SubSelect
Guidance for using the tool

Contents

1 Who can use SubSelect and for what?

SubSelect[1] is intended but not limited to be used by **FORMULATORS OF MIXTURES** and **DOWNSTREAM USERS** of substances or mixtures.

SubSelect aims to support you in your **SUBSTITUTION** activities. It can be used to **PRIORITISE SUBSTANCES** for substitution if you are unsure about where to start. Its main intention is, however, to support you in **ASSESSING**, which of the **SUITABLE ALTERNATIVES** you identified are the most sustainable[2] ones and should enter either the next assessment step or be tested in your production or use.

SubSelct can help:

- **EVALUATING** the sustainability of a substance or mixture **AND**
- **COMPARING** the **SUSTAINABILITY** of up to 5 substances and mixtures.

The comparison of sustainability will result in a ranking of the (maximum 5) substances or mixtures you compare with regard to their sustainability. As the tool is designed to be "quick and simple" it may be useful and necessary to further assess those alternatives that qualify as substitute, e.g. the alternatives ranked first and second.

The guidance will lead you through the entire process of using SubSelect and includes several illustrations and screenshots to facilitate understanding. Explanations about the general functions of SubSelect are provided in Section 4.

The figures of this guidance were derived from the English tool version. The Estonian, Latvian and Lithuanian versions have exactly the same design and functions but the menues are translated.

☺ When you see this symbol the information is not necessary but useful to understand the programme and how it works. Quick readers can skip these sections.

Before you start using the programme, it is useful that you get an overall idea of what it does. This is explained in brief in the following.

2 Idea of the assessments

SubSelect evaluates the sustainability of substances and mixtures using several „*main criteria*":

- Inclusion in lists of priority substances
- Physical-chemical hazards
- Hazardousness for humans
- Hazardousness for the environment
- Mobility
- Greenhouse gas emissions
- Resource consumption
- Responsibility in the supply chain

[1] SubSelct was developed in the fame of a research project of the Germen Environment Agency (UBA)

[2] In most cases (and tools), only the toxicity or risk of a substance or mixture is identified and compared. However, it is also important to consider if substitution could negatively affect human health and the environment by other means than their toxicity, e.g. because their production is disproportionately resource intensive (e.g. some nanomaterials) or because they are excavated under unacceptabel working or enviornmental conditions (e.g. gold). Therefore, SubSelect incudes a few criteria that aim to approximate other enviornmental impacts than toxicity.

Some of the main criteria have „*sub-criteria*“, such as the criterioun “hazardousness to human health”, which considers separately:

- hazards via inhalation, ingestion and eye contact;
- hazards via dermal contact and
- hazards from endocrine disrupting properties.

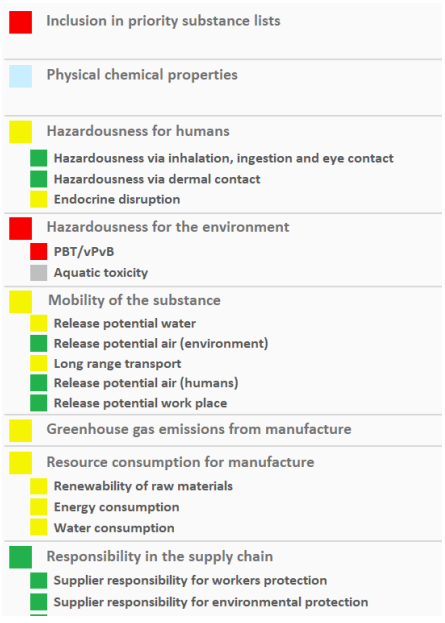
SubSelect requests data from the user to determine a value for each main criterion and sub-criterion. This value can be

- Red
  substance performs bad for the criterion (e.g. is lethal if ingested in low amounts)
- Yellow
  substance performs medium for the criterion (e.g. substance irritates the skin)
- Green
  substance performs very well for the criterion (e.g. substance is not hazardous to human health)
- Grey
  no data is available to evaluate the criterion (this is an indicator of uncertainty and an incentive for you to look for information to complete the assessment)

If there are sub-criteria, SubSelect will develop the value of the main criterion from these. For mixtures, SubSelect will for most criteria calculate the values for the mixture based on the information and values of the individual substances.

In its logics, SubSelect is biased against substances with very severe hazardous properties. This means for example, that mixtures containing a carcinogen are evaluated as “red” even though it may be contained in very low concentration (i.e. no “dilution of severe hazards”). Therefore, SubSelect always enable you to look at all individual assessments.

If you assess the sustainability of a substance or mixture, the result is a *sustainability profile*, which shows you the evaluation results using a colour code. If you make a comparison, you get the profiles of all compared substances next to each other and also can see numbers that indicate the *sustainability ranking* (1 is best rank).



Example sustainability profile (not complete)

Example comparison of substainability (not complete)

3 Getting started

3.1 Obtain SubSelect

Download SubSelect. For the Estonian, Latvian and Lithuanian Version you will be asked to provide name and e-mail address, so the tool providers can contact you in case of updates.

- Estonia: http://fitreach.eu/et/authentication-content
- Latvian: http://fitreach.eu/lv/authentication-content
- Lithuanian: http://fitreach.eu/lt/content/irankiai
- English https://www.umweltbundesamt.de/en/document/subselect-guide-for-the-selection-of-sustainable
- German Version: https://www.umweltbundesamt.de/dokument/subselect-instrument-zur-auswahl-nachhaltiger

Unpack the zip file into a separate folder on your computer. The zip-file containes: a folder called „data“, a file called Readme_EN.txt and a file SubSelect_Vxxx[3]_English.accdb.

