June 2025
12th French Biennial of Applied and Industrial Mathematics

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Understanding, modeling and controlling **wine fermentation**

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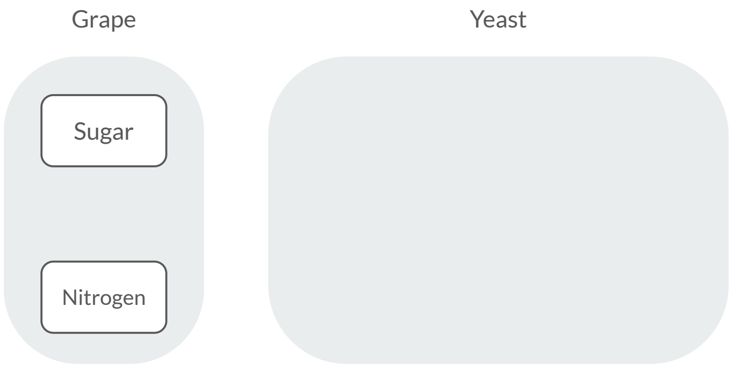
Introduction

The **wine fermentation** process



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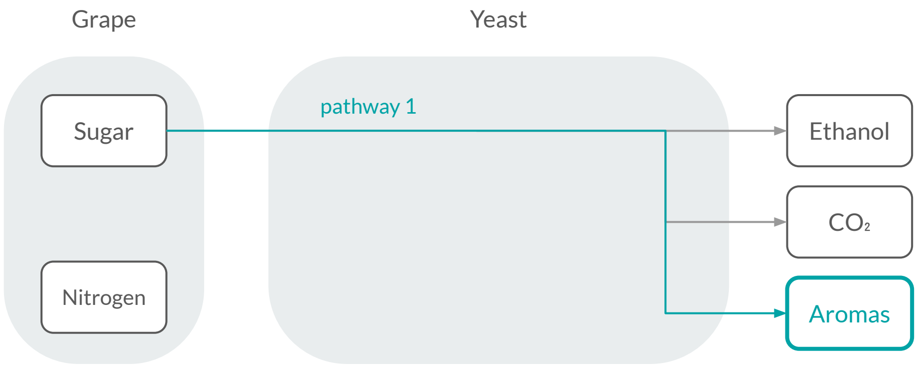

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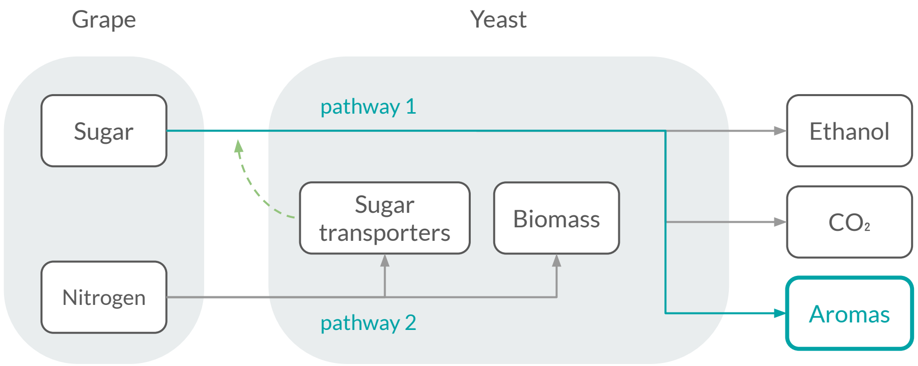

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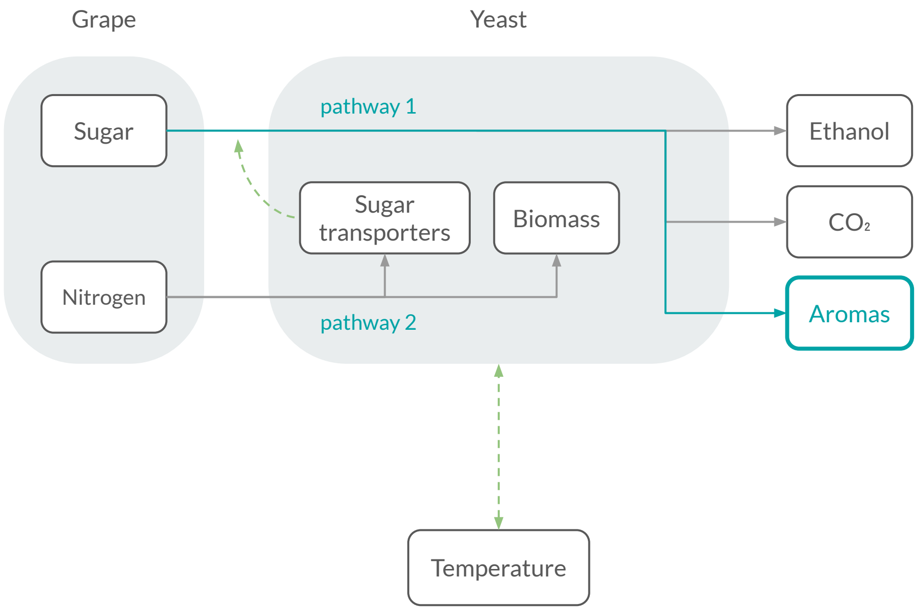

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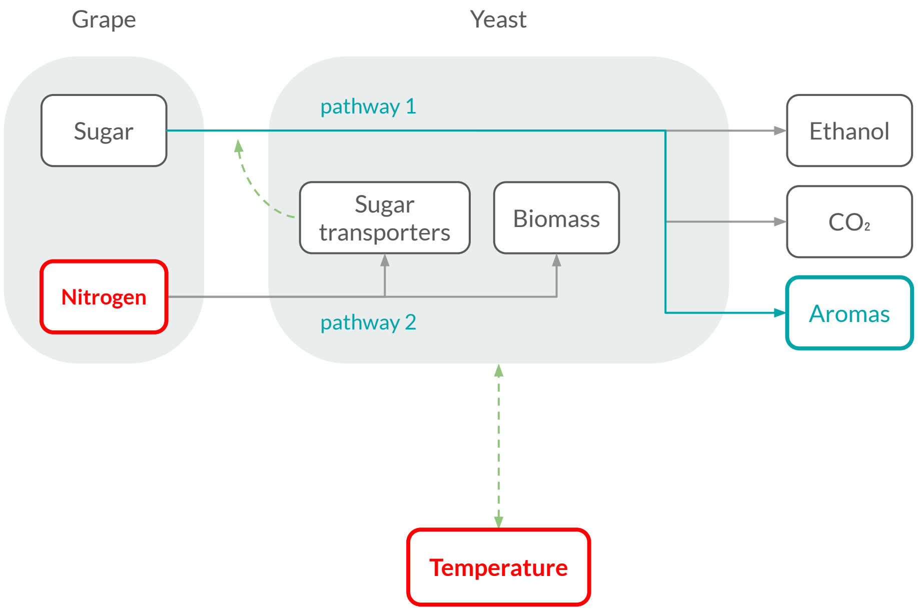
Objectives:

- Understand and model the impact of **nitrogen** and **temperature** on **aroma** synthesis.



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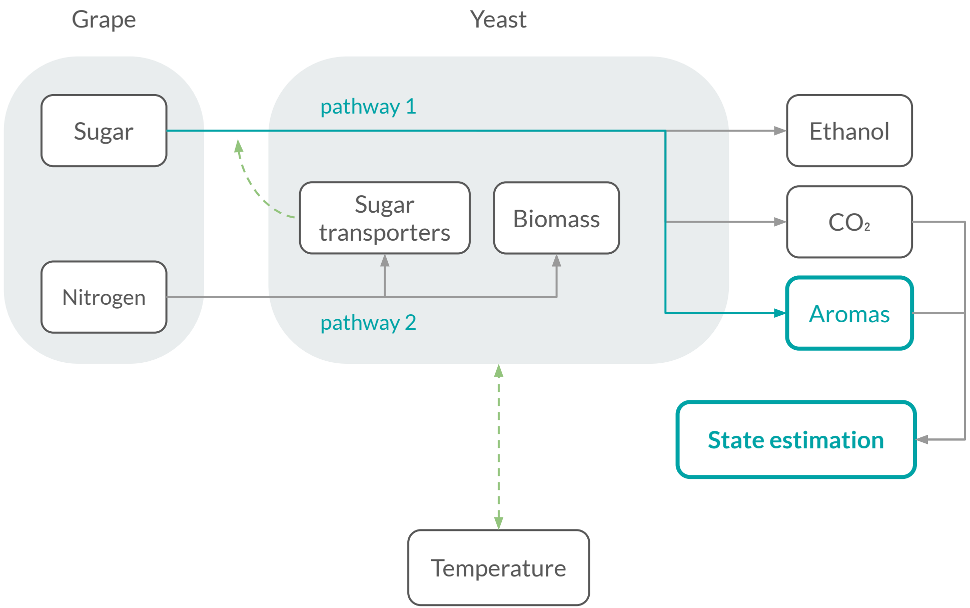
- **Estimate** internal states from measurements.



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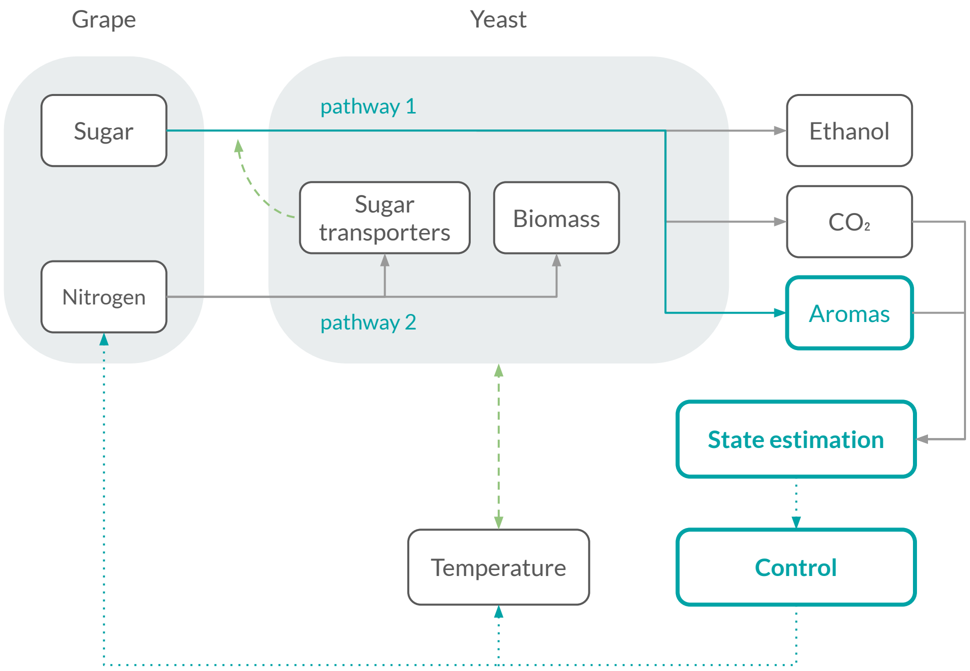

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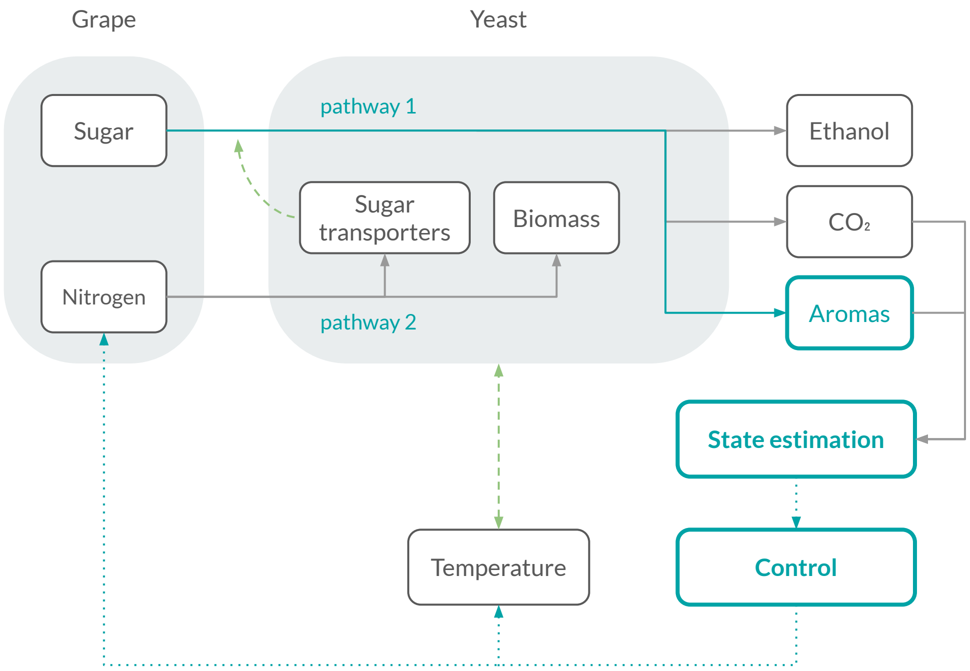

State of the art

- Lack of mechanistic models.

- Lack of comprehension of the biological process.

- Almost **no control theory** in the past.

