



A mixture experimental design with 6 components and the effects on smoke constituents

**1) Experimental design and some initial
results on physical and chemical
characteristic of cigarettes and blends**

**2) Hoffmann analytes behaviour through a
mixture experimental design**

**Gilles Figuères*, B. Vidal*, J.P. Biesse*,
B. Brégeon*, F. Louvet**, L. Muzellec*****

*** ALTADIS Research Center, Fleury-les-Aubrais, France**

**** ENSCI, Limoges, France**

***** Université de Bretagne, Brest, France**

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**A mixture experimental design with 6 components
and the effects on smoke constituents**

1) Experimental design and some initial results on physical and chemical characteristic of cigarettes and blends

**J.P. Biesse^{*}, B. Vidal^{*}, Gilles Figuères^{*},
B. Brégeon^{*}, F. Louvet^{**}, L. Muzellec^{***}**

*** ALTADIS Research Center, Fleury-les-Aubrais, France**

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General Objectives

- **Understanding the influence of each component (preblend of 6 types of tobacco) in complex blend on the chemical and physical characteristics of blends and cigarettes and particularly on the mainstream smoke yields of “Hoffmann” compounds.**

Analysing and comparing their importance on the physical, chemical and smoke properties.

- **Using model with the knowledge of observed response variations in order to contribute to the conception of new blend with lower yields of “Hoffmann” compounds.**

1) Experimental design and some initial results on physical and chemical characteristic cigarettes and blends

Objectives

■ Objectives of this presentation

→ EXPERIMENTAL STRATEGY

→ MATERIAL: Cigarettes manufacturing

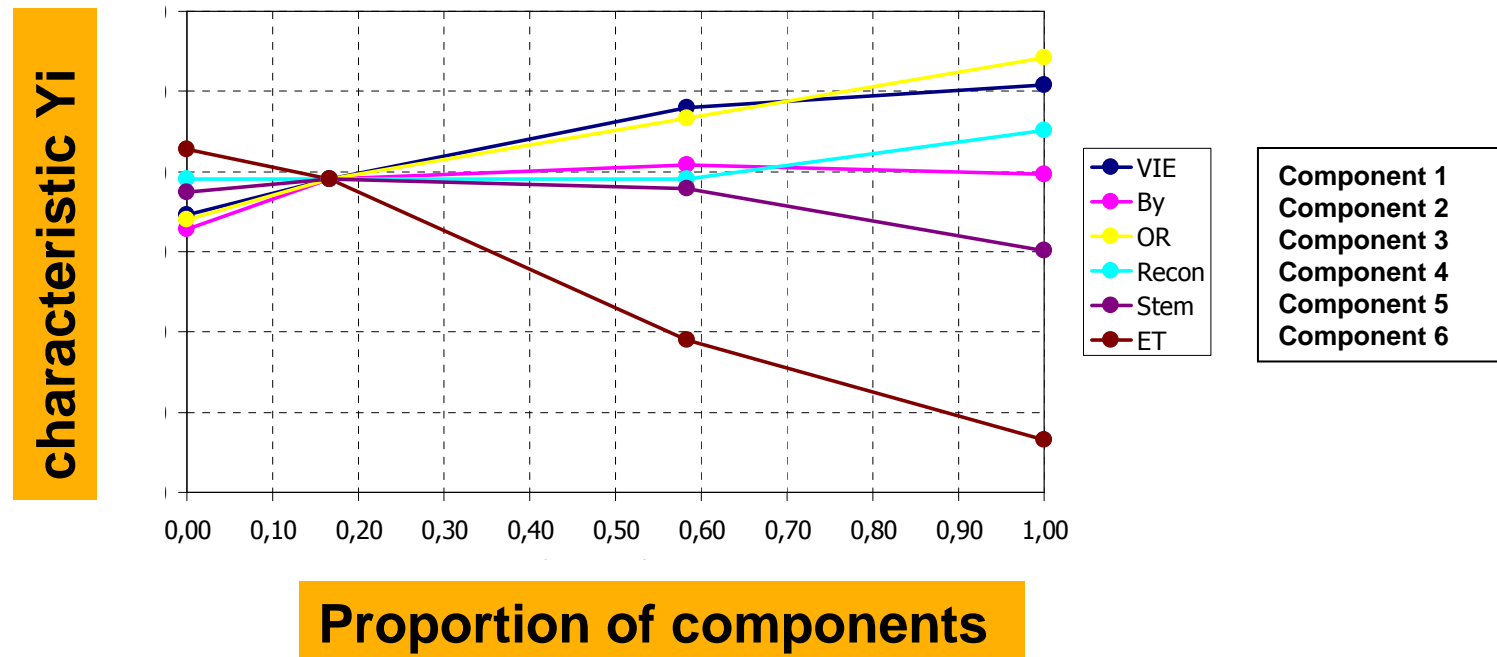
→ MEASUREMENTS

**→ SOME RESULTS ON PHYSICAL, COMMON SMOKE
CONTITUENTS**

■ FIRST CONCLUSIONS

Experimental Strategy

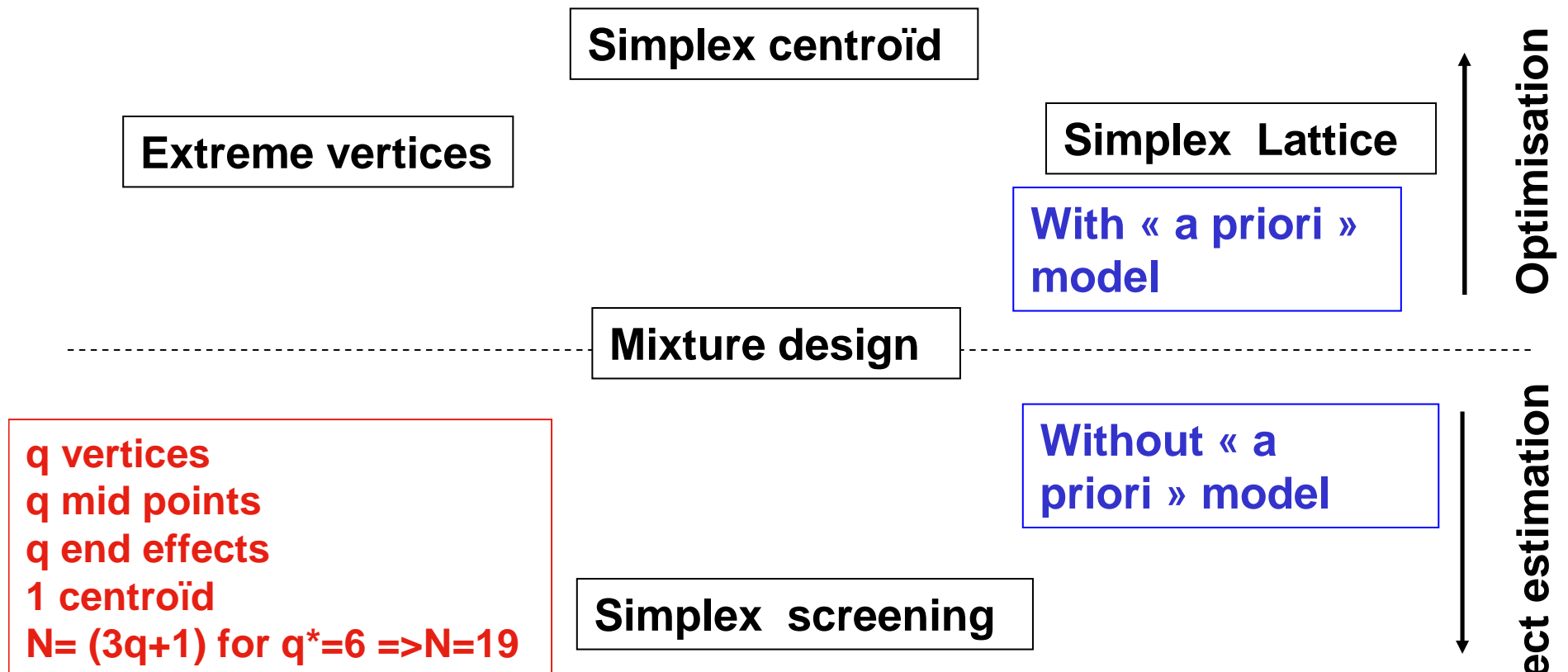
Result expression :



