1. Tutorial of usage

The main concern in the design of this tool was to develop a user-friendly software, able to simulate the response surface modelling that conventional design of experiment software does. On the following pages, it is explained how to use the tool and the options that DSODE offers.

In Table 1, it is shown the tool interface. This will be displayed when the user opens the program.

Table 1. Tool interface: initial sheet

Three different functions have been enabled on this sheet. Users can access them by clicking on the button.

- **New design**: The user will be able to create his experimental design. It is important to highlight that DSODE can create any number of designs, but if two of them have the same number of parameters and the same type of design, the second design will delete the first one. If the user is interested in keeping both, it is recommended to create it in a new file.
- **Clear all**: The user will be able to undo all the changes that could have been done. This button will reset the program. All the designs will be deleted and the susceptible code retyped to its origins.
- **View/Hide code**: The user will be able to display the hidden excel sheets where calculations are done. In an advanced level, it is useful in order to understand the unlikely errors that can arise. These sheets are protected and cannot be modified.

In Table 2, are shown the screens that will be displayed by clicking the new design button. In three easy steps, DSODE will request for all the information needed to prepare the template of the experimental design.

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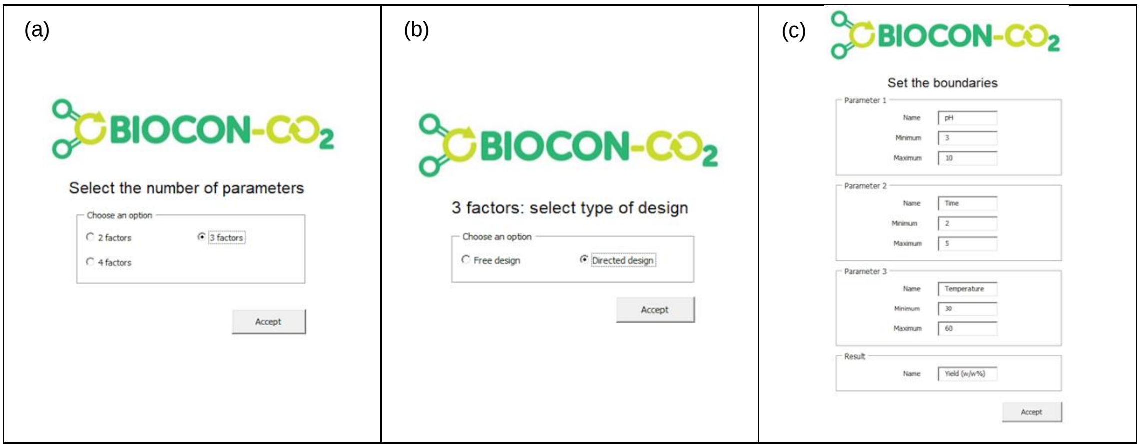
Table 2. Creation of a new design: (a) number of parameters selection, (b) type of design selection, and (c) boundaries and nomenclature.



First, the user will be asked to select the number of variables that will be tested (Table 2.a). Tick the appropriate checkbox and then click the accept button. In the next step, the user will select if the tool will suggest the experiments to do, or if it will be a free design instead (Table 2.b). Do not forget that directed CCC designs are only available for 2 and 3-factors. Otherwise, if the user selects a 4-factor design, only the free design will be available. Tick the checkbox and click accept as in the previous step. In the last step, the user will be able to select the maximum and minimum boundaries for each parameter, as well as the variables and result names (Table 2.c). The response surface will be displayed according to the limits set. Click the accept button after filling all the boxes. Then, a new excel sheet will be displayed as shown in Table 3.

