

MIR spectroscopy and chemometrics to characterize probiotic fermentation processes

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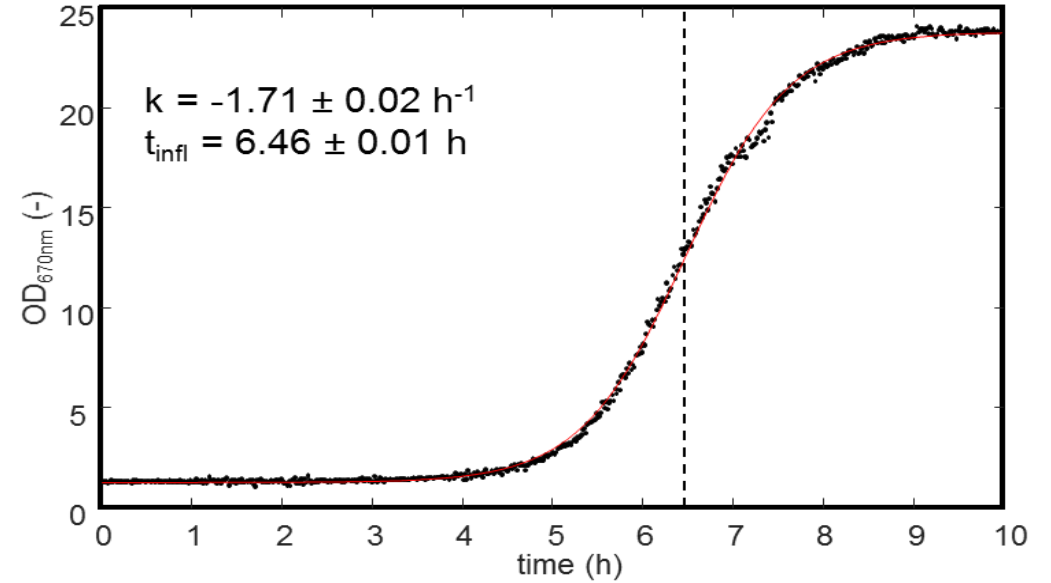
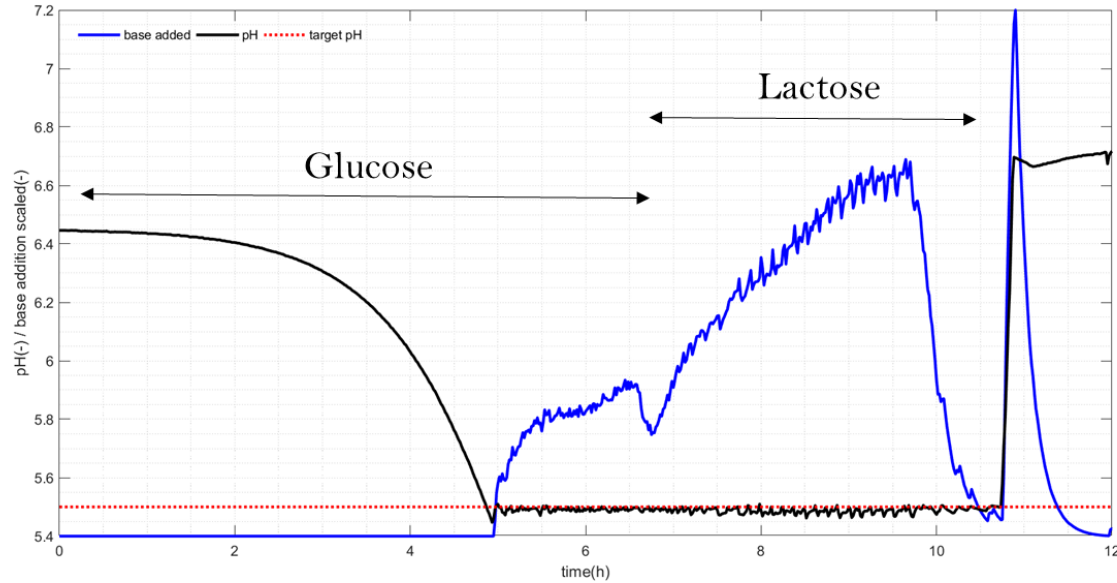
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Aim:

