration results. The MC scenario *enforces* the ‘no rainout’ option and therefore it will never predict rainout even for heavy mixtures. We recommend that you have warnings visible in the Output View when running Scenarios with MC modelling, as one particular warning - UDM 1015 – will be generated if there is still liquid in the cloud when the cloud centreline hits the ground. If this happens, it is likely the cloud would have rained out and you should consider running the Scenario using PC modelling.

APPENDICES

Appendix A Basic principles for phase equilibrium

The mole balance equation for vapour / liquid equilibrium is:

$$z_i = \alpha y_i + (1 - \alpha)x_i$$

If we define the equilibrium constant (K value) as

$$K_i = \frac{y_i}{x_i}$$

then the mass balance equation can be rearranged to compute the equilibrium compositions:

$$x_i = \frac{z_i}{1 + \alpha(K_i - 1)}$$

$$y_i = K_i x_i$$

Therefore, the essence of solving the equilibrium is one of determining the K values.

The fundamental equation governing the vapour / liquid equilibrium of a mixture is very simple – it states that the fugacity of each component must be equal in both phases:

$$f_i^v = f_i^l \quad (i = 1 - n)$$

The problem therefore is one of relating the fugacity of the component in each phase to the independent variables of Temperature (T) and Pressure (P).

The methods are as follows:

1. The Ideal Solution

The simplest method for calculating fugacity is the “ideal” solution which uses a combination of Raoult’ law and Daltons’s law, such that:

$$f_i^v = y_i P$$

$$f_i^l = x_i P_i^{sat}$$

When written in terms of the equilibrium constant we obtain:

$$K_i = \frac{y_i}{x_i} = \frac{P_i^{sat}}{P}$$

This is clearly reasonable in that, for a pure component, the K value is unity (and hence equilibrium is established) when the saturated vapour pressure equals the system pressure – in other words, the component boils.

It is also very convenient because the K value depends only on temperature and pressure, and not on the composition of the phases.

The ideal solution model is certainly the most appropriate model for pure components because the saturated vapour pressure equation is normally a correlation of experimental determined data.

It also gives reasonable results for mixtures of non-polar components (e.g. hydrocarbons) at low pressures where the temperatures required to achieve equilibrium will not be far removed from the component boiling points. When these conditions are no longer applicable, different methods of calculating fugacity need to be employed.

2. Deviation from Ideal Solution

The ideal solution makes the following assumptions:

- the vapour obeys the ideal gas law ($PV = nRT$)
- the liquid is incompressible.
- there are no energy interactions between the components.

There are therefore two main reasons for deviations from ideal behaviour:

- volumetric effects – arising largely from operating at elevated pressures
- energetic effects – arising largely from the polar nature of one or more of the components

Historically, these deviations have been tackled in different ways. The volumetric effects have been addressed by using Equations of State to represent the PVT behaviour of the mixture. The energetic effects have been addressed through energy-interaction models (usually only for the liquid phase) leading to the Activity Coefficient models.

Therefore, the appropriate choice of model can be illustrated diagrammatically as:

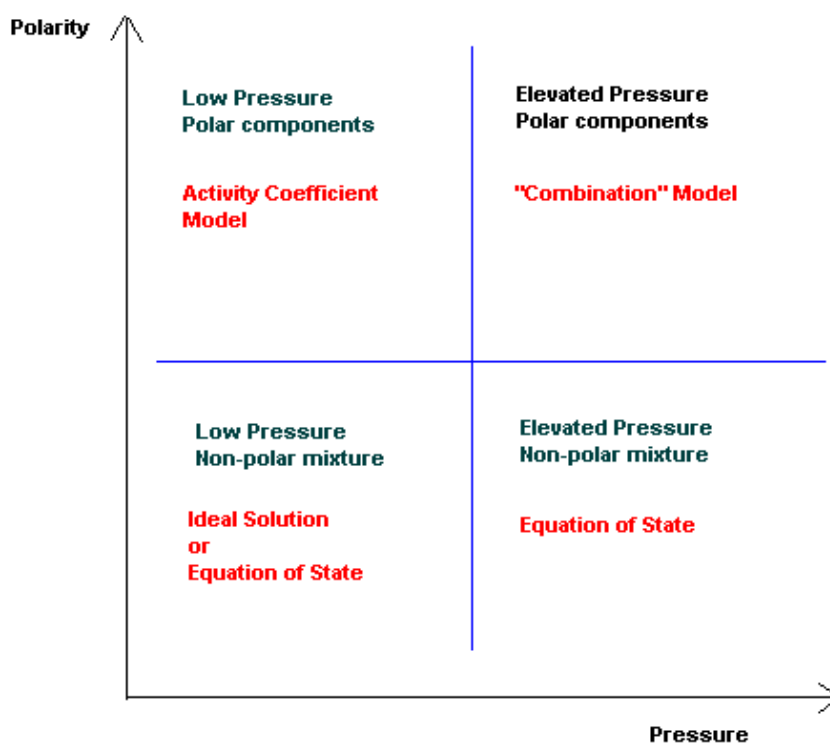


Figure 4. Choice of model for phase equilibrium.

3. Equations of state

The most frequently used equations of state, because they combine relative simplicity with a good degree of accuracy, are the cubic equations of state. Of these, the commonly used ones (all supported in Phast) are:

- Redlich-Kwong (RK)
- Soave-Redlich-Kwong (SRK)
- Peng-Robinson (PR)

These equations are able to represent the PVT behaviour of both the vapour and liquid phases. They are therefore able to completely describe the behaviour of the system at all conditions providing the same EOS is applied to both phases and this would be strongly recommended.

