

Modelling VOC/pollutant transport in DELPHIN 6

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List of Symbols

Symbol	alt. Symbol	Unit	Description
ϱ		kg/m^3	A mass density
j		kg/m^2s	A mass flux density
σ		kg/m^3s	A mass production rate
T		K	Temperature
t		s	Time
x		m	Coordinate
$\varrho^{voc,g}$		$kg(VOC)/m^3_{(REV)}$	Gas phase VOC mass density
$\varrho^{voc,s}$	c_m	$kg(VOC)/m^3_{(REV)}$	Adsorbed VOC mass density (often also used as total VOC mass density, since it is generally much larger than the gas phase VOC mass density)
ϱ_g^{voc}	c	$kg(VOC)/m^3_{(gas)}$	Gas phase VOC concentration, or density of VOC with respect to gas volume in porous medium
$\varrho_{g,sat}^{voc}$		$kg(VOC)/m^3_{(gas)}$	Saturation gas phase VOC concentration, or saturation density
$\sigma_{g \rightarrow s}^{voc}$		kg/m^3s	Phase transition rate/condensation/adsorption rate (from gas phase to solid phase)
σ_{vent}^{voc}		kg/m^3s	Mass production/removal rate due to ventilation
j_{diff}^{voc}		kg/m^2s	Diffusive VOC mass flux density
j_{conv}^{voc}		kg/m^2s	Convective VOC mass flux density
R		$J/molK$	Ideal gas constant = 8.3144598 J/molK
R_{voc}		J/kgK	Specific gas constant of the VOC/pollutant
M_{voc}		kg/mol	Molar mass of VOC/pollutant
p_{voc}		Pa	Partial pressure of VOC
K_g		s	Gas permeability of the material (with respect to gas pressure gradient), typically measured for dry air and used as dry air permeability
K_m		kg/kg	Partition coefficient, or ratio of adsorbed VOC mass over equilibrium gas phase VOC mass
K_{voc}		s	VOC permeability of the material with respect to a gradient of VOC partial pressure
$D_{voc,air}$		m^2/s	Diffusion coefficient of the VOC in air with respect to a gas phase VOC concentration gradient
D_m		m^2/s	Diffusion coefficient of the VOC in the material with respect to an adsorbed/-total VOC mass density gradient
μ_{voc}		—	VOC diffusion resistance factor of the material (similar to the vapor diffusion resistance factor)
β_{voc}		s/m	Exchange coefficient for VOC diffusion mass flux across a surface with respect to difference in VOC partial pressures
h_{voc}		m/s	Mass transfer coefficient with respect to gas phase VOC concentration
n_{vent}		$1/s$	Ventilation rate
k_m		—	Transfer coefficient for phase transition rate, with respect to difference in gas phase VOC concentration

Table 1: List of Symbols

1 Introduction

DELPHIN includes balance equations for pollutant transport¹ in porous media. When simulating pollutant transport, DELPHIN only considers a single compound/pollutant. When investigating different VOCs in the same construction, different simulation models have to be set up, usually just by replacing the VOC/pollutant of interest.

As with other balance equations, the VOC balance is enabled on demand, with the following balance equation combinations implemented so far.

¹This includes VOCs. In the rest of the document we will sometimes use VOC as alternative term.

1.1 Balance Equation Combinations

1.1.1 Isothermal VOC balance (P)

When only the pollutant balance is used, the temperature across the calculation domain, and also of the ambient air, is always 23 °C. Only two balance equations are simulated in the program, one for the gas phase VOCs and one for the adsorbed VOCs. This is also the fastest method of simulating VOC transport in porous media. For this method, only very few VOC related parameters are needed and there are no additional requirements on other material data.

1.1.2 Isothermal VOC balance with air flow (AP)

In addition to enabling the pollutant balance, the quasi-steady air flow model can be enabled. Since this is still an isothermal simulation (again with constant 23 °C), it is only meaningful for forced-flow conditions, i.e. when the construction or part of it is exposed to a pressure gradient and air flow through the construction leads to convective VOC transport. For this variant, still only two balance equations need to be solved, since the air flow pattern is only updated when necessary (quasi-steady approach). Material property K_g (gas permeability) is needed for all materials with air flow enabled.

