Suivi en temps réel de l'évolution de la qualité organoleptique des pommes lors d'un procédé thermomécanique par SPIR

Auteurs

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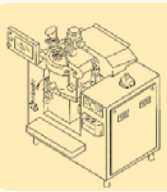
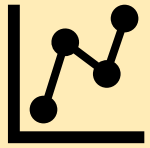
Context



Thermomechanical operation (Grinding + heating) : Information and understanding ?

Need for decision-support tools to adapt processes to raw materials variability



Monitoring rapid changes in apple puree quality

To identify during processing markers or properties explaining the final characteristics of apple puree and to predict them

Experiments

Design of experiments: full two-level factorial design

Preleminary tests

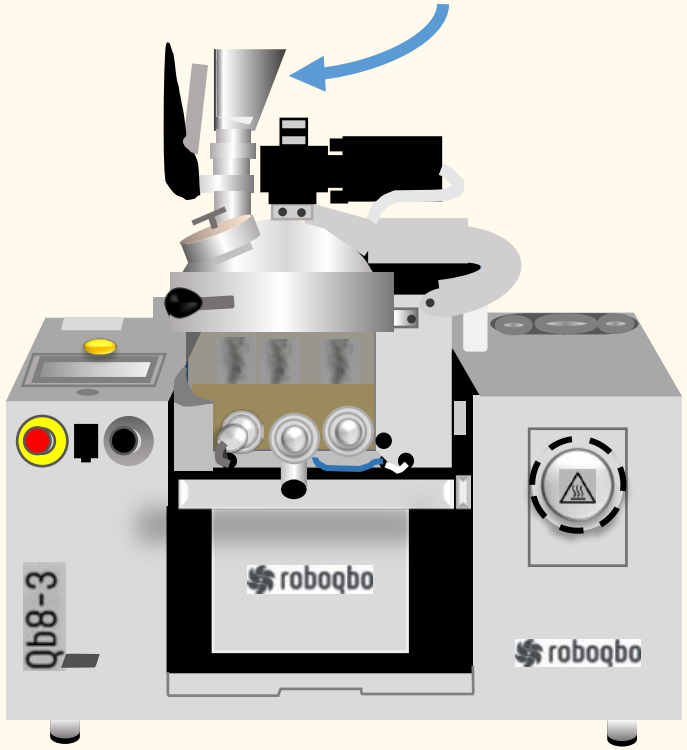
- *Defining factor choices*
- *Defining factor levels*
- *Sampling feasibility test*
- *Control of apple oxidation*

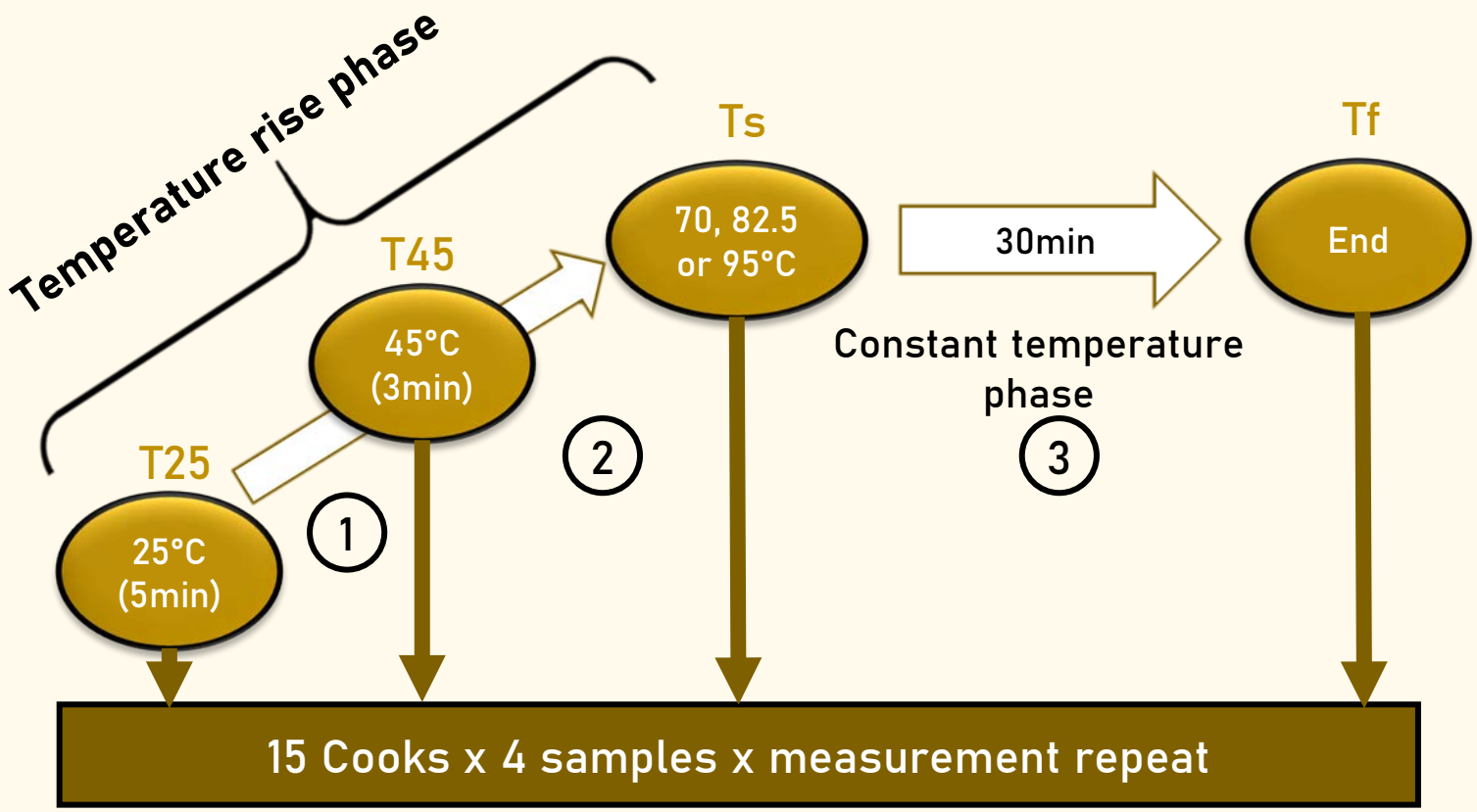
Condition	Speed (rpm)	Temperature (°C)
1	300	70
2	1000	95
3	300	95
4	1000	70
5*	**650**	**82.5**

