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A chemometric approach to minimise the diffusive effect of the biomass when using near infrared spectroscopic measurements for the monitoring of bioprocesses.

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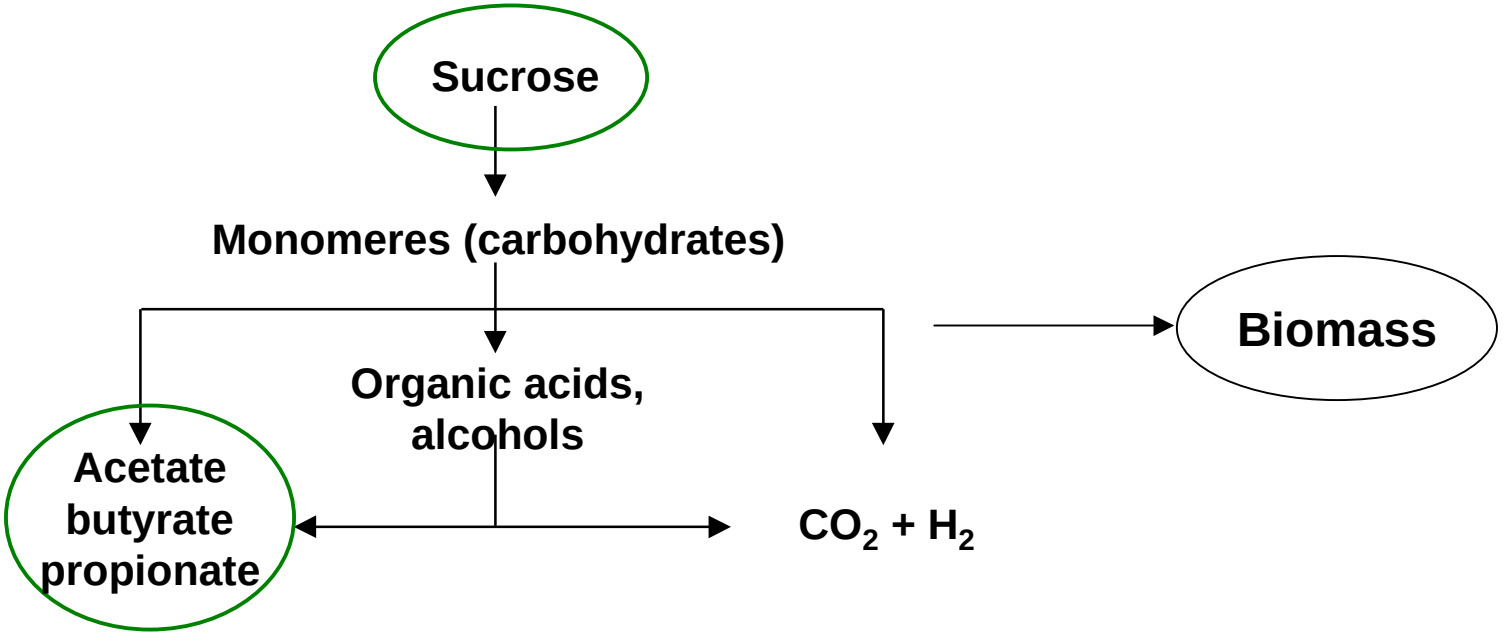
Introduction and Context

Objective : Monitoring the biomass, VFA (Volatile Fatty Acids) and sucrose.