1.1.3 Temperature-dependent VOC transport (HP)

Enabling energy and pollutant balances gives a coupled simulation, where temperature in the construction has an impact on VOC emission and diffusion speed. In this combination, three coupled balance equations are solved, two pollutant balances (gas and adsorbed phase) and the energy balance.

1.1.4 Temperature-dependent VOC transport with air flow (HAP)

In this variant, the quasi-steady air flow model is enabled in addition to the energy and pollutant balances. Again, only three balance equations need to be solved. The air flow can now be buoyancy-driven, so there will be an even stronger interaction between thermal transport and temperature conditions, air flow and convective VOC transport. This variant is also the slowest method.

Section 4.1 describes how these balance equations are selected in the DELPHIN user interface.

2 Model description

The VOC transport model is a mechanistic transport model where VOCs are transported via diffusion and convection. The model comprises several sub-models with individual parameter sets:

- balance equation and calculation algorithm that related conserved quantities to intrinsic states and material/voc properties (e.g. calculation of gas-phase VOC concentration, partial pressure of VOCs, VOC permeabilities, etc.)
- VOC diffusion boundary condition
- Initial condition calculation model
- contact condition for specifying mass transfer coefficient between normal and air materials within the construction
- VOC sources/sinks resulting from air change with ambient air
- phase transition between gas phase and adsorbed VOCs (emission/adsorption)
- during initialization of the simulation model, the mechanistic model parameters are computed from standardized VOC and VOC-material-parameters

2.1 Conservation equations (balance equations)

Two balance equations are defined for pollutant transport, one for the gas phase VOC mass density $\varrho^{voc,g}$ (eqn. 1) and for the adsorbed VOCs $\varrho^{voc,s}$ (eqn. 2). These quantities are the conserved quantities². Both balance equations are coupled via emission (transfer of VOCs from adsorbed to gas phase) and adsorption (from gas to solid phase) processes, described by a mass production term $\sigma_{g \rightarrow s}^{voc}$.

Transport only occurs in the gas phase, hence this is a classical mobile-immobile-phase model. Transport occurs via diffusion and convection, denoted with subscripts *diff* and *conv*, respectively.

$$\frac{\partial \varrho^{voc,g}}{\partial t} = -\nabla (j_{diff}^{voc} + j_{conv}^{voc}) - \sigma_{g \rightarrow s}^{voc} + \sigma_{vent}^{voc} \quad (1)$$

$$\frac{\partial \varrho^{voc,s}}{\partial t} = \sigma_{g \rightarrow s}^{voc} \quad (2)$$

The optional source term σ_{vent}^{voc} arises when air change with ambient air is considered in the model (see section 2.4).

2.2 Intrinsic quantities

The conserved quantities are related to intrinsic quantities, like gas phase VOC concentration ϱ_g^{voc} (density of VOC with respect to gas volume in porous medium)³ and partial pressure of VOCs.

The gas phase concentration/mass density is related to the adsorbed phase VOC through a storage relation, commonly expressed as:

$$\varrho^{voc,s}(\varrho_g^{voc}) = f(\varrho_g^{voc})$$

Typically, this is a linear function using the partition coefficient K_m as factor (eqn. 3).

$$\varrho^{voc,s} = K_m \varrho_g^{voc} \quad (3)$$

This corresponds to $c_m = K_m c$ (a formulation typically found in literature). With the ideal gas law we can express the partial pressure of the VOC (eqn. 4).

$$p_{voc} = \varrho_g^{voc} R_{voc} T \quad (4)$$

with $R_{voc} = R/M_{voc}$ (gas constant divided by molar mass of VOC).

2.3 Flux equations

2.3.1 Mass diffusion flux

Mass diffusion of VOCs is typically written in relation to a concentration gradient. However, from thermodynamics follows that the partial pressure gradient is the driving potential for gas diffusion processes⁴, which also includes the temperature effect. With increasing temperature, the partial pressure increases (related to the kinetic energy of the VOC molecules) and diffusion is accelerated.

