

Context

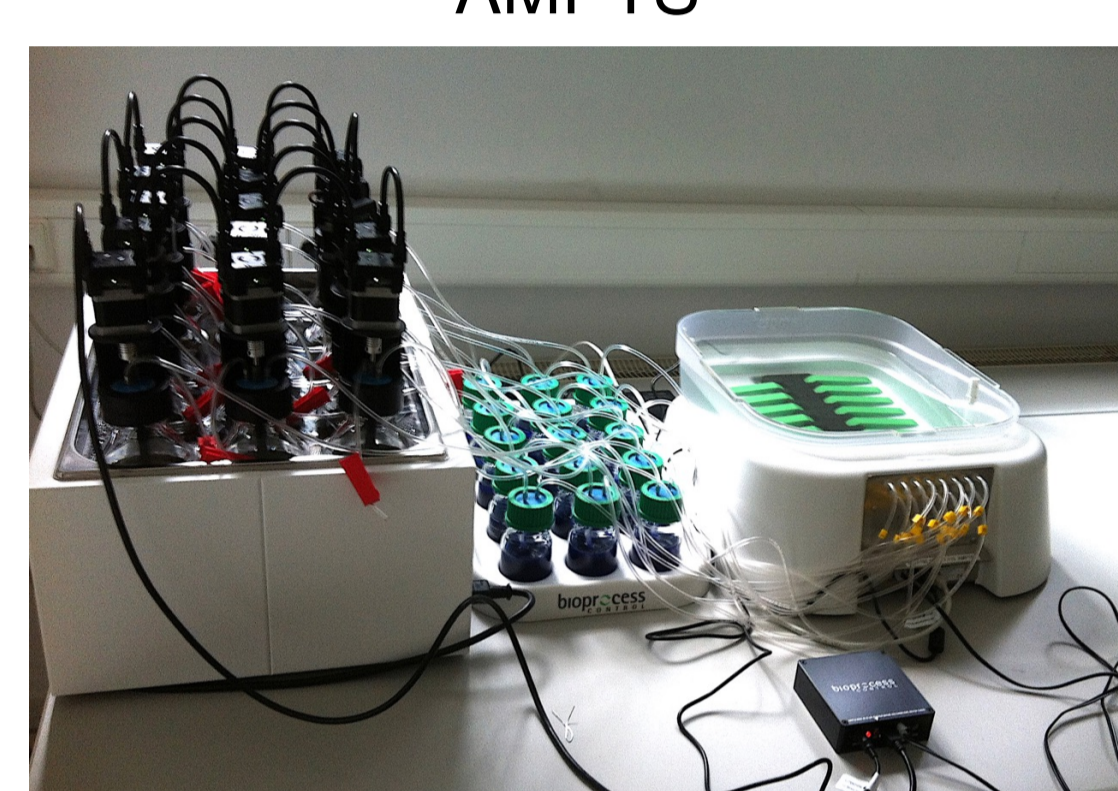
Besides the classical measure of BMP can need as long as 15 days, the dynamics of the production can be identified during the first few days if rigorous test methodology is respected and a biologically inspired mathematical model is used. This approach can provide accurate predictions of BMP value with shortened experimentation duration.

But finding mathematical models that are simple enough to be used for process control and prevision is particularly important. In this study we have used the modified AM2 model, calibrated and then validated with 90 different experiments as triplicates of 30 different substrate/inoculum mixes of sludge coming from the Paris' conurbation WWTP.

The obtained model allows a good prediction after only 4 days with an acceptable error and at the same time gives the possibility to understand the influence of the initial proportion of substrates on the production profile.