1. Follow trends over time
2. Identify batch-to-batch variations



Process details



10 hour fermentation process

Product = bacterial cells

Sugars (glucose, lactose) consumed
Lactic acid produced

Non linear regression fitting model:

$$S_x(t) = A_x / (1 + \exp[k_x \cdot (t - t_{x,\text{infl}})])$$
$$y_x(t) = S_x(t) + b_0$$

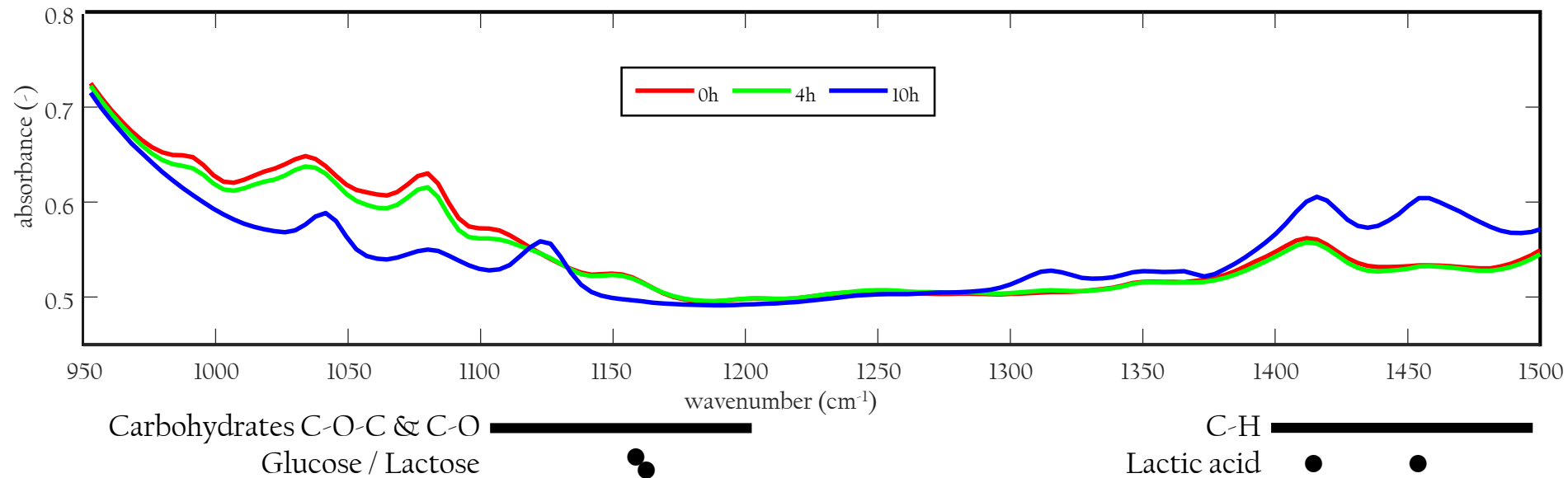
Rate constant and time of inflection to describe the “dynamics”

Mid-Infrared Spectroscopy

Vibrational spectroscopy

Infrared region of EM spectrum (400 cm^{-1} to 4000 cm^{-1})

PAT approach to process monitoring



The study

Bacterial fermentation, collect IR spectra



PCA / PARAFAC / MCR



Scores profiles



Fit a non-linear regression model



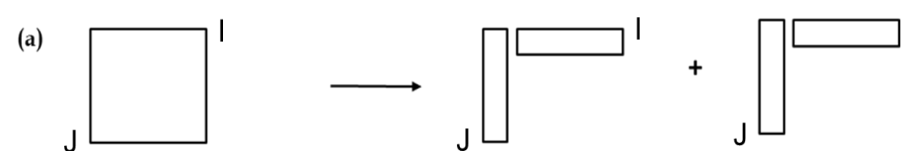
Extract rate constant (k) and time of inflection (t)



