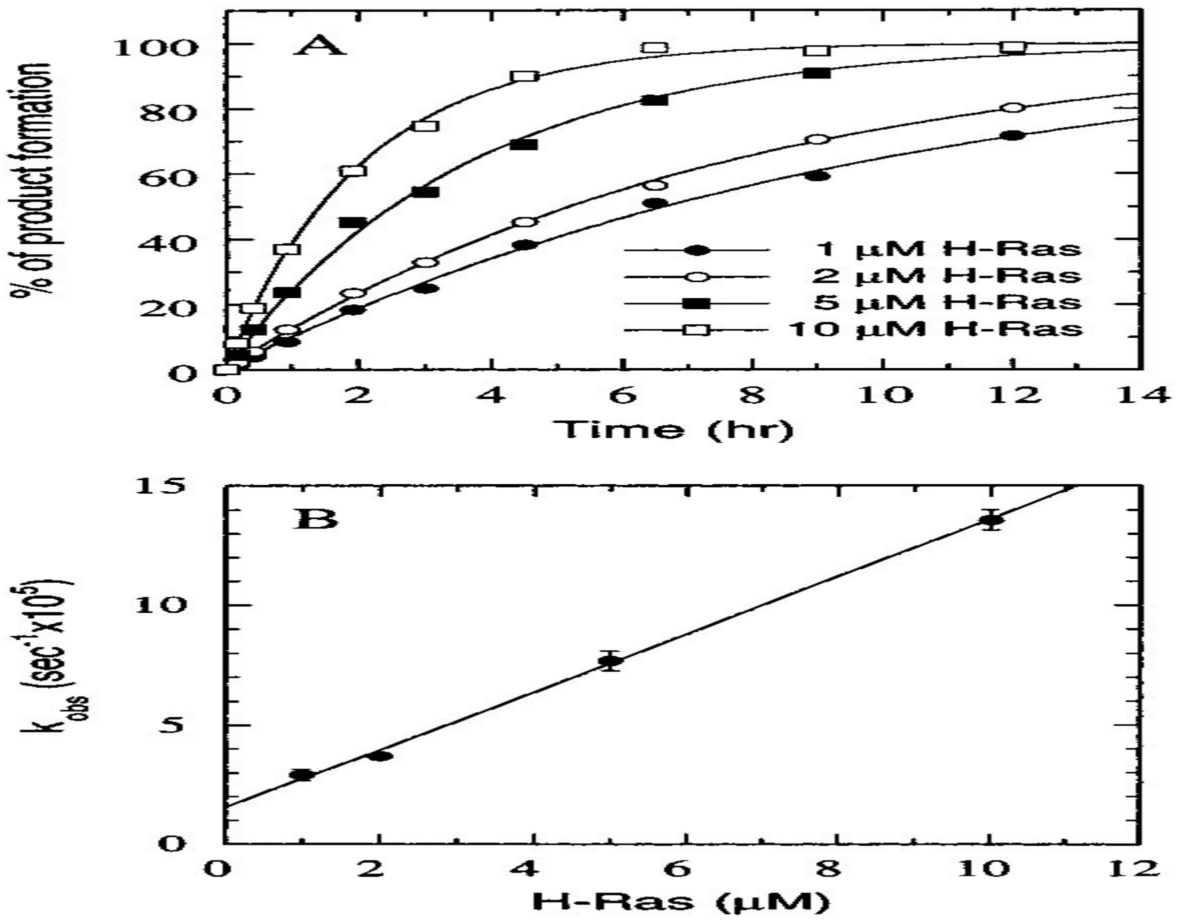
Experimental Design and Modeling

- Major topics:

- Principles of the design of experiment (DoE)
- Full factorial design
- Models
- The role of economic designs
- More complex experimental designs
- Optimization methods

Single-at-a-time experimental work



Common case in experimental studies

- One factor is selected and the scientist carries out series of experiment indication the impact of the selected factor on an output being of interest;
- After obtaining some type of relationship between the input factor and the output signal (at keeping other possible influencing factor at a constant level), another single factor is selected and included into one-at-a-time experimental scheme

The experimental reality and the disadvantages of the single factor strategy

- Usually, the value considered as “optimal” is not real since it reflects the impact of only one factor;
- Possible interaction between different impacting the signal factors is a priori excluded – there is no experimental evidence for interaction;
- In order to reach a possible optimal signal value (minimal or maximal) one needs too many real experiments if the goal is to check all factors influence;
- The single factor approach eliminates other factors from the optimization task.