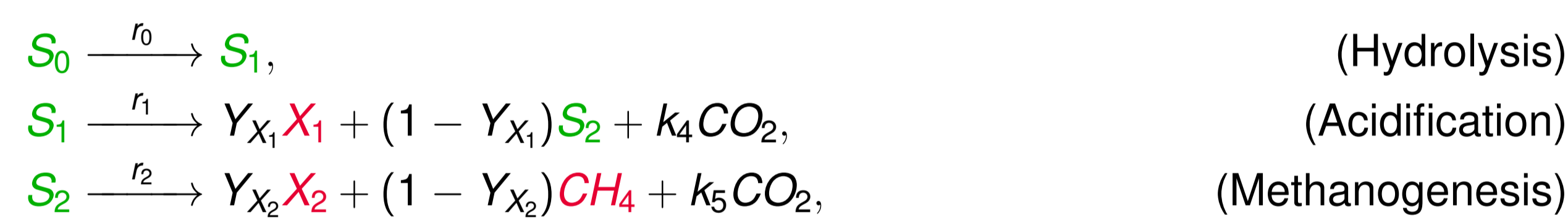
Experimental protocol

- ▶ 500 ml reactors, I/S ratio=3
- ▶ CO₂ trapping
- ▶ Mean flow measurement by ≈ 10ml throttles
- ▶ Full compliance with experts recommendations [1]
- ▶ 36 batches in triplicates
- ▶ VSS, TSS, COD, BOD measurements
- ▶ BMP obtained after 20 days



Modified AM2 model

Reaction scheme [2, 3, 4] :



S_0 : insoluble organic molecules, S_1 : simple compounds (fatty acids, peptides, amino acids, ...),
 S_2 : volatile fatty acids

Differential equations system :

- ▶ Perfectly mixed batch reactor, states of the sytem : S_0, S_1, S_2, X_1, X_2

$$\begin{aligned} S_0' &= -r_0, & S_1' &= r_0 - r_1, & S_2' &= (1 - Y_{X_1})r_1 - r_2, \\ X_1' &= Y_{X_1}r_1, & X_2' &= Y_{X_2}r_2, & CH_4' &= (1 - Y_{X_2})r_2 \end{aligned}$$

- ▶ initial conditions : $S_0(0) = S_0^0, S_1(0) = S_1^0, X_1(0) = X_1^0, X_2(0) = X_2^0$.

- ▶ reaction rates :

$$r_0 = \mu_0 S_0, \quad r_1 = \frac{\mu_1^{max} S_1 X_1}{S_1 + K_{S_1}}, \quad r_2 = \frac{\mu_2^{max} S_2 X_2}{S_2 + K_{S_2} + S_2^2/K_I}$$

- ▶ Parameters $\theta = (\underbrace{Y_{X_1}, Y_{X_2}, \mu_0, \mu_1^{max}, \mu_2^{max}, K_{S_1}, K_{S_2}, K_I}_{\theta_c : \text{kinetic parameters}}, \underbrace{X_1^0, X_2^0, S_0^0, S_1^0, S_2^0}_{\theta_b : \text{batch parameters}})$

Identification of parameters

Goals

Obtain a mathematical model allowing to reproduce the methane rate of all experiences, without necessarily uniquely describe state variables (X_1, X_2, S_1, S_2, S_0) and being able to use this model to predict the BMP from new data measured after only 4 days

Available measurements

For each batch #i we have

- ▶ $(t_k^i)_{k=1...m_i}$ the times of throttle switches
- ▶ $(D_k^i)_{k=2...m_i}$ the mean CH₄ flow rate measured at $t = t_k^i, k = 1 \dots$

Simulations

For $\theta = (\theta_c, \theta_b)$ we can simulate the mean flow of CH₄ :

$$d_k^i(\theta_c, \theta_b) = (CH_4(t_k^i) - CH_4(t_{k-1}^i)) / (t_k^i - t_{k-1}^i),$$

The function

$$J_i(\theta_c, \theta_b, T) = \sum_{\substack{k=2 \\ t_k^i \leq T}} (t_k^i - t_{k-1}^i) (D_k^i - d_k^i(\theta_c, \theta_b))^2$$

evaluates the misfit between measurements of batch #i and the simulation with parameters $\theta = (\theta_c, \theta_b)$ at horizon T

Learning phase $T = \infty$, batches #1 ... #69

Minimize with respect to $\xi = (\theta_c, \theta_b^1, \dots, \theta_b^{69}) \in \mathbb{R}^{353}$

$$\hat{\xi} = \arg \min_{\xi} J(\xi) = \sum_{i=1...69} J_i(\theta_c, \theta_b^i, \infty) + \lambda \|\xi\|^2,$$

We only keep $\hat{\theta}_c \in \mathbb{R}^8$ which is used for the prediction.