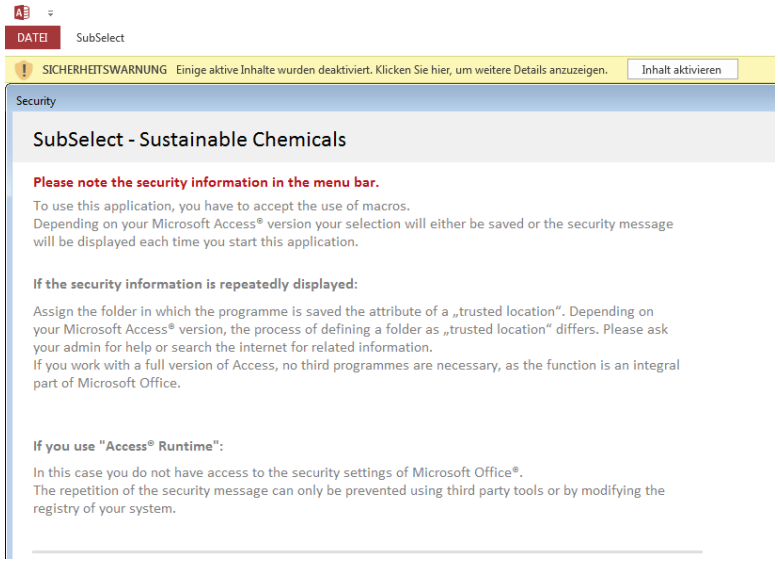
3.2 Check for MS Access®

SubSelect is based on Microsoft® Access® and you need to have either the full program or the so called “run-time” version. Check if MS Access is installed on your computer.

- If you have MS Access® (version 2010 or newer), do yan directly continue
- If you do not have MS Access® or your version is older than 2010, you can use SubSelect if you install Runtime Access®, which is available without charge under: https://www.microsoft.com/de-de/download/details.aspx?id=50040

3.3 Enter SubSelect

Doubleclick the file SubSelect_Vxxx3_English.accdb and you may see the following window.



Read the text, it informs you what you should do if you do not want to see this message every time you open the file.

To proceed with SubSelect, click on the button „activate content“ in the yellow safety warning message.

Depending on your MS Access® version, you may or may not be asked to *select the data file* (**SubSelect_Dat.accdb**). This is the file where all data that is entered into the programme is

[3] The xxx is a place holder for the version number. Currently it is version 112

stored into. It is provided with the programme and contained *in the folder „data“*. Please follow the request.

SubSelect can only work with one data file at a time but it is possible to exchange files, e.g. with colleagues. If you rename the data file or remove it from the folder, SubSelect will not find it and open same window to re-connect the data file. If you want to open a different file (that was generated by SubSelect), you can click on “open” on the very left side of the menue bar to access this window and exchange the data you are working with.

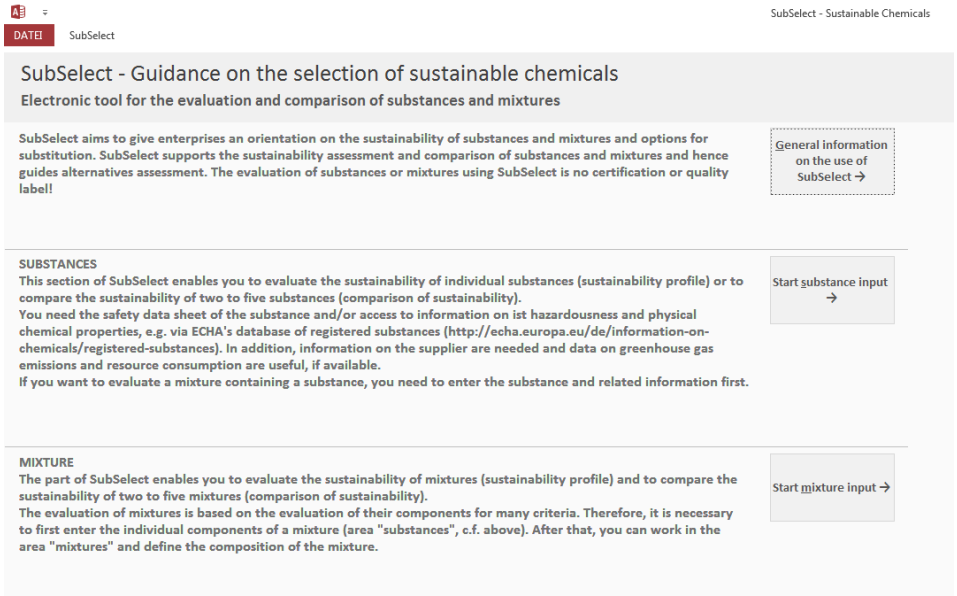
Then you will see the following screen and can actually start…

Click on the picture to continue

4 Overview of basic programme functions

4.1 Start page

This is the start page that you will see after clicking on the image. *Read* the information that is provided *before you start*!



As you can see, you the tool consists of a section for assessing substances and one for assessing mixtures.

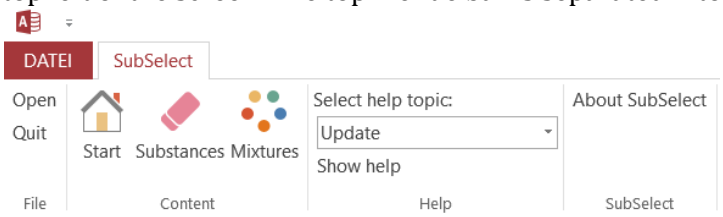
As a general principle, substance information is the basis for any assessment by SubSelect; hence, also if you assess or compare mixtures, the information about the individual substances contained (that you are aware of and) is most important and must be entered first.

Click on the button "*start substance assessment*" in parallel to reading the guidance. The next sections will explain some general options how to navigat in the tool.

4.2 Navigation within the tool

4.2.1 Top menue bar

The menue bar at the top of you screen facilitates interchanging between *basic functions*. If you do not see the top menue bar, click on "SubSelect" at the top left of the screen. The top menue bar is separated into four areas.



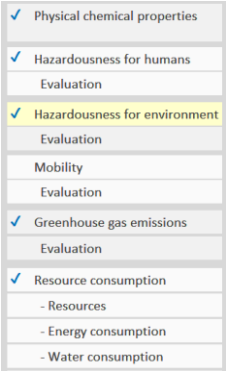
- *Open/quit*:
  allows opening a new data file or quitting the programme
- Selection of substance or mixture assessment:
  if you click on "substance" or "mixtures" you are directed to the respective start window of either assessment. The butoon "start" brings you back to the very first page of the programme
- *Help*: Providing help according to different topics
- *About* SubSelect: basic programme information

4.3 Moving forward step by step

The assessment can be done step by step following the questions and instructions of the programme. To walk-through in this way, you best use the „*forward arrow*" (looking right, middle) which is provided on almost all screens. To go back, use the „*backward arrow*" and to close the window, use the „*x on red*" button (far right)[4].