Determination of trial number and their organisation in the experimental space?

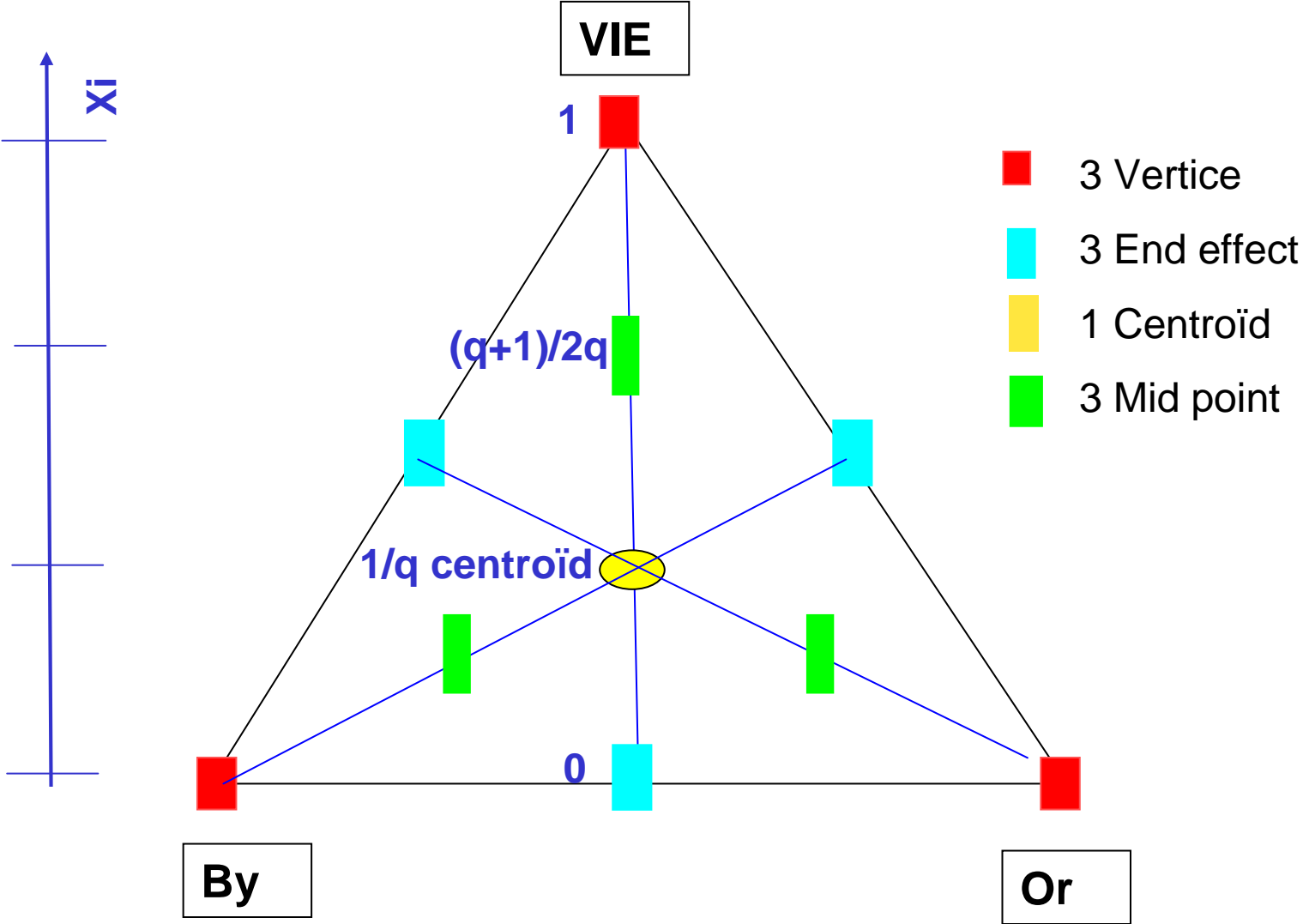
Experimental Strategy

■ The different mixture design

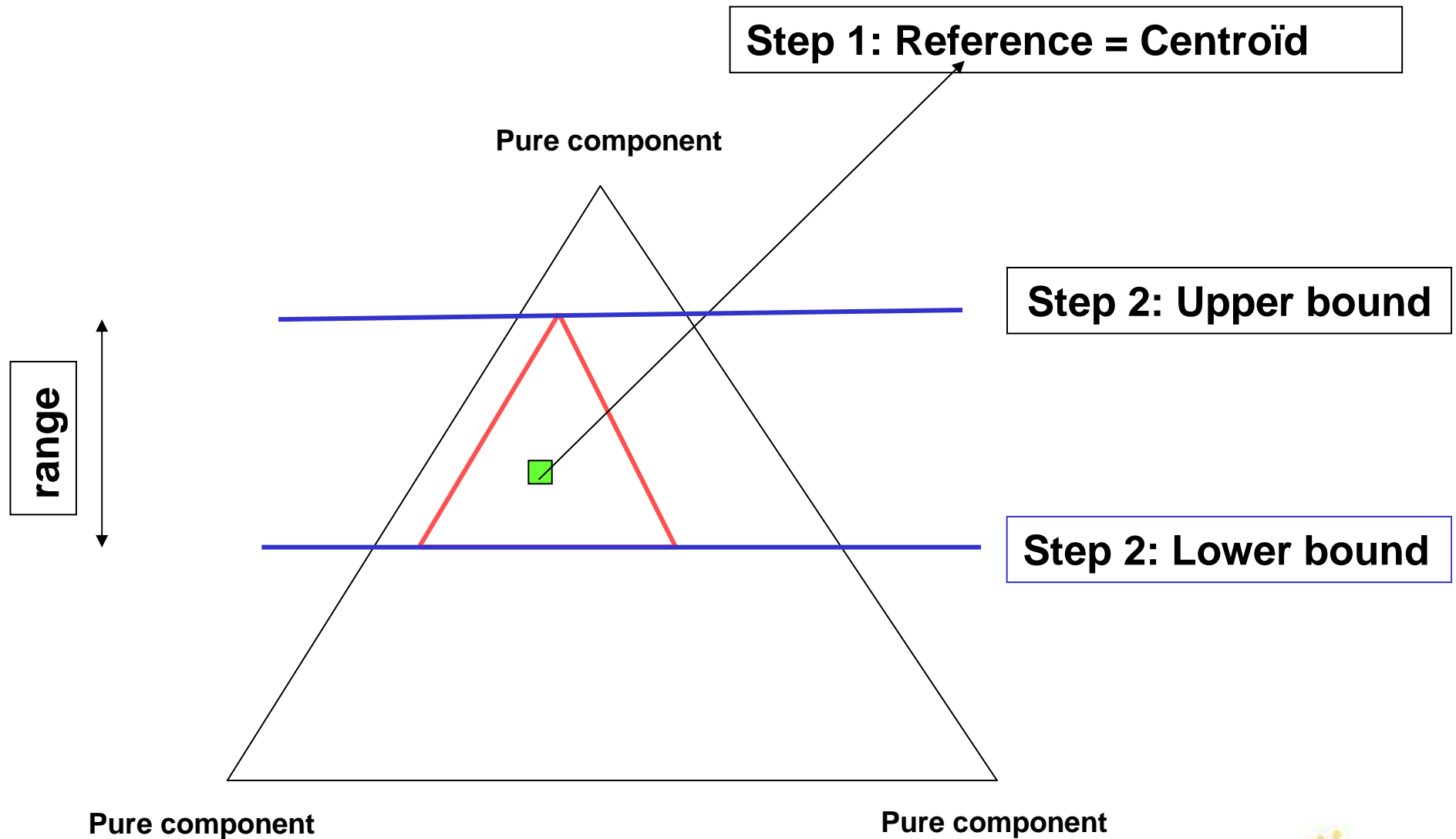


Disposition for 3 components

$q=3 \Rightarrow N=10$



Construction of experimental space



Composition of blends

Mathematical space (pseudo-component)

	essai	VIE	BY	OR	RECON	STEM	ExpandedTob
Vertex	GV1	1,0000	0,0000	0,0000	0,0000	0,0000	0,0000
Vertex	GV2	0,0000	1,0000	0,0000	0,0000	0,0000	0,0000
Vertex	GV3	0,0000	0,0000	1,0000	0,0000	0,0000	0,0000
Vertex	GV4	0,0000	0,0000	0,0000	1,0000	0,0000	0,0000
Vertex	GV5	0,0000	0,0000	0,0000	0,0000	1,0000	0,0000
Vertex	GV6	0,0000	0,0000	0,0000	0,0000	0,0000	1,0000
End effect	GEE1	0,0000	0,2000	0,2000	0,2000	0,2000	0,2000
End effect	GEE2	0,2000	0,0000	0,2000	0,2000	0,2000	0,2000
End effect	GEE3	0,2000	0,2000	0,0000	0,2000	0,2000	0,2000
End effect	GEE4	0,2000	0,2000	0,2000	0,0000	0,2000	0,2000