The diffusive mass flux is proportional to the VOC permeability K_{voc} of the material (eqn. 5).

$$j_{diff}^{voc} = -K_{voc} \frac{\partial p_{voc}}{\partial x} \quad (5)$$

$$= -\frac{D_{voc,air}(T)}{\mu_{voc} R_{voc} T} \frac{\partial p_{voc}}{\partial x} \quad (6)$$

²Note that $\varrho^{voc,s}$ corresponds typically to symbol c_m but $\varrho^{voc,g}$ is *not* the gas phase VOC concentration c .

³Typically, the symbol c is used for the gas phase VOC concentration ϱ_g^{voc} with respect to gas volume.

⁴This can be derived from the gradient of chemical potential that appears in the Gibbs energy equation.

The permeability is proportional to the diffusion coefficient of the VOC in air $D_{voc,air}$, which is a temperature-dependent function. The tortuosity/pore structure of the material is incorporated in the diffusion resistance factor μ_{voc} (eqn. 6).

For a diffusion flux between two adjacent materials (or rather elements), the VOC permeability is averaged using a weighted, arithmetic average. If one of the materials is inert/tight for VOC diffusion (see section 4.2.2 for details on material-VOC property mapping), the flux is set to zero.

In case of isothermal conditions, the partial pressure gradient simplifies to a concentration gradient. First, the chain rule is applied since p_{voc} is a function of T and ϱ_g^{voc} (see equation 4).

$$\frac{\partial p_{voc}}{\partial x} = \underbrace{\varrho_g^{voc} R_{voc} \frac{\partial T}{\partial x}}_{=0 \text{ in isothermal conditions}} + T R_{voc} \frac{\partial \varrho_g^{voc}}{\partial x}$$

Then, the partial pressure gradient is replaced in equation 6.

$$\begin{aligned} j_{diff}^{voc} &= -\frac{D_{voc,air}(T)}{\mu_{voc} R_{voc} T} T R_{voc} \frac{\partial \varrho_g^{voc}}{\partial x} \\ &= -\frac{D_{voc,air}(T)}{\mu_{voc}} \frac{\partial \varrho_g^{voc}}{\partial x} \end{aligned} \quad (7)$$

2.3.2 Convective VOC transport

When air/gas phase moves through the porous media, the VOC is transported alongside it. For a known gas mass flux j_{conv}^g the corresponding VOC mass flux is expressed simply by multiplication with the intrinsic gas phase VOC concentration ϱ_g^{voc} (eqn. 8).

$$j_{conv}^{voc} = \varrho_g^{voc} j_{conv}^g \quad (8)$$

2.3.3 Boundary flux for VOC diffusion

VOC diffusion across the boundary is described as driven by a difference in partial pressures between surface and outside air (eqn. 9).

$$j_{diff}^{voc} = -\beta_{voc} (p_{voc,s} - p_{voc,e}) \quad (9)$$

However, to simplify use with established parameter sets, the boundary condition definition in DELPHIN requires a mass transfer coefficient h_{voc} to be provided, instead (see section 4.5.1). The mass transfer exchange coefficient β_{voc} can be computed from the mass transfer coefficient h_{voc} , as described in section 3.4.

2.3.4 Boundary flux for convective VOC flux

Convective VOC mass flux across the material boundary is described exactly the same as convective flux within the calculation domain.

2.3.5 Contact condition for VOC diffusion flux across material-air interfaces

When the calculation domain includes an air space (an air material, not a VOID), this material is identified by the AIR flag in the material file, and also when it is mapped to an Air material in the VOC database (see section 4.2.2).

Instead of calculating the diffusion flux from a material to the air space via an averaged VOC permeability, the flux can be computed with a model that corresponds to the diffusion mass boundary flux (eqn. 9).

The exchange coefficient is given, in this case, via a contact condition and overrides the calculation of the averaged permeability (see section 3.4 for information on how the mass transfer coefficient is converted into an exchange coefficient).