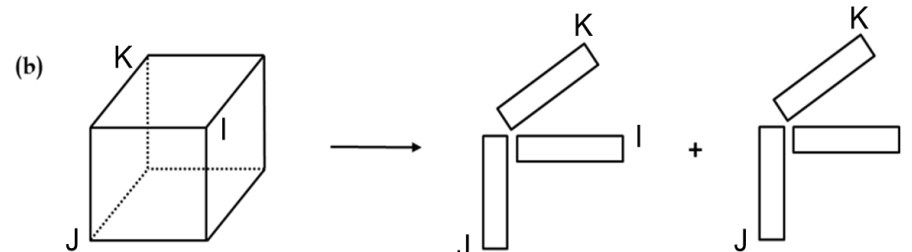
Compare the performance of the batches

Data organization

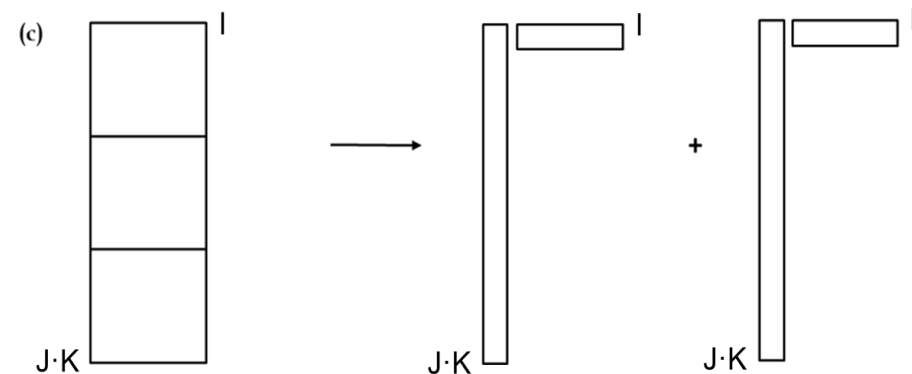
PCA / MCR(i)