End effect	GEE5	0,2000	0,2000	0,2000	0,2000	0,0000	0,2000
End effect	GEE6	0,2000	0,2000	0,2000	0,2000	0,2000	0,0000
Centroïd	TEGCEN	0,1667	0,1667	0,1667	0,1667	0,1667	0,1667
Mid point	GMID1	0,5833	0,0833	0,0833	0,0833	0,0833	0,0833
Mid point	GMID2	0,0833	0,5833	0,0833	0,0833	0,0833	0,0833
Mid point	GMID3	0,0833	0,0833	0,5833	0,0833	0,0833	0,0833
Mid point	GMID4	0,0833	0,0833	0,0833	0,5833	0,0833	0,0833
Mid point	GMID5	0,0833	0,0833	0,0833	0,0833	0,5833	0,0833
Mid point	GMID6	0,0833	0,0833	0,0833	0,0833	0,0833	0,5833

Materials and measurements

Experimental Cigarettes

- Constant cigarette design
 - Same Non Tobacco Materials with filter tip
 - Constant Pressure Drop.
 - No casing, no flavour
- 19 tobacco blends used for Mixture Design with tobacco preblends in various proportions.
- + 6 tobacco preblends ⇔ pure components (blend of Virginia, Oriental, Burley, Stems, Expanded and Reconstituted tobacco).