2.4 Source/sink due to air change with ambient air

A field condition (source/sink) can be used to model air change with the ambient air. The air change rate due to mechanical ventilation n_{vent} is a model parameter. The model is applied to each selected element individually, resulting in a VOC source/sink σ_{vent}^{voc} (eqn. 10).

$$\sigma_{vent}^{voc} = n_{vent} (\varrho_{g,e}^{voc} - \varrho_g^{voc}) \quad (10)$$

σ_{vent}^{voc} is positive, when the ambient VOC concentration $\varrho_{g,e}^{voc}$ is higher than the concentration in the element.

2.5 Phase transition between adsorbed and gaseous VOCs within the porous medium

The mobile-immobile phase model for VOCs in DELPHIN 6 includes a phase transition term $\sigma_{g \rightarrow s}^{voc}$. The phase transition is based on the equilibrium concentration above the adsorbed phase, defined by the storage relation and hence by the partition coefficient. For a given adsorbed VOC concentration $\varrho^{voc,s}$ we obtain the equilibrium gas phase concentration $\varrho_{g,eq}^{voc} = \varrho^{voc,s} / K_m$.

The key idea of the immobile-mobile phase model is, that the actual gas phase concentration may deviate from the equilibrium concentration. It will, however, in time approach the equilibrium concentration. This is modeled by defining the phase transition mass source/sink based on the difference between actual and equilibrium gas phase concentration (eqn. 11).

$$\sigma_{g \rightarrow s}^{voc} = k_m (\varrho_g^{voc} - \varrho_{g,eq}^{voc}) \quad (11)$$

When the actual gas phase concentration is higher than the equilibrium concentration, than some gaseous pollutants will be adsorbed. The $\sigma_{g \rightarrow s}^{voc}$ is then positive and acts as a sink in the gas phase VOC balance equation, while acting like a source in the adsorbed VOC balance equation.

In a coupled simulation with the energy balance, the equilibrium gas phase concentration becomes a temperature dependent quantity. Typically, for higher temperatures, the equilibrium gas phase concentration for the *same adsorbed VOC mass density* will be higher. This is considered in the model by multiplying the equilibrium relation with a ratio of saturation densities (eqn. 12).

$$\varrho_{g,eq}^{voc} = \frac{\varrho^{voc,s}}{K_m} \frac{\varrho_{g,sat}^{voc}(T)}{\varrho_{g,sat}^{voc}(23^\circ\text{C})} \quad (12)$$

The model is based on the observation, that the partition coefficient is obtained at 23 °C and thus indirectly includes the saturation density at 23°C. Using this model requires the saturation density of the VOC as function of temperature (see section ??).

2.6 Calculation of diffusion resistance factor from model parameters

The mass diffusion equation (6) requires the VOC diffusion resistance factor μ_{voc} . The VOC parameter database contains the diffusion coefficient D_m with respect to a gradient of the adsorbed VOC mass density $c_m = \varrho_s^{voc}$ (eqn. (13)).

$$j_{diff}^{voc} = -D_m \frac{\partial c_m}{\partial x} \quad (13)$$

Inserting the relations introduced above, the flux equation can be rearranged.

$$\begin{aligned}
 j_{diff}^{voc} &= -D_m \frac{\partial \rho_g^{voc} K_m}{\partial x} \\
 &= -D_m \frac{\partial \frac{p_{voc}}{R_{voc} T} K_m}{\partial x} \text{ (isothermal conditions)} \\
 &= -\frac{D_m K_m}{R_{voc} T} \frac{\partial p_{voc}}{\partial x}
 \end{aligned}$$

Through coefficient comparison we get an equation for the VOC diffusion resistance coefficient (eqn. 14).

$$\begin{aligned}
 \frac{D_m K_m}{R_{voc} T} &= \frac{D_{voc,air}(T)}{\mu_{voc} R_{voc} T} \\
 \mu_{voc} &= \frac{D_{voc,air}(T)}{D_m K_m}
 \end{aligned} \tag{14}$$

3 Parametrization of the model and VOC database

3.1 Database file

The VOC and VOC - material parameters are stored in a VOC database file, usually with the extension `.vdb`. The header file has the following structure:

```

1 # DELPHIN6 VOC Database File
2 #
3 # Lines beginning with a hash character '#' are comments and ignored
4 # Use the keyword 'undefined' for all _string_ entries to indicate missing information
5 # For constant "linear splines" simply store one x and one y value.
6 # Use -1e-100 for undefined/unknown values.
7
8 TABLE: VOC_DATA
9
10 .... VOC parameter sets
11
12 TABLE: VOC_MATERIAL_DATA
13
14 .... VOC - material parameter sets

```

The first line is a comment and must contain the keyword DELPHIN6 to indicate that the new format for DELPHIN 6 is being used.

