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 prediction 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/noculum mixtures of sludge coming from the Paris’ conjuration 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 ~ 10 ml 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] :
- S0 −→ S1, (Hydrolysis)
- S1 −→ Y0 X1 + (1 − Y0) S1 + k1 CO2, (Acidification)
- S1 −→ Y0 X1 + (1 − Y0) CH4 + k2 CO2, (Methanogenesis)

S0 : insoluble organic molecules, S1 : simple compounds (fatty acids, peptides, amino acids, . . .), S2 : volatile fatty acids

Differential equations system :
- Perfectly mixed batch reactor, states of the system : S0, S1, S2, X1, X2
- Reaction rates :
  \[ \frac{dS_i}{dt} = -r_{S_i} - \sum_{j=1}^{2} r_{S_i \to S_j} \]
  \[ r_{S_i \to S_j} = \frac{S_i}{K_{S_i} + S_i} \theta - \frac{S_i}{K_{S_i} + S_i} \theta \]
- Initial conditions : S0(0) = S0, S1(0) = S1, X1(0) = X1, X2(0) = X2
- Parameters \( \theta = (Y_0, \mu_k, \mu_m, \mu_{mmax}, \mu_{CII}, \mu_{CH4}, K_B, K_X, \theta) \)

Identification of parameters

Goals
- Obtain a mathematical model allowing to reproduce the methane rate of all experiences, without necessarily uniquely describe state variables \( (X_1, X_2, S_1, S_2, S_3) \) 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
  \( \{z(k), (\theta), (\mu) \} \), i.e. the times of throttle switches
- \( \{z(k), (\theta), (\mu) \} \), the mean CH4 flow rate measured at \( t = \delta_k, k = 1 \ldots \)

Simulations
- For \( \theta = (\theta_0, \theta_0) \) we can simulate the mean flow of \( CH_4 \) :
  \[ \frac{dCH_4(t)}{dt} = \left( CH_4(\delta_k) - CH_4(\delta_{k-1}) \right) / (\Delta t) \]

The function
  \[ J(\theta_0, \theta_0, T) = \sum_{k=1}^{T} \left( \sum_{i=j}^{2} \left( \frac{S_i(Y_0, \mu_k, \mu_m, \mu_{mmax}, \mu_{CII}, \mu_{CH4}, K_B, K_X, \theta)}{K_{S_i} + S_i} \theta - \frac{S_i(Y_0, \mu_k, \mu_m, \mu_{mmax}, \mu_{CII}, \mu_{CH4}, K_B, K_X, \theta)}{K_{S_i} + S_i} \theta \right) \right)^2 \]

evaluates the misfit between measurements of batch i and the simulation with parameters \( \theta = (\theta_0, \theta_0) \) at horizon \( T \)

Learning phase \( T \to \infty \), batches \#1 \ldots \#69
- Minimize with respect to \( \xi = (\xi_0, \ldots, \xi_{69}) \in \mathbb{R}^{69} \)
  \[ \xi = \arg \min_{\xi \in \mathbb{R}^{69}} J(\xi_{68}, \xi_0, \theta) \]

We only keep \( \xi_0 \in \mathbb{R} \) which is used for the prediction.

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

Prediction/validation phase \( T = 4 \) days, batches \#70 \ldots \#108
- Independently minimize with respect to \( \theta \) in \( \mathbb{R}^7 \)
  \[ \theta = \arg \min_{\theta \in \mathbb{R}^7} J(\xi_{70}, \theta, 4) \]

Results

- Learning on batches \#1 to \#69
  \( \mu_k = 5.58 \)
  \( \mu_{CII} = 12 \)
  \( \mu_{CH4} = 2.99 \)
  \( \mu_{mmax} = 3.63 \)
  \( \mu_{mmax} = 2.67 \)
  \( K_B = 1.02 \)
  \( K_X = 3.45 \)
  \( \theta = 1.44 \)

- Prediction on batches \#70 to \#108 at \( T = 4 \) days
  \( \theta = (Y_0, \mu_k, \mu_m, \mu_{mmax}, \mu_{CII}, \mu_{CH4}, K_B, K_X, \theta) \)

- Prediction on batches \#70 to \#108
  \( \theta = (Y_0, \mu_k, \mu_m, \mu_{mmax}, \mu_{CII}, \mu_{CH4}, K_B, K_X, \theta) \)

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