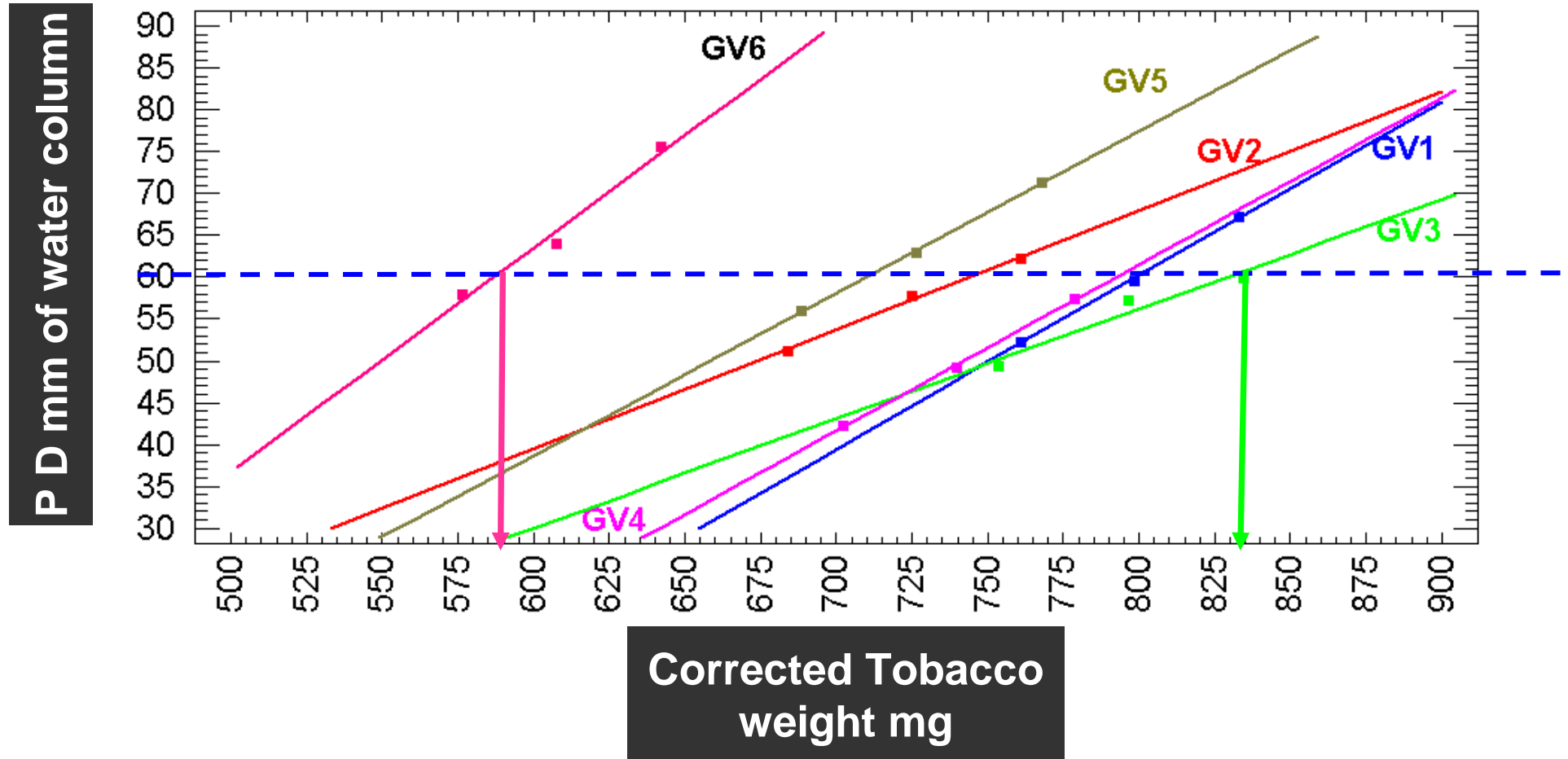
Measurements

Physical measurements: 18 variables (free burning rate, hardness, tobacco weight, tobacco filling power...)

Current smoke constituents of the mainstream smoke: 6 compounds of interest (Nico, Tar, CO, Puff,...)

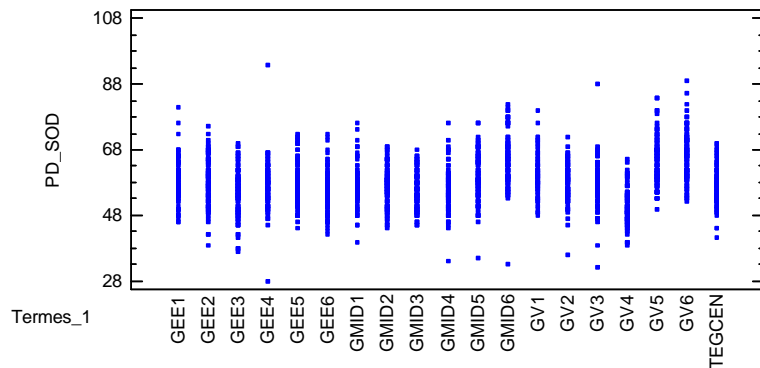
Smoking tests in compliance with ISO conditions

Pressure drop function of weight of tobacco rod

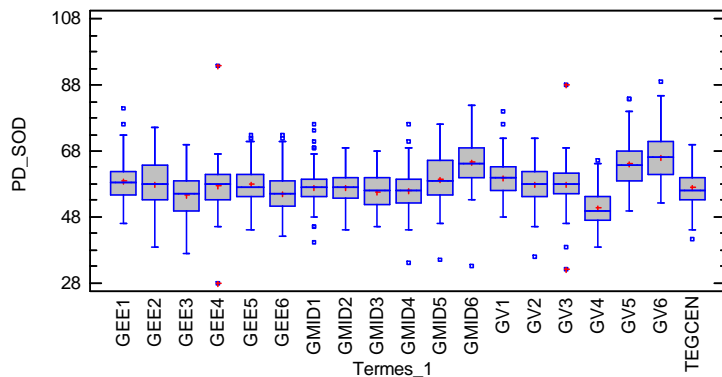


Checking of Pressure Drop of tobacco rod after cigarette manufacturing.

Scatter plots



Box and Whisker plots



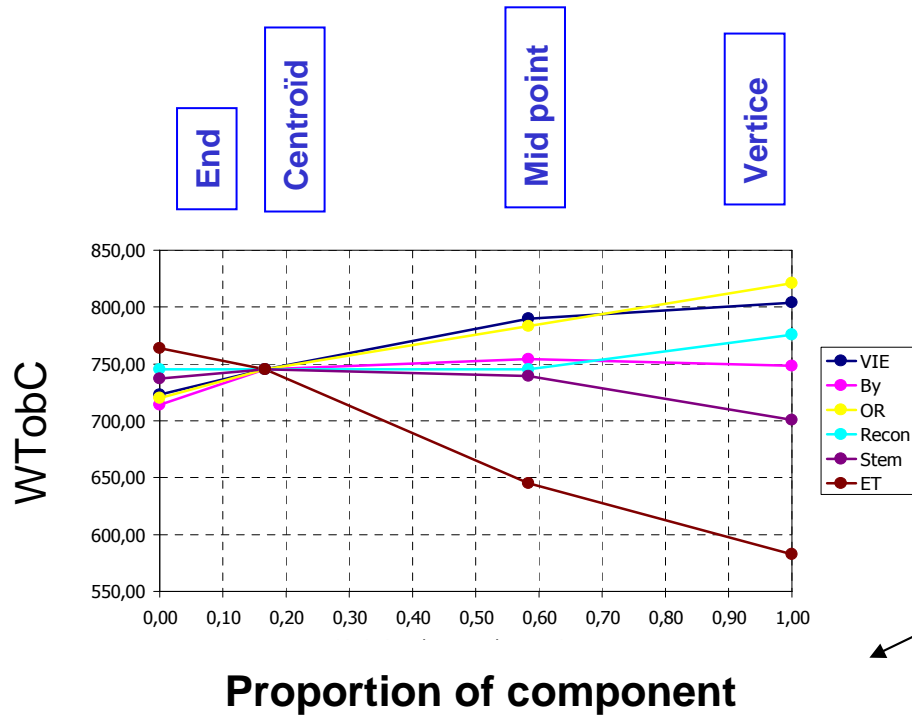
Trials	Average	SD
GEE1	58,7	6,3
GEE2	58,2	7,1
GEE3	54,8	7,0
GEE4	57,3	6,8
GEE5	57,8	6,2
GEE6	55,1	6,4
GMID1	57,1	5,9
GMID2	56,9	5,7
GMID3	55,7	5,4
GMID4	55,9	6,2
GMID5	59,5	7,2
GMID6	64,5	7,6
GV1	60,1	6,2
GV2	57,9	5,6
GV3	57,9	6,8
GV4	50,6	5,4
GV5	64,3	7,1
GV6	66,1	7,1
TEGCEN	56,8	5,7

