A new methodology for early BMP assessment using a mathematical model

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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.

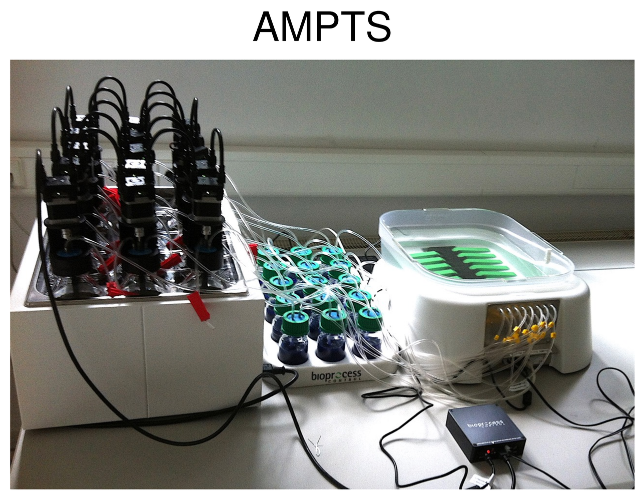
But finding mathematical models that are simple enough to be used for process control and prevision is particularly important. In this study we have used the modified AM2 model, calibrated and then validated with 90 different experiments as triplicates of 30 different substrate/inoculum mixes of sludge 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
- CO_2 trapping
- Mean flow measurement by ≈ 10ml throttles
- Full compliance with experts recommendations [1]
- 36 batchs in triplicates
- VSS, TSS, COD, BOD measurements
- BMP obtained after 20 days

AMPTS



Modified AM2 model

Reaction scheme [2, 3, 4] :

$$S_0 \xrightarrow{r_0} S_1, \qquad \text{(Hydrolysis)}$$
$$S_1 \xrightarrow{r_1} Y_{X_1} X_1 + (1 - Y_{X_1}) S_2 + k_4 CO_2, \qquad \text{(Acidification)}$$
$$S_2 \xrightarrow{r_2} Y_{X_2} X_2 + (1 - Y_{X_2}) CH_4 + k_5 CO_2, \qquad \text{(Methanogenesis)}$$

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

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

- 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 :

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

- 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
  - $(t_k^i)_{k=1 \ldots m_i}$ the times of throttle switchs
  - $(D_k^i)_{k=2 \ldots m_i}$ the mean CH_4 flow rate measured at $t = t_k^i$, $k = 1 \ldots$

- **Simulations**

  For $\theta = (\theta_c, \theta_b)$ we can simulate the mean flow of CH_4 :

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

  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 $T = \infty$, batchs #1 ...#69**

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

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

  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, batchs #70 ...#108**

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

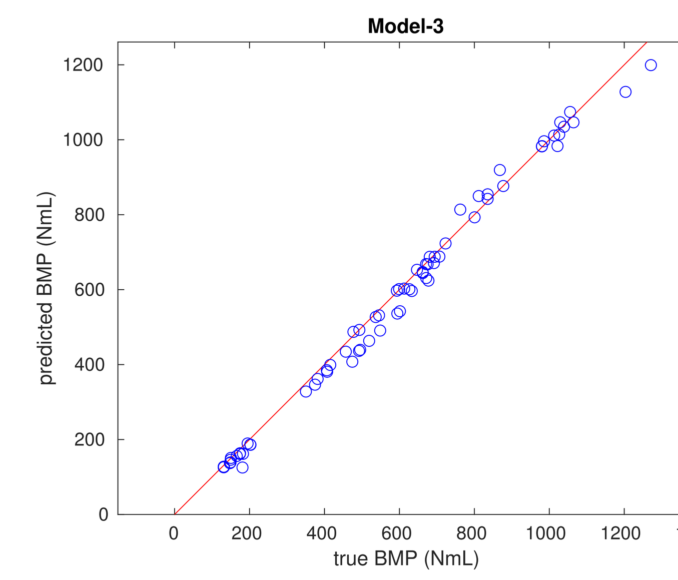
$$\hat{\theta}_b^i = \arg\min_{\theta_b} J_i(\hat{\theta}_c, \theta_b, 4), \qquad i = 70 \ldots 108$$

