

Industrial Processes Design

CFD in Industrial Processes

KEYWORDS: Energy efficiency / Process enhancement / Reactors Design/ Power Transformers

LSRE-LCM has a well-established team on Fluid Dynamics and Mixing phenomena with solid expertise in Computational Fluid Dynamics (CFD). This knowledge has been shared over the last 15 years with the national industry through various partnerships. In the reporting period, a major project on Thermal Simulation of Power Transformers was concluded in collaboration with EFACEC, a worldwide leading manufacturer of power transformers, and a project for the design of microalgae production units. In addition, several collaborations with other research groups were conducted to develop industrial technologies.

Introduction

One of the main fields of cooperation with industry, which was at the origin of this research line, was the design of Power Transformers (PT) based on CFD. This line started with a challenge posed by EFACEC to Prof. José Carlos Lopes to have the academia using their know-how to improve the design of PT. This research was concluded during the period of this report. Currently, EFACEC has internalized CFD and a mechanistic Thermo-Hydraulic Network Model (THNM – developed at LSRE-LCM) in their group for PT design and development.

During the period of this report, another main project was related to the design of microalgae production units within the scope of a contract made with company A4F. This contract aimed to design raceways, horizontal photobioreactors and deaeration and heat transfer units.

Additional research was also conducted in cooperation with CoLab NET4CO2 to advance NETmix. This research included the study of the thermal design of NETmix in the MSc thesis on Computational Mechanics of Nelson Lorenzoni, the study of combustion in NETmix carried within the PhD thesis of Joana Matos, and on the multiphase flow in NETmix studied under the PhD thesis of Isabel Fernandes.

Last, this group has actively sought cooperation with other research lines on developing industrial processes from their technologies. Particularly active cooperation was kept with the environmental group on Advanced Oxidation Processes, with the materials group on the design of photocatalytic reactors, and with LEPABE on CFD simulation of indoor air quality and oscillatory flow reactors (OFR) for microalgae cultivation.

Current Development

PT – Power transformers

Most of the work on PT focused on heat transfer and flow distribution in the windings. Part of this research was published in the journal Electric Power Systems Research. In the final part of the cooperation with EFACEC, the PTs were studied as a whole, with a 3D CFD simulation of the flow in several parts of the reactor. The geometry was assessed in decouplable regions because the PT is too complex to be simulated in a single model. Fig 1 shows the PT components and a study of the oil distribution on the basis of the PT. This study devised some rules for the design of the several components. In the bottom oil tank, the CFD simulations enable the distribution of pressure and flow at the inlets of the windings. The flow rate in the windings was related to the inlet pressure as an outlet Boundary Condition. This model has direct application to the optimization of the oil tank design.

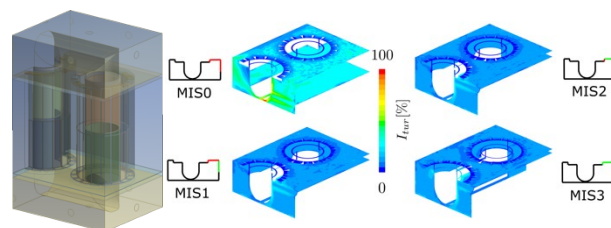


Fig 1. Power transformer geometry with the identification of several parts that can be decoupled for flow simulation. CFD simulation of the bottom oil tank that distribute the oil through the windings.

Microalgae

Microalgae units need to keep liquid circulating to have the biomass suspended. This operation poses a large energy penalty to the process. The two main types of units are raceways and photobioreactors (PBRs). Raceways are generally agitated by paddle wheels, with very low energy efficiencies, less than 20%. PBRs are transparent pipes where the microalgae culture flows. Since these are internal flows, they heat up over time and accumulate oxygen. So, PBRs need to be coupled with cooling and deaeration units.

