Modelling butanol production in anaerobic mixed microbial cultures

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Introduction

Butyrate and hydrogen are common intermediates of anaerobic digestion and can be converted into butanol (Eq.1) using anaerobic mixed microbial cultures [1]. Butanol is an energy-rich C4 alcohol which is used in various industries, ranging from coatings to cosmetics. With an energy density 50% higher than ethanol, it is one of the most promising transport biofuels.

\[
2 \text{H}_2 + \text{Butyrate} \rightarrow \text{Butanol} + \text{H}_2\text{O} \quad \Delta G^{\circ} = -13.6 \text{kJ/mol}
\]

More recently, butanol production was observed in an anaerobic enrichment under bicarbonate limiting conditions [2]. These observations highlight the concept that certain operating conditions can trigger butanol formation from waste streams.

Objectives

- To predict optimum conditions for waste-based butanol production in a continuous full-scale anaerobic digester
- To study the impact of thermodynamics
- To determine an upper theoretical limit for butanol productivity

Methodology

The anaerobic digestion process is described using the ADM1 BSM2 implementation [3] of the Anaerobic digestion model No.1 (ADM1) [4]. The model is upgraded by implementing:

- Butanol formation from butyrate and hydrogen (see Eq.1)
- Hydrogen supply to the reactor headspace
- Butanol gas-liquid mass transfer
- Thermodynamic limitation of acetogenesis, methanogenesis and butanol formation following [5] under consideration of a minimum energy quantum of 20 kJ/mol
- An improved description of the physicochemical processes (e.g. reactant activities instead of concentrations) according to [6].

Biomass yields on substrate are estimated according to the Gibbs energy dissipation method [7] and maximum biomass-specific conversion rates are calculated according to [8]. In all estimations, an average error of 15 % is assumed.

Results

The energy gain from butanol formation cannot sustain microbial life under standard conditions. However, thermodynamic analysis reveals feasible conditions at low pH and increased hydrogen partial pressure (Fig. 1).

\[\Delta G = \text{Gibbs energy change, } \Delta G_1 \text{ (kJ mol}^{-1} \text{ butanol), of butanol formation as a function of the hydrogen partial pressure and pH. A temperature of 35°C and a butyrate/butanol ratio equal to one are assumed.}\]

A pronounced thermodynamic impact becomes apparent upon implementing thermodynamic limitations and additional hydrogen supply (Fig. 3). The default ADM1 implementation upgraded only by the butanol forming reaction overestimates butanol productivity by 120% as compared to the thermodynamics based implementation. External hydrogen supply results in a 66% increase in butanol productivity. A theoretical upper productivity limit is reached at 3.0 MWh-butanol d⁻¹, where 96.9% of the butyrate available from acidogenesis are channeled towards butanol formation.

Conclusions

- Butanol productivity is maximized at pH 5, where between 6% and 12% of the biodegradable influent COD fraction. Butanol productivity is almost doubled (2.61 MWh-butanol d⁻¹) at 1.4 bar, which results in 11.7% COD recovery.

Elevated hydrogen partial pressures increase butanol productivity (Fig. 4). The lowest indicated partial pressure (0.47 bar) is reached without external hydrogen supply and results in the formation of 1.36 MWh-butanol d⁻¹, corresponding to 6.1% of the biodegradable influent COD fraction. Butanol productivity is almost doubled (2.61 MWh-butanol d⁻¹) at 1.4 bar, which results in 11.7% COD recovery.

- Butanol productivity is overestimated by 120% when neglecting thermodynamic constraints.
- We propose a two-stage process for butanol/methane production in the frame of anaerobic digestion.

References


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