3.2 VOC parameters

The VOC database defines basic properties of VOCs/pollutants. However, these properties are not needed for all balance equation combinations. The diffusion coefficient of the VOC in air $D_{voc,air}$ must only be provided when air materials are being used in the construction. Otherwise, if the diffusion coefficient of air is not known, a value can be estimated ($10^{-6} \text{ m}^2/\text{s}$), since μ_{voc} is computed from D_m first (see section 2.6). The same is true for the mass transfer coefficient M_w .

For non-isothermal calculations, the saturation density of the VOCs must be provided as temperature dependent function. At least a single value must be given, in which case the temperature effect on the emission will be disabled.

The VOC parameters are specified in the VOC database, in table VOC_DATA in the following format:

```

1 # ENTITY <string: VOC name>
2 #   <string: alternative descriptive name(s)>
3 #   <string: molecular formula>
4 #   <string: source information, quality measure, reference>
5 #   <double: molar weight in kg/mol>
6 #   <double vec: temperatures for saturation densities in K>
7 #   <double vec: saturation densities in kg/m3(gas), one for each of the temperatures in the previous line>
8 #   <double vec: temperatures for diffusion coefficients in K>
9 #   <double vec: diffusion coefficients in air in m2/s, one for each of the temperatures in the previous line>

```

For example, the data entry for Formaldehyde looks like:

```

1 ENTITY Formaldehyde
2   50-00-0
3   CH2O
4   Literature, ref. author and author2 (2011)
5   1083
6   253.15  258.15  263.15  268.15  273.15  278.15  283.15  288.15  ...
7   1.393   1.698   2.052   2.458   2.922   3.449   4.042   4.707   ...
8   296.15
9   1.455E-05

```

whereby Formaldehyde is the unique VOC identification name.

3.3 VOC - material properties

For isothermal calculations the transport model requires only its diffusion coefficient with respect to the material D_m and the partition coefficient K_m . These are stored in the table VOC_MATERIAL_DATA, for combinations of a material and a VOC, in the following format:

```

1 # ENTITY
2 #   <string:VOC name>
3 #   <string:Material ID name>
4 #   <string: source information, quality measure, reference>
5 #   <double:   diffusion coefficient D_m w.r.t material concentration in m2/s>
6 #   <double:   partition coefficient, K_ma in [m3(gas)/m3(REV)] >
7 #   <double:   initial total VOC mass density, Cm0 in [kg(VOC)/m3(REV)] >
8 #   <double:   water vapor diffusion resistance factor mu in [--] if known for this material >

```

Such an entry must exist for each material and VOC parameter set. There must not be an Air material in the database, since air materials are handled separately, already. The following example shows data for Particle board and Hexanal:

```

1 ENTITY
2   Hexanal
3   Particle Board
4   Literature, Deng et al. (2003), An analytical model for VOC emission from dry building materials. Building
   and Environment.
5   7.65E-11
6   3289
7   1.15e-11
8   -1e-100

```

The last line of this data block is optional and contains the water vapor diffusion resistance factor μ . Since this value may not be available for all materials, it is indicated as *missing* by the special value -1e-100 in this example.