Optimization is done with interior points method (fminc, MATLAB) and computation time is small despite problem size (computer with 20 processors Xeon E5-2660-v2).

Prediction/validation phase $T = 4$ days, batches #70 ... #108

Independently minimize with respect to $\theta_b^i \in \mathbb{R}^5$

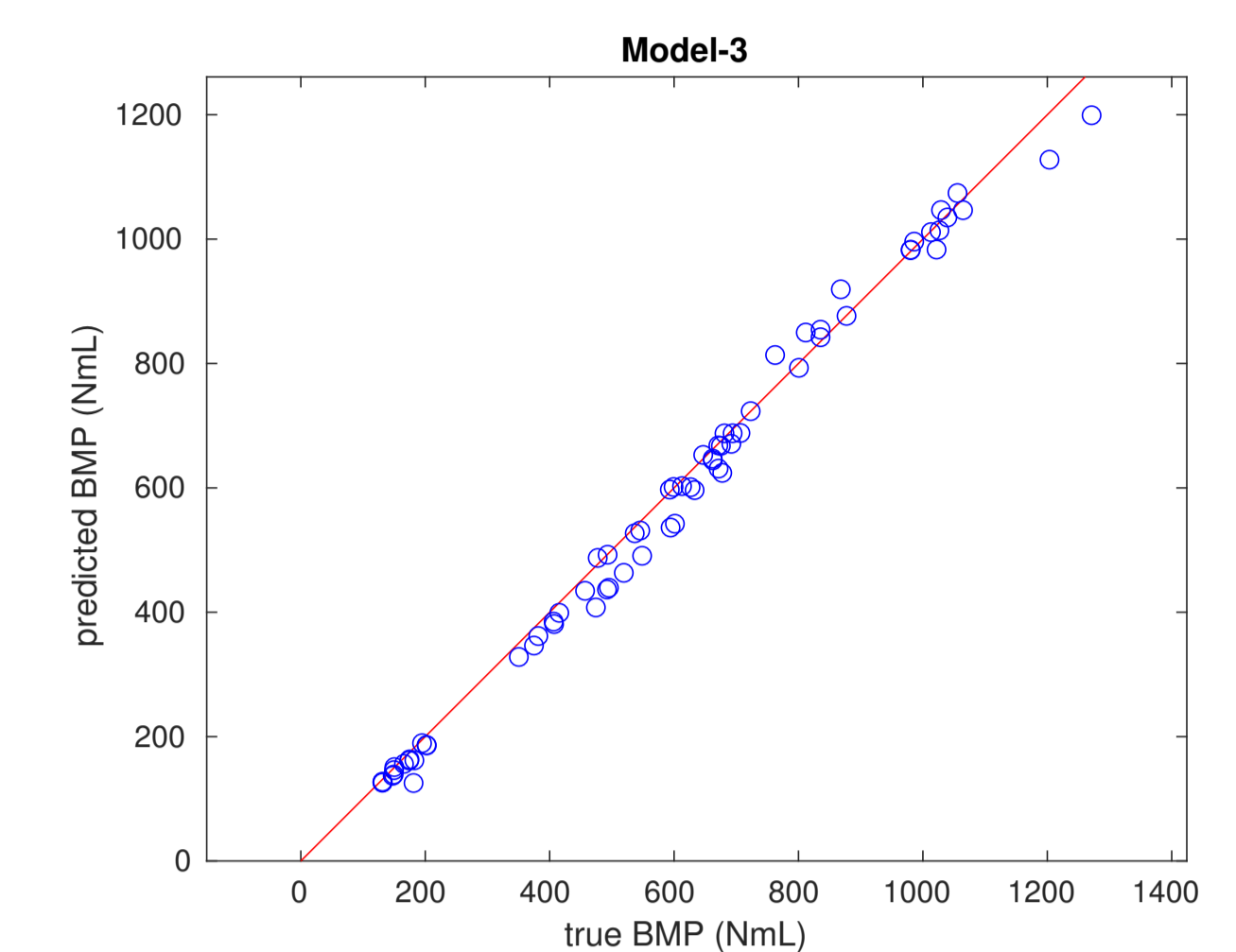
$$\hat{\theta}_b^i = \arg \min_{\theta_b} J_i(\hat{\theta}_c, \theta_b, 4), \quad i = 70 \dots 108$$