Mechanistic modeling

First approaches: extracellular modeling

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$$\dot{S} = -XN_{ST}(N_0 - N, X, T)\nu_{ST}(S, E, T)$$ (Sugar)

$$\dot{N} = -X\nu_N(N, E, T)$$ (Nitrogen)

$$\dot{X} = k_1(T)X\left[1 - \frac{X}{X_{\max}(N_0)}\right]$$ (Biomass)

$$\dot{E} = -\mu\dot{S}$$ (Ethanol)

- Admits nitrogen addition
- Isothermal fermentations
- No aroma compounds

$$CO_2(t) = E(t), \forall t \geq 0$$

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$$\mathrm{CO}_2(t) = E(t), \forall t \geq 0$$

where:

$$\nu_{ST}(S, E, T) = \frac{k_2(T)S}{K_S + S(1 + K_{Si}E^{\alpha_S})}$$

(Ethanol-inhibited glucose absorption)

$$\nu_N(N, E, T) = \frac{k_3(T)N}{K_S + N(1 + K_{Ni}E_N^{\alpha})}$$

(Ethanol-inhibited nitrogen absorption)

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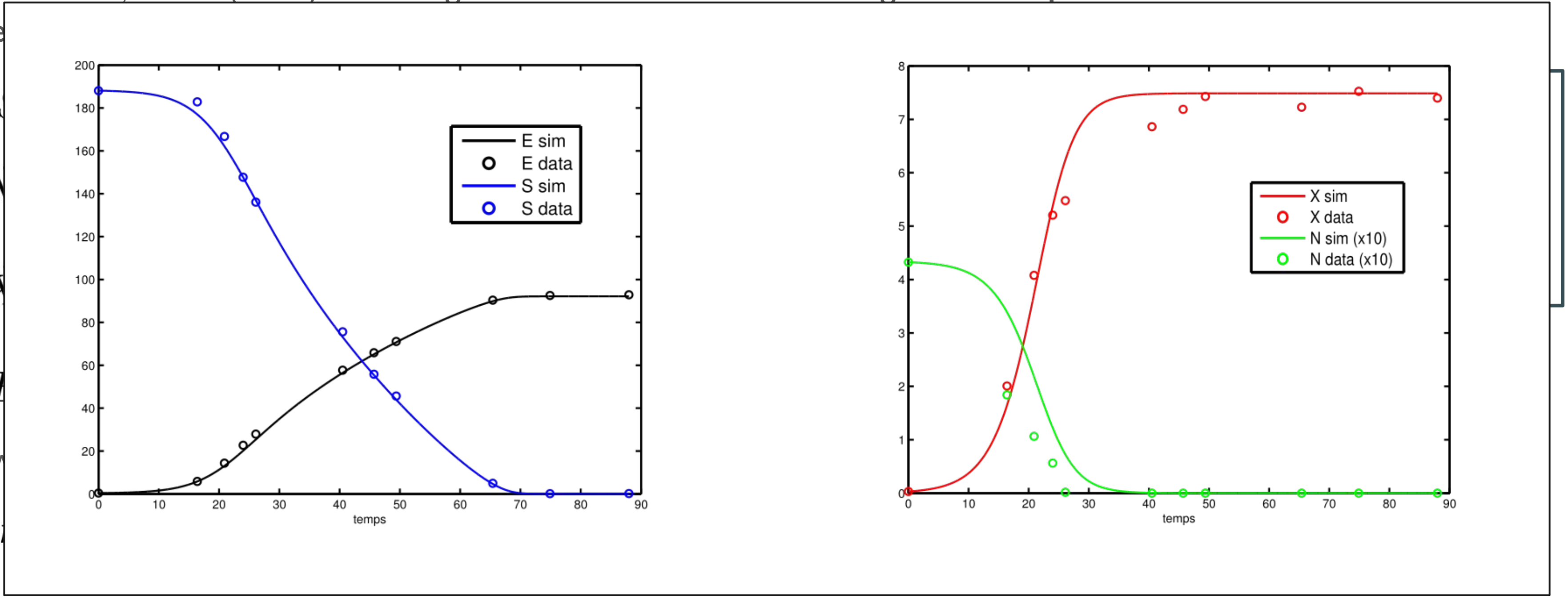


(Ethanol-inhibited glucose absorption) (Ethanol-inhibited nitrogen absorption)

Main fermentation kinetics

$$\dot{S} = -X\,\nu_{st}(S, E, N_{st}, T),$$ (Sugar)

$$\dot{N} = -\nu_N(N, E, A, T)X,$$ (Nitrogen)

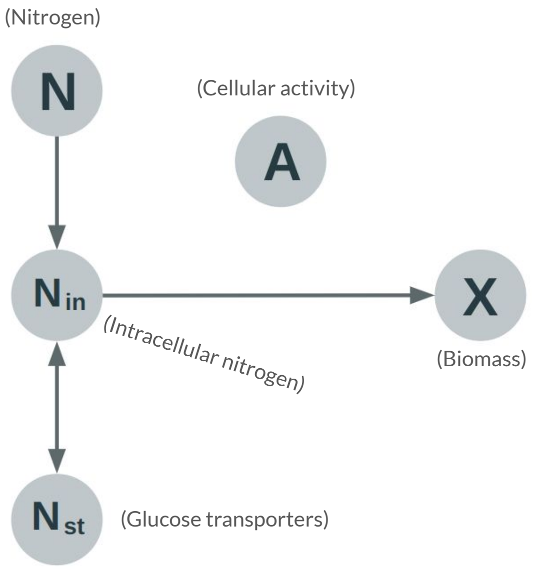
$$\dot{X} = \mu(N_{in}, E, A, T)X,$$ (Biomass)

$$\dot{N_{in}} = \nu_N(N, E, A, T) - \frac{1}{Y_{N_{st}}}\nu_{\mathrm{tr}}(N_{in}, N_{st}, T) - (N_{in} + \alpha_1)\,\mu(N_{in}, E, A, T),$$ (Intracellular nitrogen)

$$\dot{N_{st}} = \nu_{\mathrm{tr}}(N_{in}, N_{st}, T) - N_{st}\,\mu(N_{in}, E, A, T),$$ (Glucose transporters)

$$\dot{A} = \mu(N_{in}, E, A, T)\,(A^* - A) - \kappa(T)A.$$ (Cellular activity)

$$CO_2 = E = (S(0) - S)/2.17$$



Beaudeau *et al.* (2023). Dynamic modelling of the effects of assimilable nitrogen addition on aroma synthesis during wine fermentation. Chemical Engineering Transactions.

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Temperature-dependent reaction rates

$$\nu_{st}(S, E, N_{st}, T) \doteq k_2(T) N_{st} \frac{S}{K_S + S(1 + K_{Si} E^{\alpha_S})},$$

(Glucose transport rate)

$$\nu_N(N, E, T) \doteq k_3(T) \frac{N}{K_N + N(1 + K_{Ni} E^{\alpha_N})}$$

(Nitrogen assimilation rate)

$$\nu_{\mathrm{tr}}(N_{in}, N_{st}, T) \doteq k_{N_{st}}(T) \left(1 - \frac{Q_0}{N_{in}}\right)^+ - k_{d,N_{st}} \left(\frac{N_{st}}{k_{N_{st}} + N_{st}}\right),$$

(Sugar transporter synthesis rate)

$$\mu(N_{in}, E, A, T) \doteq k_1(T) \left(1 - \frac{N_{in,0}}{N_{in}}\right)^+ \left(1 - \frac{E}{E_{\max}}\right)^+ A$$

(Yeast growth rate)

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(Yeast growth rate)

$$\begin{aligned} k_1(T) &= a_1 T + b_1, \\ k_2(T) &= a_2 T^2 - b_2 T + c_2, \\ k_3(T) &= a_3 T^2 - b_3 T + c_3, \\ \kappa(T) &= a_4 T - b_4, \\ k_{N_{st}}(T) &= a_5 T^2 - b_5 T + c_2, \end{aligned}$$

Heuristic model for synthesis of aroma compounds

The model is based on the relationship between sugar consumption and production of aromas

$$\frac{dAroma}{dt} = -Y_{aroma}\frac{dS}{dt}$$

The conversion yield changes when the nitrogen is added:

$$\ln(Y_{aroma,1}) = D_1 + D_2N_0 + D_3T + D_4N_0^2 + D_5T^2 + D_6N_0T$$

(before nitrogen addition)

$$\ln(Y_{aroma,2}) = D_7 + D_8(N_0 + N_{ad}) + D_9T + D_{10}(N_0 + N_{ad})^2 + D_{11}T^2 + D_{12}(N_0 + N_{ad})T$$

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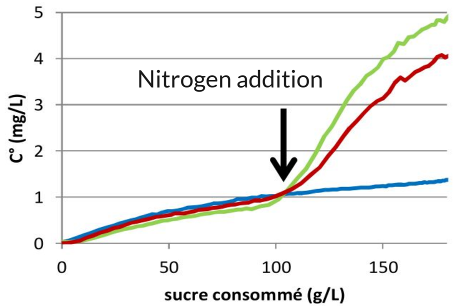

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$$\frac{dAroma}{dt} = -Y_{aroma}\frac{dS}{dt}$$

The conversion yield changes when the nitrogen is added:

- General and comprehensive (5 aroma compounds)
- Very variable performance

$$\ln\left(Y_{aroma,1}\right) = D_1 + D_2N_0 + D_3T + D_4N_0^2 + D_5T^2 + D_6N_0T$$

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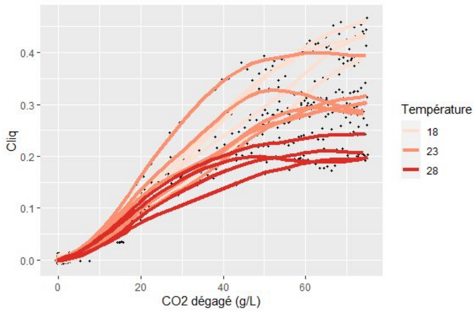
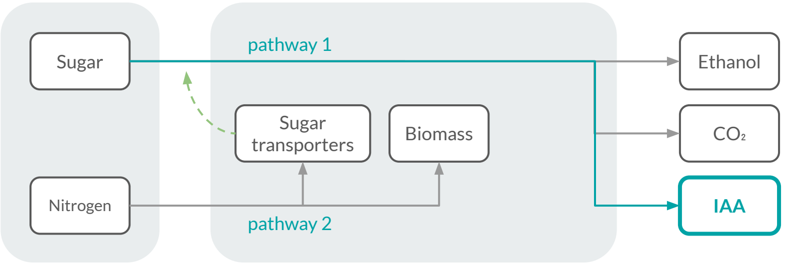
Mechanistic modelling of isoamyl acetate synthesis

The objective: to develop mechanistic models of aroma synthesis based on the experimental data





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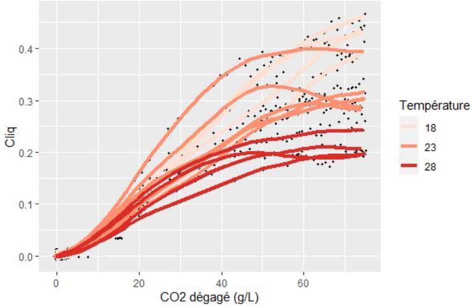

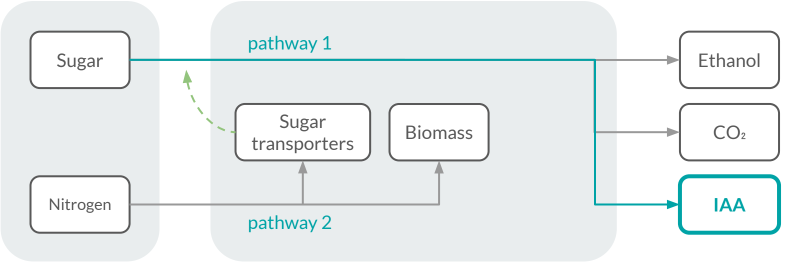

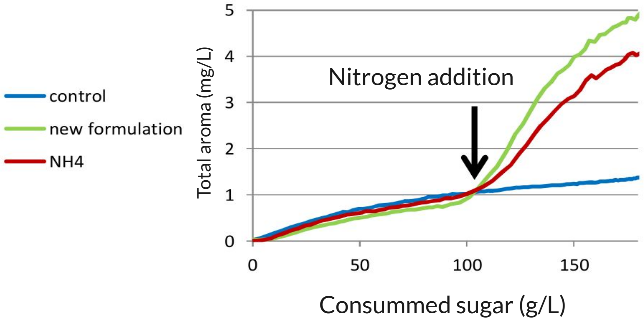

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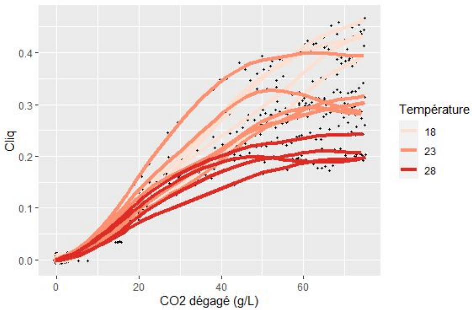
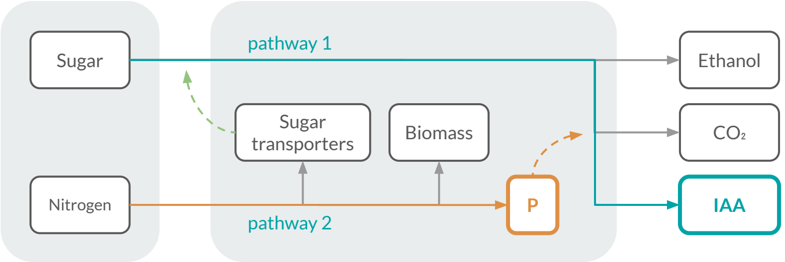
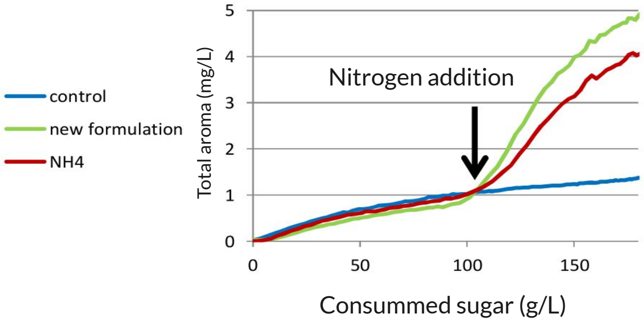


