Infrared spectroscopy to guide food formulation: an innovative concept applied on apple puree

Weijie Lan[1], Benoit Jaillais[2], Catherine Renard[1], Alexandre Leca[1], Sylvie Bureau[1]

[1] INRAE - Université d'Avignon et des Pays de Vaucluse, UMR408 SQPOV, Avignon, France
[2] INRAE-ONIRIS Unité Statistiques, Sensométrie, Chimiométrie (Stat SC), Nantes, France

Apple puree

- 2nd largest market of fruit puree after banana puree.
- 2,000 million USD annual global market value.
- 14% of the French harvested apples processed into puree.
- 46% pure apple purees and 54% mixed purees in France.
- Popular from all ages of people.

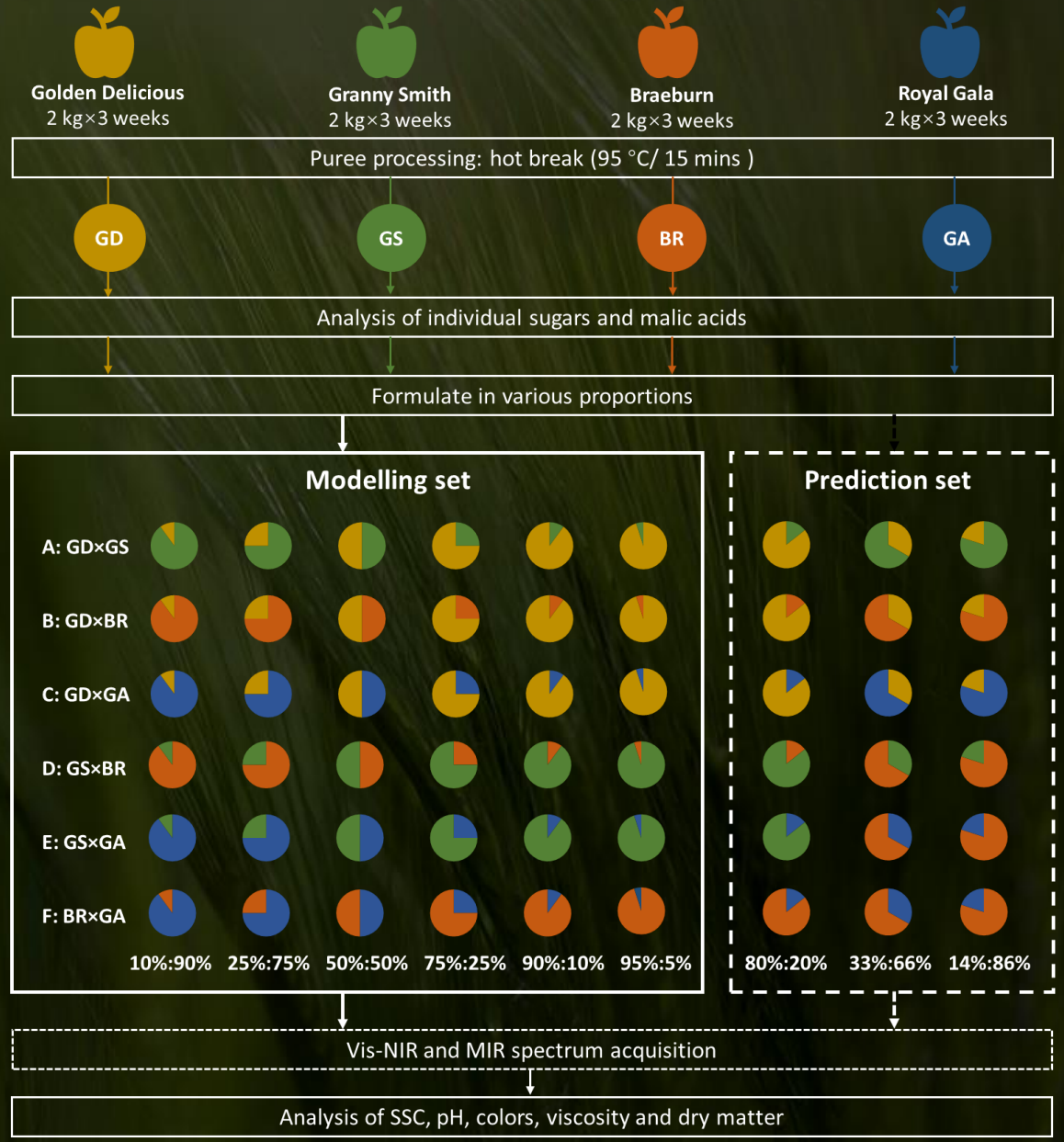
A large variability of raw apples impacts the quality of cooked purees.

We need to know how to formulate apple purees:

- Produce sustainable purees
- Facilitate and optimize choices of raw apples
- Limit losses and wastes
- Use variability to enhance the puree quality

Objectives and plan

- Trace the proportions of each apple variety in formulated purees
- Predict quality of formulated purees from spectral information of initial single-variety purees



Variety traceability by infrared techniques

Infrared information
(Vis-NIR 400-2500 nm, MIR 900-1800 cm^{-1})

Model A

What proportions of each variety in the formulated purees?