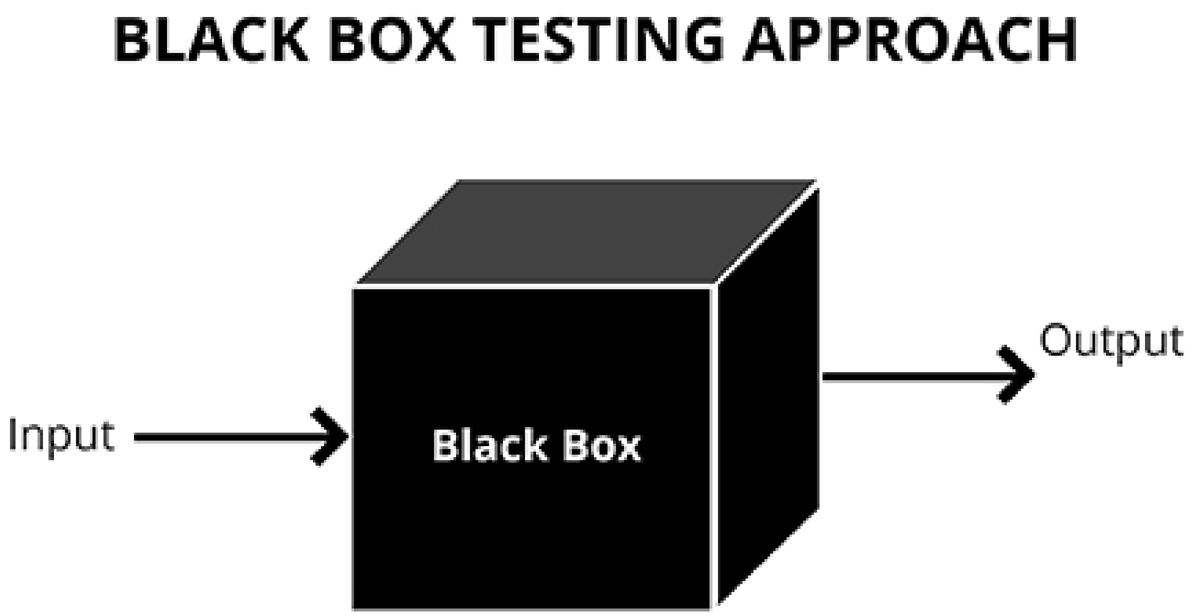
Multifactor strategy

- In the real experimental environment not one but many factors influence simultaneously the output signal – e.g. time, concentration, temperature, distance, length, volume and many others;
- Therefore, another strategy is needed in order to get an adequate model of the system of interest or to reach desirable optimal output;
- According to this strategy all chosen factors should be involved in the experimental scheme at the same time, not one by one;
- This strategy is usually considered as “EXPERIMENTAL Design” since it requires careful planning of the experiments to be carried out.

General scheme of the experimental design approach

- Design of the specific experiment - selection of factors and output;
- Realization of the experiments according to the design;
- Statistical analysis and modeling;
- Assessment and interpretation of the model;
- Decision making and problem solving.

What is BLACK BOX approach ?



Why black box?

- In general, it seems like a magic box of professional magicians – the input is, let's say, a plastic spoon and the output – white rabbit. We are not interested of the mechanisms of changes into the box.
- A similar tactics is foreseen for experimental design; it is important to have well defined inputs (several factors) and a correctly measured output

What is needed in advance

- Problem to be solved
- Choice of input factors (independent variables) Xi
- Output function (dependent variable) Y
- Type of model, usually $y = f(x_i)$
- Interpretation of the relationship “input – output”
- Solutions expected
- Optimization goals

Full factorial design on two levels of the input factors

- It is a simple but very effective approach requiring relatively small number of real experiments;
- Selection of number of inputs – depending on the system in consideration; at least two input factors; the maximal number should not be too big since the increase of factors hinders the model interpretation of mixed interactions and needs high number of real experiments;
- The maximal number of real experiment for this design is 2^n, where n is the number of inputs.

Output function

- There are many options for choice of output – it has to be relatively simple, reproducible, reliable, sensitive to input changes and easy to be measured;
- Very often (especially in analytical chemistry) the output is the analytical signal;
- Yield, specific material properties, physicochemical parameters. Power and information parameters are also possible;
- In some experimental schemes more than one output could be used as dependent variable.

Factor values scaling and standardizing

- In order to construct a simple but effective design allowing a rapid performance of the experiments foreseen a preliminary scaling of the input values for each selected factor is recommendable. It allows easy organization of the whole design and eliminates the differences of the dimensions of the different input factors (concentration, temperature, electric potential etc.) turning them into dimensionless figures, usually + 1 or -1 .

How to select input factors and output function

- The type and the number of input factors depends generally on own experience (expertise, preliminary experiments) and
- On collected a priori information about the system (black box) being studied
- Not recommendable: too many factors (significant number of real experiments are required) or small number of factors (not enough to describe the system of interest) – the responsibility of the experimentalist
- One or more output functions? The most important thig is the output to be easy to measure!

What next?

- The experimental design itself!
- For each input a HIGH level and a LOW level of variation is selected; the values selected for both levels are normalized to + 1 and – 1 in a simple way;
- The interval between HIGH and LOW level of variation is called “spread” ; it has an average level (middle of the interval); the distance between the middle level and the high (or low) level is called “variation step”;
- The selection of all these parameters is responsibility of the experimentalist (information and previous experience)