[4] The „x on red" button only closes the window and brings you back to the start page either for substances or for mixtures, depending on what you are working on. It does not close SubSelect – to close the programme click on "quit" at the far left of the programmes top menue bar.

4.4 Where you are



Once you start entering information on a substance or mixture, the menue bar shown at the left will appear. It lists all windows for entering data (e.g. physical chemical properties, Resource consumption – resources, Resource consumption – energy consumption etc.) and the windows, where you can access the results (evaluation).

If there is a tick at the left side of the data entry windows, data has already been entered.

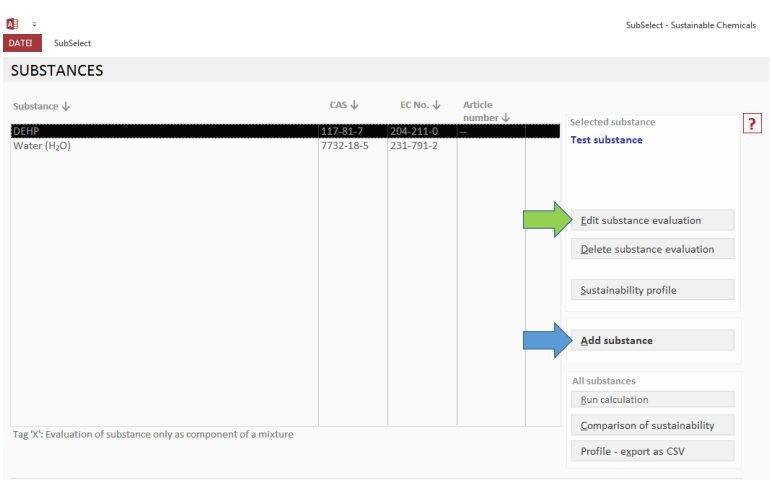
If the title of a page is highlighted in right yellow, this is the one you are on at the moment.

5 Assess a substance

5.1 Management of substances

If you click on „substances“, you will see the following screen, which is the starting point for any activities you do with the programme on substances.

On this page, you see the *full list of all substances* that are already enterd into the datat file. When you first start the programme, only water is included in the list. As you enter further enter substances they will be added to the list. From here, you can start any activity for one substance:



If you want to add a substance, you simply *click on „add substance“* (blue arrow), if you want to delete one, click on “*delete substance evaluation*” and if you want to edit data of an existing substance, click on „*edit substance evaluation*“ (green arrow) after having marked the specific substance you want to work on.

Mark a substance and click on *“sustainability profile”* to the the evaluation of sustainability. You can compare several substances by clicking on „*comparison of sustainability*“, which will bring you to a window, where you can select the substances that you want to compare (maximum of 5!).

SubSelect also enables you to export data as CSV (last button on the page). The button “run calculation” should be used, when you import a data file into a new version of SubSelect to ensure that any changes of the REACH-Candidate list are considered in the evaluations.

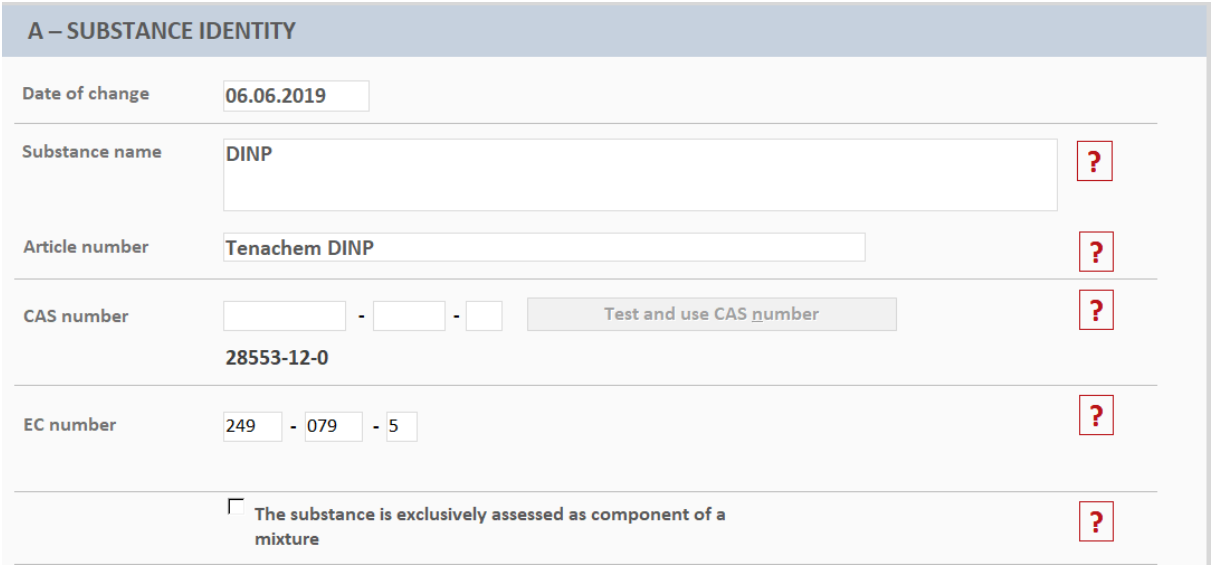
5.2 Add a substance

If you click on „add substance“ you will see the follwing screen.

Whenever you see a red questionmark in a box you can click on it and get some help/information on the question that you are currently working on.

Enter the sustance name and, if you have an internal number for it, an article number.