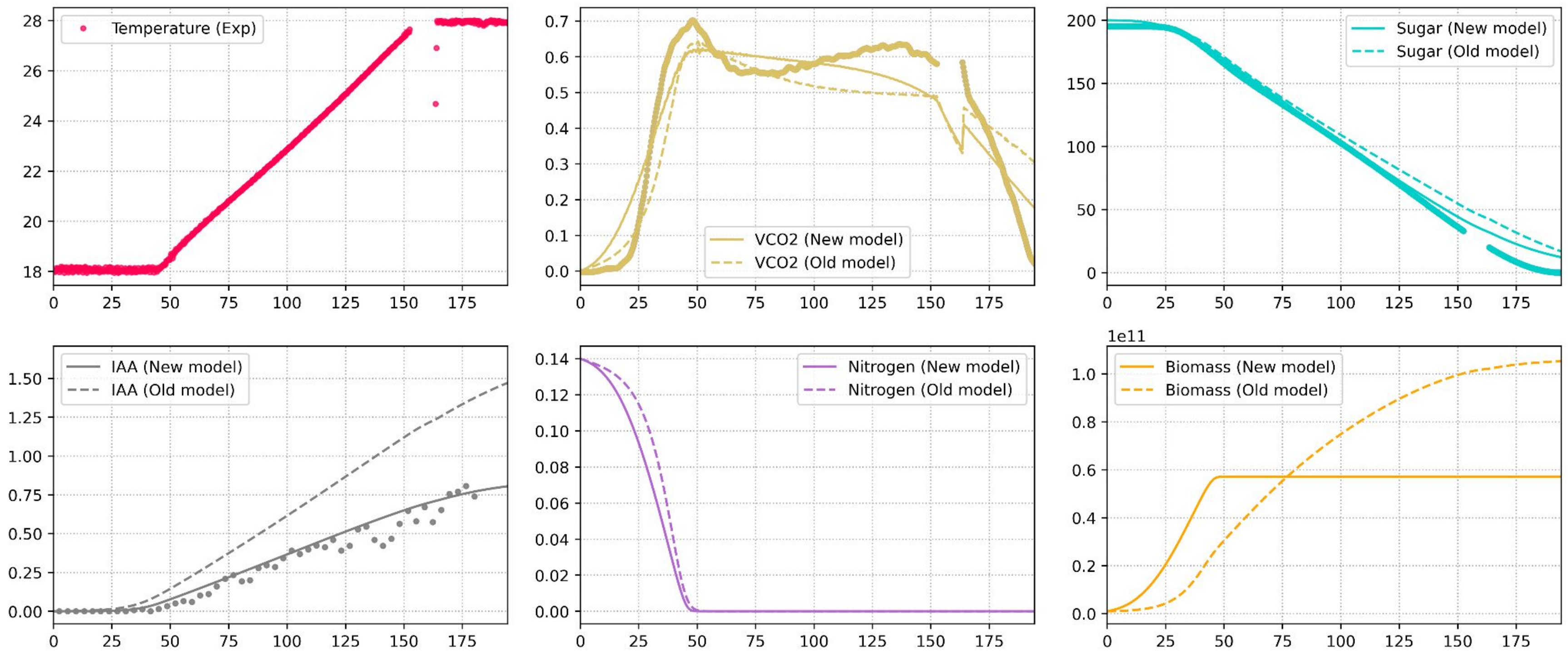




$$\dot{P} = \underbrace{-k_P(T)\, r_S(S)\, \dot{N}}_{\text{Enzyme synthesis}} - \underbrace{k_{m,P} P}_{\text{Degradation}}, \qquad \text{(Enzyme)}$$

$$\dot{X} = \underbrace{P}_{\text{Enzyme catalyzing effect}} \nu_X(S, E, T) \qquad \text{(IAA)}$$

Simulations of mechanistic model of IAA



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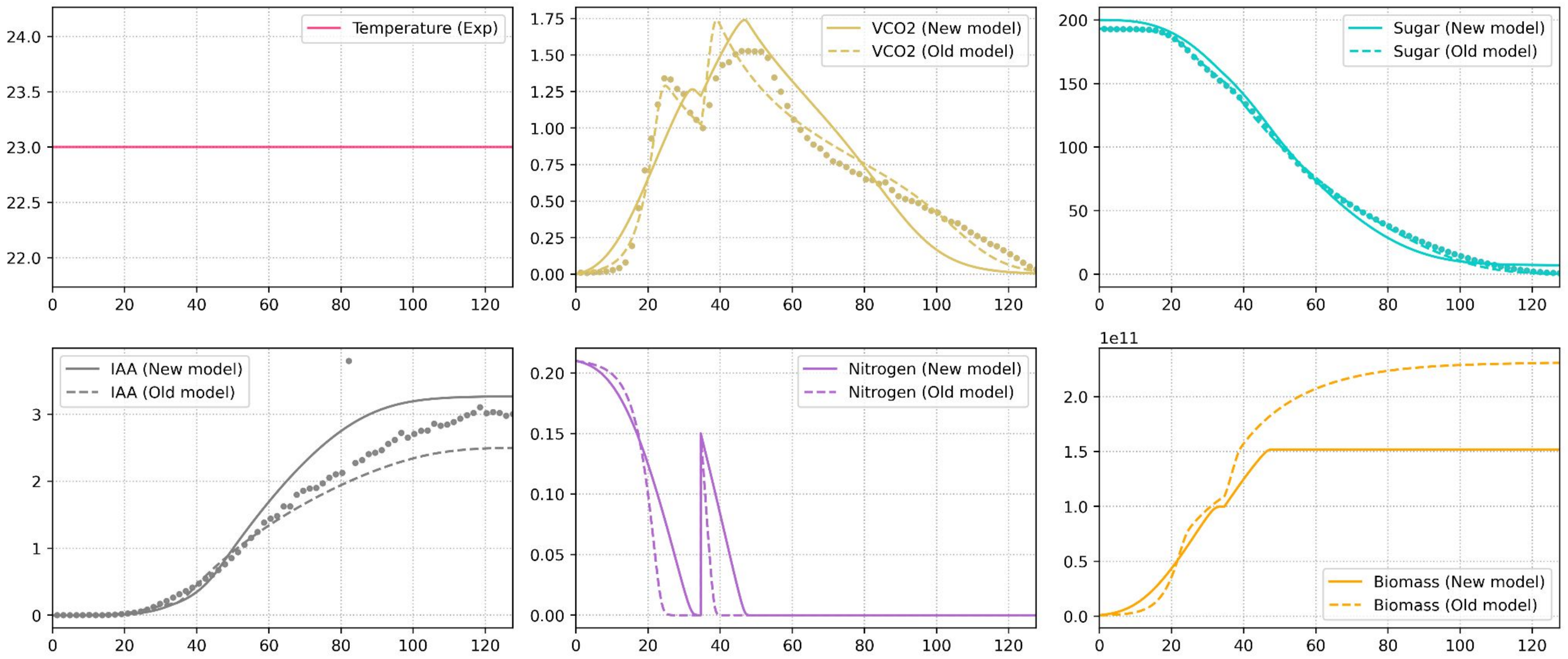

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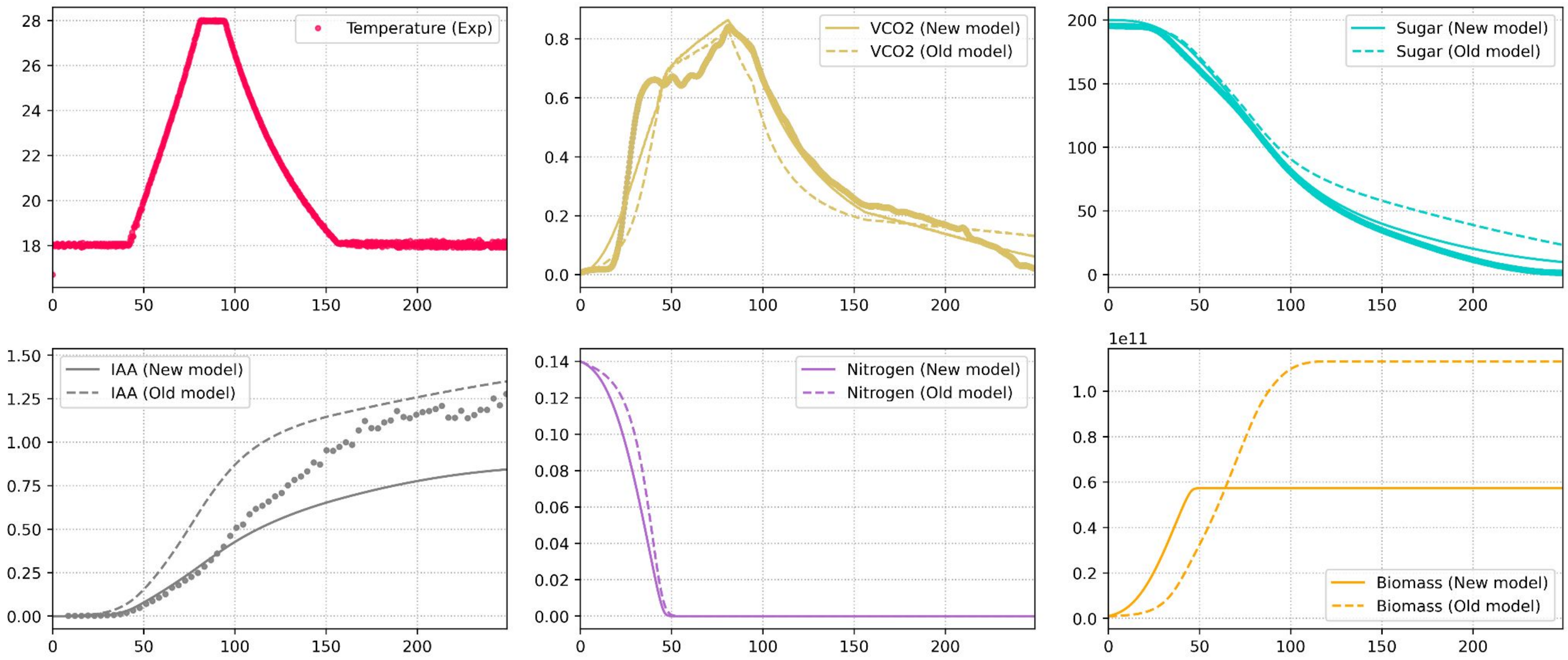


Another point of view of ester synthesis

Understanding regulation of the ratio ACoA/CoA

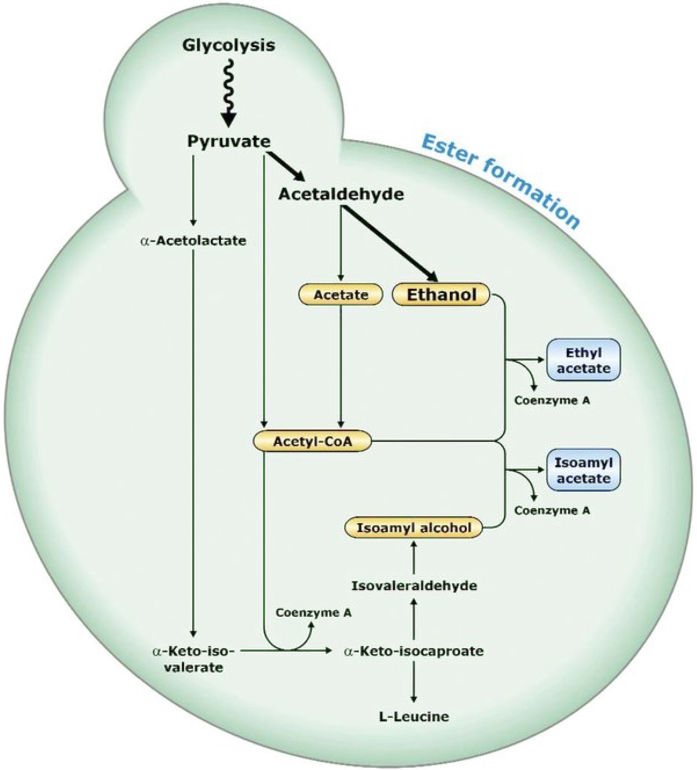
$$IAOH + ACoA \xrightarrow{Enzyme} IAA + CoA$$

Hypotheses:

- Since IAOH does not limit the reaction, ACoA is the limiting quantity.

  Extend the model with ACoA

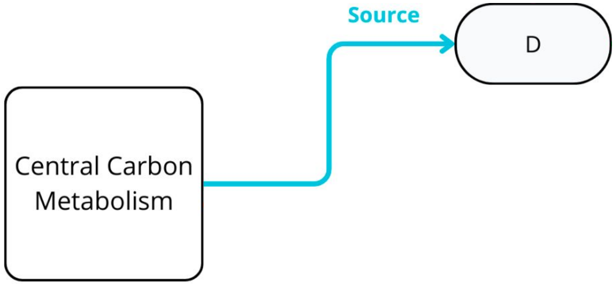
- Yeasts tries to keep a ratio ACoA/CoA "optimal". The reaction tries to get rid of the excess of ACoA to clean the cells.