Some results: effect of each component:

Weight Tobacco Humidity Corrected

Observed data

Objective 1: effect estimation

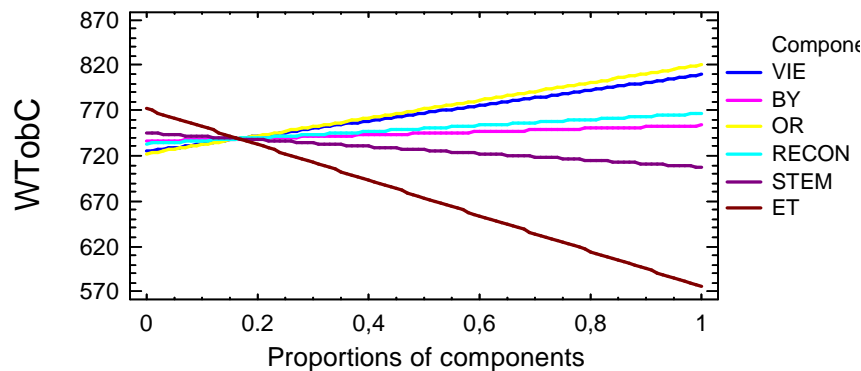


Linear model is well adapted for objective 2.

Linear Model

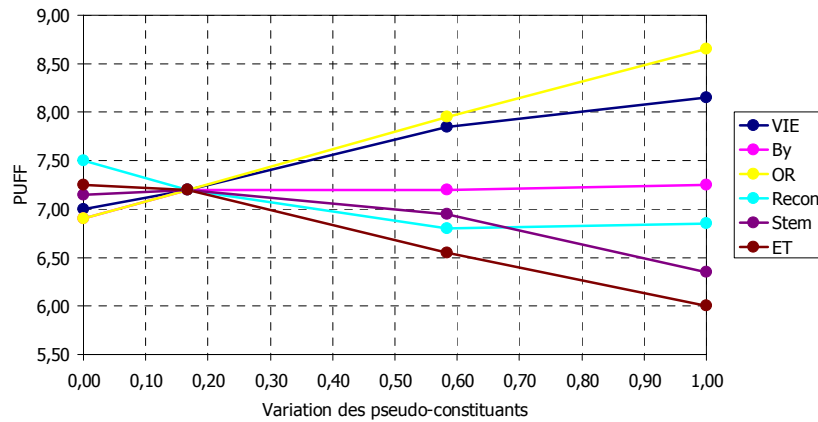
$R^2_{adj}=95.3\%$

Objective 2: optimum determination



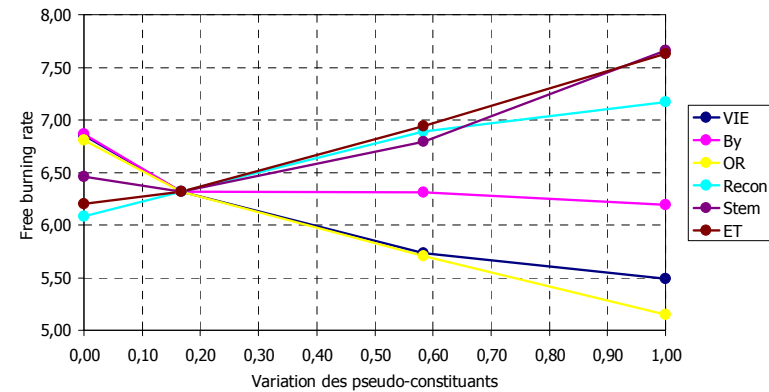
Some results : effect of each component

Puff/cig



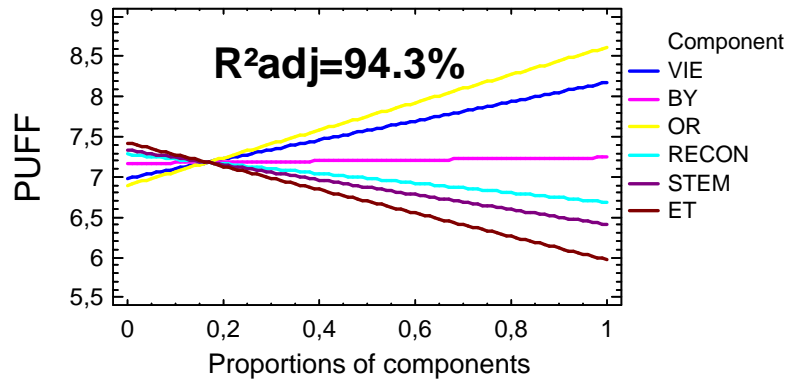
Objective 1: effect estimation

Free Burning Rate

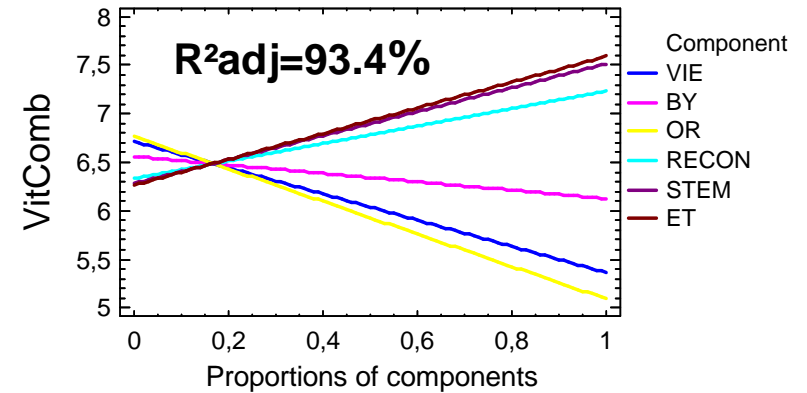


Objective 2: optimum determination

Trace graph for PUFF

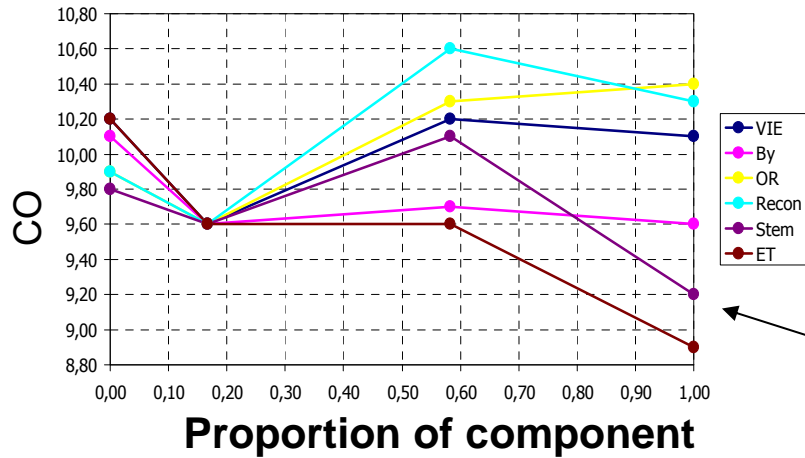


Trace graph for VitComb

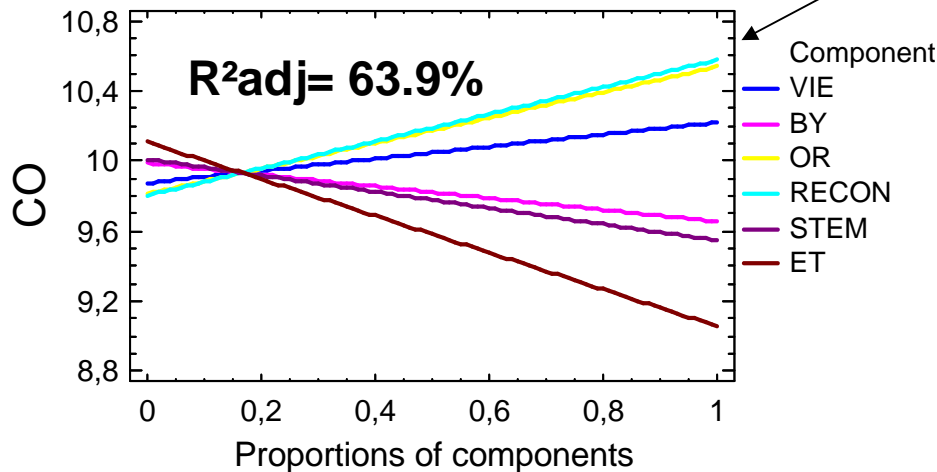


Some results : effect of each component

Characteristic: CO



Trace graph for CO



Objective 1: effect estimation

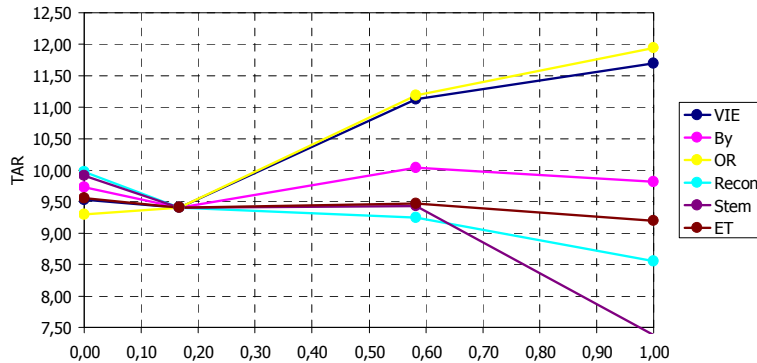
Linear model is insufficient for good description of response variation.

Objective 2: optimum determination

The degree of the model has to be increased (stepwise regression).