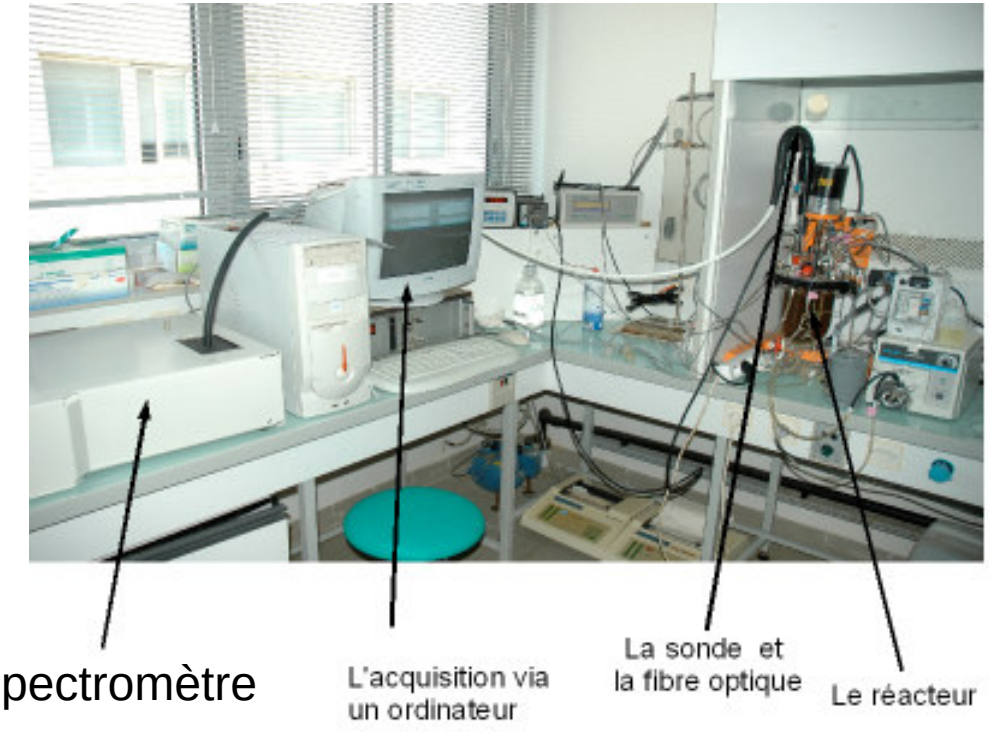
Context of sustainable development: wastes are valorised in energy production.

Production of H_2 by micro-organism in anaerobic conditions.

Need of sensors *in situ* for the monitoring of some inhibitory compounds.



Introduction and Context



The on-line monitoring by Near Infrared Spectroscopy with a fibre probe.

1000-2500 nm ;
resolution : 3 nm

Substrate : sucrose

Detection limit: low range values for the molecules monitored.

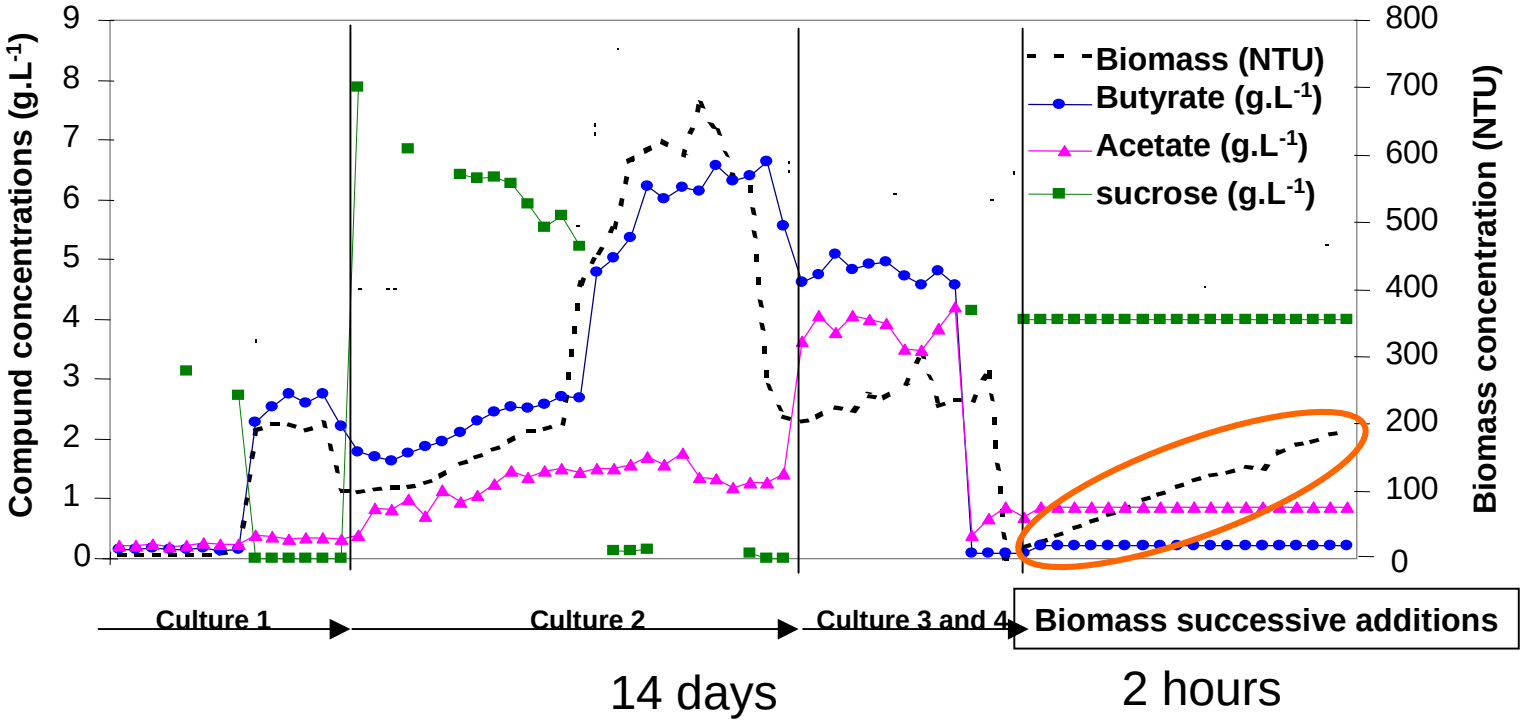
Correlations between biomass, VFA and sucrose concentrations cause wrong regression: experimental design.