Another point of view of ester synthesis

Modeling the production of IAA as a product of the excess of ACoA

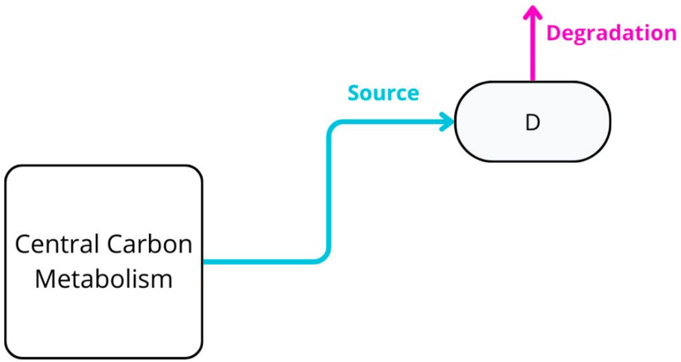
$$\dot{D} = k_D(T).\phi(S).(-\dot{S})$$



Another point of view of ester synthesis

Modeling the production of IAA as a product of the excess of ACoA

$$\dot{D} = k_D(T).\phi(S).(-\dot{S}) - \eta(T).D$$

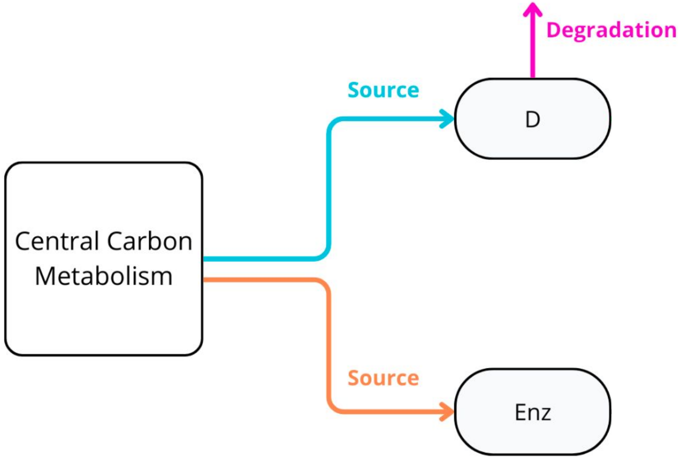


Another point of view of ester synthesis

Modeling the production of IAA as a product of the excess of ACoA, catalyzed by the enzymes **ATF1p/ATF2p**,

$$\dot{D} = k_D(T).\phi(S).(-\dot{S}) - \eta(T).D$$

$$\dot{Enz} = k_{Enz}(T).\phi(S).(-\dot{N})$$



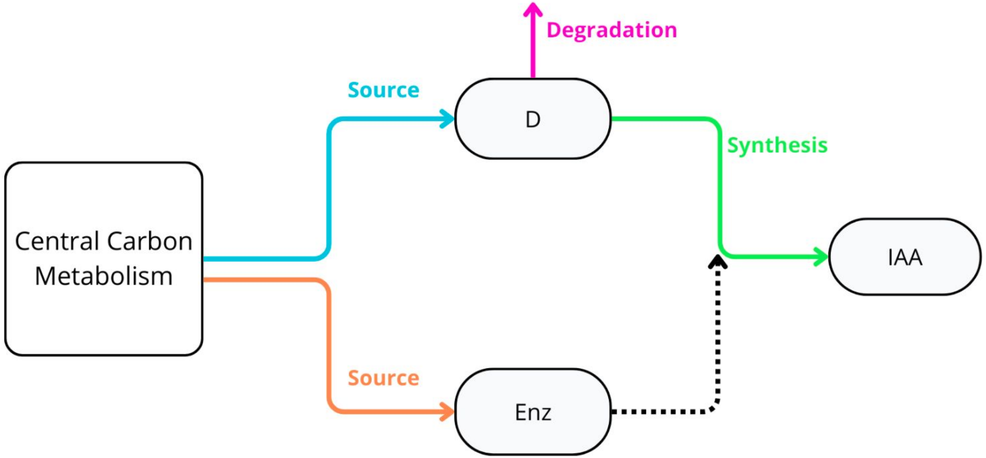
Another point of view of ester synthesis

Modeling the production of IAA as a product of the excess of ACoA

$$\dot{D} = k_D(T).\phi(S).(-\dot{S}) - \eta(T).D - k_{IAA}(T).\frac{D^h}{K_m^h + D^h}.Enz$$

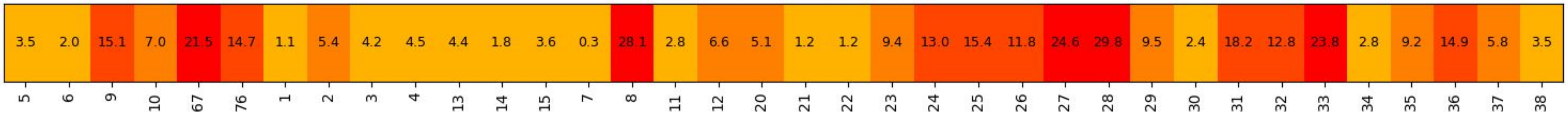
$$E\dot{n}z = k_{Enz}(T).\phi(S).(-\dot{N})$$

$$I\dot{A}A = k_{IAA}(T).\frac{D^h}{K_m^h + D^h}.Enz$$

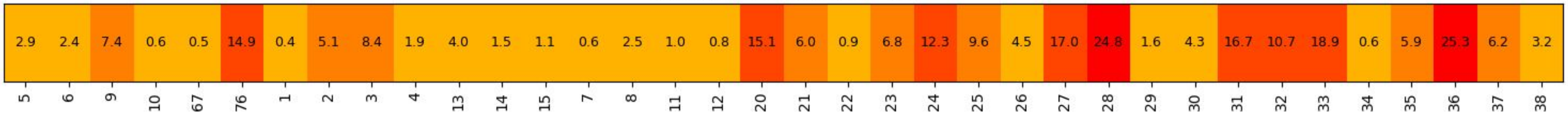


Comparison of models (simple vs ACoA/CoA)

Relative error for simple model



Relative error for ACoA/CoA model



Promising approach but still mixed results

Heat-transfer dynamics

The equation for the conservation of power gives the time-evolution of the temperature:

$$P_f(\dot{CO_2}) = \tilde{P}_a(CO_2, T)\dot{T} + P_w(T - T_e) + P_e(CO_2, \dot{CO_2}, T) + Q_c$$

Colombié, S., Malherbe, S., & Sablayrolles, J. M. (2007). **Modeling of heat transfer in tanks during wine-making fermentation**. Food control, 18(8), 953-960.

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$$\underbrace{P_f(\dot{CO_2})}_{\text{Fermentation}} = \underbrace{\tilde{P}_a(CO_2, T)\dot{T}}_{\text{Accumulation}} + \underbrace{P_w(T - T_e)}_{\text{Wall}} + \underbrace{P_e(CO_2, \dot{CO_2}, T)}_{\text{Evaporation}} + \underbrace{Q_c}_{\text{Refrigeration system}}$$

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Refrigeration system (Q_c)

We define the function:

$$v_{T_{\mathrm{nc}}}(CO_2, \dot{CO_2}, T_{\mathrm{nc}}) = \frac{1}{\tilde{P}_a(CO_2, T_{\mathrm{nc}})}\left(P_f(\dot{CO_2}) - P_w(T_{\mathrm{nc}} - T_e) - P_e(CO_2, \dot{CO_2}, T_{\mathrm{nc}})\right)$$

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Thus, the temperature is a new state of the system governed by the equation:

$$\dot{T} = v_{T_{\mathrm{nc}}}(CO_2, \dot{CO_2}, T) - \frac{Q_c}{\tilde{P}_a(CO_2, T)}$$

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Refrigeration system

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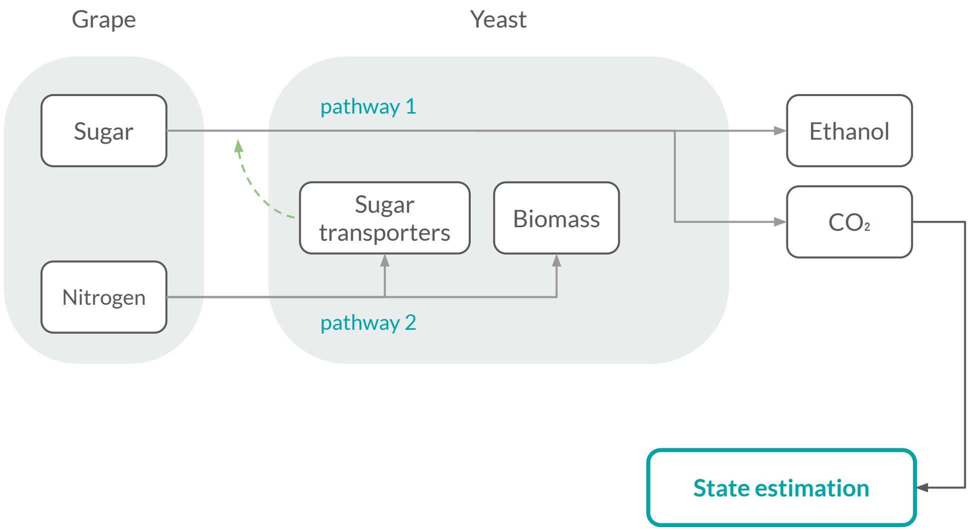
The temperature regulation scheme is subject to the following constraints:

$$Q_c(t) > 0 \qquad 18°C \leq T \leq 28°C \qquad \left|\frac{\mathrm{d}T}{\mathrm{d}CO_2}\right| \leq \Delta T_{\max}$$

The state estimation problem

State estimation of the main kinetics

Features of the fermentation process:



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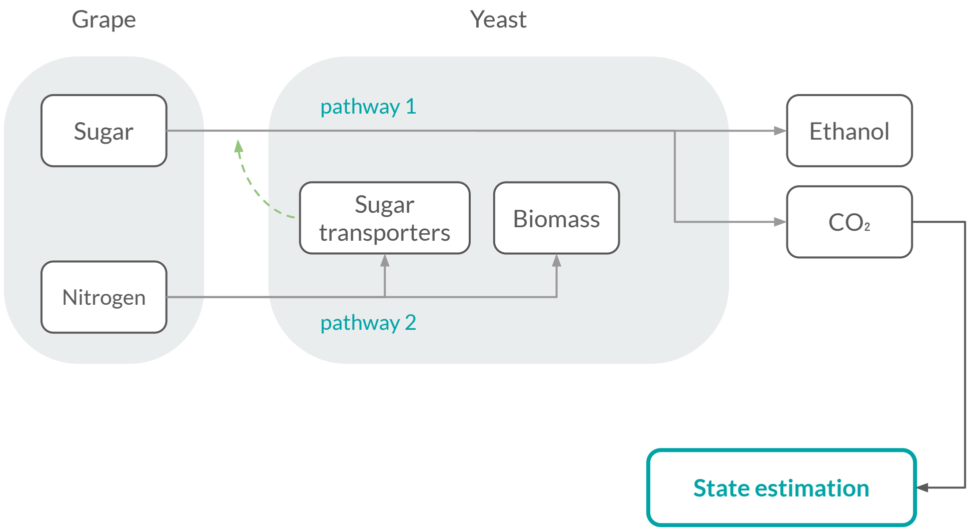

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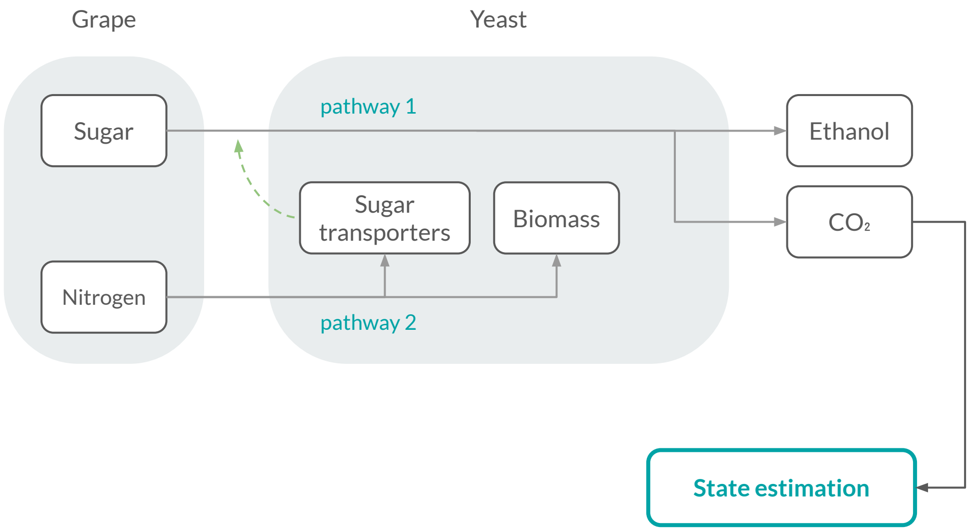
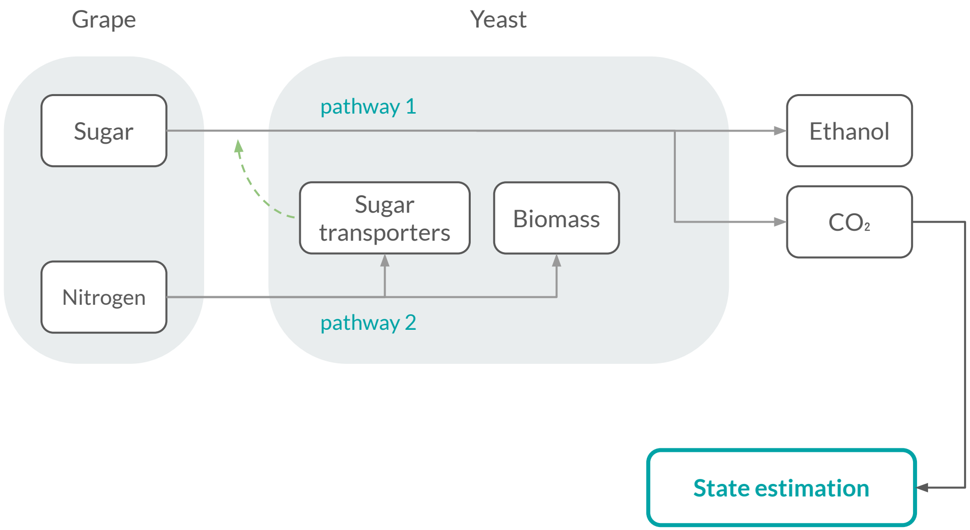
- Biomass and nitrogen measurements require manual sampling.



State estimation of the main kinetics

Features of the fermentation process:

- We can easily measure CO_2 through the weight difference.
- Biomass and nitrogen measurements require manual sampling.
- **Low**-frequency sampling time (= **high** computation time).