Results

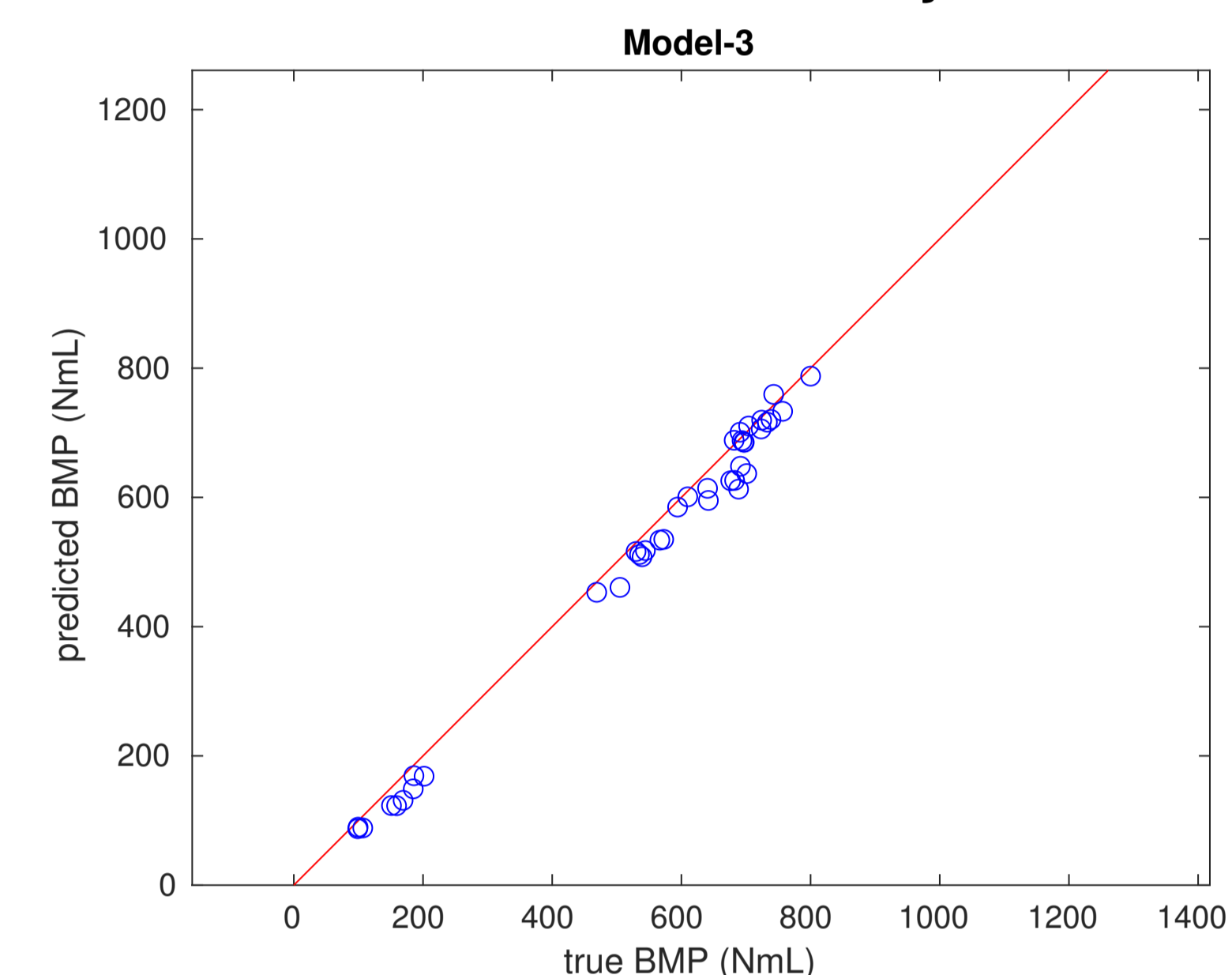
Learning on batches #1 to #69

Kinetic parameters $\hat{\theta}_c$