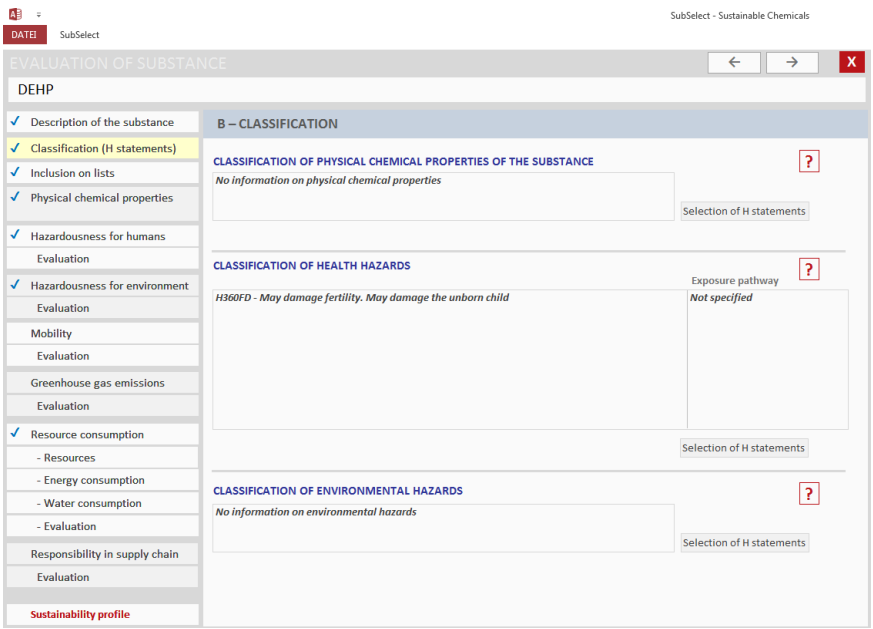
The *CAS number* is used as unique identifier of the substance in the programme. Therefore, the correctness of the CAS number is checked and you cannot go to the next step without having entered a correct number. *Click on „Test and use CAS number", otherwise you cannot proceed.*



Then you just answer all the questions that you are asked when you walk through the programme (forward arrow button). After information for a criterion is completely entered (tick in the left navigation bar), you will be shown the assessment results in a separate screen.

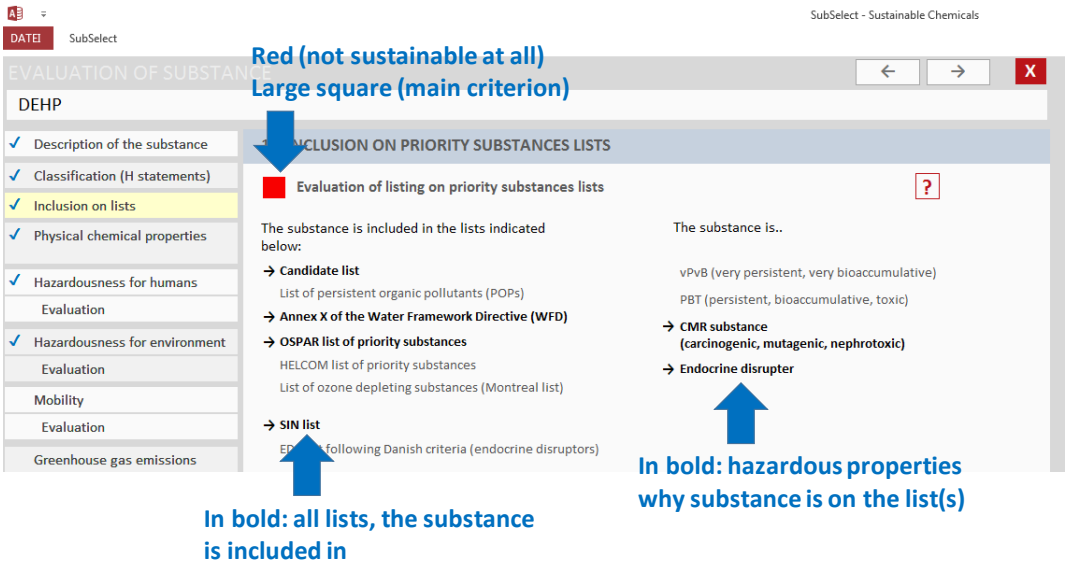
5.3 Enter substance data

5.3.1 Hazard classification



Use the safety data sheet of the substance or, if not available, any public database to obtain the classification of the substance, such as ECHA's classification and labelling inventory. Enter the *H-statements* for all three areas from the drop-down lists. If the substance is *not classified* check if this is due to data indicating that *no classification applies* (first option in the lists) *or* if it is not classified because there is a *lack of data* (third option in the drop-down list).

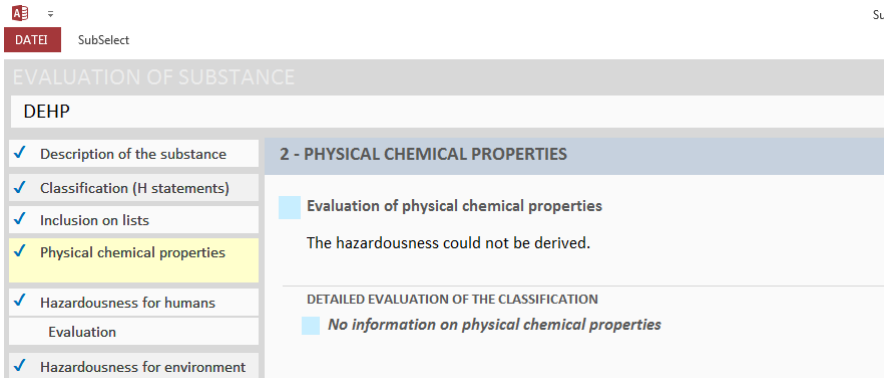
Some parameters are *automatically assessed* by SubSelect, such as the *inclusion on priority lists* (based on the CAS-Number) and *substance hazards* (H-statements). The next figure shows the evaluation result: the red dot shows that DEHP is not sustainable with a view to the toxicity; it is included on several lists and has CMR and EDC properties.



The screen as shown in the above figure informs you of the evaluation of the criterion for which you just entered information. If you notice a mistake, you can directly go back (backwards arrow).

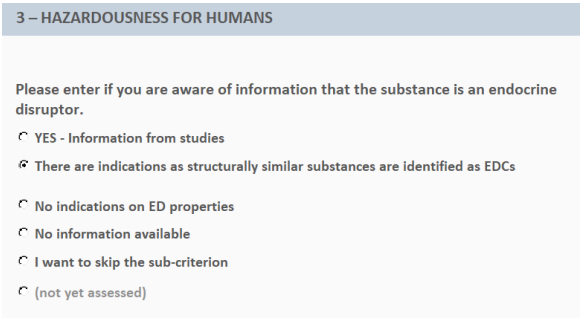
You do not have to save anything, the programme automatically saves all data you enter!