Triplicate

Apple puree processing

Apple slices + Ascorbic acid



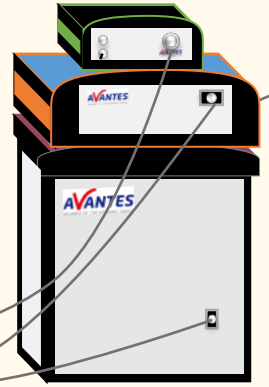


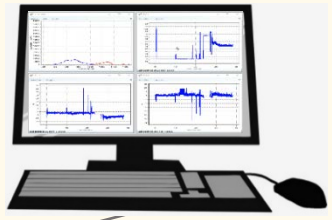
5 Operating conditions

3 repetitions of each Operating conditions
(3.5 kg of raw apples per batch)

In-line and off-line Measurements

1-In-line and off-line measurements to monitor the characteristics of puree during processing





IN LINE

Continuous data acquisition every 10s
Spectra visible and NIR
(3818 spectra)

OFF LINE

60 reference data

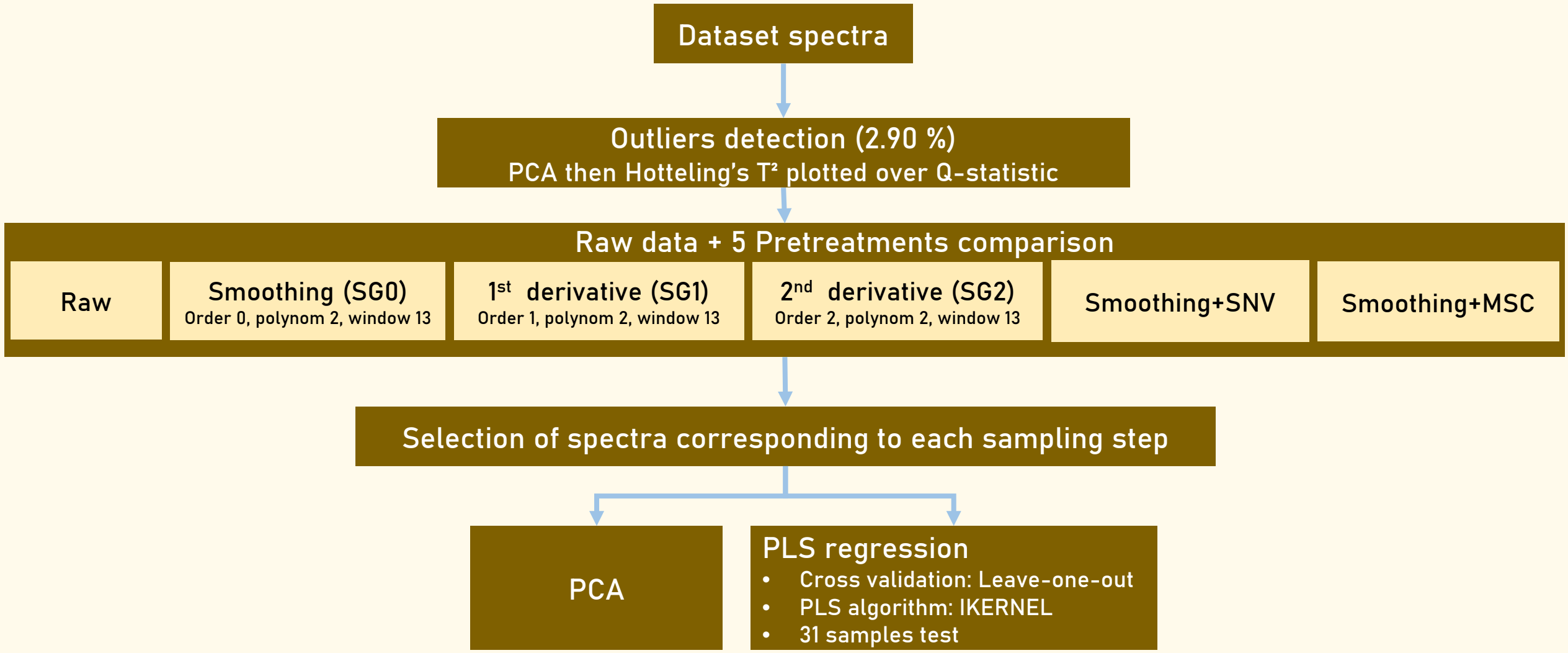
