# Modelling fermentative hydrogen production of cheese wastewater

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**HIGHLIGHTS:**

- Bio-hydrogen recovery during secondary fermentation
- Lactate plays a fundamental role in carboxylic chain elongation
- Modified ADM1 simulated the syntrophism between species

**BACKGROUND**: Brazilian agroindustry has an expressive, but not exploited, source of energy in its wastewaters and by-products. For instance, cheese whey (CW) disposed from the dairy industry represents a high residual sugar-content (lactose) with potential to energy recovery by anaerobic bioprocess[1,2]. In anaerobic microbiomes, sugar and other substrates are commonly hydrolyzed and fermented to short-chain mono-carboxylic acids (SCCAs), such as: acetic, propionic and butyric acids. In turn, the reverse β-oxidation pathway might transform SCCAs into medium-chain monocarboxylic acids, also known as chain elongation process (CE).

Despite organic acid outputs, both processes are well established as high biological hydrogen (bio-$H_2$) yielders. Also they are affected by carbon-source, key electron donors, partial hydrogen pressure ($P_{H2}$), pH, reactor microbiomes and temperature conditions[3,4]. Additionally, the feasibility of electron donor source implies on CE-capable microorganisms activity, which can recover $H_2$ through SCCA consumption[5]. Conversely, $P_{H2}$ can determine both fermentative and CE pathways, acting as thermodynamic inhibitor[6]. In addition, pH can also act as inhibitor in both processes, leading to electron control via disruption of bio-$H_2$ production pathways[7].

Mathematical modelling is a powerful tool to better understand complex interactions amongst microbiomes and inhibition factors, as presented so far. Thus, the aim of the present study is to develop a mathematical model to depict microbiome interaction between dark fermentative and CE biomasses. Experimental data to calibrate the model was gathered on a previous study of dark fermentative bio-$H_2$ production, in which batch essays of synthetic cheese whey wastewater were inoculated with continuous flow experiment biomass[8]. In order to consider chain elongation biomass ($X_{CE}$), kinetics and balances, along with $P_{H2}$ and pH effects, a modified version of Anaerobic Digestion Model n.1 (ADM1)[9] is proposed.

**RESULTS & DISCUSSION**: The model was successfully implemented in MatLab®. In order to evaluate different microbial communities, biomass was split onto dark fermenters ($X_{SU}$) and $X_{CE}$. Latter was considered to grow

during lactose fermentation and CE[10]. To avoid early CE synthesis (*i.e.* bio-$H_2$ and *n*-butyrate), $X_{ce}$ was inhibited by a competitive lactate function. Which implied on four new parameters to be estimated (Table 1).

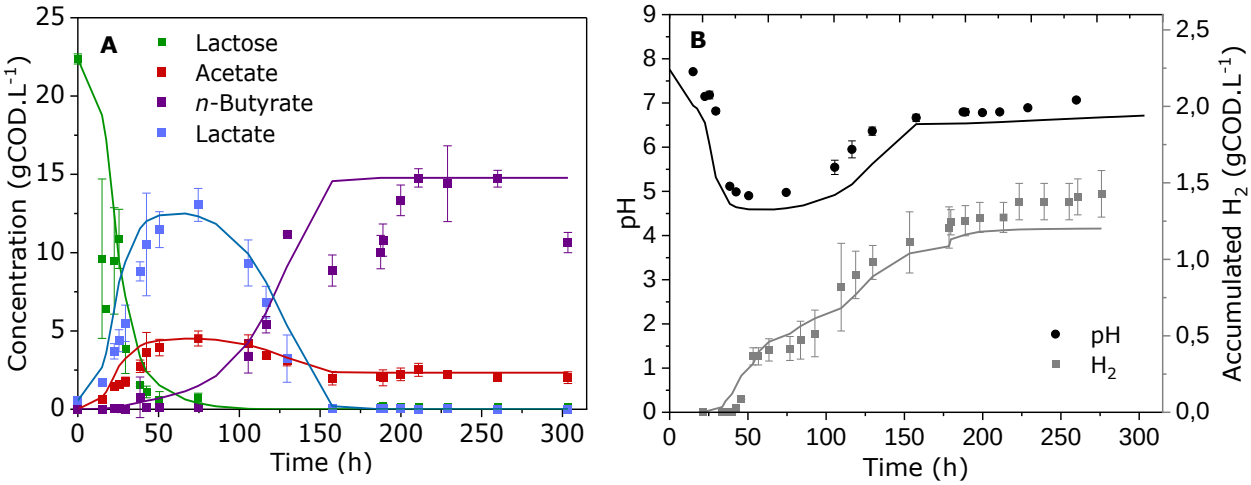
Table 1. Petersen matrix of proposed model, estimated parameters in bold.

| Proc.↓ Comp.→ | $S_{su}$ | $S_{bu}$ | $S_{ac}$ | $S_{lac}$ | $S_{H_2}$ | $X_{su}$ | $X_{CE}$ | Rate |
|---|---|---|---|---|---|---|---|---|
| Uptake of sugar | -1 | | $f_{ac,su}$<br>$f_{bu,su}$ | $f_{lac,su}$<br>$f_{lac,su}$ | $f_{h2,su}$<br>$f_{bu,su}$ | $Y_{su}$ | $Y_{CE}$ | $k_{m,su}\frac{S_{su}}{K_{s,su}+S_{su}}\mathbf{X_{su}}I_{pH}$<br>$\mathbf{k_{m,lac}}\frac{S_{su}}{\mathbf{K_{s,lac}}+S_{lac}}\mathbf{X_{CE}}I_{pH}$ |
| Uptake of butyrate | | -1 | | | | | | |
| Uptake of acetate | | | -1 | | | | $Y_{CE}$ | |
| Uptake of lactate | | $f_{bu,lac}$ | $f_{ac,lac}$ | -1 | $f_{h2,lac}$ | | | $\mathbf{k_{m,CE}}\frac{S_{lac}}{K_{s,CE}+S_{lac}}X_{CE}I_{pH}I_{H_2}I_{lac}$ |
| Uptake of $H_2$ | | | | | -1 | | | |
| $X_{su}$ decay | | | | | | -1 | | $k_{dec}X_{su}$ |
| $X_{CE}$ decay | | | | | | | -1 | $k_{dec}X_{CE}$ |

Due to reduced number of data between 75 to 150 h, a β-spline interpolation was used to better fit data. The initial $X_{CE}/X_{SU}$ was kept constant on 0.167. Biomasses yields, sugar consumption kinetics and CE half saturation constants were based on literature[8,11] and other parameters were adopted from ADM1 framework.

Time dependent simulation profiles indicated good agreement with data (Figure 1), with a slight early bio-$H_2$ production and diverging pattern on *n*-butyrate production around 150 Parameters were estimated by minimizing the sum of the absolute values of the deviations, presenting the following values: carbohydrates 0.88, acetate 0.16, *n*-butyrate 0.56, lactate 0.45, $H_2$ gas 0.04, biomass (not plotted) 0.27 and 0.16 for pH.

Figure 1. Experimental data (scatters) compared to simulation data (lines) obtained by modified ADM1 structure. **A** chart represents sugar and SCCAs dynamics, and **B**, accumulated $H_2$ production and pH variation patterns.




**CONCLUSION**: The developed ADM1 model for acetate and lactate CE-coupled, considering syntrophism between two biomasses, could represent both bio-$H_2$ (%) and *n*-butyrate production.

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