If you have no information for a specific criterion, then you can select the option “no information”. This is reflected in the presentation of results by grey/light blue colour. This is exemplarily shown in the next figure.

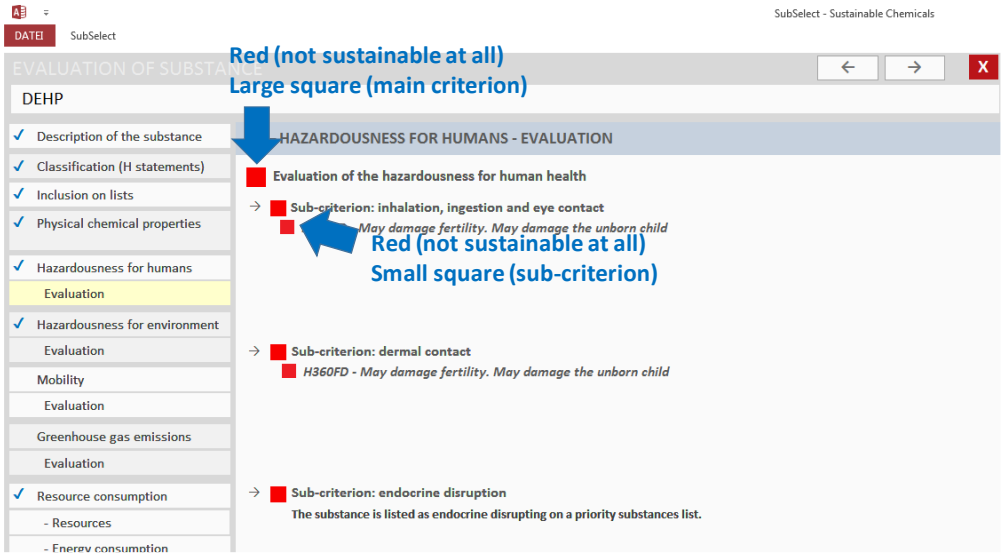


5.3.2 Hazardousness for humans

The criterion hazardousness for humans has three sub-criteria, of which the one on *endocrine disruption requires input* in addition to the classification. The screen allows you to select one of the options shown below. For the example substance, a structural similarity to an EDC exists and the respective option is selected.

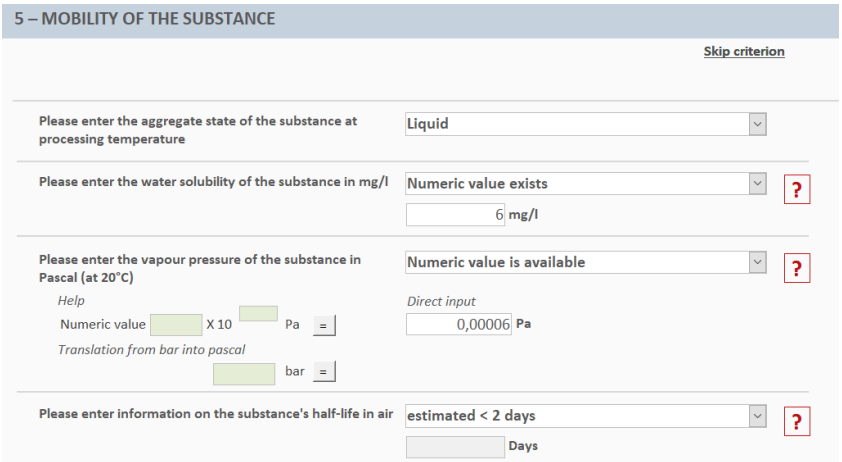


The result of an assessment of DEHP looks are shown in the following figure with explanation of the meaning of the outcome shown

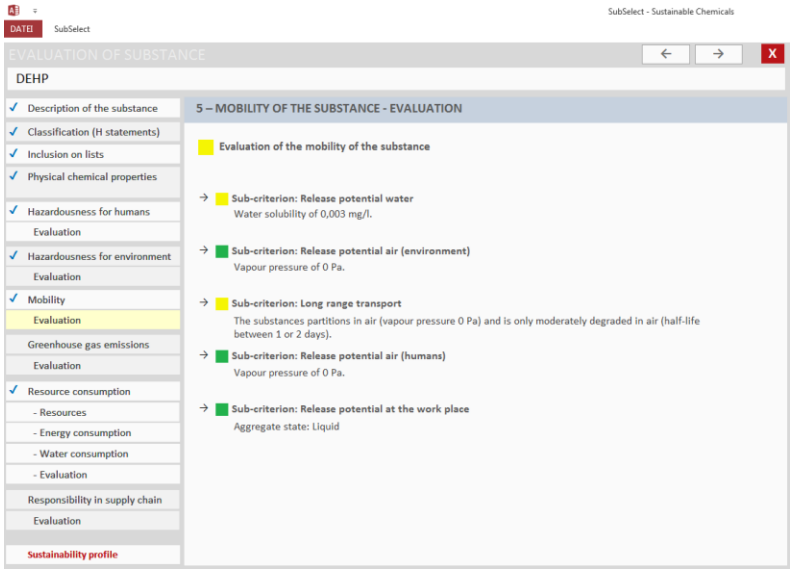


5.3.3 Mobility

SubSelect requires data on the mobility of the substance to estimate the exposure potential for humans and the environment. You can either enter qualitative or quantitative information, if that is available. Only if you select „*numeric value is available*“ from the drop down list, you are allowed to *enter these specific values*. For many substances you can find this information in ECHAs database on registered substances. Use the „key values for safety assessment“, which are frequently provided in the substance data of that data base.