Apple puree samples

VOCs analysis with ATD GC-MS
- Headspace method
- 15 volatile compounds selected

Biochemistry
- pH
- titratable acidity
- soluble solid content
- water content

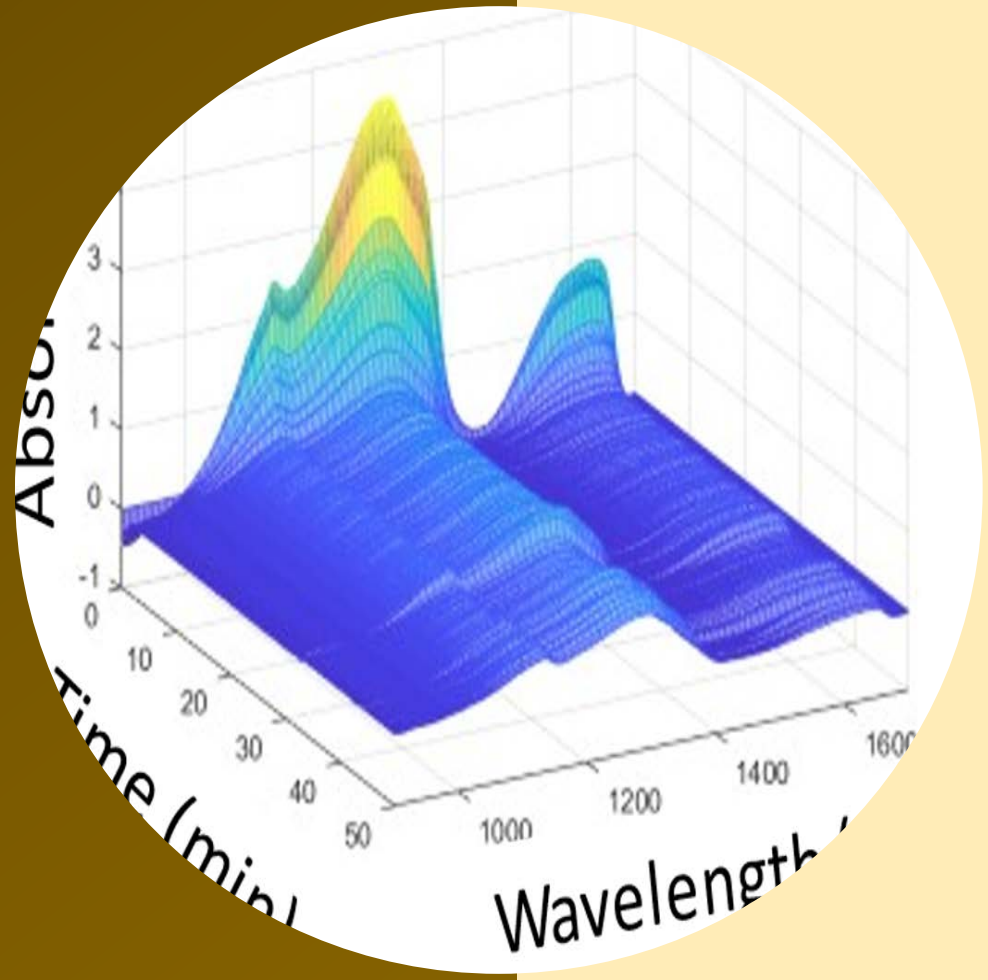
Physical parameters
- Viscosity
- Particle size analysis
  - laser diffraction (< 800µm)
  - Imagery (> 800µm)

NIR data processing



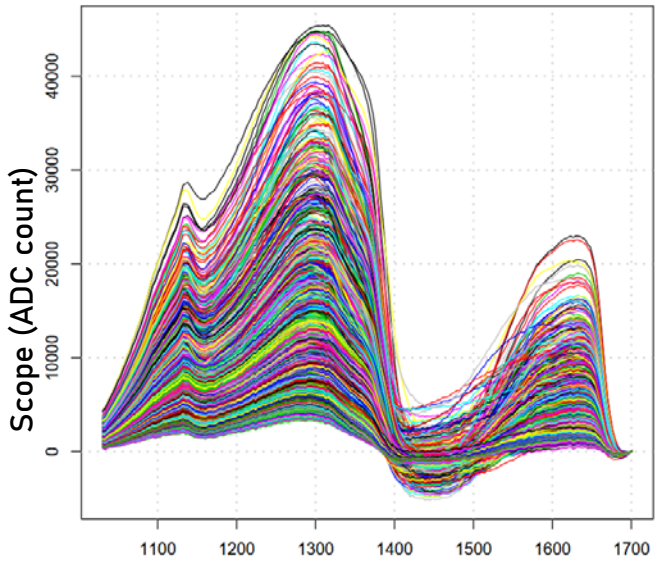
SG: Savitzky-Golay algorithm ; **PCA:** Principal Component Analysis ; **SNV:** Standard Normal Variate ; **MSC:** Multiplicative Scatter Correction