If the directed design was selected, there will be a list of experiments to do with these conditions (Table 3.a). If it is a free design, the user will introduce his conditions manually. If we are working with the directed CCC design, in some cases we will visualize impossible conditions (e.g. negative times or concentrations). As mentioned above, this occurs because its axial points are outside the factorial square. Check the experimental design created and repeat it reducing the boundaries if necessary. Equations 5 and 6 for two-factor, and equations 7 and 8 for three-factor design, are the transformations suggested to the user for the reduction:

- For two-factor design:

$$min_{new} = min_{old} + (max_{old} - min_{old}) \cdot \frac{-1 - (-\sqrt{2})}{\sqrt{2} - (-\sqrt{2})} \qquad (Eq.5)$$

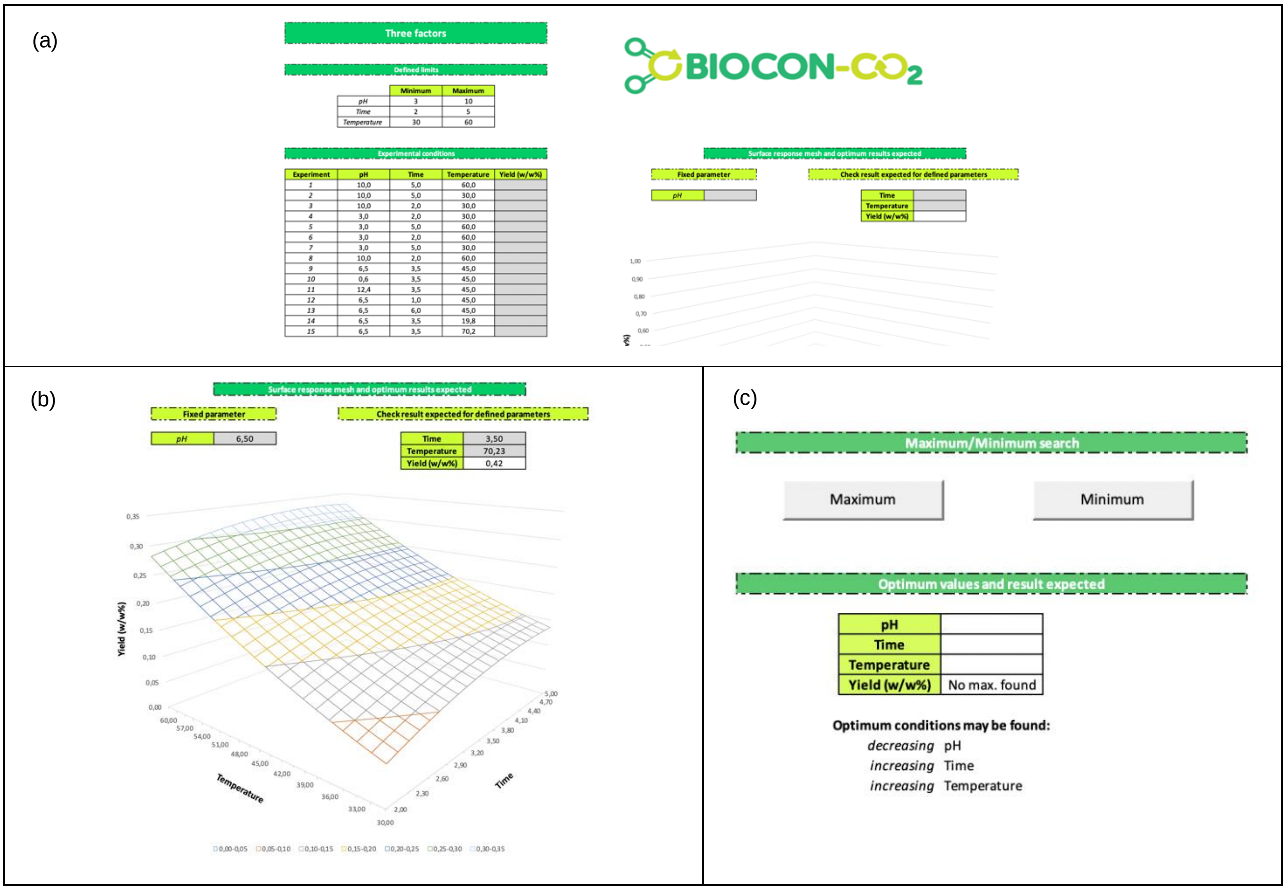
$$max_{new} = min_{old} + (max_{old} - min_{old}) \cdot \frac{+1 - (-\sqrt{2})}{\sqrt{2} - (-\sqrt{2})} \qquad (Eq.6)$$

