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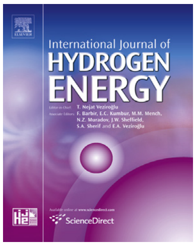

Review Article

A review of the role of hydrogen in past and current modelling approaches to anaerobic digestion processes

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ABSTRACT

Anaerobic digestion is a consolidated technology for effective waste (water) treatment and biogas production. Despite many reported studies, the complex dynamic behaviour of the process is not completely understood, hindering its full exploitation. In particular, process start-up is delicate and disturbances can deviate the process from its expected course of operation. There is evidence in literature that hydrogen might play an important role, as an early indicating factor of dynamic behavioural changes. The objective of this article is to review the existing literature on mathematical modelling of anaerobic digestion, with a special emphasis on how the dynamics of hydrogen has been considered in existing models and how it could potentially be further exploited in future work.

Contents

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Introduction

Anaerobic digestion (AD) is a well-known and established technology used to treat waste, especially in the methanization of sewage sludge from wastewater treatment plants [1]. One of the most important drawbacks of this bioprocess is its sensitivity to disturbances which can lead to some stability problems along with a diminishing biogas production flow [2]. Therefore, intense research was devoted to get more insight into the biology inside the reactor, especially in terms of the microbial communities, microbial interactions and biological pathways of the substrate and intermediates [3–5].

However, it is necessary to further investigate the control of AD processes with a view to the rejection of operational and environmental perturbations, and to the maximization of biogas production and waste treatment. In this connection, mechanistic mathematical models could be a good basis to develop more advanced control strategies. A review of general modelling and identification issues is available in Ref. [6].

Nevertheless, little attention has usually been paid to the dynamics of hydrogen in modelling and control applications. This is the motivation behind this review paper, which discusses the importance of hydrogen in the AD process using thermodynamics, kinetics, and mass transfer arguments. Moreover, existing models and control approaches, which include the dynamic evolution of hydrogen, are briefly presented, along with a critical analysis. Finally some conclusion and future prospects are suggested.

Role of H_2 in AD

Hydrogen is an intermediate metabolite present in most of the reactions that take place during the AD process. Some of these reactions are listed in Table 1 and a schematic representation is shown in Fig. 1. The main reactions include:

1. Conversion of organic monomers to hydrogen, bicarbonate, acetic, propionic, and butyric acids and other organic products such as ethanol and lactic acid.
2. Oxidation of reduced organic compounds to hydrogen, bicarbonate, and acetic acid by obligate hydrogen producing acetogens (OHPA).
3. Non-syntrophic homoacetogens where hydrogen and carbon dioxide are used to produce acetate.
4. Oxidation of hydrogen by nitrate-reducing bacteria (NRB).
5. Methane production from hydrogen-utilizing microorganisms called hydrotrophic methanogens.

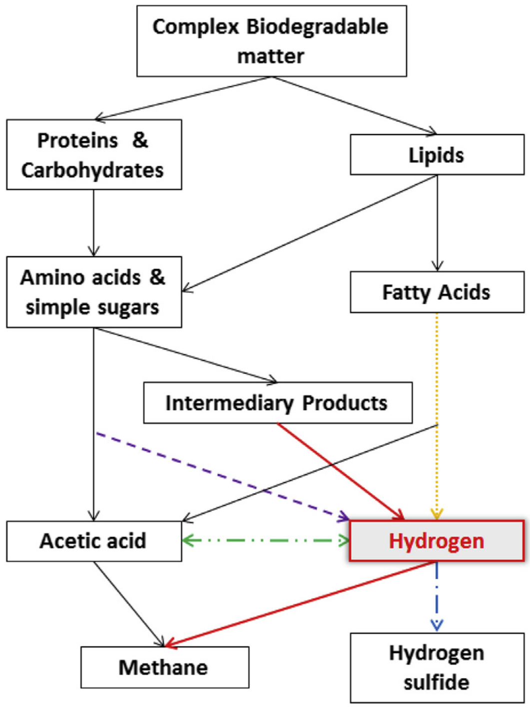

Fig. 1 – Suggested routes for hydrogen production and consumption. Solid red lines: common route for all models. Dash-dot-dot green line: route suggested by Refs. [9–12], Dashed purple line: route suggested by Refs. [9,12–18]. Dotted yellow route suggested by Refs. [9–11,13,17]. Dash-dot blue line: hydrogenotrophic sulfidogenesis considered by Ref. [19]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1 – Anaerobic digestion reactions involving H_2. Free energy ΔG_r^0 values are calculated at pH 7, 1 atm pressure, and 1 M concentrations of reactants and products in aqueous solution a) 30 °C and b) 25 °C.

Reaction	ΔG_r^0 [KJ/mol]
$2CO_2 + 4H_2 \rightarrow acetate^- + H^+ + 2H_2O$	-138.2^a
$2Lactate^- + H^+ \rightarrow n - butyrate^- + 2CO_2 + 2H_2$	-71.8^a
$Lactate^- + acetate^- + H^+ \rightarrow n - butyrate^- + CO_2 + H_2$	-21.3^a
$n - butyrate^- + H^+ + 2H_2O \rightarrow 2acetate^- + 2H^+ + 2H_2$	48.1^a
$Glucose + 2H_2 \rightarrow 2propionate^- + 2H^+ + 2H_2O$	-308.5^a
$Glucose + 2H_2O \rightarrow 2acetate^- + 2H^+ + 4H_2 + 2CO_2$	-292.3^a
$Glucose \rightarrow n - butyrate^- + H^+ + 2H_2 + 2CO_2$	-309.4^a
$Propionate^- + 3H_2O \rightarrow acetate^- + HCO_3^- + H^+ + 3H_2$	76.1^b

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