3.4 Mass transfer exchange coefficient for diffusion boundary condition

The VOC diffusion mass flux across a boundary requires definition of a mass transfer coefficient h_{voc} with respect to differences in gas phase VOC concentrations. It is then converted to a VOC diffusion exchange coefficient as follows:

$$\begin{aligned}
 j_{diff}^{voc} &= h_{voc} (\varrho_{g,s}^{voc} - \varrho_{g,e}^{voc}) \\
 &= h_{voc} \left(\frac{p_{voc,s}}{R_{voc}T} - \frac{p_{voc,e}}{R_{voc}T} \right) \\
 &= \frac{h_{voc}}{R_{voc}T} (p_{voc,s} - p_{voc,e})
 \end{aligned}$$

Comparing coefficients gives an equation for the mass diffusion exchange coefficient (eqn. 15).

$$\beta_{voc} = \frac{h_{voc}}{R_{voc}T} \quad (15)$$

4 Definition of VOC models in the DELPHIN 6 user interface

4.1 Enabling pollutant balance equation

Open the simulation model view and check the respective balance equations, as shown in Figure 1 for the balance equation combination HAP.

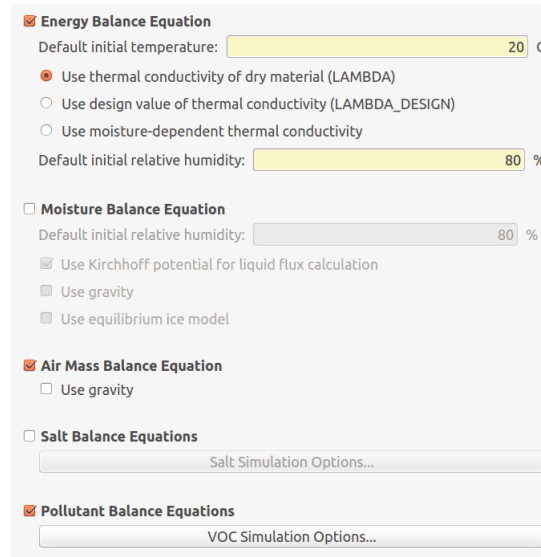


Figure 1: Screenshot of the Simulation Model Options in DELPHIN 6, with energy and pollutant balances and quasi-steady air flow model enabled

The corresponding balance equation keywords in the project file are: `BEPollutant`, `BEHeatPollutant`, `BEAirPollutant`, `BEHeatAirPollutant`

4.2 VOC model settings

4.2.1 Selection of VOC database and VOC to be calculated

Once the pollutant balance equation has been enabled, the button to open the VOC simulation options is enabled. Pressing this button opens the dialog shown in Figure 2.

In the dialog, first a VOC database file has to be selected. Once the database file has been chosen, it will be automatically read. Alternatively, or in case of database errors, you can click on “Update list from database”, to refresh the VOC data table.

Next, select the row with the VOC to be used for calculation.

Lastly, specify the DELPHIN 6 material to VOC DB material mapping as described below.

The VOC modeling data is store in the project file in the following XML block within the Init section:

```

1  <ModelSettingsVOC>
2    <VOCDatabase>/tmp/demonstration/VOCEmissionTest/voc_data.vdb</VOCDatabase>
3    <VOCID>Hexanal</VOCID>
4    <MaterialMapping>Air gap 50 mm (vertical) [18] == Air</MaterialMapping>
5    <MaterialMapping>Particle board [348] == Particle Board</MaterialMapping>
6  </ModelSettingsVOC>

```

4.2.2 Material-material mapping

The VOC database is maintained independently of the DELPHIN 6 database. Also, materials that are tested for VOCs are often not tested for moisture transport and storage parameters. Therefore, the materials in the VOC database may not correspond to materials from the DELPHIN 6 database.