Results

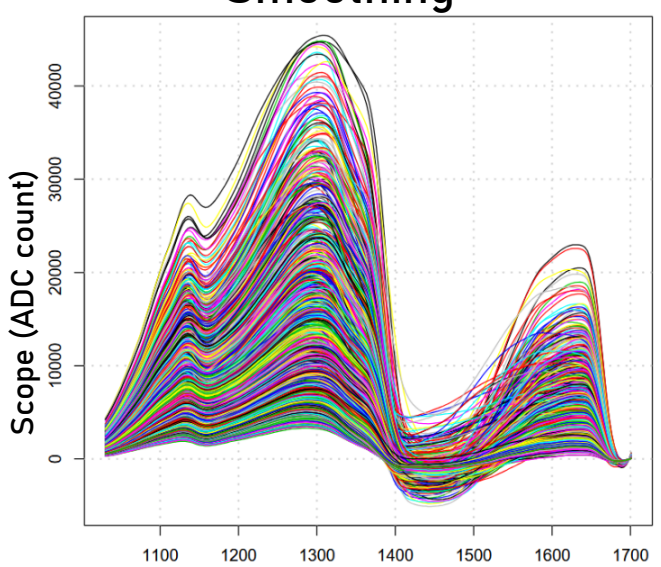


NIR Spectra (1000 – 1700 nm): Pretreatments comparison

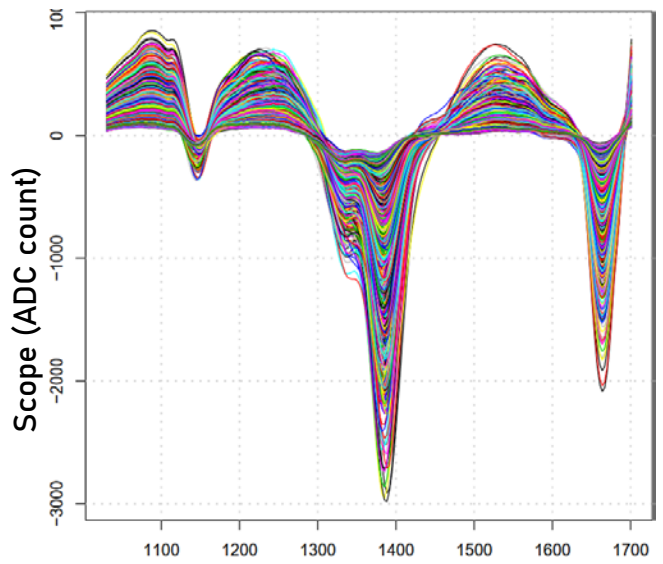
Raw



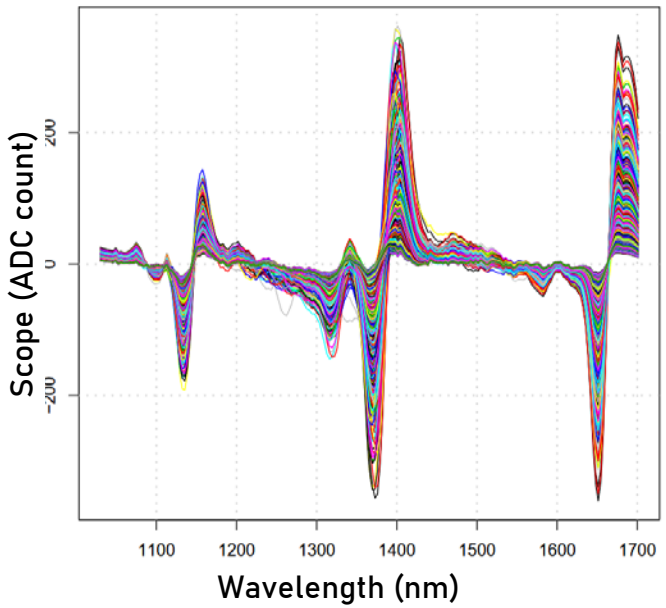
Smoothing



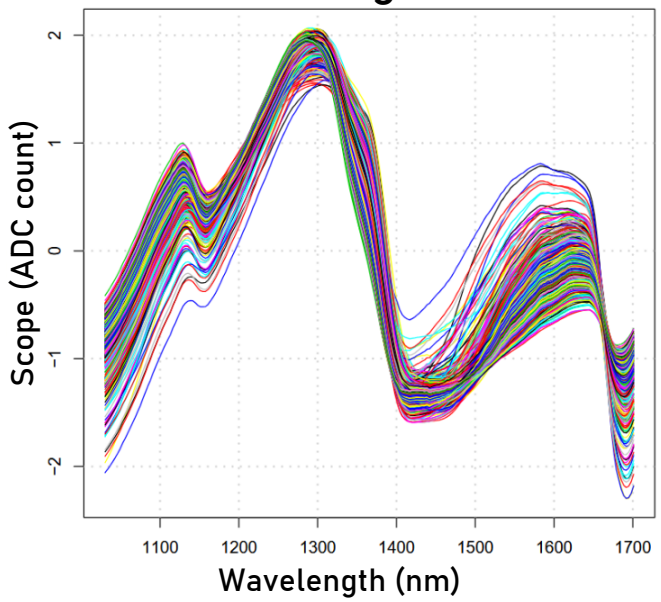
1st derivative



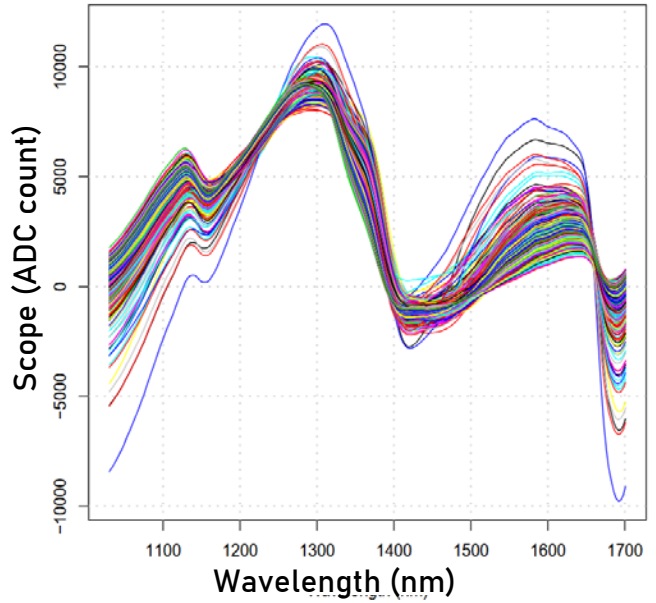