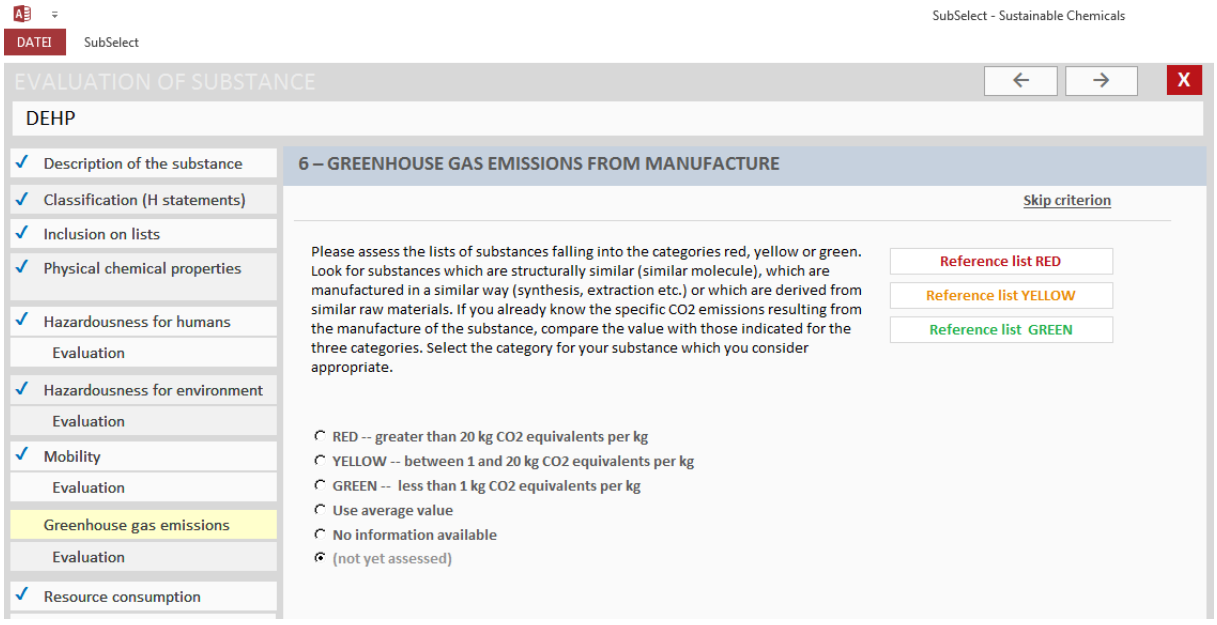


From the results of the evaluation of the „overall mobility“ (main criterion), you can see that the programme does not average the results of the sub-criteria (e.g. two yellow and three green sub-criteria does NOT result in light green but in yellow) but takes the worst result to derive the main criterion.



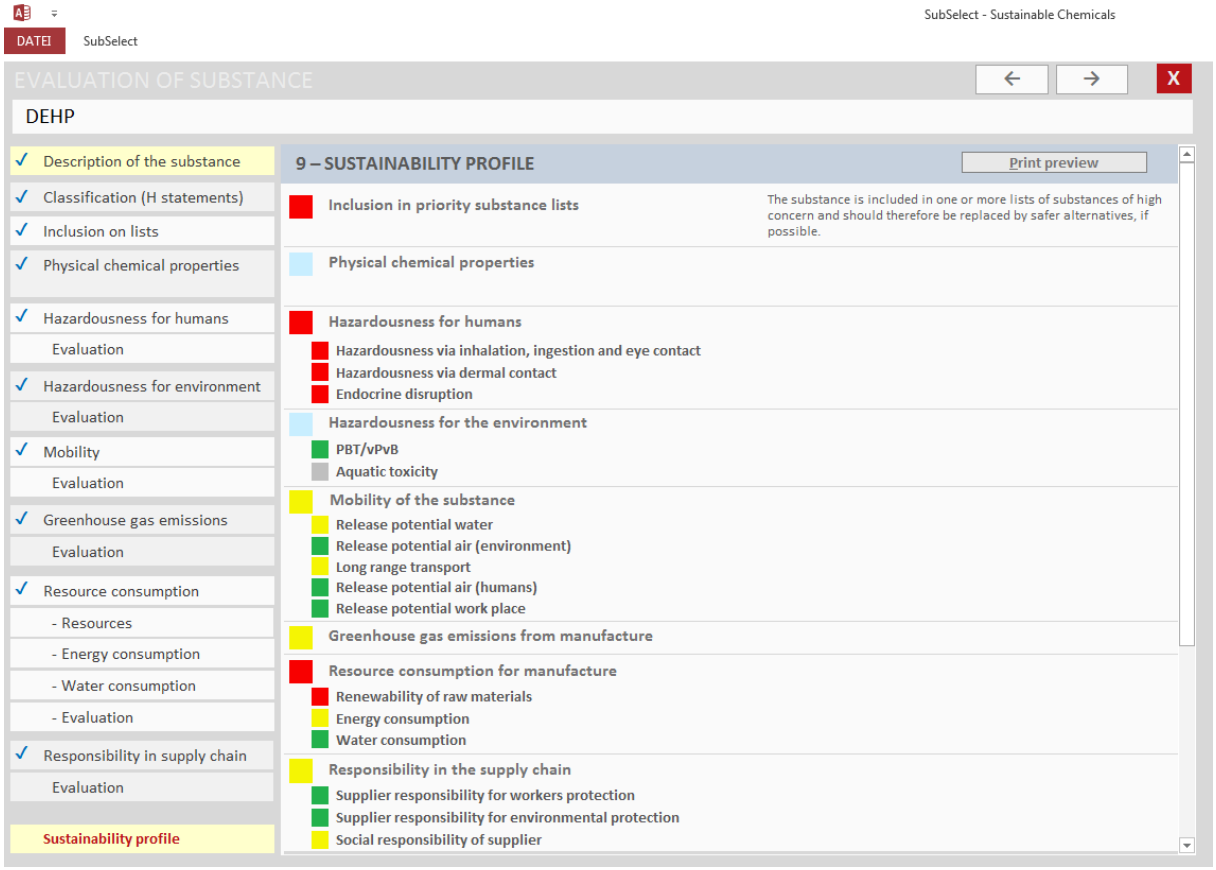
5.3.4 Greenhouse gas and resource consumption

The information input for the following criteria require non-chemical information. If you find this data, *select the colour as indicated* in the options to select (e.g. more than 20 kg; between 1 and 20 kg and below 1 kg CO2 per kg. Substance in the figure shown below). If you do not have this data, you can skip the question or select „*average value*“ or select information from similar substances. *Reference lists* to see substances which would be evaluated as red, yellow or green can be opened by clicking on the respective buttons.