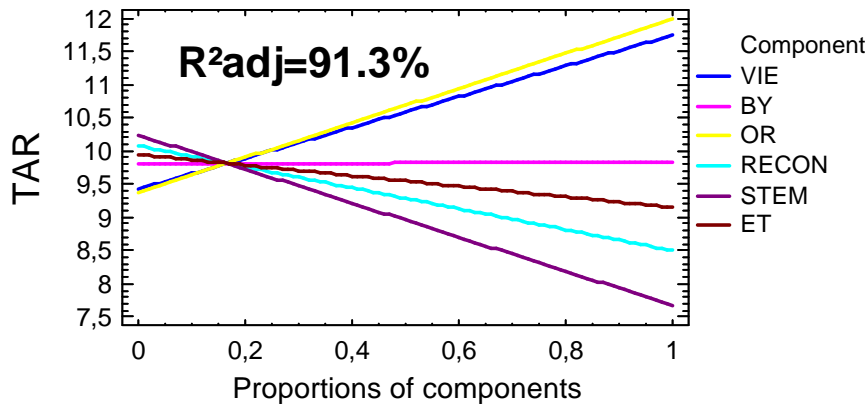
Some results : effect of each component

Tar/cig

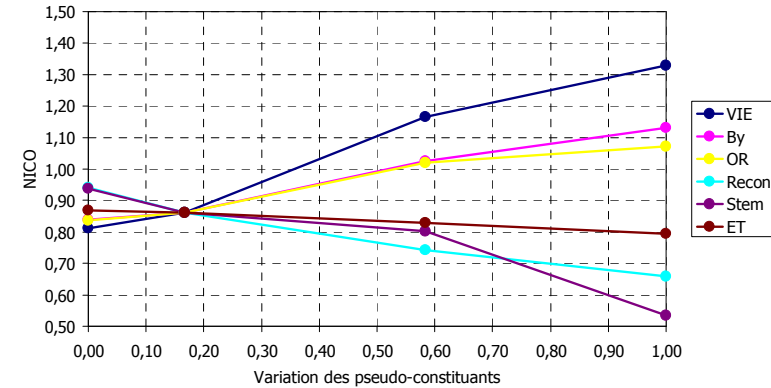


Proportion of component

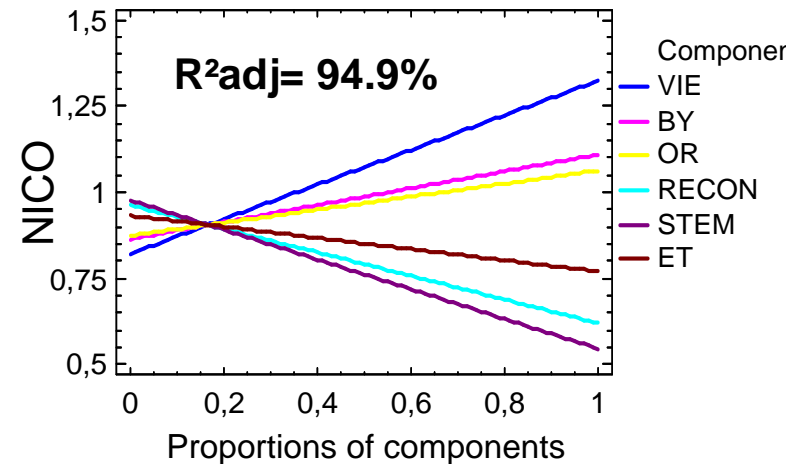
Trace graph for TAR



Nicotine/cig



Trace graph for NICO



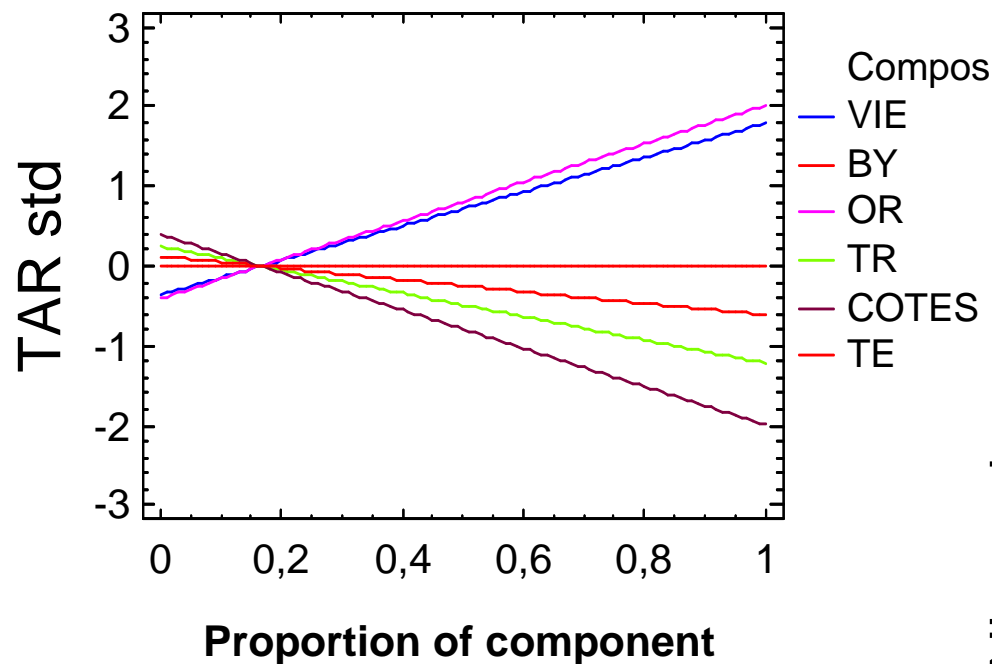
Objective 1: effect estimation