A4F wanted an optimized design for a raceway unit and a set of horizontal PBRs with a deaeration and heat transfer unit. The raceway was based on an alternate design to the paddlewheel, based on recirculation pumps with distribution units. A novel deaeration and cooling unit was developed for the horizontal PBRs. Fig 2 shows a simulation of this unit. These units were designed for an industrial park to produce microalgae, representing a 22M€ investment.

NET4CO2

One of the goals of CoLAB NET4CO2 is the establishment of

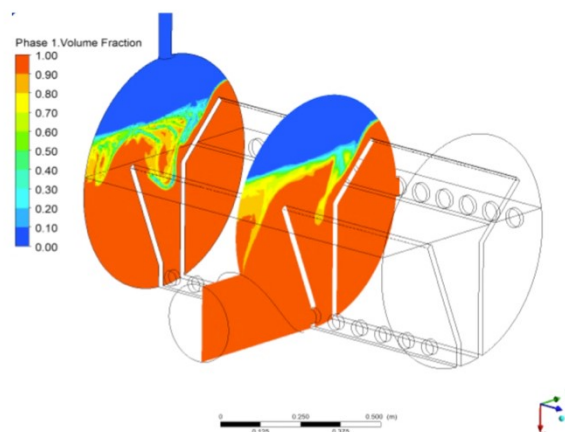


Fig 2. Deaeration unit for horizontal PBRs for microalgae production with integrated cooling.

NETmix as an industrial standard for mixing applications. LSRE-LCM has contributed significantly to the dissemination of this technology. Multiphysics simulations of NETmix, comprising structural simulation, heat and mass transfer, were carried out (see Fig 3). The complete study on the best designs for NETmix at high pressure and high temperature is presented in Nelson Lorenzoni's MSc thesis. One of the main applications of NETmix is on processes with large heat transfer ratios. In the

case of endothermal processes, for example, Steam Methane Reforming, this can be coupled with combustion. CFD simulations of combustion in NETmix performed in Joana Matos's PhD thesis show excellent control of mixing and temperature, which reduces NO_x formation.

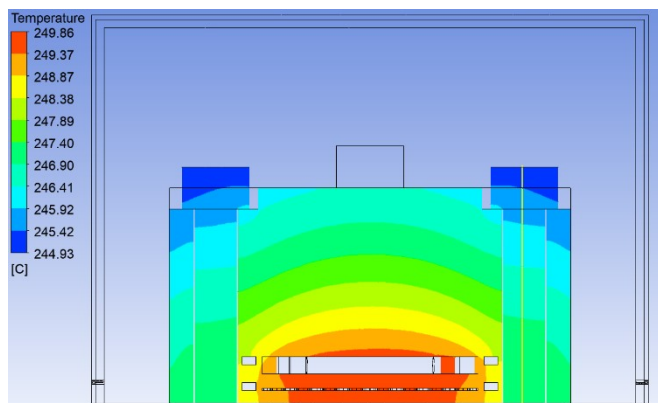


Fig 3. Temperature of the solid components of a NETmix plate with an heatexchange plate.

The development of NETmix was also made within the scope of the European High-Performance Computing Joint Undertaking framework, which is promoting a super-cluster in Portugal. Tests were made at the Minho Advanced Computing Center (MACC). The MACC cluster has been used to implement CFD software to simulate transport phenomena and reaction processes in NETmix. These resources have enabled results for fully resolved 3D CFD simulations of multiphase flows and combustion in NETmix. This work was an initial effort to take advantage of the Deucalion cluster.

Internal cooperations

CFD simulations were carried out in joint work with the Thermodynamics and Environment group, namely for ozonation processes using NETmix and optimization of tube-in-tube reactor. This collaboration enabled to assess industrial designs for ozonation units and UV disinfection.

An MSc thesis was also conducted on the optimization of the deflectors in primary settlers. This thesis was conducted in collaboration with Dr. Anna Karkinska from Southern Water in the UK. This work gave the best deflector design at the mixing region of primary settlers. A model was developed to assess the removal efficiency per particle size based on the flow field simulated with CFD. State-of-the-art methodology for removal efficiencies of settlers for wastewater is based on average values from industrial facilities or laboratory tests, which do not account for the actual flow field.