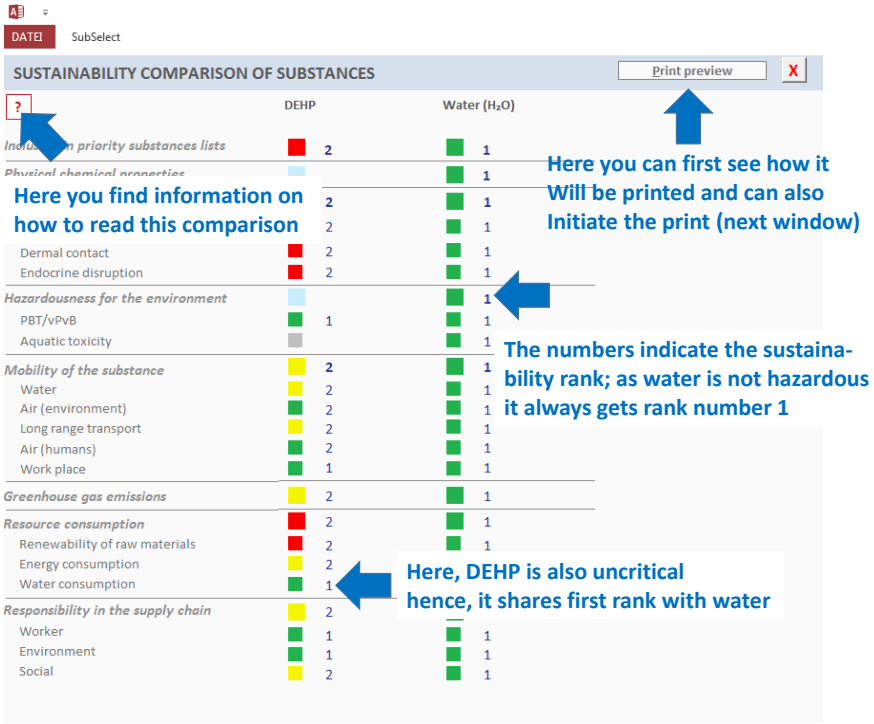
5.4 Evaluation

When you finished data entry, you can get a sustainability profile by clicking on the respective button. It chould look like this.



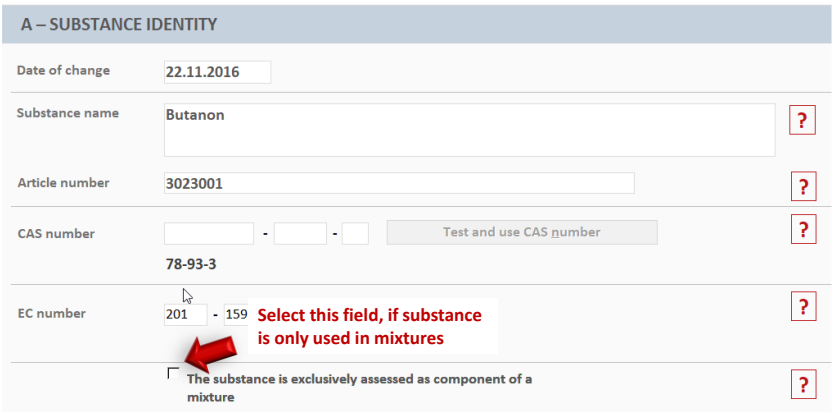
Use the scroll bar on the right to see the results at the bottom of the window.

If you make a comparison, e.g. with water the the result looks like this.



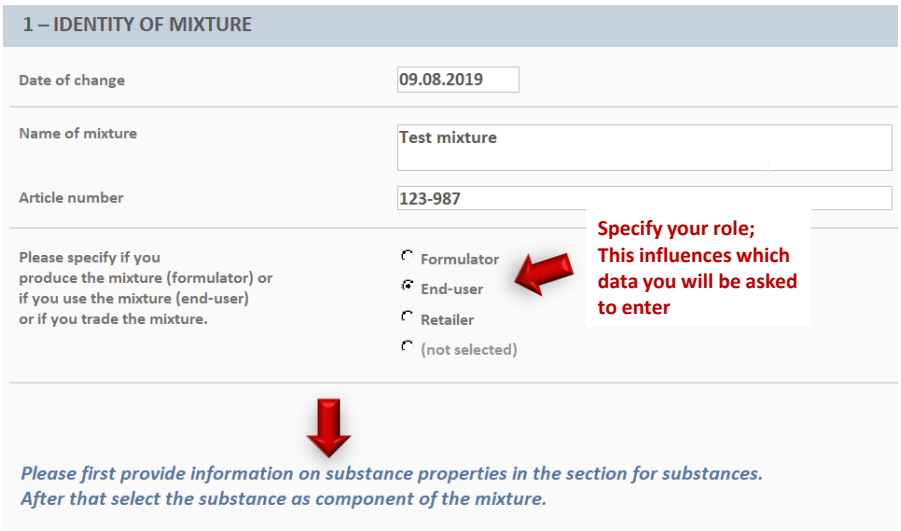
6 Assessing mixtures

If you want to assess a mixture, *you first insert information on the substances contained* in the mixture. For this, enter all substances that you know are contained (safety data sheet of the mixture) in the substances section (c.f. Chapter 5). You may select the box „*substance is exclusively used in mixtures*“ because then you are not asked to enter some of the information, which is not needed in the mixture assessment at the level of individual substances.



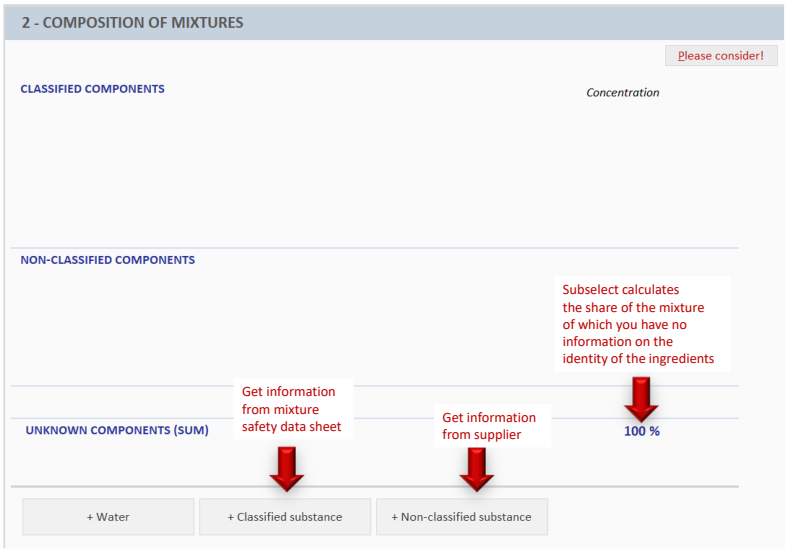
6.1 Define a new mixture

Select the mixture section and click „*add mixture*“ in the starting window. Then you assign the name and also select *your role* in relation to the mixture (the knowledge of some information differs when you are a formulator or a downstream user. This is consididered in some questions by the programme). If you produce mixtures, check formulator, if you use them end-user and if you sell them only, make a tick in the box for the reltailer.