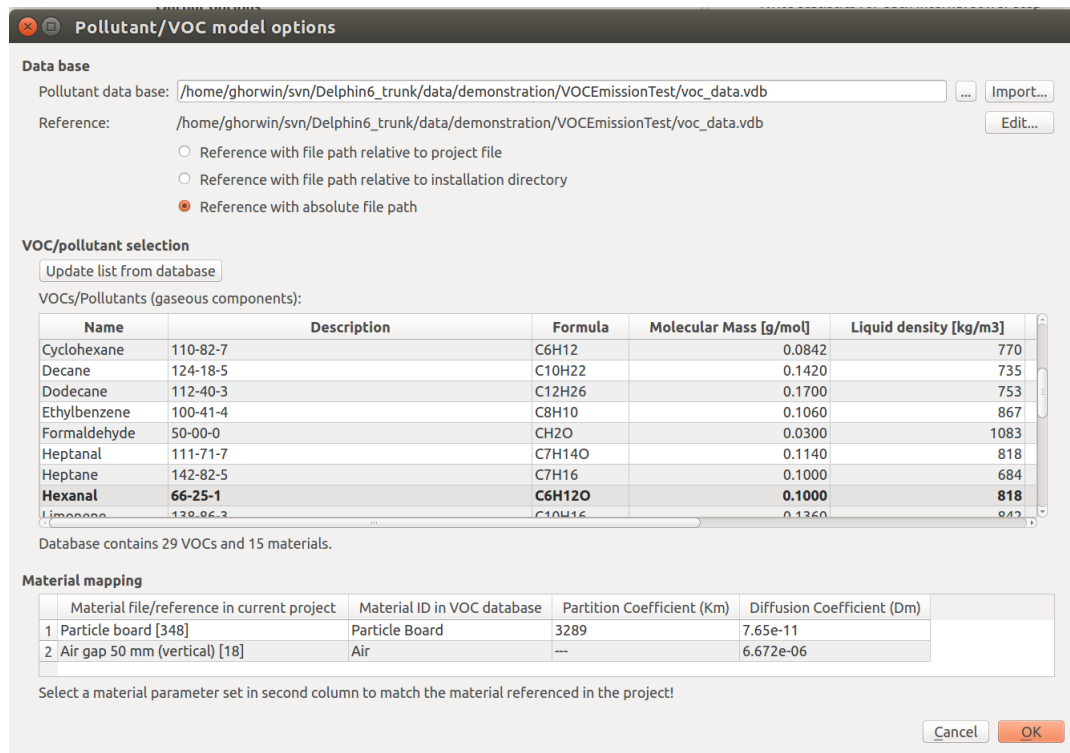


Figure 2: VOC/pollutant model settings; selection of database file, selection of VOC to be calculated, and material-material mapping

The VOC model settings dialog allows to assign specific VOC - material database materials to materials used in the DELPHIN project. In the table, the first column lists the material reference names of all materials used in the project (mind, also unused materials are shown here). The second column can be edited and a material used in the VOC database can be selected. The list of available materials includes only those materials, that appear in dataset defined for the combination of the material and the currently selected VOC.

Therefore, changing the current VOC in the database may require re-mapping materials!

In addition to parametrized voc/materials combinations, an *Air* material and an *Inert/VOC-tight* material is offered for mapping. These special cases are interpreted as follows:

- Air materials only hold gas phase VOCs (no adsorbed phase) and a partition coefficient and material diffusion coefficient is not required
- Inert/VOC-tight materials do not contain VOCs; fluxes and source are ignored for such materials

4.3 Defining initial conditions

Initial concentration of VOCs are defined via initial conditions. Hereby, the initial adsorbed VOC concentration C_{m0} is defined and assigned to the element range of interest (default method as for custom temperature/moisture conditions). VOC initial conditions are of type VOCMass.

4.4 Defining air change rates

When simulation chamber tests, the air volume elements beside the VOC emitting material receive a field condition of type AirChange.

4.5 VOC related boundary conditions

Generally, the engineering interfaces do not consider VOC diffusion, hence surfaces with plain engineering interfaces are tight with respect to VOCs. If VOC transfer shall be permitted, a DETAILED interface type has to be used and VOC related boundary conditions have to be specified manually.

4.5.1 VOC diffusion boundary condition

A boundary condition of type VOCDiffusion can be defined to model VOC emission from a material surface. The only parameter expected is the mass transfer coefficient h_{voc} of the VOC with respect to the gas phase VOC concentration and given at 23°C. According to equation (15), the exchange coefficient with respect to partial pressure of the VOC is then at 23°C:

$$\beta_{voc} = \frac{h_{voc}}{R_{voc} 296.15 K}$$

Currently, this transfer coefficient is kept constant in the model regardless of the surface/air temperature.