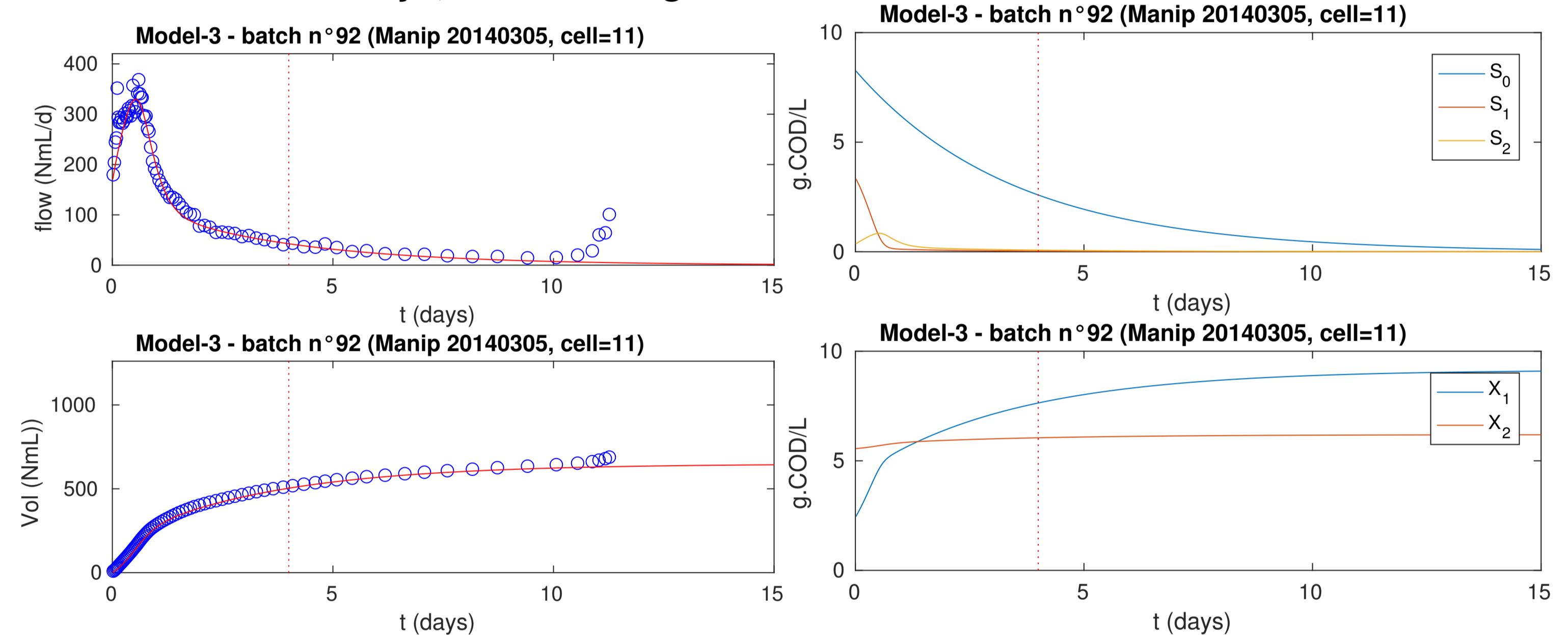
Y_{X_1}	0, 58
Y_{X_2}	0, 12
μ_0	0, 29
μ_1^{max}	3, 63
μ_2^{max}	2, 67
K_{S_1}	1, 02
K_{S_2}	3, 45
K_I	1, 44