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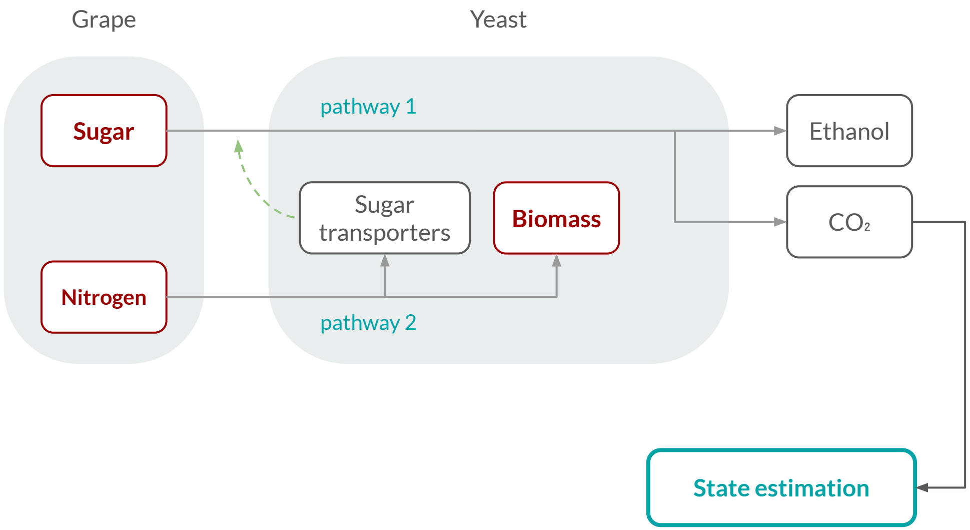
Objective: estimate the concentrations of sugar, nitrogen and biomass from **CO_2** measurements



The simple case: Malherbe *et al.* model

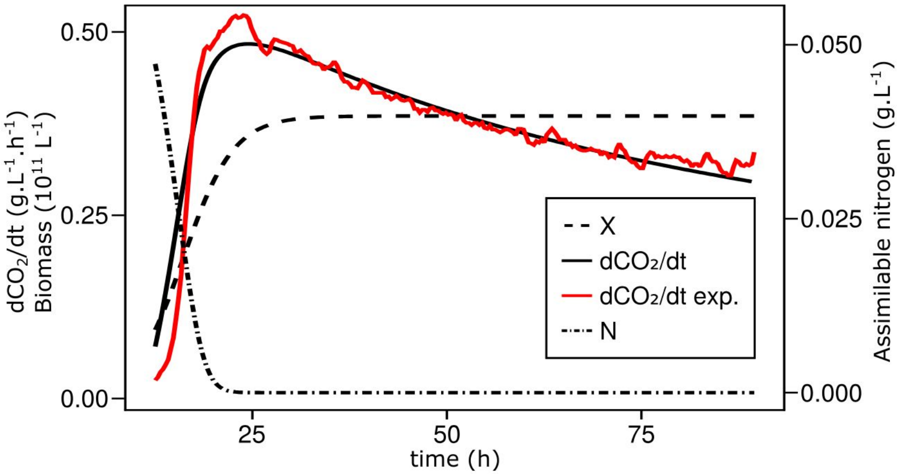
Malherbe, S. *et al.* (2004). **Modeling the effects of assimilable nitrogen and temperature on fermentation kinetics in enological conditions.** Biotechnology and bioengineering.

$$\dot{S} = -XN_{ST}(N_0 - N, X, T)\nu_{ST}(S, E, T)$$

$$\dot{N} = -X\nu_N(N, E, T)$$

$$\dot{X} = k_1(T)X\left[1 - \frac{X}{X_{\max}(N_0)}\right]$$

$$\dot{E} = -\mu\dot{S}$$



where:

$$\nu_{ST}(S, E, T) = \frac{k_2(T)S}{K_S + S(1 + K_{Si}E^{\alpha_S})}$$

(Ethanol-inhibited glucose absorption)

$$\nu_N(N, E, T) = \frac{k_3(T)N}{K_S + N(1 + K_{Ni}E_N^{\alpha})}$$

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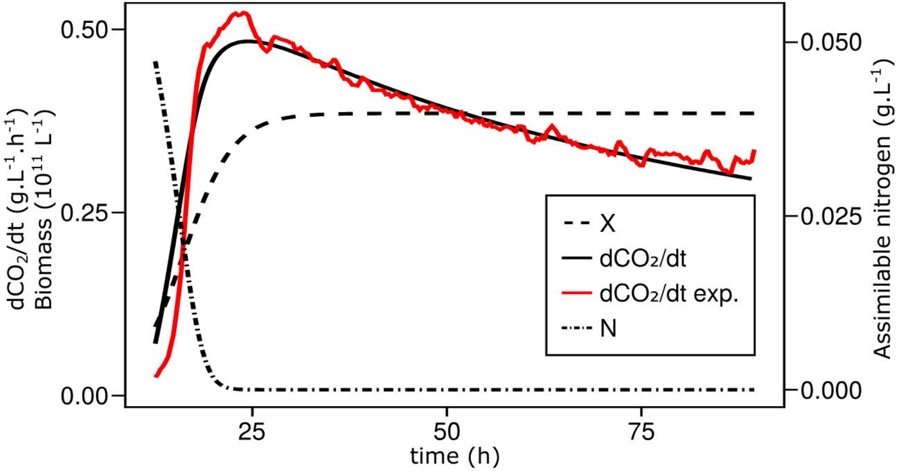
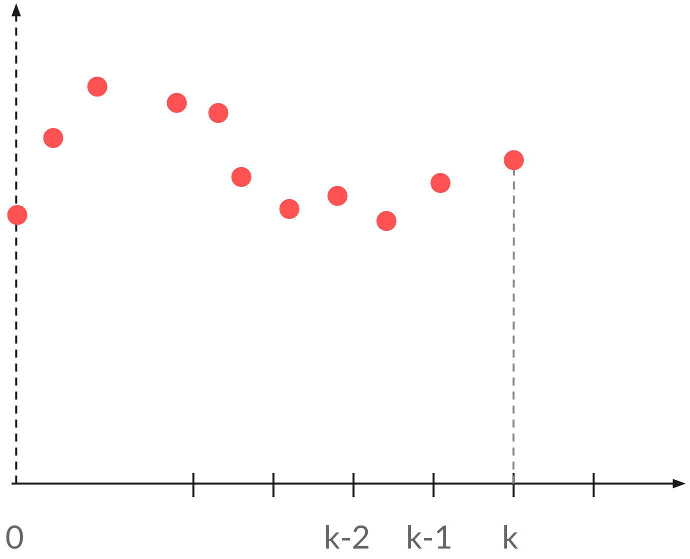


Proposition 1: Under isothermal conditions (T constant), for any $0 \leq t_1 < t_2$, System (1)-(4) is observable over $[t_1, t_2]$. That is, for any two trajectories of (1)-(4) with initial conditions such that $(S_0, N_0, X_0,), (\tilde{S}_0, \tilde{N}_0, \tilde{X}_0) \in \Omega$, $E_{|[t_1,t_2]} \equiv \tilde{E}_{|[t_1,t_2]}$ implies $(S_0, N_0, X_0) = (\tilde{S}_0, \tilde{N}_0, \tilde{X}_0)$.

Non-linear **Full Information Estimator (FIE)**

Given the state $\xi = (S, N, X, E)$ and the dynamics:

$$\dot{\xi} = f(\xi)$$
$$\mathbf{y} = E + v$$



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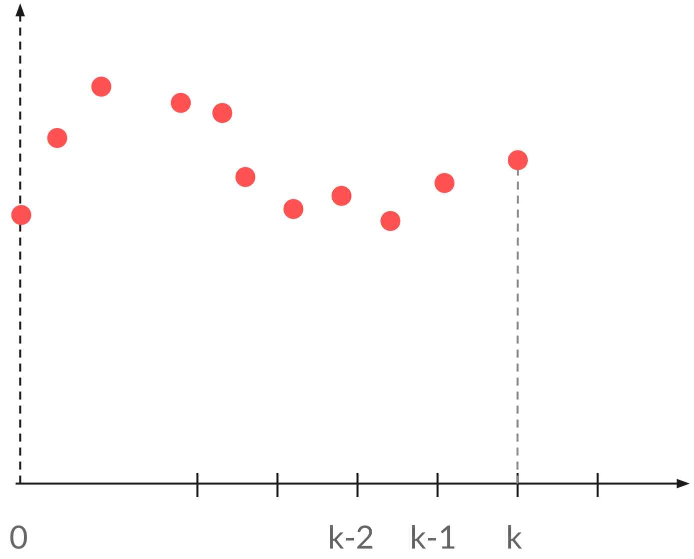

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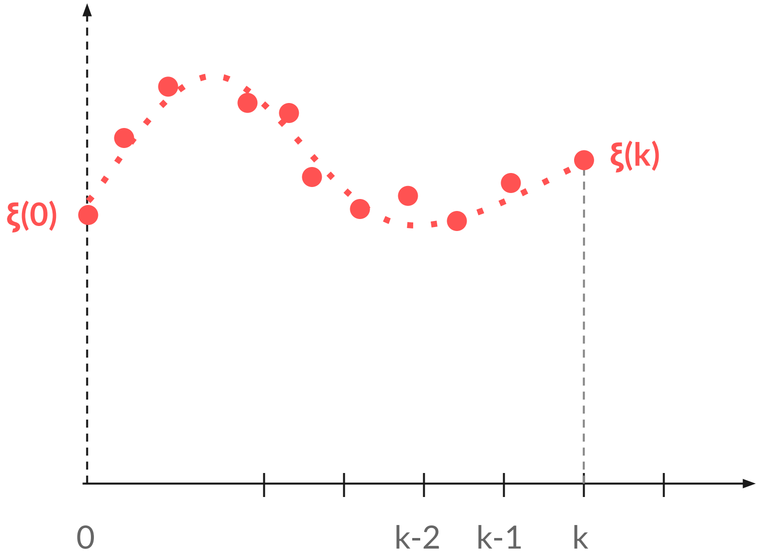

The Full Information Estimation problem is to solve the optimization problem:

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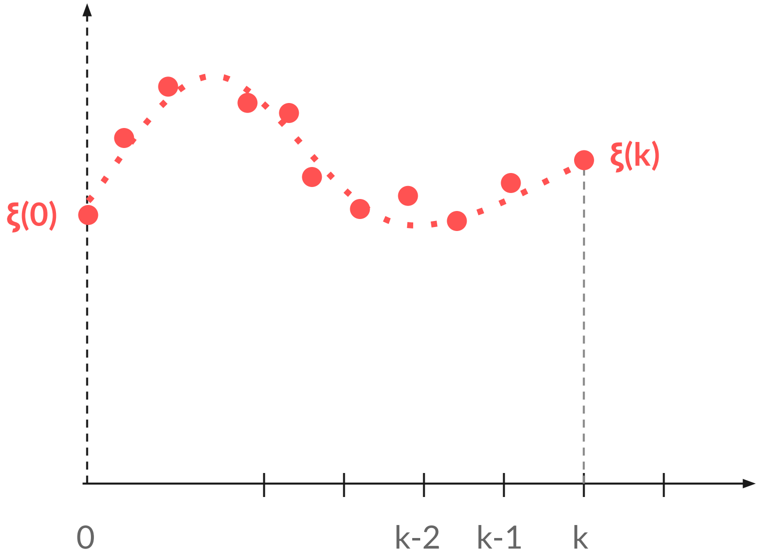

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At each time instant, we take into account **all the data**.

FIE convergence result

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time (h)

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Proposition 5: Under the above assumptions, there exists a $\mathcal{K}$-class function ω such that

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In particular, $\xi = \hat{\xi}^k$ on $[0, T_k]$ if $v = 0$. Furthermore, if $\|v\|_{L^2(T_k,+\infty)} \to 0$ as $k \to 0$, then $\hat{\xi}^k(0) \to \xi_0$.

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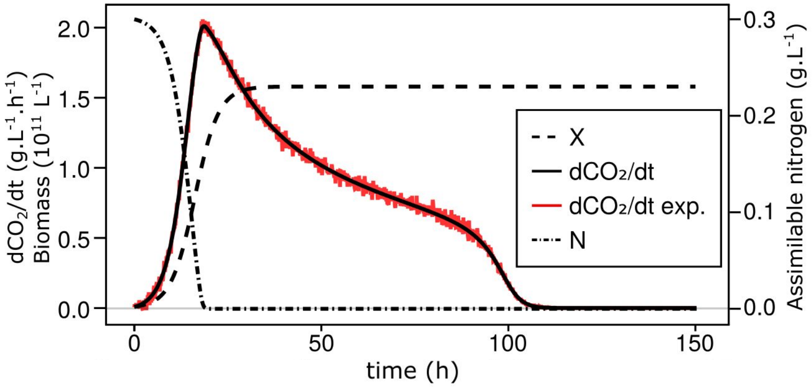

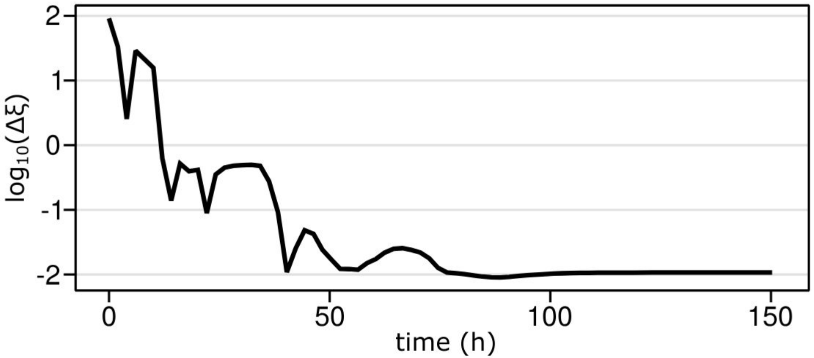

The control problem

Numerical results

Minimize total energy consumption:

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Maximize final liquid concentration of IAA:

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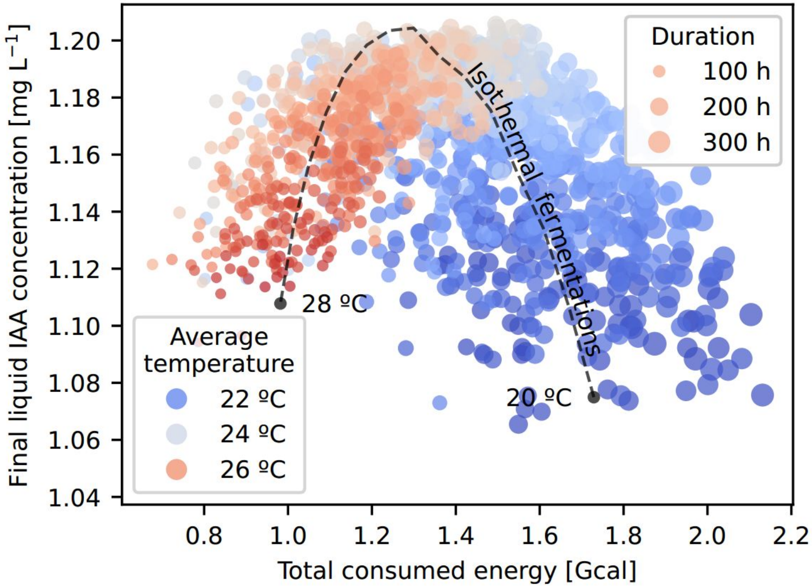

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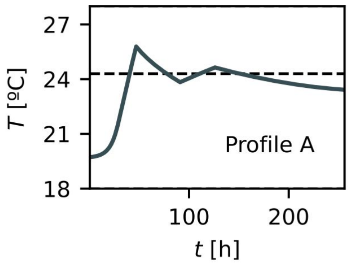