Biomass produces scattering effects: pretreatment of spectra.

How to delete the scattering effect?

Results

Evolution of compounds and biomass concentrations during the cultures and the biomass addition phase.

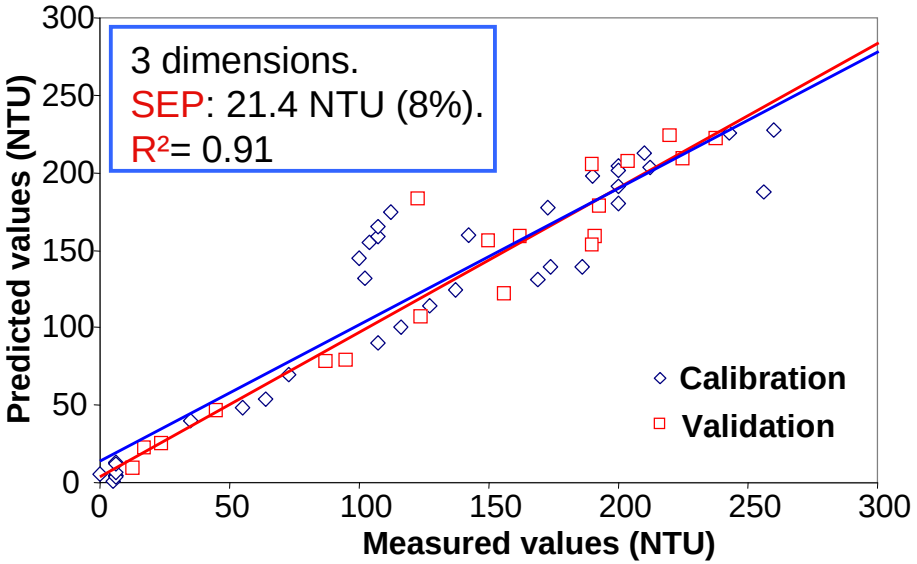


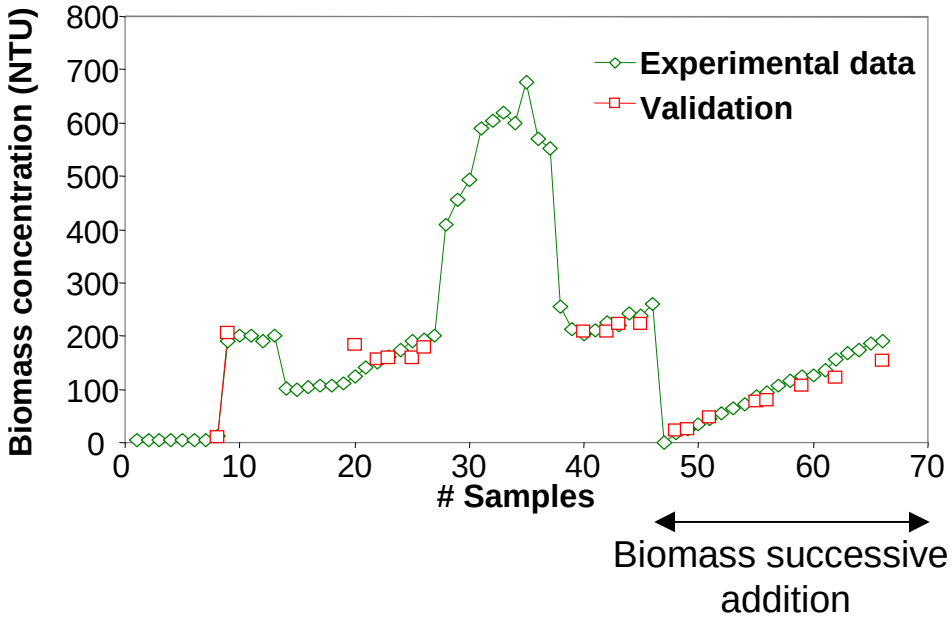
Biomass concentration