Before you can assess the mixture, please enter all substances that you are aware of which are contained in it via the “substance” section of SubSelect. Check the safety data sheet of the mixture and/or ask your supplier about the main (hazardous) ingredients to get the information.

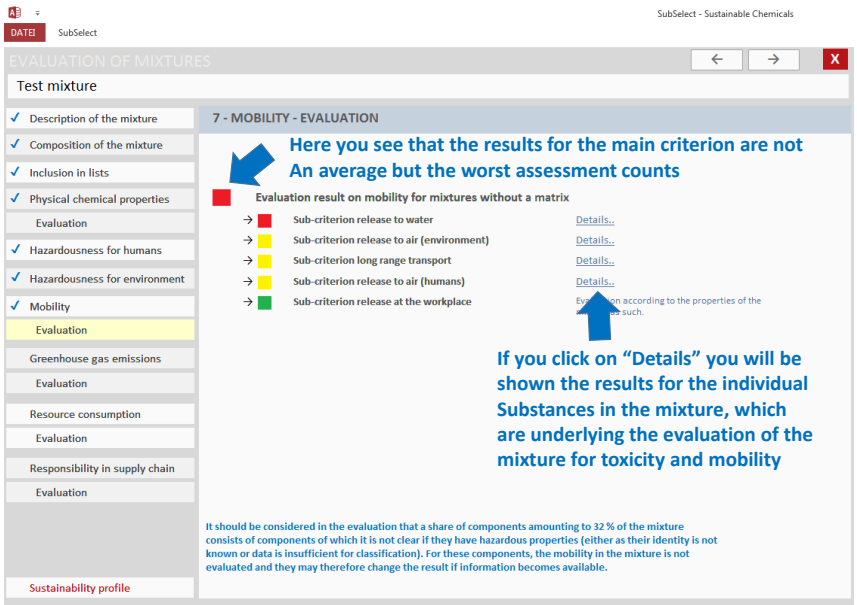
6.2 Enter the mixture composition



You have to click on the buttons at the bottom to add the components of the mixture. SubSelect differentiates between *water*, *classified ingredients* and *non-classified ingredients*. The latter are most likely to be unknown to end-users of chemicals, where formulators may have at least some knowledge of these substances.

When you click on one of the three buttons, a new window opens allowing you to enter their concentration or concentration range in the mixture.

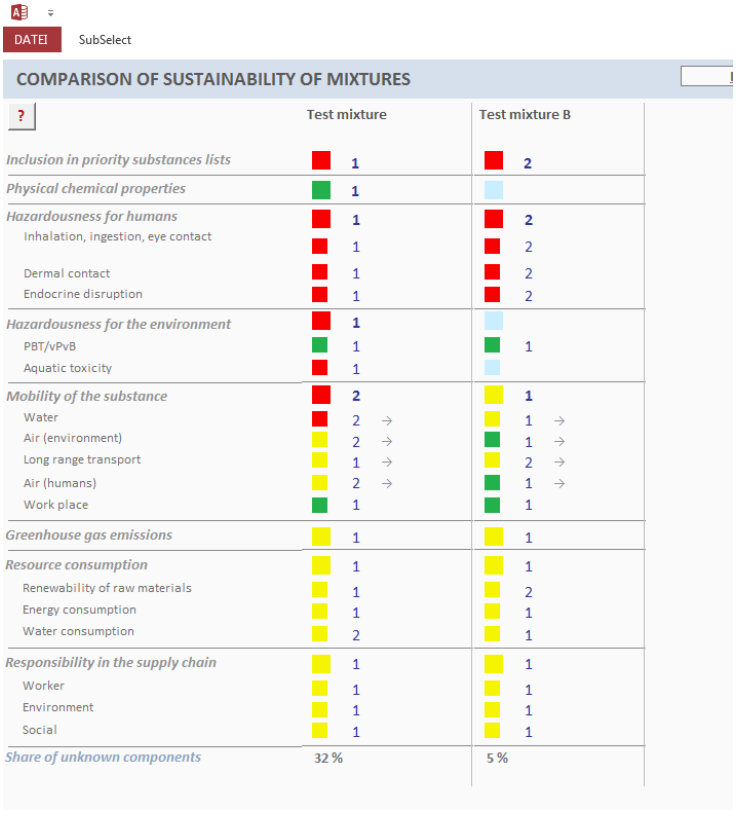
Then you simply continue entering the requested information, just as for the substances using the "forward arrow". As for the substances, you are shown the interim result per each main criterion. As the mixtuer results are based on the evaluations of the components and not all of these can be shown, you have the possiblity of looking them up by clicking on „Details".



6.3 Comparison of sustainability

If you want to compare mixtures, you first enter the mixtures and then select the compare sustainability function, which allows you to select up to 5 mixuters the sustainability performance of whic can be evaluated.

As for the substances, the results of the main criteria and the sub-criteria for are shown for the mixture. The numbers next to the coloured squares indicate the sustainability rank. In the case of lists of substances e.g. the ranking is worse for mixture B, because the concentration of listed substances is higher than in test mixture B. In teste mixture B less substances are contained that are soluble in water and hence, here the rank is better than for the other, however still not good (yellow).



7 Updates

Unfortunately, the tool cannot (yet) automatically run an update, when the candidate list of REACH is updated. Therefore, a new version is provided after every update of the candidate list. If you download and use a new version of SubSelect, keep your „old“ data file and connect it to the programme (click „open“ in the main top menue!).

Then click „run calculation“ on the overview page of substances and mixtures to ensure that if you entered substances that were just included on the candidate list are evaluated with the most recent version of the candidate list!