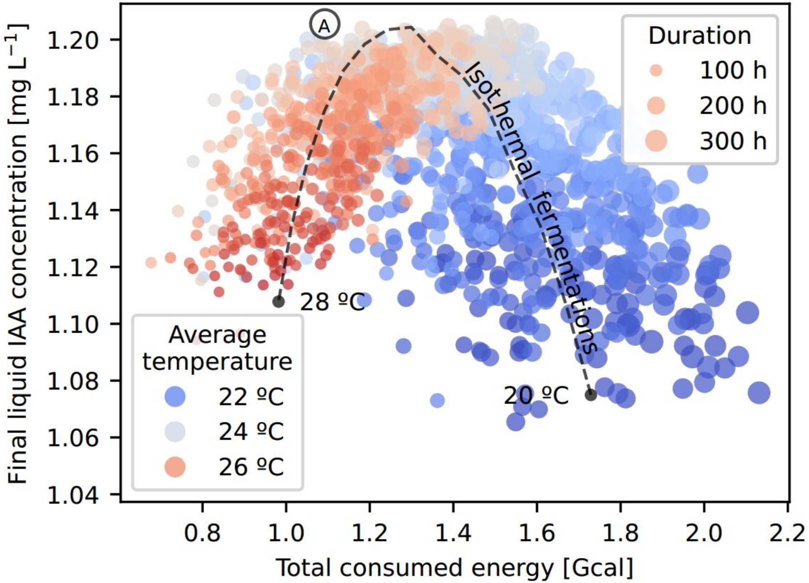

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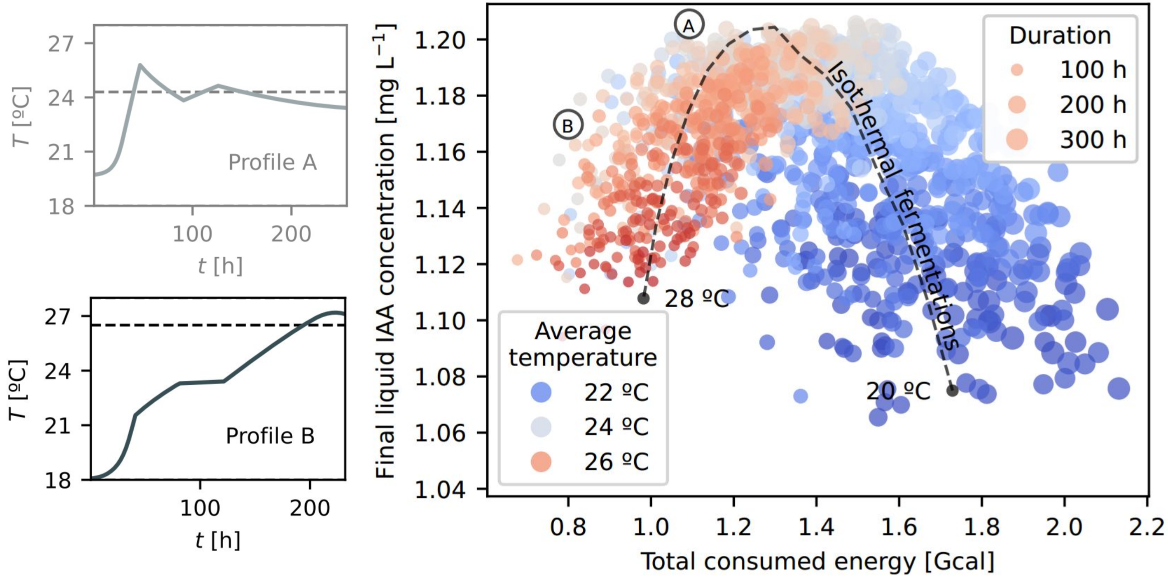

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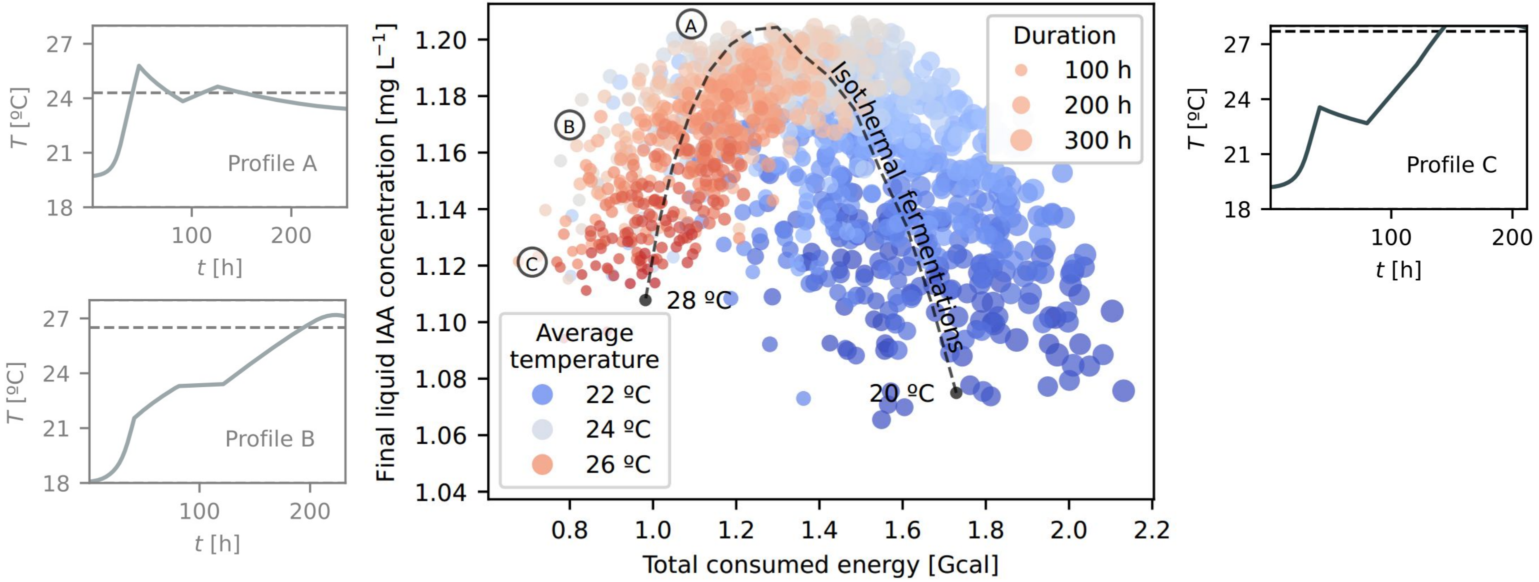

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The approach can easily include:

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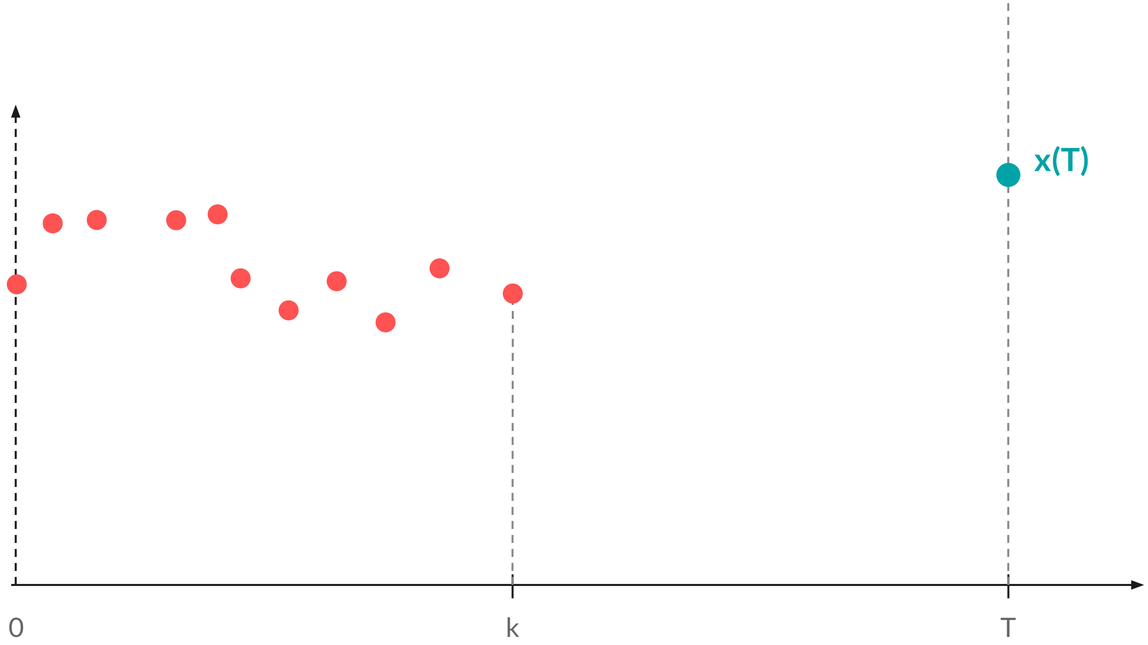

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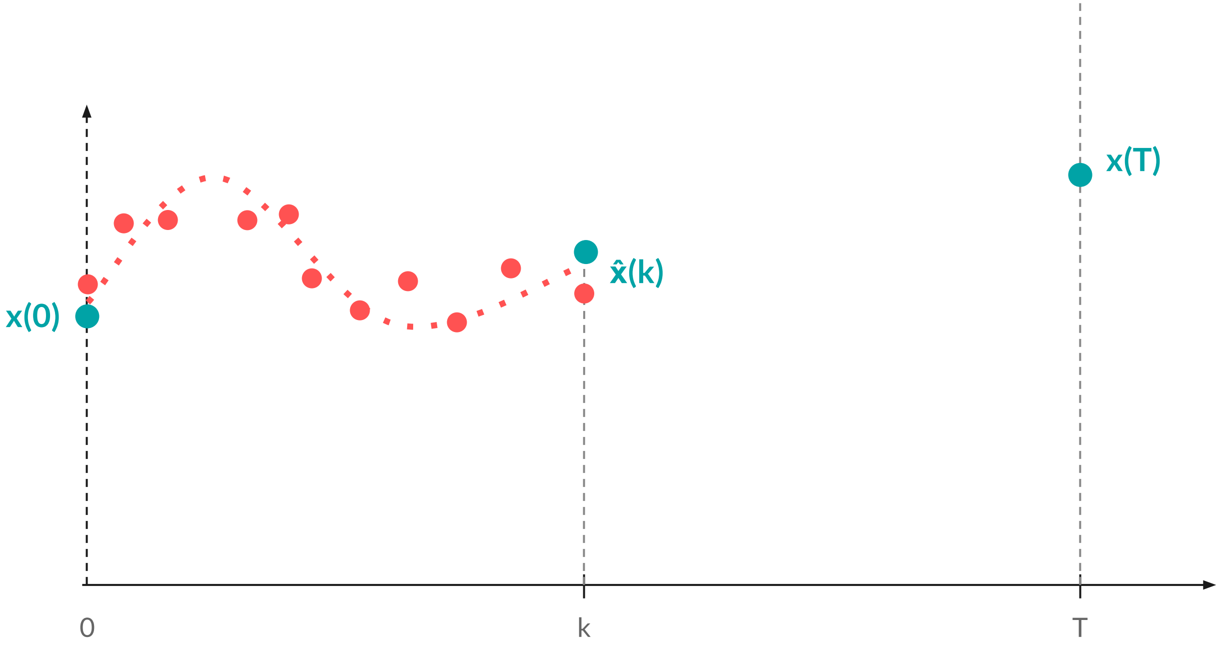

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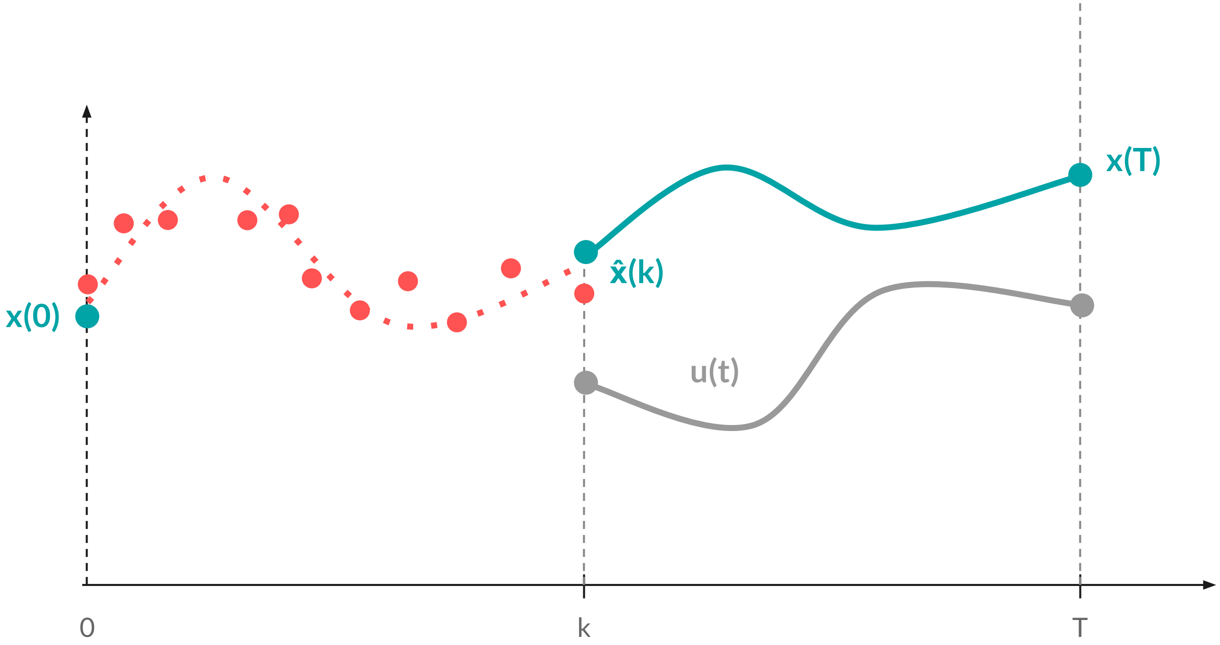