Better regression for low values (< 260 NTU)

Biomass prediction using PLS regression.

39 samples in calibration, 17 samples in validation.





Butyrate concentration

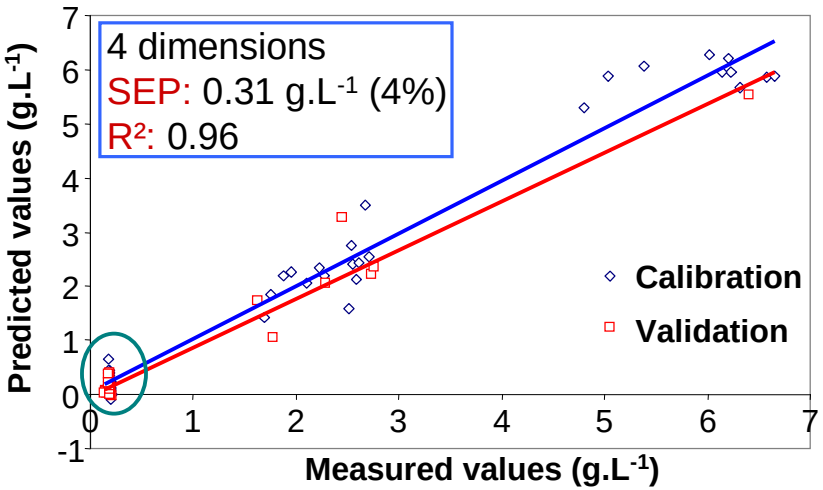
SNV applied on transmittance values: good prediction

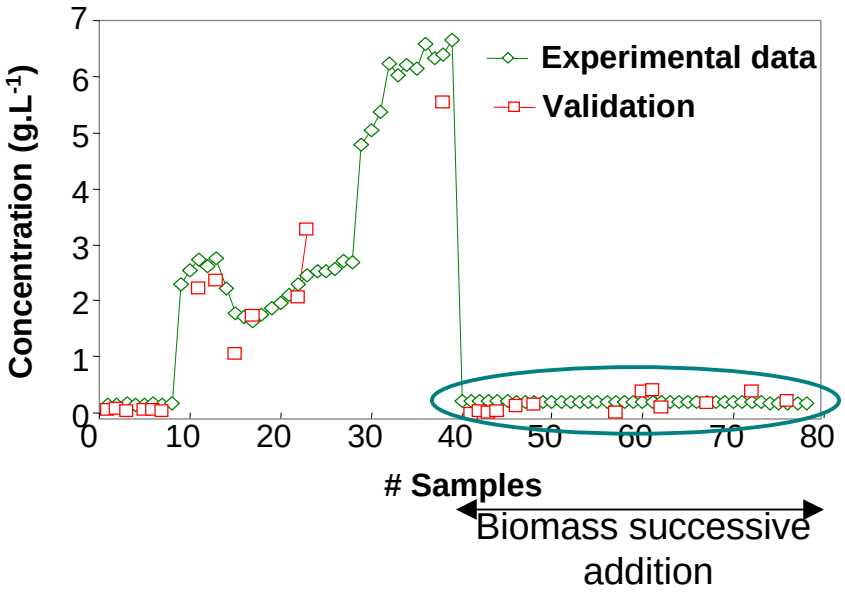
Scattering effect of the biomass is mainly additive.