2nd derivative



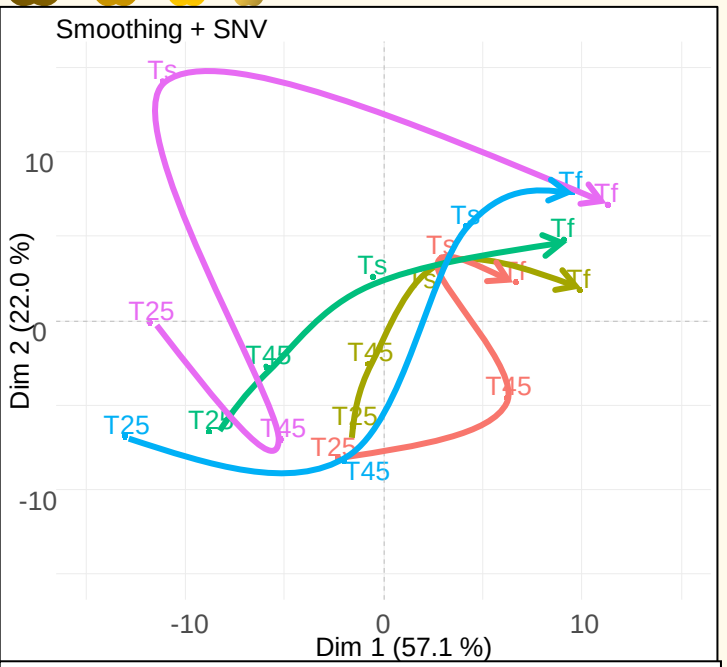
Smoothing+SNV

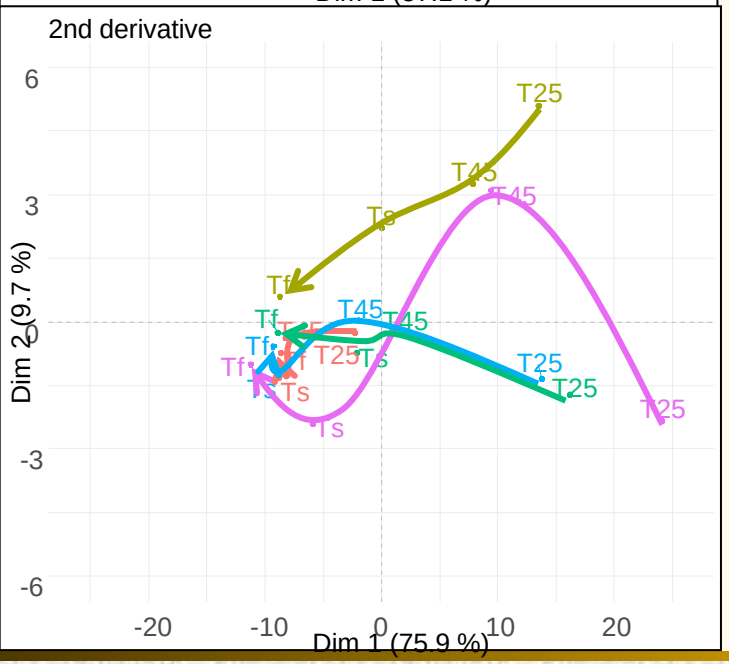


Smoothing+MSC



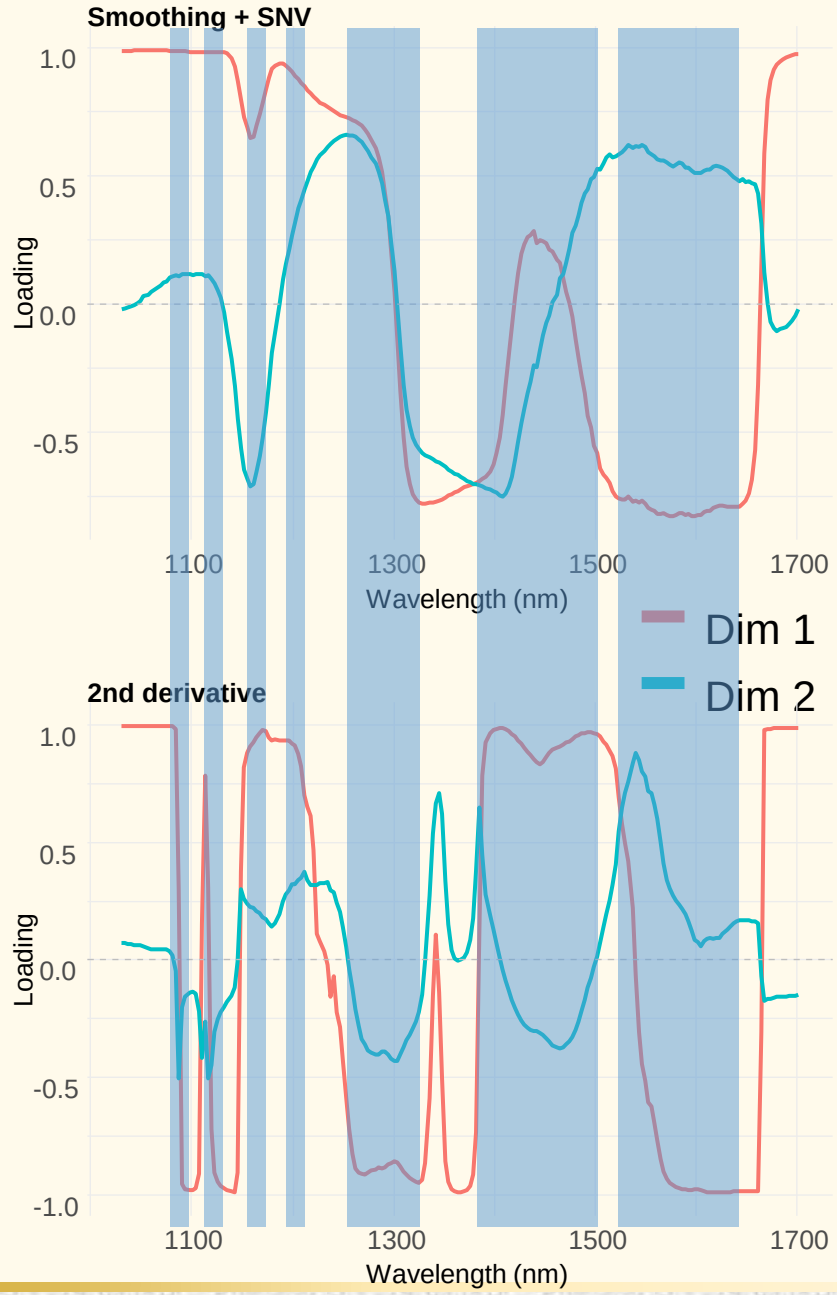
NIR Spectra (1000 – 1700 nm): PCA and loadings





Processing conditions

- 70/300
- 70/1000
- 82.5/650
- 95/300
- 95/1000



1100 and 1250 nm : sugar content (*Ma T. et al., 2018*), **1180-1210, 1239, 1290 – 1330 nm** (*Lan W. et al., 2022*)

1139, **1180-1210**, **1307-1330 nm**: Dry matter content (*Lan W. et al., 2022*)

1386–1392 nm : combination of O–H bonds of waters and C–H bonds of sugars and organic acids in apples (*Kemps B. et al., 2010*)