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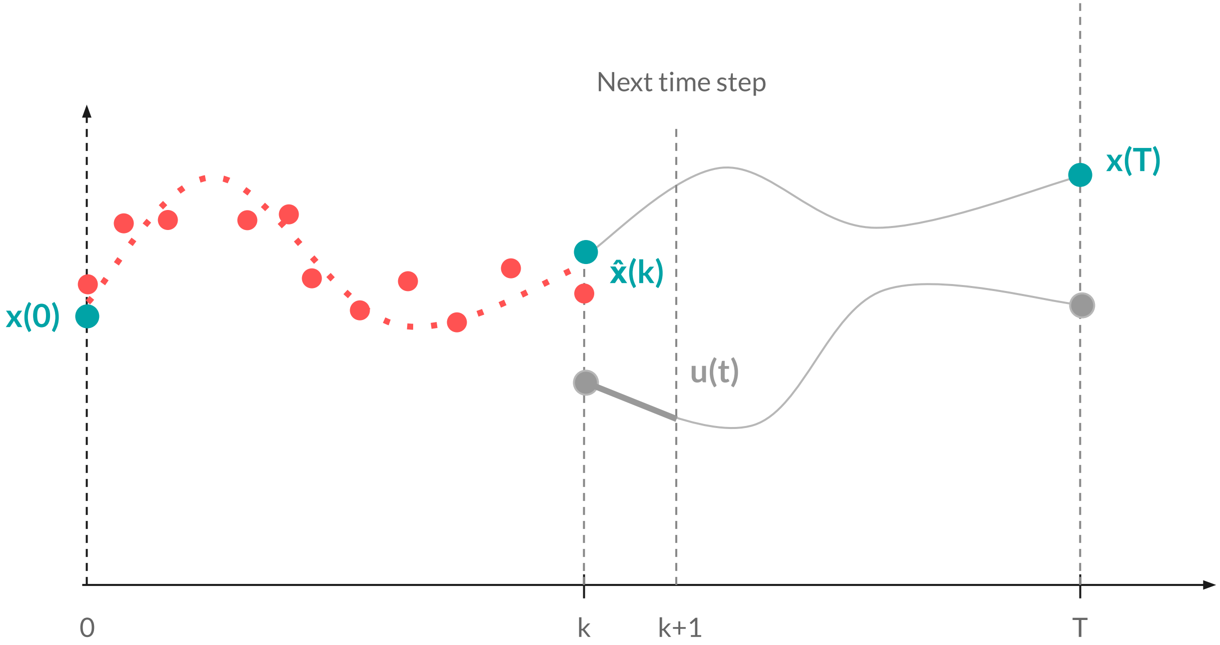

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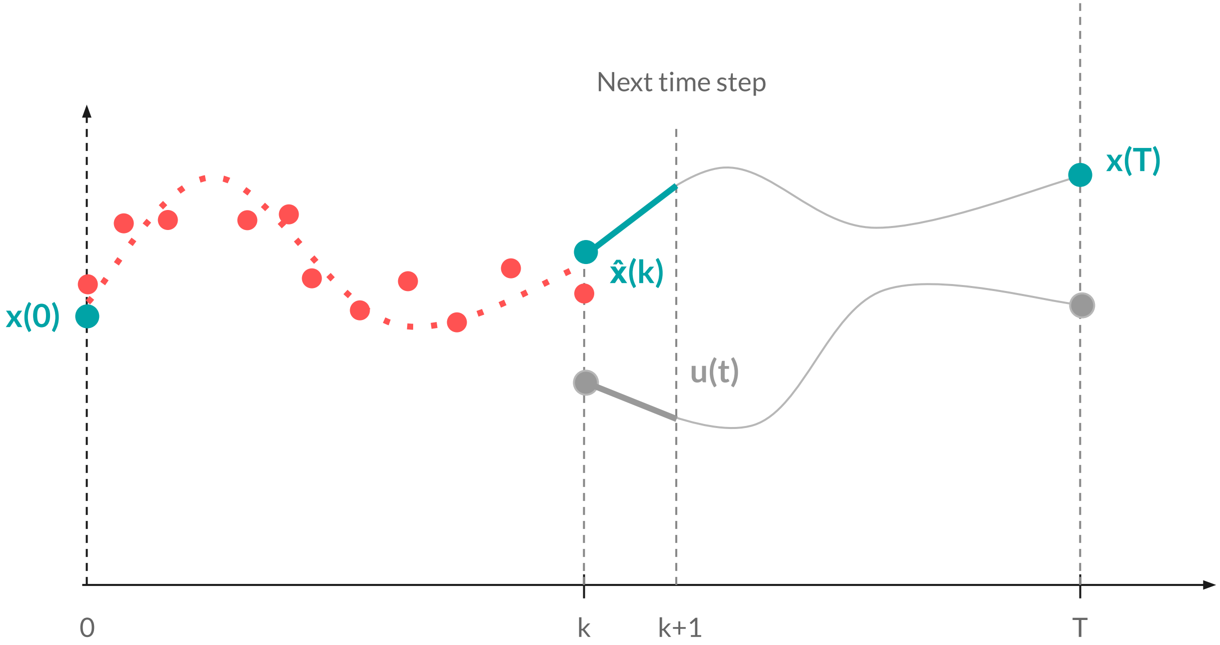

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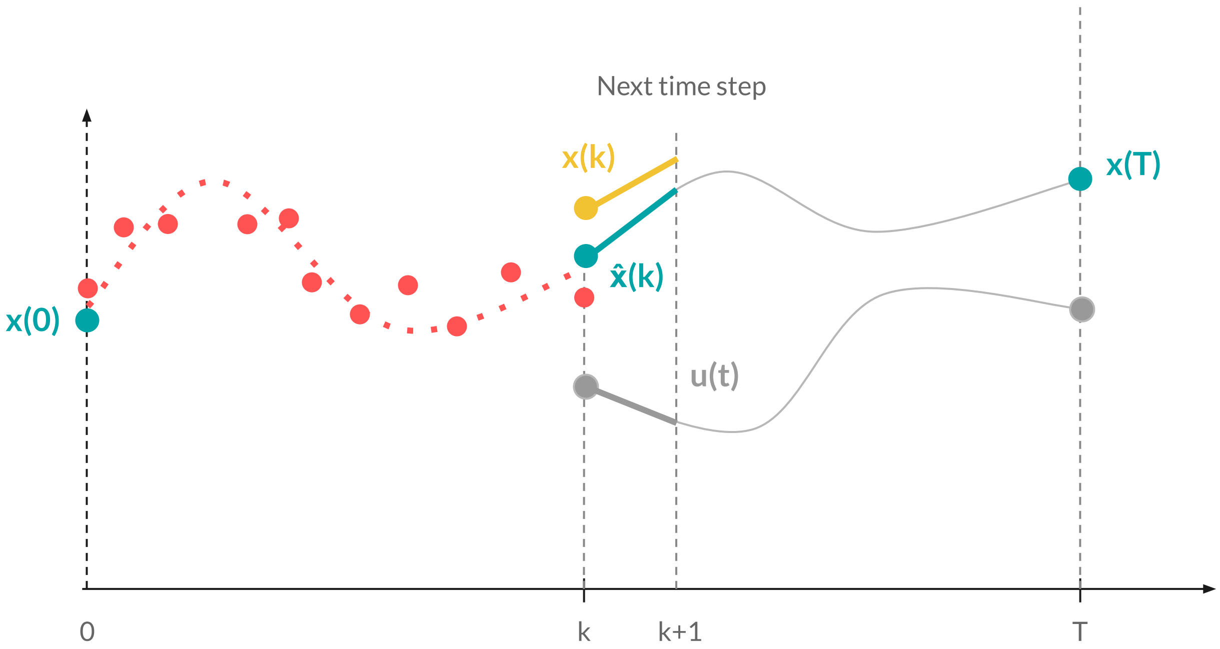

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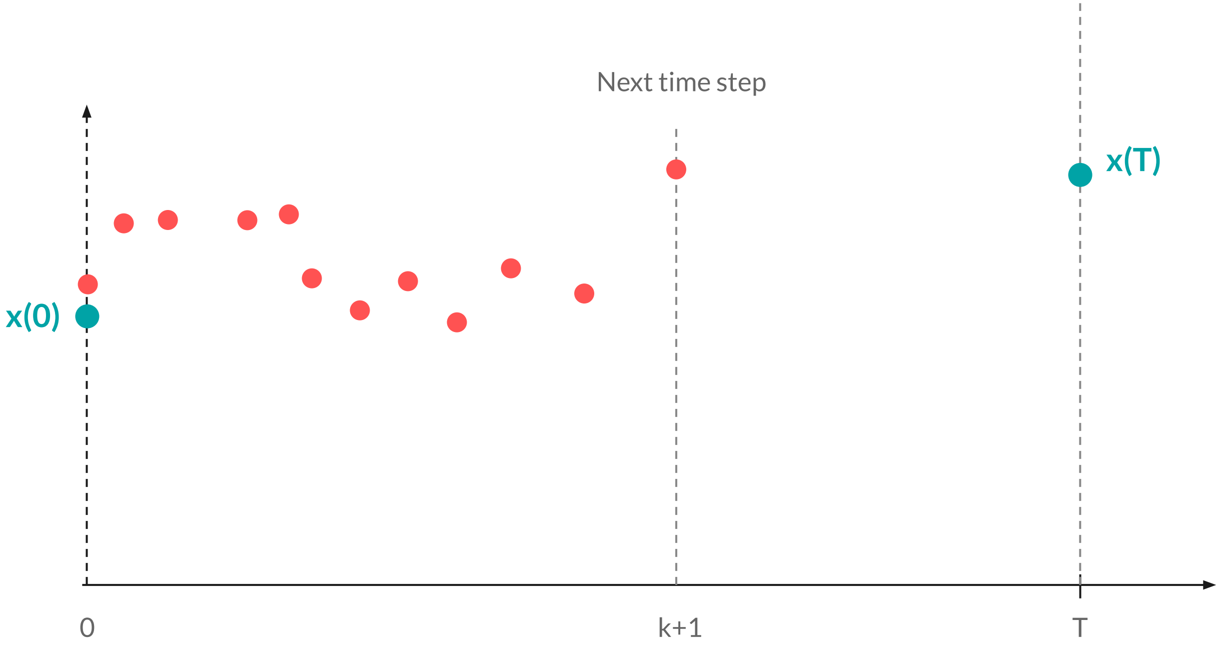
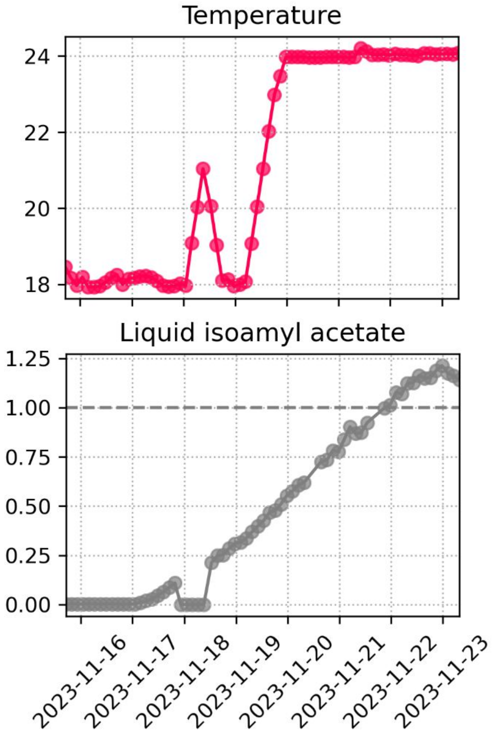
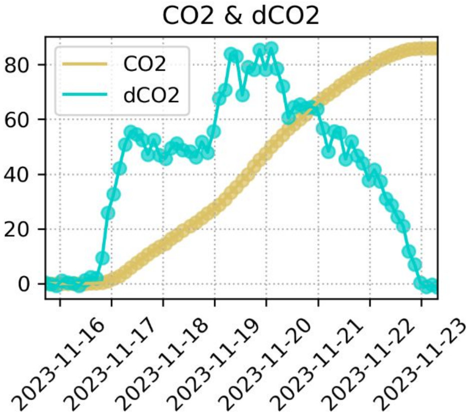


Experimental results





Experimental 100L fermenter

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Campo, P. J., & Morari, M. (1987, June). **Robust model predictive control**. In 1987 American control conference. IEEE.

