UNIVERSITÉ Clermont Auvergne

CLERMONT AUVERGNE INP

ÉCOLE DOCTORALE DES SCIENCES POUR L'INGÉNIEUR

LABO – Institut Pascal, GePEB group

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Title :

Contribution of physics-informed neural networks to multiphase reactors dedicated to anaerobic bioprocesses for the production of energy vectors

Summary

Anaerobic bioprocesses dedicated to the production of energy carriers (such as anaerobic digestion, dark fermentation for biohydrogen production, and biological methanation) represent key technological building blocks for the energy transition. They play a central role in the valorization of organic waste, the decarbonization of energy systems, and the storage of surplus renewable electricity through power-to-gas strategies, particularly in the case of biological methanation.

The types of bioreactors used to operate these processes notably include mechanically stirred tanks or gas-driven systems such as bubble columns and their variants. These systems are characterized by complex, often turbulent flows and strong spatial heterogeneities, which can significantly affect performance and even lead to operational issues. The prediction of these heterogeneities is traditionally based on computational fluid dynamics (CFD) approaches, relying on the solution of the Navier–Stokes equations coupled with species transport equations. However, achieving accurate results requires fine computational meshes, leading to high computational costs in terms of memory and processing time. Despite recent advances, such as the use of GPU processors, these approaches remain difficult to directly couple with experimental data.

A promising alternative is provided by physics-informed neural networks (PINNs). These machine learning methods allow physical laws—typically expressed as differential equations—to be explicitly incorporated into the loss functions, thereby guiding the learning process toward physically consistent solutions. The mesh-free nature of PINNs gives them a decisive advantage in terms of computational efficiency. Moreover, they can be used in inverse approaches to reconstruct flow or concentration fields from a limited number of experimental measurements. Nevertheless, introduced only recently (2017), PINNs are still under development, and their application to complex cases remains limited.

The GePEB group (Process Engineering, Energy and Biosystems) at Institut Pascal has a substantial body of experimental data on anaerobic processes. Regarding stirred tank reactors dedicated to biohydrogen production, studies conducted during several PhD theses (Trad 2017, Chezeau 2018, Danican 2021, Li 2024) have enabled the characterization of flows of both Newtonian and non-Newtonian fluids, using imaging-based measurements of velocity and concentration fields, complemented by local measurements. A CFD model has been developed for Reynolds numbers above 200, making it possible to generate additional three-dimensional data for training purposes. In parallel, an experimental database is currently being developed for a bubble column, as part of an ongoing PhD project (Essid 2026) and a postdoctoral project including CFD developments. The objective of this PhD thesis is to leverage these experimental and numerical datasets to incrementally develop a PINN-based simulation tool for modeling the fluid behavior in these bioreactors. The approach will consist of successively addressing velocity fields, concentration fields, and then gas–liquid mass transfer phenomena (and potentially transfer-limited reactions), each of these stages representing an increasing scientific challenge and an original contribution compared to the current state of the art.

Initially, the study will focus on a mechanically stirred tank in an axisymmetric configuration, for which the flow will be considered single-phase as a first approximation, given the low gas production rates. After validating the approach, the research will move on to a three-dimensional configuration. Depending on the results obtained, the work could be extended to a bubble column dedicated to biological methanation. The final objective is to develop a robust, fast, and reliable tool for optimizing operating conditions by balancing mass transfer, mixing quality, and energy consumption.

The desired candidate profile corresponds either to a background in process engineering with a strong interest in numerical approaches (Python, CFD, etc.), or to a background in computer science or applied mathematics with a strong interest in physical phenomena. Although the PhD is primarily focused on numerical modeling, participation in experimental work is envisaged in order to better understand the studied phenomena and their orders of magnitude.