PARAFAC

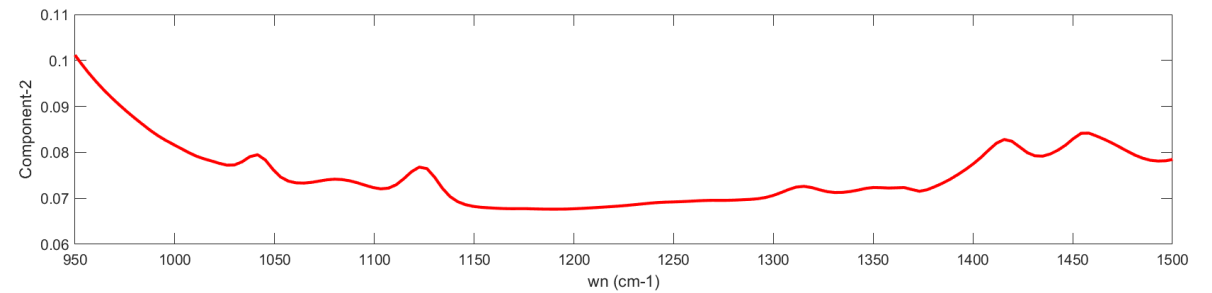
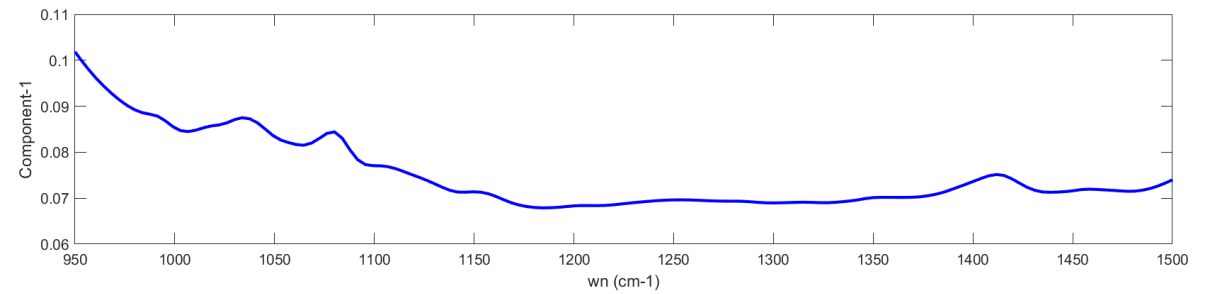
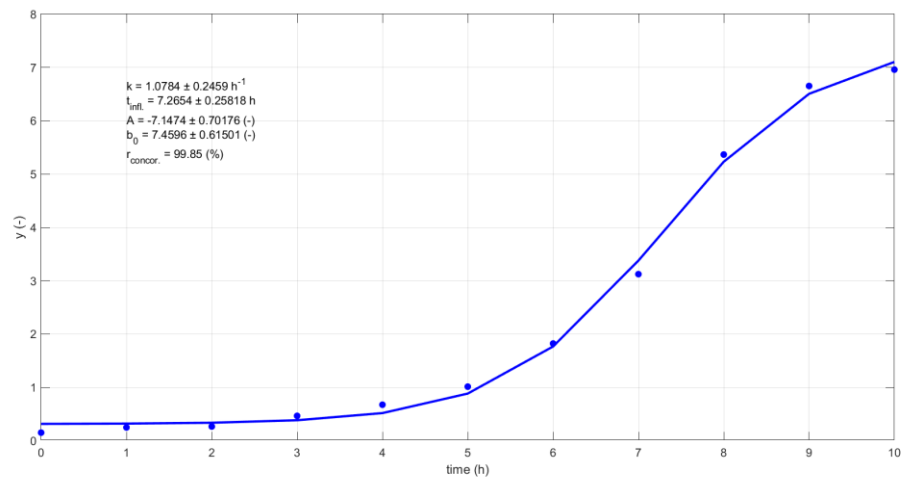
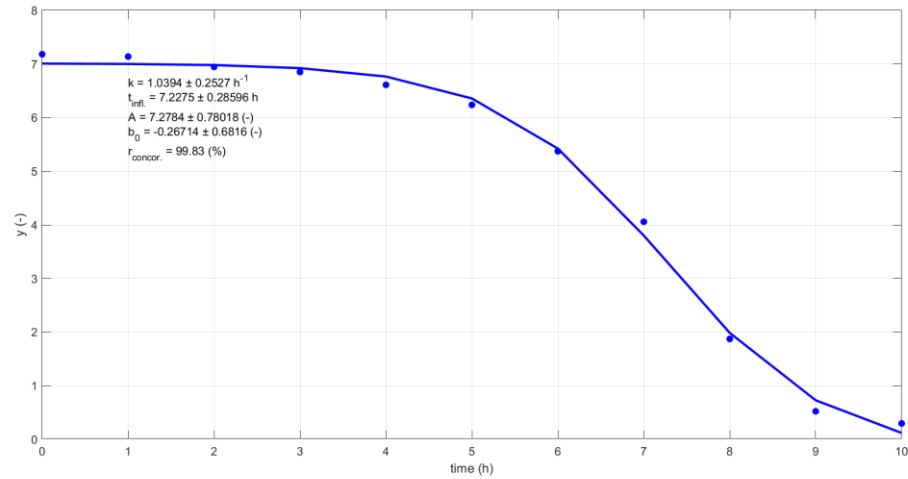


MCR(a)



Results – MCR(a)