Objective 2: optimum determination

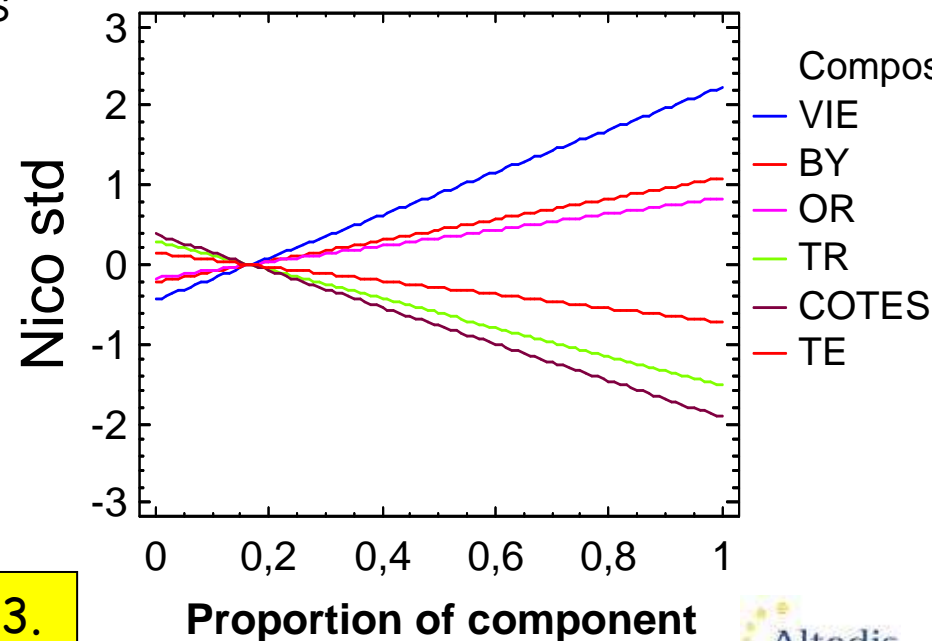
Comparison of effect of each component. Data normalization (by centering and reducing)

TAR & Nicotine

Trace graph for Puff std



Trace graph for NICO std



the range of the effect varies from -3 to +3.

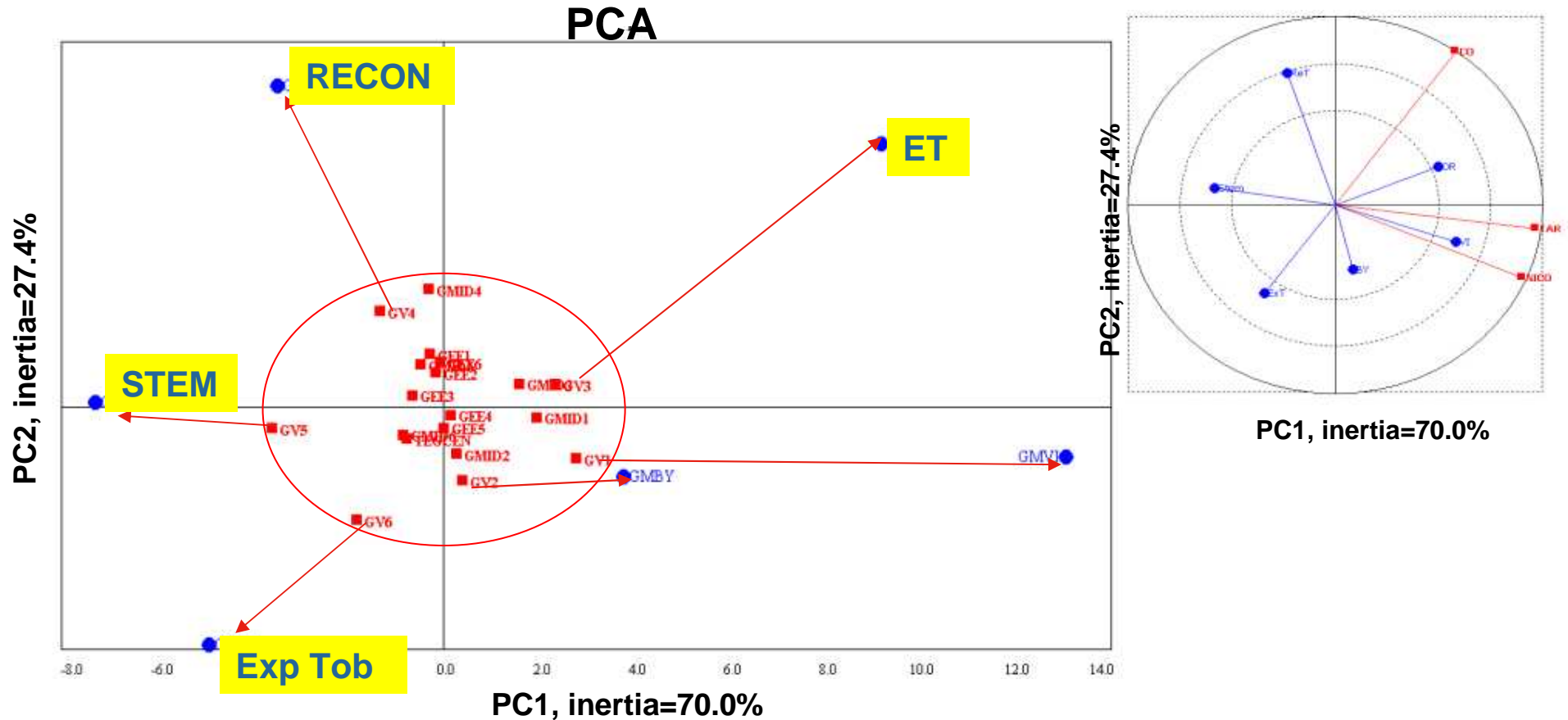
Table for R^2_{adj} (linear model)