Results

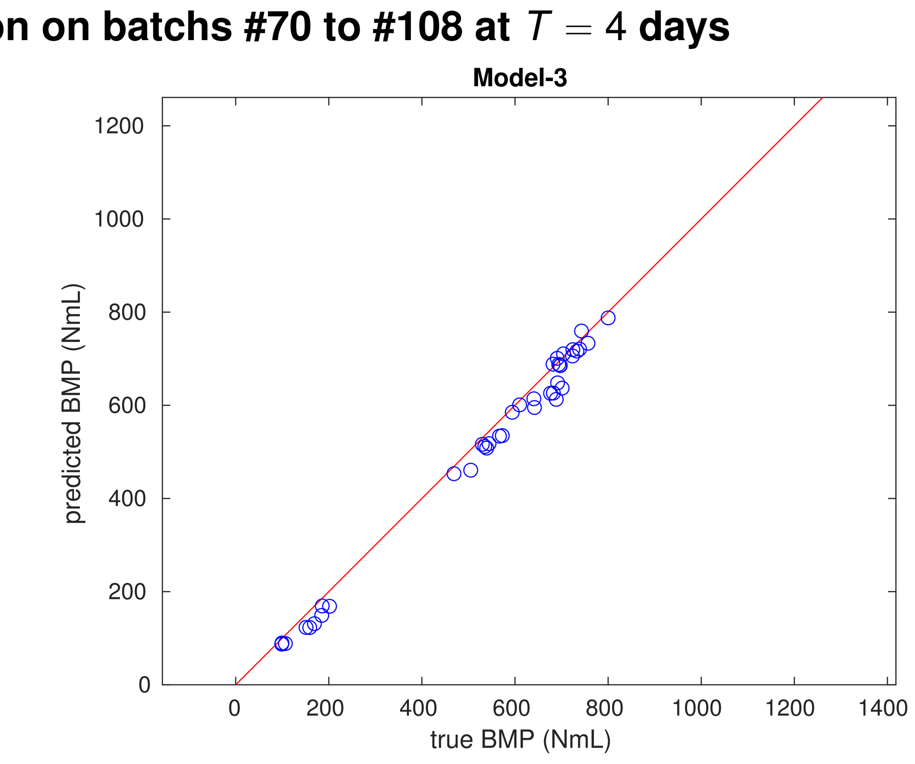
- **Learning on batchs #1 to #69**

Kinetic parameters $\hat{\theta}_c$

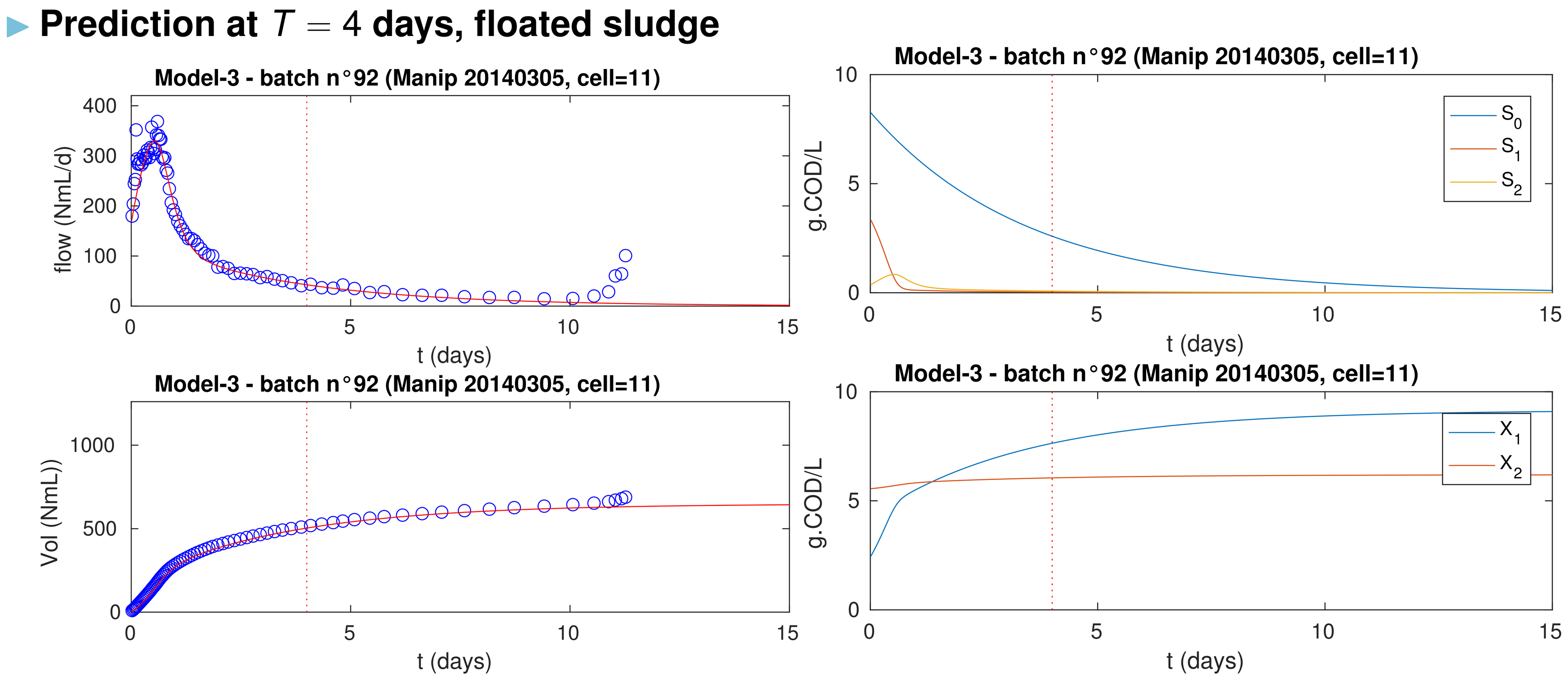
Y_{X_1}	0,58
Y_{X_2}	0,12
μ_0	0,29
μ_1^{max}	3,63
μ_2^{max}	2,67
K_{S_1}	1,02
K_{S_2}	3,45
K_I	1,44