In terms of calculating fugacity, the Soave modification to the RK equation to produce the SRK equation significantly improved its accuracy in predicting vapour / liquid equilibrium and so would normally be used in preference to RK.



The choice between SRK and PR is less clear cut. The performance of both is very similar, and it is usually a question of user preference.

Very often the SRK and PR equations are used without binary interaction parameters with adequate accuracy. Interaction parameters (determined from experimental data, and sometimes available in published literature) can improve the accuracy further for specific circumstances. They can also be used to extend the applicability of the equations to the light gases and slightly polar components that are frequently present in hydrocarbon mixtures e.g. Hydrogen, Nitrogen, Hydrogen Sulphide, Carbon Monoxide, and Carbon Dioxide.

4. *Activity coefficient and "Combination" models*

These are used where there are significant concentrations of polar components present in a mixture. They are not currently supported in Phast, but further details are included in the XPRP Theory manual.

Thus where polar components are present Phast will not typically give accurate results for MC calculations.

Appendix B Property calculation methods and ‘templates’

Available Templates

A variety of different methods are available to calculate some properties in Phast. Rather than select these individually Phast users have available a number of predefined sets of methods called ‘templates’.

Template Name	Description
Phast64	A set of properties and methods mimicking the behaviour of the property system in PHAST version 6.42. Note that for mixtures, many properties were ‘constant’ and did not vary once set. For MC logic this is incorrect as mixture compositions can vary. It uses ideal fugacity calculations which are more robust particularly in the dispersion calculations, but give less accurate flash calculations at elevated pressures. This is the only template available for property calculations to users without the MC add-on.
Phast64-SRK Phast64-PR Phast64-RK	These templates differ from Phast64 only in the equation of state that is used. They represent the set of methods used if the corresponding ‘equation of state’ flag is selected for users without the MC add-on.
PhastMC	A set of properties and methods based largely on using Soave Redlich Kwong where applicable and using simple mixing rules for other properties. There are no ‘constant’ properties so changes in composition will correctly be reflected in property calculations. It uses ideal fugacity calculations which are less accurate at elevated pressures, but more robust than the equation of state fugacities used in the Soave Redlich Kwong and Peng Robinson templates. This is the default template when using the program in MC mode.
Peng Robinson	Peng Robinson is used where applicable (including for fugacity calculations) and simple mixing rules are used for other properties
Soave Redlich Kwong	Soave Redlich Kwong is used where applicable (including for fugacity calculations) and simple mixing rules are used for other properties
Ideal and SRK	Soave Redlich Kwong is used where applicable, but fugacities are set to ‘ideal’. Simple mixing rules are used for other properties.
Acid Association	This should only be used for HF

Table 4. Available ‘template’ sets of property methods in Phast.

Equations of state

Equations of state are generally applicable over a wide range of temperature and pressure and find wide use in gas processing and refining applications and some petrochemical applications. They can be used to predict phase behaviour close to the critical point. The equations of state offered here are not applicable when polar components are present or when the concentrations of gases such as H₂, N₂, CO₂, CO and H₂S in the liquid phase are higher than a few percent.

Redlich Kwong has largely been superseded and is included for reasons of backward compatibility. When an equation of state is to be used the choice between Soave Redlich Kwong or Peng Robinson is largely a matter of user preference. The results are very similar except for liquid densities where Peng Robinson is marginally better. In general however, none of the available equations of state are recommended for liquid densities, and normally the DIPPR saturated liquid density is used for these calculations.

Water handling

Water is not treated in any special way. Water is a DIPPR component like any other. Its properties are calculated using whatever methods are selected for a particular property. There are no supported ASME Steam Table or other specialised methods.

Pure component streams

Phase behaviour within the range of the vapour pressure data should be modelled using vapour pressure i.e., ideal fugacities. At temperatures or pressures above the limit of the vapour pressure equation it will be better to use an equation of state such as Soave Redlich Kwong.

Polar mixtures

Polar mixtures that form azeotropes, more than one liquid phase or mixtures that contain different types of components cannot be modelled accurately using the methods offered here.

At low pressure, phase behaviour for mixtures such as methanol, ethanol, propanol, etc should be modelled using vapour pressure data, i.e., ideal fugacities. These kinds of mixtures are quite well behaved with little interaction between the component species.

Hydrocarbon applications with light gases

Use Soave Redlich Kwong or Peng Robinson as long as there are no polar components present. If gases such as N₂, CO₂, H₂S, H₂ or CO are present then interaction parameters between these components and the hydrocarbons should also be supplied. Use the Costald liquid density method.

Petrochemical applications

1. *Light hydrocarbons*

Use Soave Redlich Kwong or Peng Robinson as long as there are no polar components present. If gases such as N₂, CO₂, H₂S, H₂ or CO are present then interaction parameters between these components and the hydrocarbons should also be supplied. Use the Costald liquid density method.

2. *Aromatics*

At low pressures when the components are similar (e.g., xylene isotopes) you can use Ideal fugacity calculations but with increased CPU time you can also use Soave Redlich Kwong or Peng Robinson. Use the Costald liquid density method.

If non-aromatics are also present the system cannot be accurately modelled using the equations of state currently available here.



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