Scores (fitted) and loading profiles



Augmented matrix

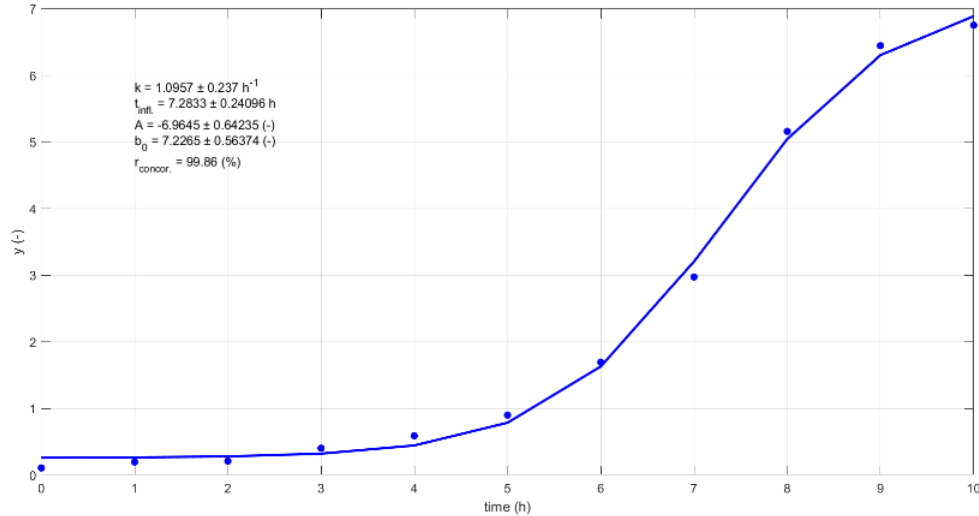
2-component model

Non-negativity in spectral and time direction

Results – MCR(a)

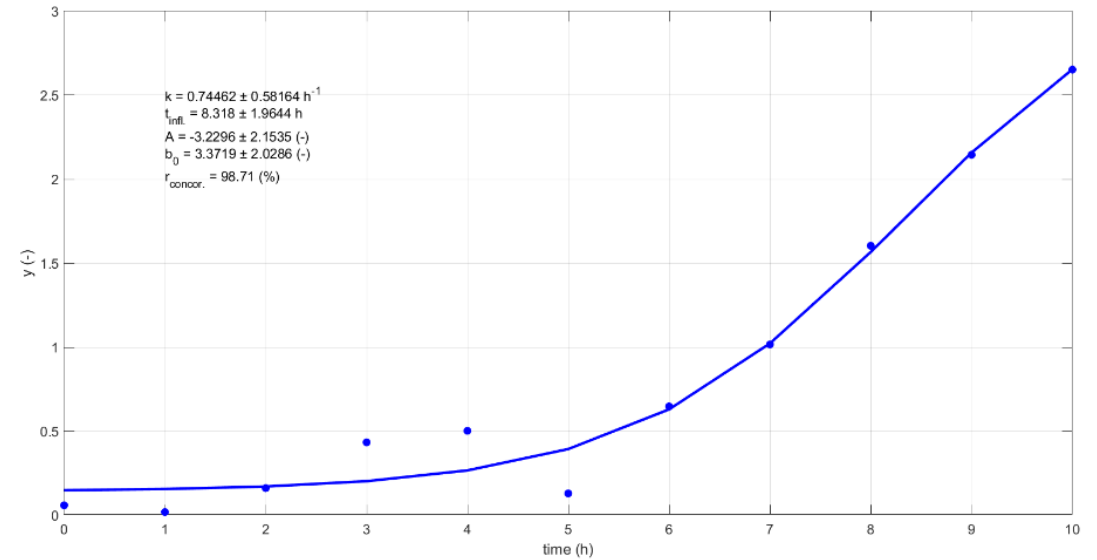
Scores profiles from component 2 fitted

Normal batch



$$k = -1.09 \pm 0.23 \text{ h}^{-1}$$
$$t = 7.2833 \pm 0.24 \text{ h}$$

Deviating batch



$$k = -0.744 \pm 0.58 \text{ h}^{-1}$$
$$t = 8.318 \pm 1.96 \text{ h}$$