In consideration of the determination of the Regione Piemonte – Direzione Coesione sociale No. 445 of August 3, 2021 which approved the following apprenticeship position for the PhD project proposal submitted by the Politecnico di Torino in the framework of a specific regional call for proposals (Apprendistato di Alta Formazione e Ricerca 2016-2018 - Avviso Pubblico per la realizzazione dei percorsi formativi di: Laurea triennale e magistrale, Diploma Accademico di primo e secondo livello, Master di primo e secondo livello Universitario, Dottorato di ricerca e Diploma accademico di formazione alla ricerca, Attività di ricerca approvato con Determinazione 537 del 3/8/2016 e s.m.i.):

PhD in Chemical Engineering

Research project “Simulazioni numeriche di reattori tipo Trickle Bed per metanazione biologica”

Politecnico di Torino – Optimad engineering srl

Indicare anche un titolo progetto abbreviato (max 5 parole) che verrà utilizzato per la pubblicazione del posto sul sito della Scuola di Dottorato

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Numerical Modelling of Trickle Bed Reactor

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|----------------------|--------------------------------------------------|
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http://www.optimad.it/phd-thesis-numerical-simulation-trickle-
bed-reactors/         |
|----------------------|--------------------------------------------------|
Trickle bed reactors (TBR) are three-phase reactors where gas and liquid flow through a bed of fixed packing elements (solid phase). The liquid phase enters the reactor at the top and flows downwards. The gas phase is conducted either from the top (co-currently) or from the bottom (counter-currently). Examples of large industrial applications can be found in chemical industries and oil-refinement processes.

Due to the increasing demand for sustainable energy supply with low greenhouse gas emissions, an emerging application for TBR is biological methanation which transforms renewable hydrogen (H2) and carbon dioxide (CO2) into methane (CH4), thus achieving a higher volumetric energy density and the possibility of feeding large amounts of methane into the gas grid. In TBR for biological methanation, the gaseous reactants dissolve into water (the liquid phase) due to concentration gradients between the different phases. Microorganisms members of the family Archaea present in a stabilized microfilm over the packing elements absorb the dissolved H2 and CO2 and convert them into CH4. Within the microorganism, enzymes catalyze the methanation reaction (Sabatier reaction) biochemically.

Performances of TBRs are not solely determined by the reaction kinetics and operation pressure and temperature. Hydrodynamics, and transport phenomena in general, have a strong influence on the overall reactor efficiency and productivity. Additionally, different flow regimes can be encountered depending on the operating conditions and geometry of the reactor. Therefore, an adequate understanding of multiphase hydrodynamics is of paramount importance in order to develop better reactor technologies. The main challenge with the numerical simulation of trickle bed reactor is the inherent multiscale nature of the problem due to the two-way coupling between the main flow characteristics and the hydrodynamics occurring at the smallest geometrical scales of the packing elements and the small time-scales of reaction kinetics.
A numerical simulation capable of resolving the fluid-dynamics at the smallest scales would require tremendous computation effort, therefore a number of models of have been developed in the past two decades based on different concepts to properly account for the effect of the flow features at the smallest scales while resolving only the main flow. Sàez and Carbonell (1985) developed a model based on the concept of relative permeability. The interfacial force model presented by Attou and Ferschner (1999) accounts for the drag force resulting from both particle-fluid and fluid-fluid interactions. Lappalainen et al. (2008, 2009) introduced model equations in 2D/3D including a mathematical/semi-empirical models for interfacial and dispersion forces in different spatial directions.

The goal of the PhD thesis is to develop a mathematical/numerical model for the multiphase flow in co(counter)-current trickle bed reactor for biological methanation to predict the performances of a prototype reactor being developed by “Sistema Energetico - RSE S.p.A.” (proposal nr. 60705, 22/07/2021)

The Company Optimad Engineering has planned for the winner of this position a collaboration within a contract of high apprenticeship according to the Italian Legislative Decree 81/2015, art. 45.

Objectives

The multiphase-model will be based on the Eulerian-Eulerian framework, where solid, liquid and gas are modeled as interpenetrating continua. Within this framework the fluid-dynamics will be resolved at the larger time-space scales using an all-Mach solver for compressible multi-phase flows. The coupling between phases will be achieved through machine learning models for the inter-phase forces, mass and momentum transfer, and absorption/dilution processes.
The machine learning model for the microscale hydrodynamic will be trained based on both the results of an experimental campaign and ad-hoc fine-scale numerical simulations. Model parameters will be calibrated to reproduce the overall behavior of a prototype reactor.

Roadmap

- Investigation and critical assessment of the state-of-the-art mathematical/numerical models for the multi-phase fluid-dynamics of TBRs.
- Definition of a mathematical/numerical model for the multiphase flow of a TBR.
- Implementation of an all-Mach numerical model for compressible multi-phase flows in a CFD simulation framework based on immerse-boundary paradigm.
- Investigation and definition of suitable reduced-order models (semi-empirical, machine learning, etc.) to incorporate the effects of small-scale hydrodynamics in the main flow.
- Calibration of model parameters based on experimental results (DoE).
- (Optional) Optimization of reactor geometry (geometry and organization of packing elements within the reactor’s bed) and operating conditions (pressure, temperature, gas/liquid inlet mass flow rates) to maximize reactor’s production rate.

Skills and competencies for the development of the activity

The candidate shall be **less than 30 years old** at the moment of the hiring from the company. The **skills of the candidate** imply competences in the:

- knowledge of numerical methods for PDEs
- knowledge of C/C++
- programing skills in Bash, Python, Matlab, or similar
- problem-solving skills
- proactive attitude and willingness to learn
- motivation to work in a collaborative environment
- Communication skills in English and in a professional context (presentation of research results at scientific meetings, colloquial discussions, writing of manuscripts) across all levels of business, both verbal and written.