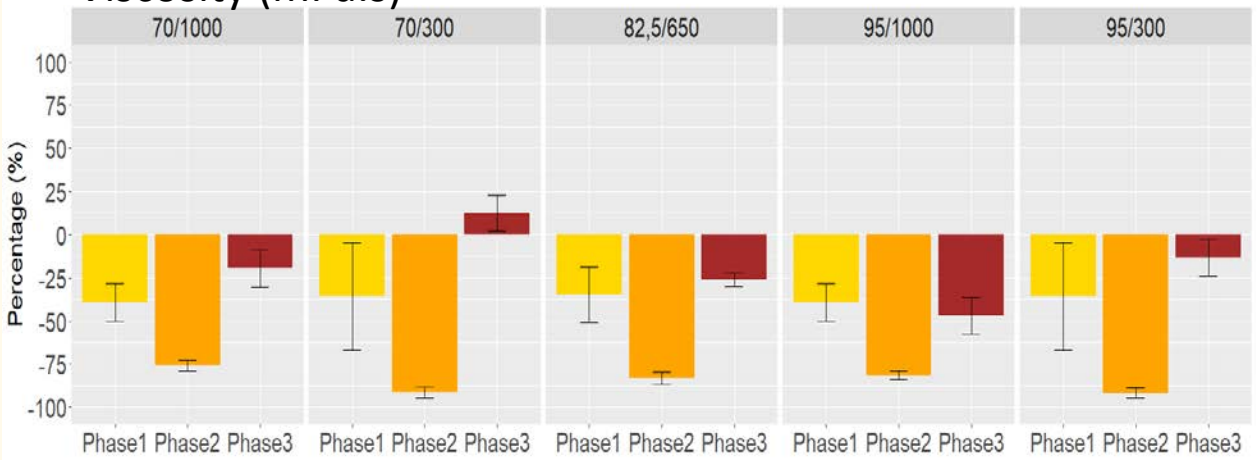
1410–1498 nm : Viscosity prediction (*Lan W. et al., 2022)*

1550–1730 nm : major variations for discrimination of apple purees, (*Lan W. et al. 2020*)

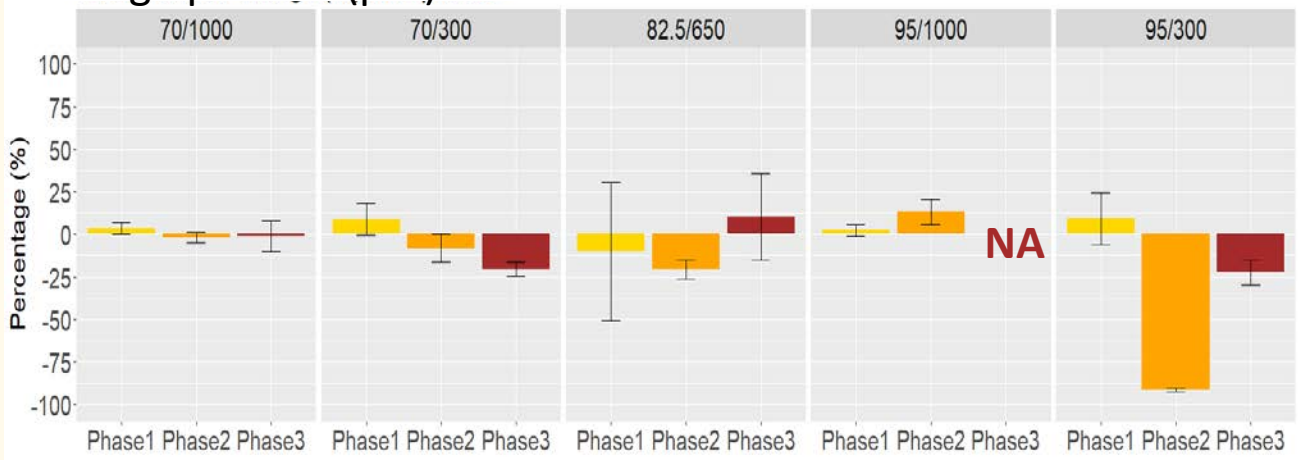
Variation (%) of apple puree quality traits over phases

The biochemical measurements : Statistically no difference. Constant over time and therefore could not be modeled using PLS.

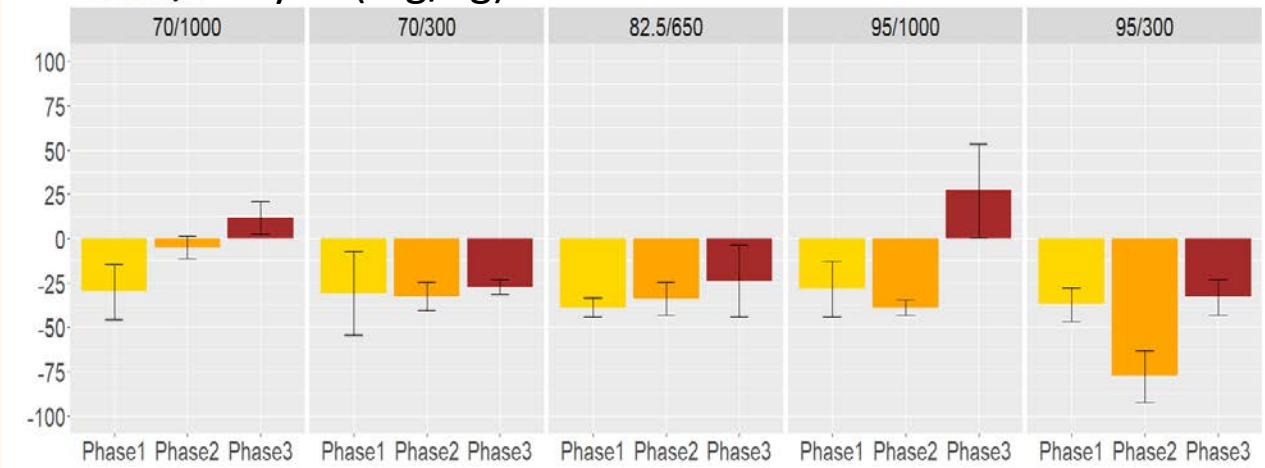
Viscosity (mPa.s)