Response	R^2_{adj}
Tar_NIC	96,59%
Wtobc	95,31%
NICO	94,91%
Ni_PUF	94,40%
PUFF	94,34%
Dry.PM	91,92%
Tar	91,31%
TPM	89,46%
Tar_PUF	74,00%
CO	63,69%
Hard C	56,84%
PD	55,87%
WATER	49,84%
PDEF	49,65%

Good ajustement

Weak ajustement

IS IT POSSIBLE to extrapolate some conclusions outside the studied space?



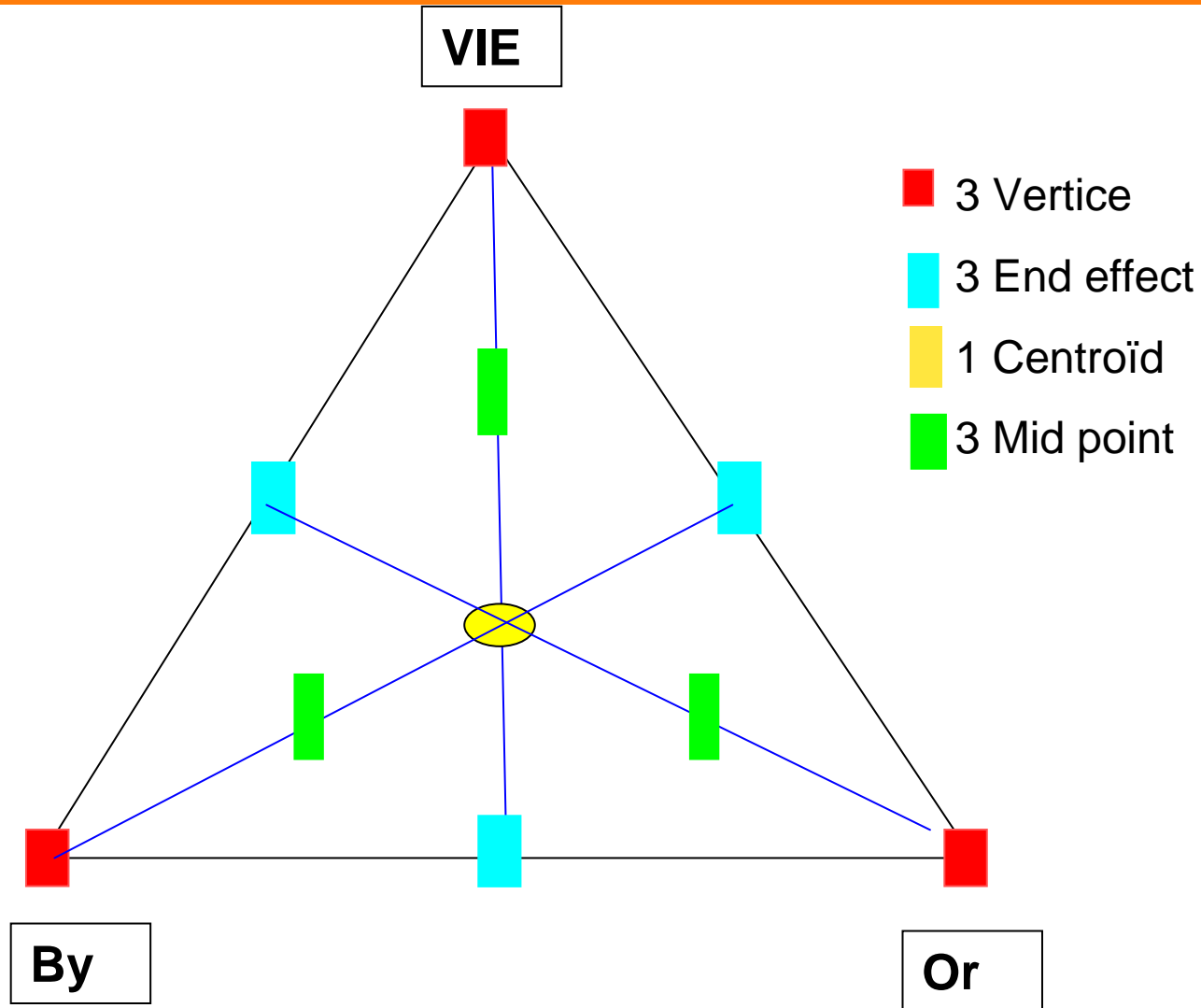
It seems possible to enlarge the conclusions of this experiment out of the framework of this design

Conclusions

- Experimental mixture design allows to measure the effect of 6 components and to model their influences.
- The number of trials is reduced and the restitution of results is easy.
- The construction of mixture design must be done carefully to achieve successful results.
- The simple multiple linear model is often adequate.
- We can enlarge the conclusions to the nearest neighbourhood
- We confirm the known effects of each component on some parameters. Yet with this mixture design, we have to consider when a component varies in proportion the others vary accordingly.
- .

Disposition for 3 components

$q=3 \Rightarrow N=10$



Yet with this mixture design, we have to consider when a component varies in proportion the others vary accordingly

Thank you for your attention !

First Internet system



Internet precursor french system, called "télégraphe de Chappe" which worked from 1823 to 1850.