

Understanding the kinetics, transfers and reactions in the biological gas desulfurization process



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Motivation

sulfur

H₂S is a toxic and environmentally harmful gas that can be found in (bio-) gas streams. Therefore, it must be removed, which is traditionally done through physio-chemical methods such as the Claus process, an energy-intensive process that uses harmful chemicals. The biological gas desulfurization process is an environmentally friendly process that converts H₂S into elemental sulfur (S⁰) using sulfur-oxidizing bacteria (SOB) under haloalkaline conditions (pH 8-9.5 and ionic strength 1-1.5 M) ^[1]. Within the process, biological, chemical and mass-transfer reactions take place simultaneously. The process consists of three steps: 1) absorption of H₂S into a (bi)carbonate solution to form dissolved HS-, 2) anaerobic uptake of HS- by SOB and 3) aerobic conversion of stored HS⁻ into S⁰.

Aside from S⁰, SO₄²⁻ (sulfate) and S₂O₃²⁻ (thiosulfate) can also be formed through biological or chemical oxidation. Theoretically, 98% of incoming S atoms can end up in S⁰, but in practice lower percentages are achieved ^[2]. Modelling can help understand the interplay between the different processes in order to improve the process design and control. Understanding can be generated at multiple scale levels, starting at single (bio)chemical reactions and cross-film mass transfer all the way up to a full-scale integrated process.

The aim of this research is to model the biological gas desulfurization process at each of these scale levels, starting at the smallest scale. Past experimental data will be supplemented with new small-scale experiments and used for model validation.

Technological challenge

Three challenges must be overcome in the modelling of the biological gas desulfurization process:

Aspects of the SOB biology, e.g. their ability to take up and store HS⁻ under anaerobic conditions. This most likely requires the development of models that go beyond Monod kinetics.

Interesting system properties to investigate after model development are observability and controllability, properties relevant to process monitoring and control. Observability is a measure of how well external outputs (i.e. sensor measurements) can be used to estimate state values (e.g. HS⁻ concentrations in the process units). Controlability is the degree to which it is possible to move state values to any value within their solution space, using only achievable control inputs.



Fig 1: process scheme for the biological gas desulfurization process

Research goals

- 1. Determine the dominant physical, chemical and biological processes and quantify their kinetics;
- 2. Develop a novel model for the SOB biological rates;
- 3. Model simultaneous chemical and biological mass transfer enhancement in the absorber column;
- 4. Model the processes that take place around the HS^{-} and O_{2} injection points and determine how the mixing pattern around these points affects the process performance;
- 5. Determine to what degree the biological gas desulfurization process is observable and/or controllable;
- Both sulfur crystals and bacteria are known to enhance mass transfer in the absorber column ^[3,4]. To date no quantitative information exists on the relative contributions of both forms of enhancement and no model exists in literature that combines both biological and chemical mass transfer enhancement.
- Investigating the hypothesis that most of the chemical conversions in the micro-aerophilic reactor take place within a gradient around the reactor O₂ and HS⁻ injection points. This necessitates the use of computational fluid dynamics (CFD).

References

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