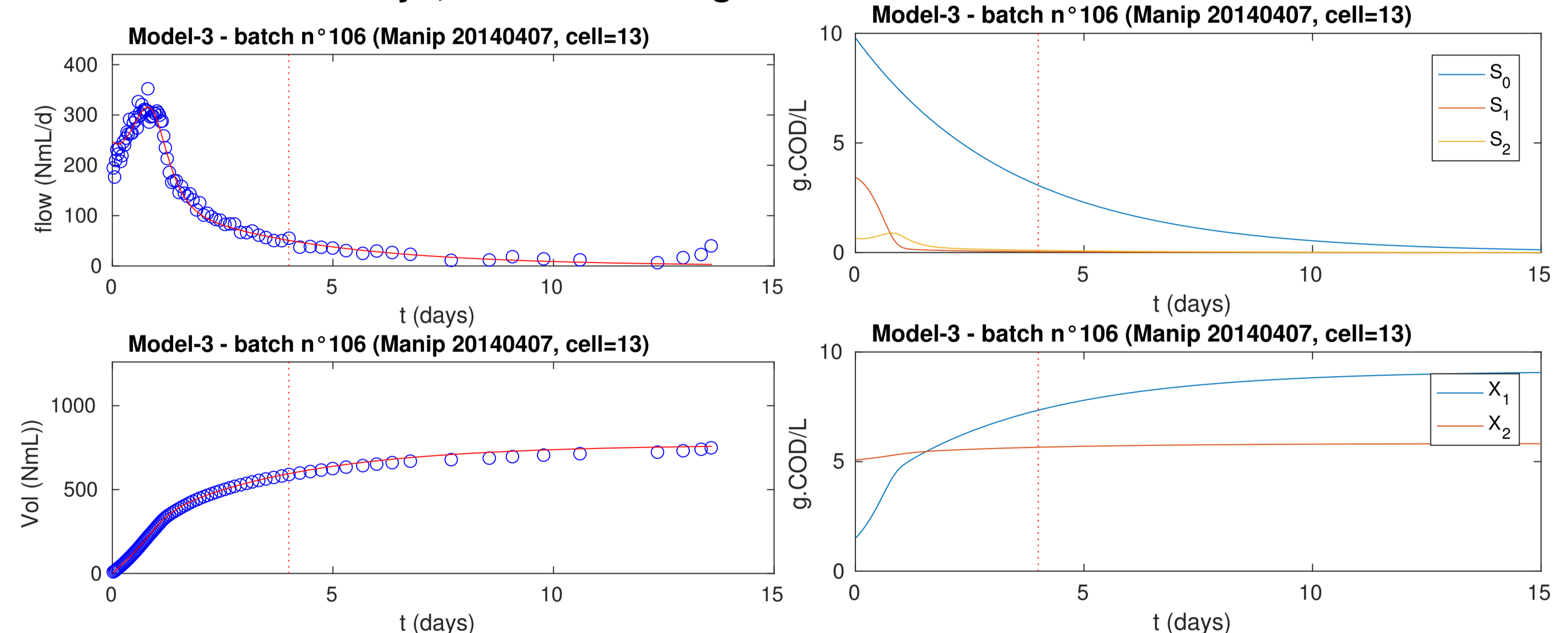
Prediction/validation on batches #70 to #108 at $T = 4$ days



Prediction at $T = 4$ days, floated sludge



Prediction at $T = 4$ days, thickened sludge



Trends and conclusions

Results :

- ▶ Well fitted kinetics in learning phase and good prediction of BMP at 4 days
- ▶ Ratios of S_0, S_1, S_2 seem to be interpretable
- ▶ Planned improvements :
 - ▶ Theoretical study of identifiability of parameters in learning phase
 - ▶ BOD and VSS measurements should be taken into account
 - ▶ Coupling between triplicates has to be considered
 - ▶ Confidence intervals should be computed for the predicted BMP
 - ▶ Actual model should be simplified and compared with other models

References

- [1] C. Holliger et al. (2016), Towards a standardization of biomethane potential tests, Water Science & Technology
- [2] O. Bernard, Z. Hadj-Sadok, D. Dochain, A. Genovesi, J. P. Steyer (2001), Dynamical model development and parameter identification for an anaerobic wastewater treatment process, Biotechnology and bioengineering
- [3] R. Fekih Salem, N. Abdellatif, T. Sari, and J. Harmand (2012), On a three step model of anaerobic digestion including the hydrolysis of particulate matter, MATHMOD 2012
- [4] A. Donoso-Bravo, S. Pérez-Elvira and F. Fdz-Polanco (2014), Simplified mechanistic model for the two-stage anaerobic degradation of sewage sludge, Environmental Technology