Golden Delicious


Granny Smith


Braeburn


Royal Gala

(First time)

Model A:
VIS-NIR or MIR spectra to trace the proportions of each variety by PLS

(RPD>=2.5 good)

Cultivars	MIR		Vis-NIR	
	RMSEP	RPD	RMSEP	RPD
Golden Delicious	8.1%	3.6	19.0%	1.5
Braeburn	4.3%	7.7	7.5%	4.4
Granny Smith	2.7%	11.4	9.2%	3.4
Royal Gala	7.4%	4.7	16.2%	2.1

MIRS with PLS is a powerful tool to estimate apple puree proportions.

An innovative strategy based on multivariate curve resolution-alternating least squares (MCR-ALS)

Formulated purees spectra matrix D

n (samples) × λ (wavenumbers or wavelengths)

MCR-ALS

Pure concentration profiles

C_{GD} C_{GS} C_{BR} C_{GA}

n (samples) × q (single variety purees)

+

Single-variety purees spectra matrix

S^T

S_1: Golden Delicious (GD)

S_2: Granny Smith (GS)

S_3: Braeburn (BR)

S_4: Royal Gala (GA)

λ (wavenumbers or wavelengths)

Reconstructed purees spectra matrix R

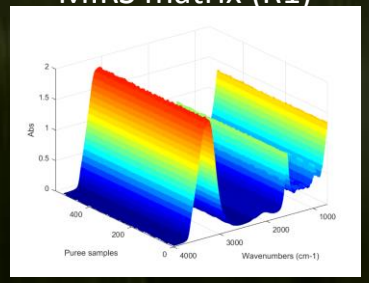
n (samples) × k (wavenumbers or wavelengths)

Spectra sample 1= $C_{GD1}S_1+C_{GS1}S_2+C_{BR1}S_3+C_{GA1}S_4$

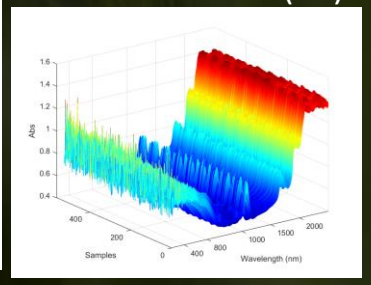
Spectra sample 2= $C_{GD2}S_2+C_{GS2}S_2+C_{BR2}S_3+C_{GA2}S_4$

Spectra sample n= $C_{GDn}S_1+C_{GSn}S_2+C_{BRn}S_3+C_{GAn}S_4$

Reconstructed MIRS matrix (R1)



Reconstructed VISNIRS matrix (R2)



Compare multivariate regression results using matrix D and R

Infrared spectroscopy to guide puree formulation

(First time)


Golden Delicious


Granny Smith


Braeburn


Royal Gala

Infrared information
(MIR 900-1800 cm^{-1})

Model B

Guide the quality of formulated purees with different composed proportions

Model B:
PLS to predict formulated purees based on raw and reconstructed MIR spectra

(RPD>=2.5 good)

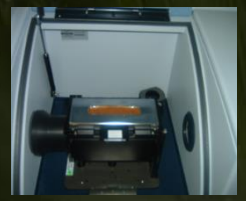
Parameters	Raw		Reconstructed	
	R_p^2	RPD	R_p^2	RPD
Viscosity (η_{50})	0.90	4.1	0.86	4.0
Soluble solids content (°Brix)	0.95	5.1	0.90	4.1
Titratable acidity (meq/kg FW)	0.96	4.3	0.91	3.4
Malic acid (g/kg FW)	0.97	5.9	0.93	4.7

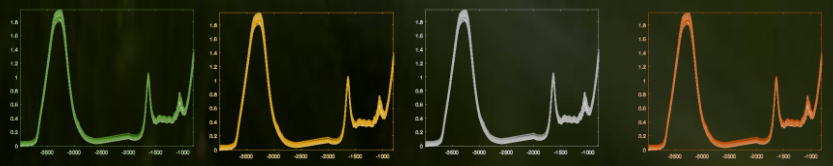
Spectra acquired on single-variety purees allow to predict the viscosity, soluble solids, titratable acidity of formulated purees

Perspectives: an innovative strategy to guide puree formulation by MIRS

single-variety purees

MIRS





single-variety spectra

Innovative chemometric strategy: spectral reconstruction

Formulation guidance

Sustainable quality

Develop new products

Reconstructed spectra of purees

Golden Delicious 33.3% + **Granny Smith** 66.6% → Low redness, High acidity, High viscosity

Braeburn 80% + **Royal Gala** 20% → More redness, Low acidity, Low viscosity

Conclusion

Infrared spectroscopy

- A powerful tool to trace variety proportions and predict quality properties in formulated purees
- An innovative strategy to guide puree formulation

Lan, W., Bureau, S., Chen, S., Leca, A., Renard, C. M., & Jaillais, B. (2020). Visible, near-and mid-infrared spectroscopy coupled with an innovative chemometric strategy to control apple puree quality. Food Control, 107546.
Lan, W., Renard, C. M., Jaillais, B., Buergy, A., Leca, A., Chen, S., & Bureau, S. (2021). Mid-infrared technique to forecast cooked puree properties from raw apples: A potential strategy towards sustainability and precision processing. Food Chemistry, 355, 129636.