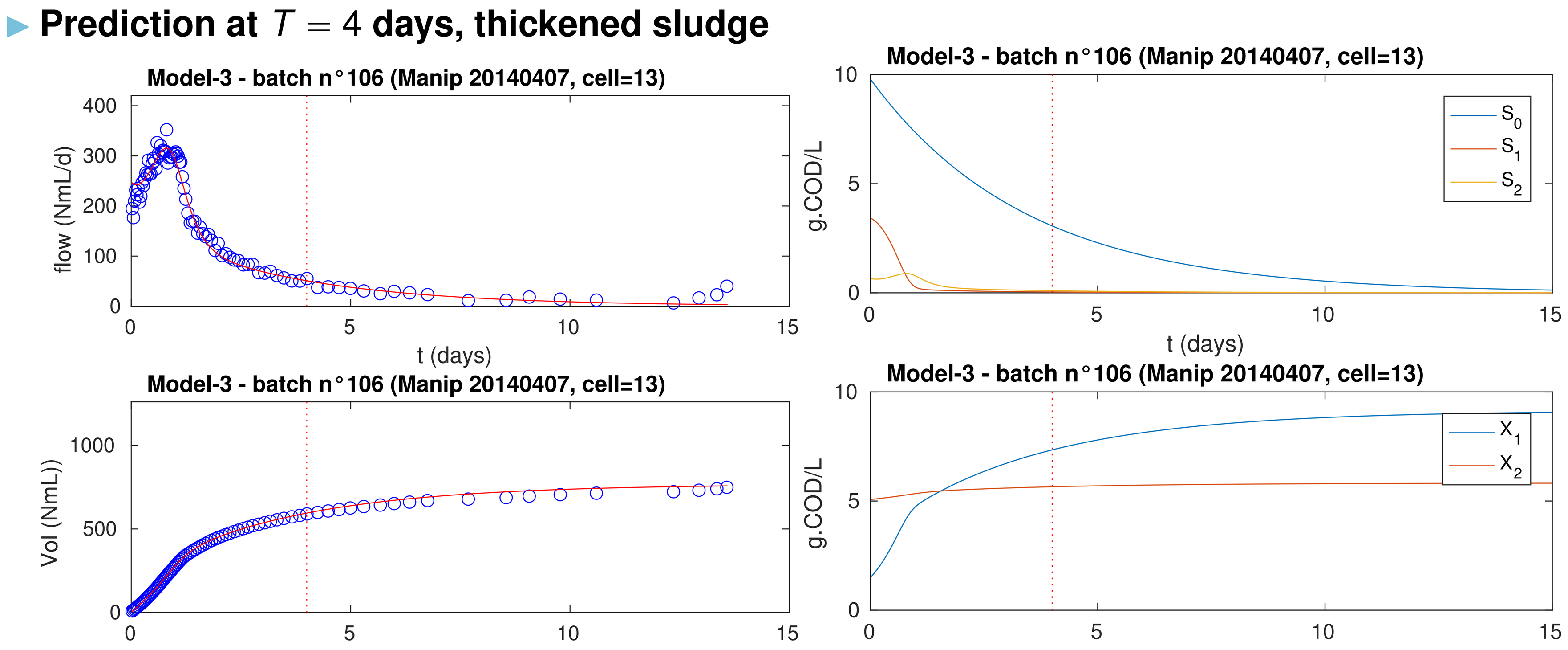
- **Prediction/validation on batchs #70 to #108 at $T = 4$ days**



- **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

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