Butyrate prediction using PLS regression.

48 samples in calibration, 26 samples in validation.

SNV applied on **transmittance** values





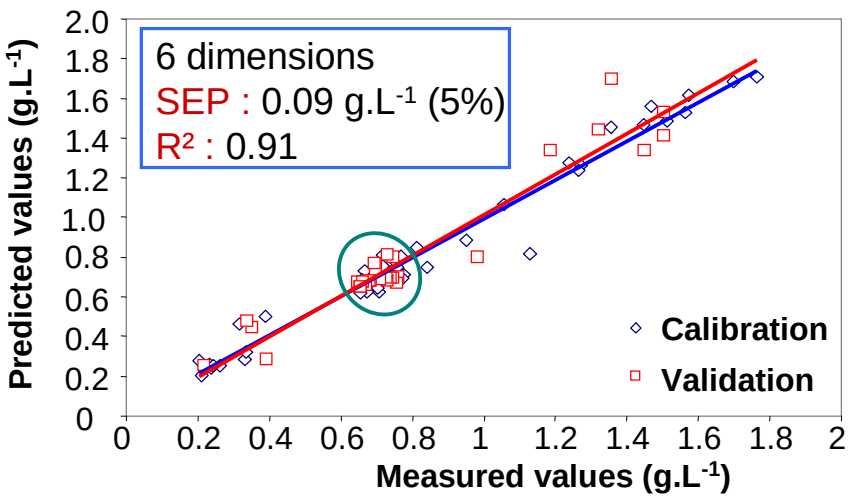
Acetate concentration

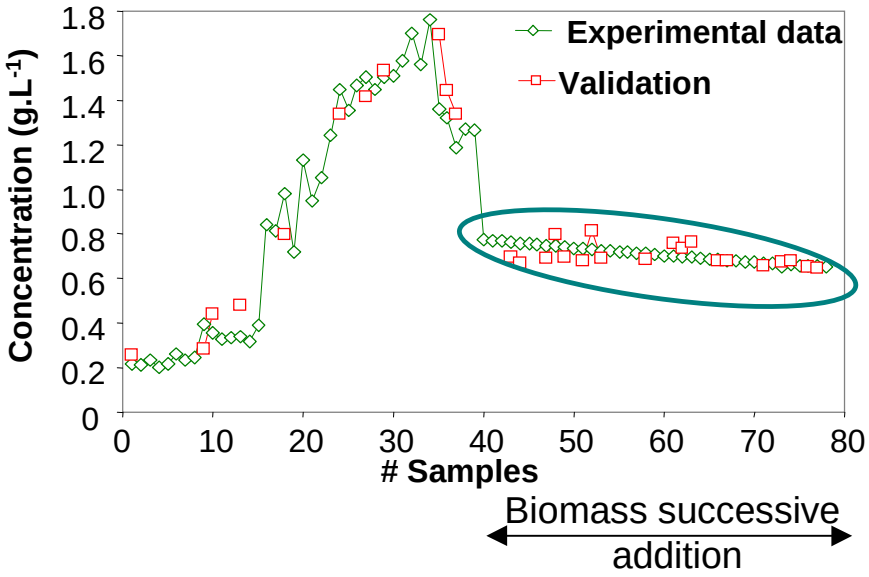
SNV applied on transmittance values: good prediction.

Acetate prediction using PLS regression.

48 samples in calibration, 30 samples in validation.

SNV applied on **transmittance** values





Conclusion and perspectives

- The **biomass prediction** is **not a linear regression** and is mainly based on **the scattering effect**.

- The SNV pretreatment, applied on **transmittance value,** improved the calibration of **butyrate** and **acetate**.

- **Sucrose is not well predicted**, whereas it is the most concentrated compound.

Perspectives:
- non-linear methods for biomass prediction.
- how to use the prediction of the biomass to improve the prediction of the molecules?

NIR: a suitable method for the monitoring of inhibitory compounds in H_2 production by fermentation of molasses.