- For three-variables design:

$$min_{new} = min_{old} + (max_{old} - min_{old}) \cdot \frac{-1 - \left(-\sqrt{2 \cdot \sqrt{2}}\right)}{\sqrt{2 \cdot \sqrt{2}} - (-\sqrt{2 \cdot \sqrt{2}})} \qquad (Eq.7)$$

$$max_{new} = min_{old} + (max_{old} - min_{old}) \cdot \frac{+1 - \left(-\sqrt{2 \cdot \sqrt{2}}\right)}{\sqrt{2 \cdot \sqrt{2}} - (-\sqrt{2 \cdot \sqrt{2}})} \qquad (Eq.8)$$

Table 3. DoE interface: (a) experimental design, (b) response surface, and (c) optimum conditions search



After completing the laboratory tasks, the user will feed the tool with the results achieved in the grey area (KPIs should be used for future comparisons). After that, it is mandatory to set the "fixed parameter" before checking the response surfaces (Table 3.b). If those cells are empty, the tool will set the conditions as zero. In the two-factor design, there are not fixed parameters as it is a unique response surface. In the three-factor design, there are three different graphs, and each one has one fixed parameter. In the four-factor design, there are six, with two parameters fixed on each. Fixed parameters can be varied to generate different surface responses. This is useful to understand the parameters interaction and its performance in the process. Moreover, it has been added a result calculator that estimates the response at certain conditions with accuracy. Finally, two buttons have been enabled to look for optimum conditions (maximums and minimums). By clicking on them, the tool will perform a search of local maximums and minimums (Table 3c). Occasionally, there will not be optimum values in the boundaries set. In those cases, DSODE will suggest the direction where optimum conditions might be found. Also, it is important to highlight that in the 3 and 4-factor designs there might be more than one local maximum or minimum, depending on the values of the parameters fixed. It is recommended to verify that the conditions suggested are the absolute maximum or minimum.

1.1. Selection of the most suitable process

Process selection is done through the comparison of techniques using KPIs. Let us assume that the user wants to compare three different processes: A, B, and C. The main process aim is to obtain a very pure product (KPI_1), but the user needs a significant recovery rate (KPI_2) and low energy consumption (KPI_4) as well, even though in a lower level of significance. He decides to give the following ponderations: KPI_1 has a 60% of relevance as purity is the main requirement of the end-user, while KPI_2 and KPI_4 have a 20% each one. Then, the user will carry out the experimentation. As a result, he will obtain three different optimal conditions, one for each process. He observes that with both, processes A and B, a high purity rate is obtained, even in process A is slightly higher. However, in terms of recovery rate and energy consumption, process B is quite better. On the other hand, process C has unsatisfactory results. He will give different scores according to these observations, as shown in Table 4.

Table 4. KPIs evaluation for different processes

Process indicator		**Ponderation**	**Scores**		
			Process A	**Process B**	**Process C**
KPI_1	*Product quality*	60%	100	90	40
KPI_2	*Separation effectiveness*	20%	80	100	60
KPI_4	*Energy consumption*	20%	70	100	35
Total		100%	90	94	43

According to the final scores, process B seems to be the best option to carry out the studied task. It is important to not set the scores randomly. They should be based on numerical values. For example, a desirable purity might be equal or higher than 99.5%, while purities lower than 70% should not be acceptable. We should set values from 0 to 100 between these conditions. Processes with lower purities than the minimum set should get a 0, while purities that fulfill the maximum requirement should get a 100. Intermediate values should get an interpolated score between the limits.