In this approach, we parametrize the parametric/system uncertainty with a set of models:

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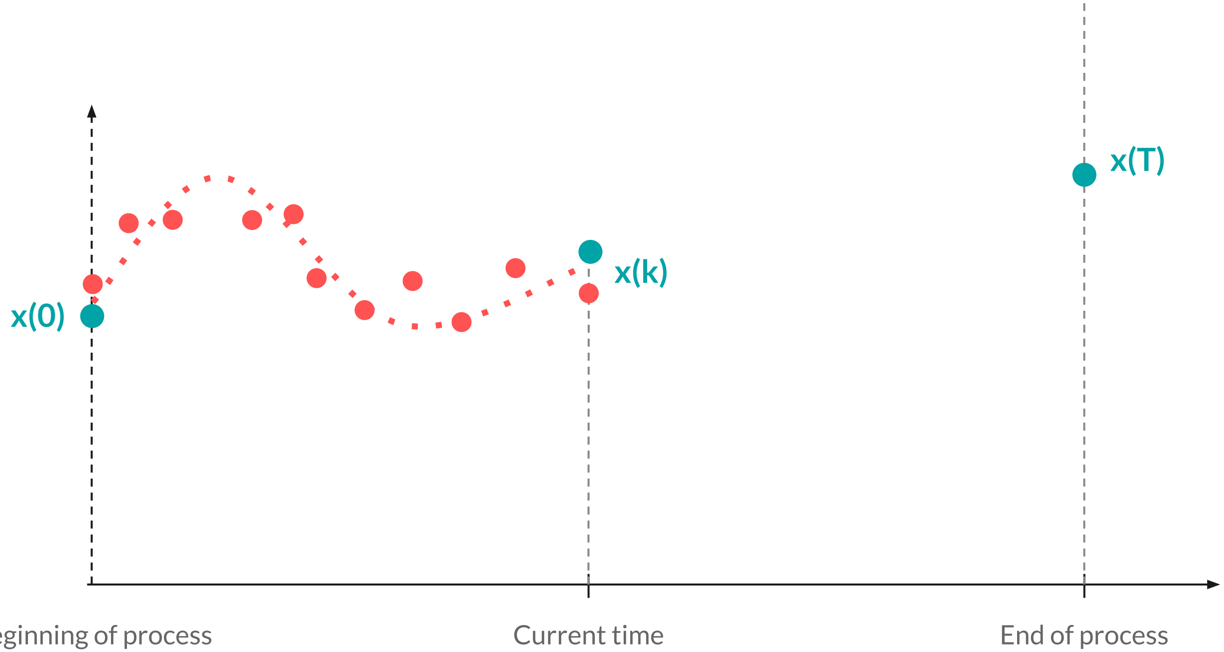

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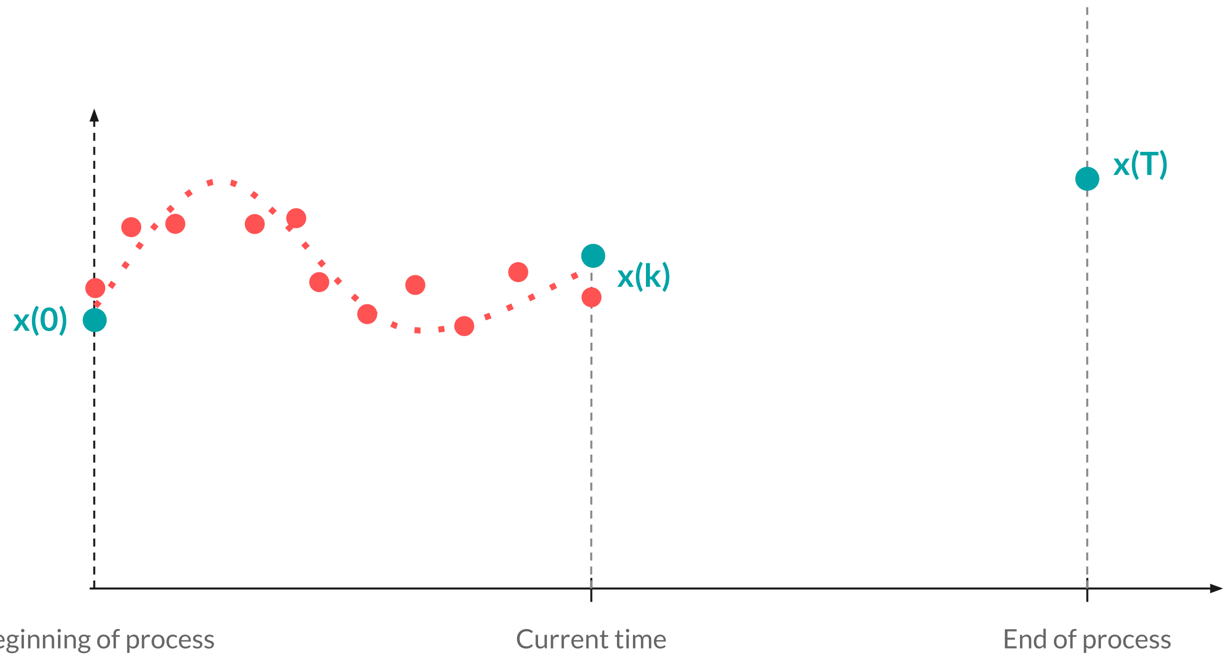

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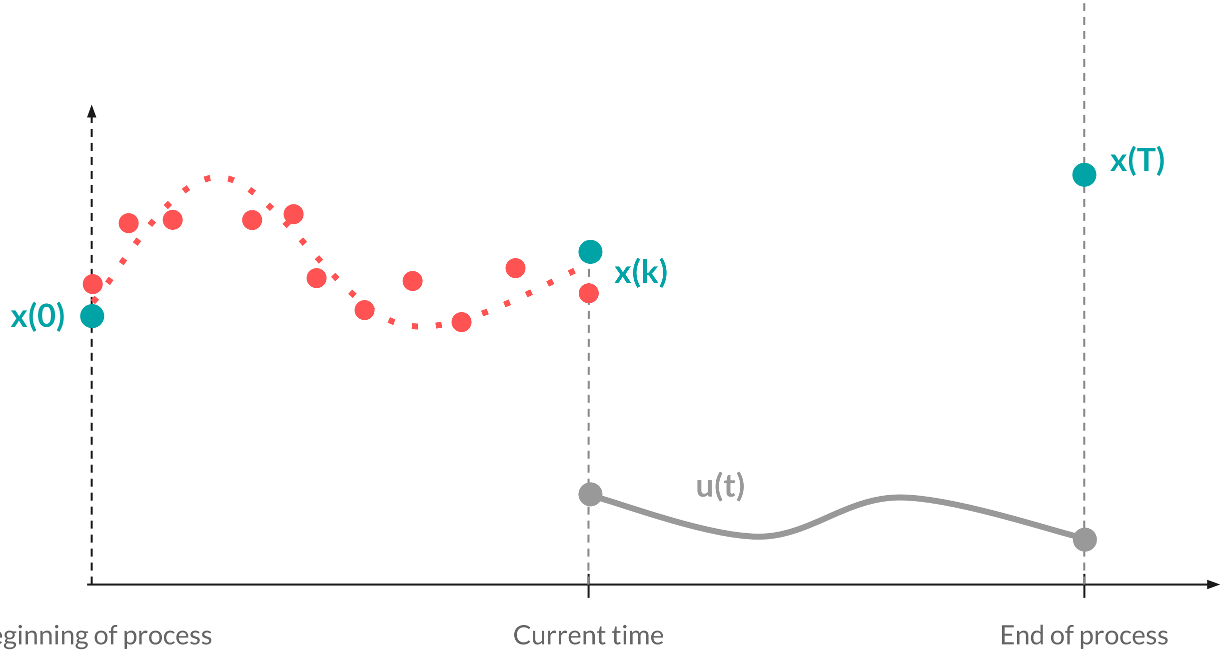

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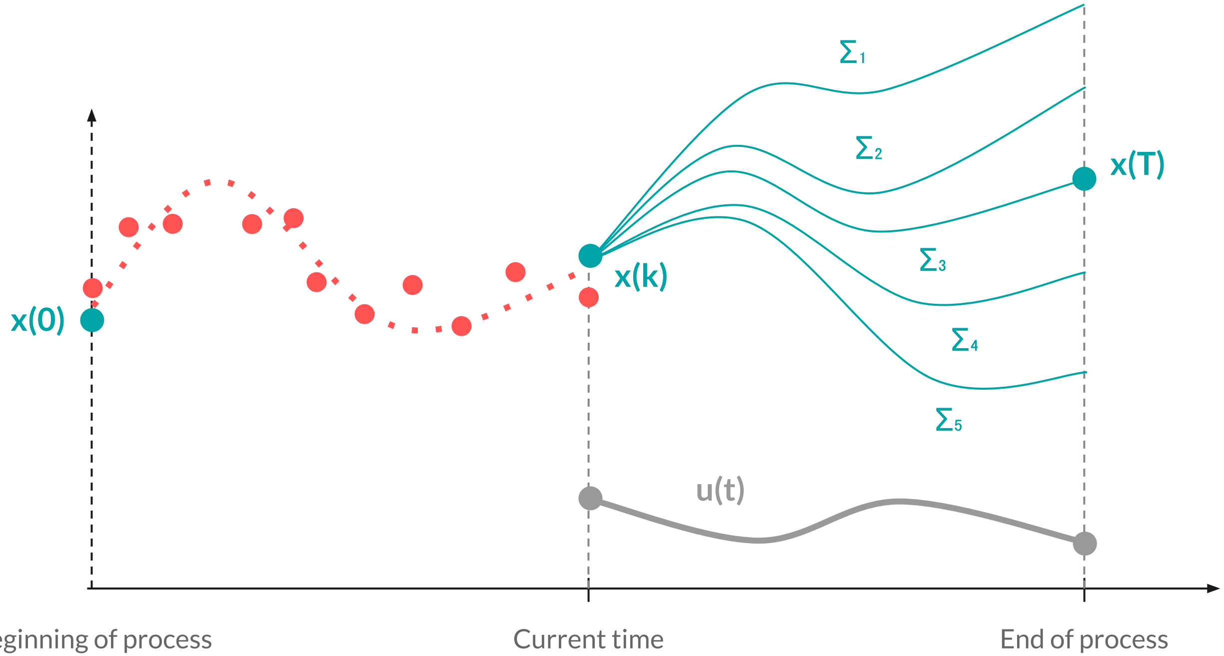

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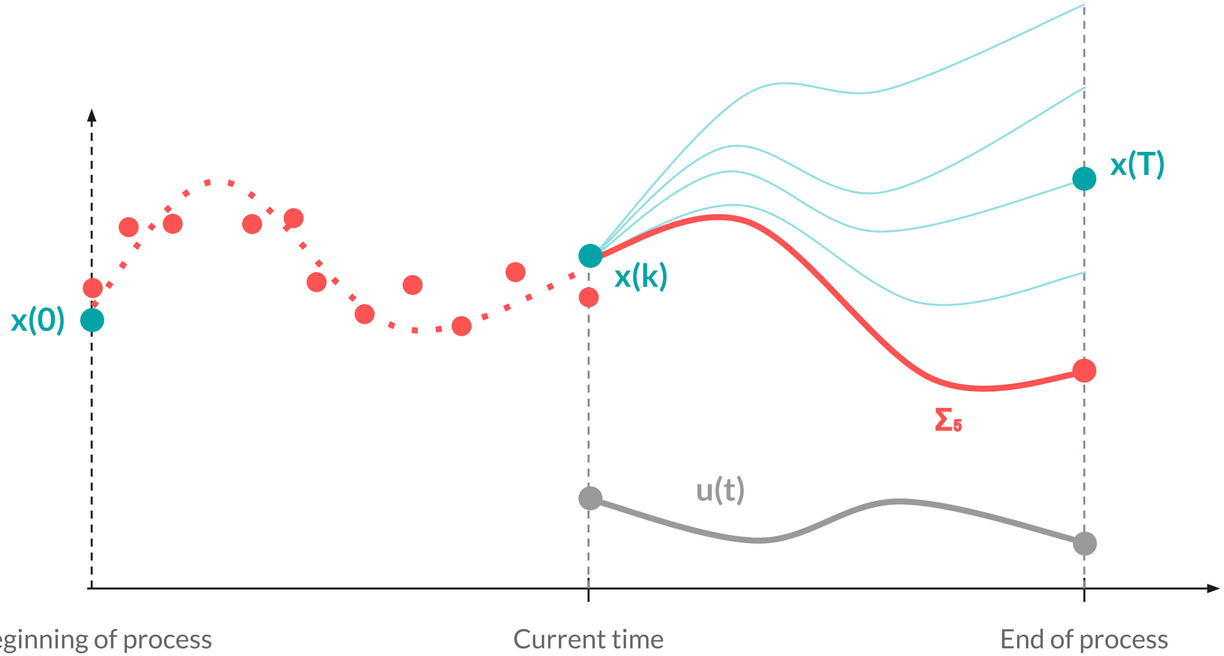
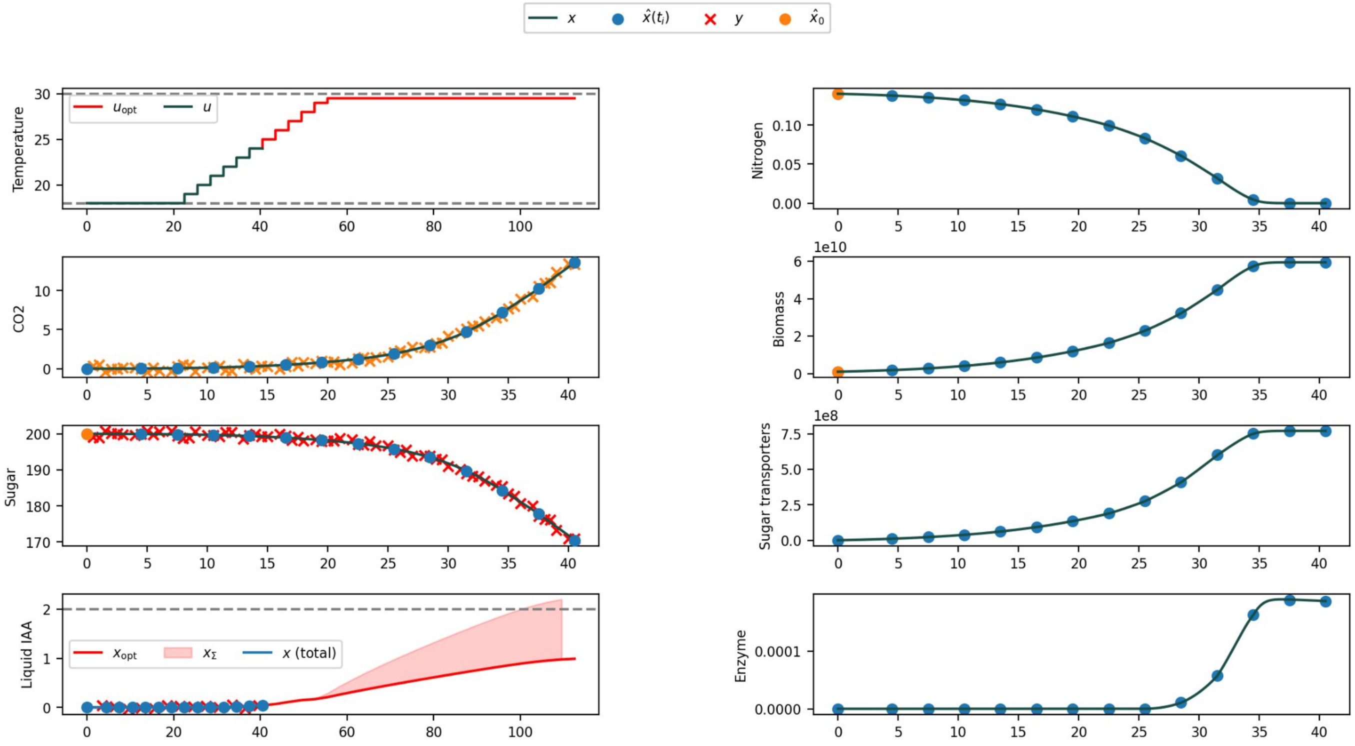


Simulations



Merci !

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