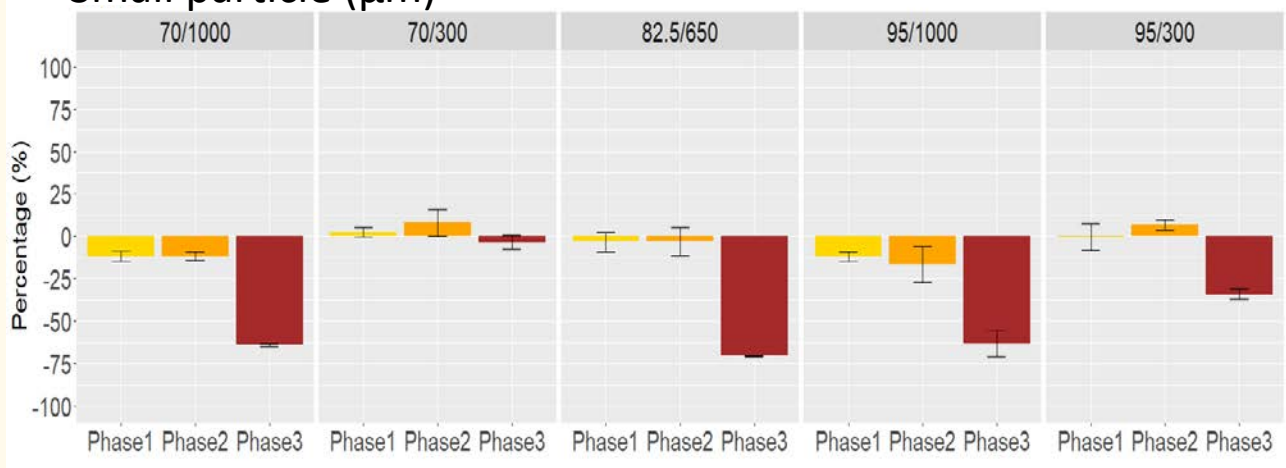
Large particle (µm)

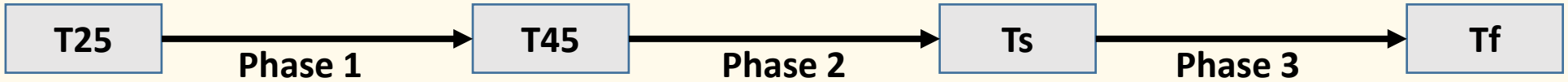


Acetaldehyde (mg/kg)



Small particle (µm)





PLSr results

Parameters	Unit	Pretreatment	Calibration parameters				Prediction parameters			Model evaluation	
			LV	*RMSEC*	*RMSECV*	R_c^2	std_p	*RMSEP*	R_p^2	*RPD*	*Comment*
Viscosity *(Shear rate: $20s^{-1}$)*	*mPa.s*	*2^{nd} derivative*	2	3511	3955	0.79	9953	7783	0.69	1.28	
		Smoothed +SNV	2	5023	5164	0.57	9953	7849	0.50	1.27	
Large particle *(Feret diameter)*	*µm*	*2^{nd} derivative*	3	1982	2055	0.57	3247	1668	0.78	**1.95**	*Discrimination low to high values*
		Smoothed +SNV	6	1996	2432	0.61	3247	1979	0.69	**1.64**	*Discrimination low to high values*
Small particle *(Mode)*	*µm*	*2^{nd} derivative*	1	208	212	0.18	220	178	0.33	1.24	
		Smoothed +SNV	4	164	182	0.53	220	168	0.51	1.30	
acetaldehyde	*mg/kg apple puree*	*2^{nd} derivative*	2	1.36	1.44	0.66	4.26	4.19	0.55	1.02	
		Smoothed +SNV	1	2.04	2.10	0.22	4.26	4.53	0.14	0.94	

Conclusion and perspectives

Conclusion :

- Possibility of discrimination of processing conditions and steps by NIRS
- Relevant parameters were identified
- The current PLSR models showed poor predictive performance
- Spectral variability and apple puree heterogeneity may have contributed to model overfitting or underfitting
- Need for alternative approaches or improvements to enhance model robustness and accuracy.

Perspectives :

- Other pretreatments → pretreatment combinations (e.g., SNV+1st derivative, SNV+2nd derivative, …)
- Model Optimization → alternative regression models (e.g., non linear: SVR, random forest,…)
- Dataset improvement → more diverse and representative samples to improve model training and validation.
- Multiblock regression → visible and NIR spectroscopy
- Variables selection → Most relevant wavelengths

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The End

Thank you !