Module 4: Response surface and mixture designs: principles and applications in R

Trainers: Prof. Romain Glèlè Kakaï, Dr. Eng. Valère Salako, Frederick Tovissodé (MSc.)

Many problems in biological science (crop science, animal rearing, food science and technology, forestry, environmental science, engineering, etc.) require the use of optimization techniques. For example, a researcher wants to extract 3-Deoxyanthocyanidins and phenolic contents from the leaf sheaths of Dye Sorghum focusing on temperature of extraction and the ethanol content of the watery extraction solvent, the aim being to identify which combination of extraction temperature and ethanol content of the watery extraction solvent optimizes the extracted quantity of 3-Deoxyanthocyanidins and phenolic contents. Another example is relative to a factory that wishes to produce juice of baobab, but would like to keep its natural nutritional properties (e.g. content in vitamin A, vitamin C, Iron and Zinc content). The factory therefore wants to operate on the temperature and time of processing. Note that the experiments could be extended to more than 2 factors.

In other cases, the above optimization problem could be expressed in term of *"what is the proportional combination"* of the factors to yield a given response. For example, one may want to optimize the tensile strength of stainless steel. The factors of interest might be the proportions of iron, copper, nickel, and chromium in the alloy. The fact that the proportions of the different factors must sum to 100 % changes the type of design. Additional examples are when one might be developing a pancake mixture that is made of flour, baking powder, milk, eggs, and oil or might be developing an insecticide that blends four chemical ingredients (A, B, C and D). In such situations, the response is a function of the proportions (not their absolute quantity) of the different ingredients in the mixture.

Response surface and mixture designs are tools developed specifically to handle such optimization issues. This module will introduce participants to the principles of Response surface and mixture designs. Next, focus will be put on Central composite design and Box-Behnken design for response surface designs and simplex centroid, simplex lattice and extremes vertice designs for mixture design. Finally the module will take the participants through generating the designs, advices in conducting the experiments, analysing the data and reporting in scientific and professional approaches. The main points to cover include:

- Response surface design
    - Central composite design
    - Box-Behnken design
    - response surface design data analysis in R
    - scientific and professional report of response surface design data modelling
- Mixture design
    - simplex centroid design
    - simplex lattice design
    - extrême vertice design
    - mixture design data analysis in R

scientific and professional report of mixture design data modelling