Collaboration was pursued with the Catalysis and Materials group on CFD simulations to enhance photocatalytic reactors for green production of ammonia. This work also focused on the nexus of CFD design studies with 3D printing technology.

A collaboration with the Environmental Sciences and Technologies research group at LEPABE was started to introduce CFD tools to assess and find strategies to improve indoor air quality, namely in classrooms. Suitable models for airflow simulation in a classroom were tested and validated numerically. This work analyzed the implementation of

chemical reactors concepts, such as the Residence Time Distribution, to the design of buildings with better indoor air quality.

A second cooperation with LEPABE assessed the Oscillatory Flow Reactor (OFR) for the cultivation of microalgae. This work evaluated the flow dynamics in OFR and the suspension of solids, a critical aspect of biocultures. This work was partially developed at the Institute Polytechnique the Toulouse with a visit of PosDoc researcher Margarida Brito from September 2022 to January 2023.

Future Perspectives

In 2023, a project with the packing sector, Packing for the Future, was started. One of the outputs of this project is creating a centre to address the sustainability of packings. One of the areas of the centre is on the development of industrial processes, aiming to increase the sustainability of packings. Within the CFD tasks, the group intends to enhance the efficiency of industrial operation units in this sector.

The collaboration works with groups that need to assess the industrial implementation of their technologies, namely on photocatalytic reactors, ozonation units, and OFRs, will carry on. New collaborations are starting, namely on the simulation of industrial electrochemical processes. The work on indoor air simulation will also be continued, aiming to broaden the cooperation to architectural/civil construction sectors.

More importantly, the group will continue to establish contacts with the industry offering services to increase the efficiency and sustainability of chemical processes.

Related Sustainable Development Goals



Outputs

Master Dissertations

- [1] Maria Carolina Duarte, Advanced Computational Methods Applied to the Design of Primary Settlers, MIEA, FEUP, 2022
- [2] Nelson Lorenzoni, Computational study of heat exchange in a mesostructured network mixer, MMC, FEUP, 2020

Selected Publications

- [1] I.S. Barbosa et al., Chemical Engineering & Technology 46, 1241 (2023)
- [2] I.S. Babosa et al., Chemical Engineering and Processing - Process Intensification, 167, 108541 (2021)
- [3] C.P. Cotas et al., Electric Power Systems Research 187, 106423 (2020)
- [4] S. Marcos et al., Journal of Supercritical Fluids 146, 65 (2019)

Team

José Carlos Lopes Professor; **Ricardo Santos**, Researcher; **Madalena Dias**, Professor; **Margarida Brito**, Researcher; **Carla Cotas**, Project Post-Doctoral researcher; **Isabel Fernandes**, PhD student; **Isabel Barbosa**, PhD student; **Nelson Lorenzoni**, Project researcher;

Funding

A4F Service Contract, FEUP/A4F/2018-72684, 2018
 GALP7 Contract, FEUP/EXPOINTEDECADA/2018-73065, 2018-2020
 NET4CO2 Service Contract, FEUP/NET4CO2/2022-79721, 2022-2023
 NET4CO2 Service Contract, FEUP/NET4CO2/2021-78270, 2021-2022
 NET4CO2 Service Contract, FEUP/NET4CO2/2020-76537, 2020-2021
 HyGreen&LowEmissions, NORTE-01-0145-FEDER-000077, 2021-2023
 2SMART, NORTE-01-0145-FEDER-000054, 2021-2023
 LSRE-LCM Base Funding, UIDB/50020/2020, 2020-2023
 LSRE-LCM Programmatic Funding, UIDP/50020/2020, 2020-2023
 LA LSRE-LCM Funding, UID/EQU/50020/2019, 2019
 LA LSRE-LCM Funding, POCI-01-0145-FEDER-006984, 2013-2018
 FCT Scholarships: UI/BD/151092/2021 (I. Barbosa)