Habilitation à diriger des recherches

Modeling as a tool for chemical and biochemical engineering

Victor POZZOBON

Jury

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Prof. Gérald Debenest *(sponsor)*
Prof. Patrick Perré *(supervisor)*

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CentraleSupélec

To Sylvain Salvador
and Patrick Perré,
the two men who made
me the researcher I am.

A Sylvain Salvador
et Patrick Perré,
les deux hommes qui
ont fait de moi le chercheur
que je suis.

Abstract

Modeling as a tool for chemical and biochemical engineering

Abstract:

In this exercise, I take a step back and consider the work I led as a researcher over the last seven years. I introduce some of my works in order to illustrate the possible uses for the tool that is modeling. These illustrations are focused on the application of modeling to chemical and biochemical engineering. Four main applications are drawn: 1. understanding - aiming at the delivery of basic blocks of knowledge -, 2. characterization - providing hard to obtain parameters -, 3. design - guiding through the difficult process of new conception - and 4. scale up - transferring the most promising designs to the industrial sector -.

The first chapter is an extended formal curriculum vitae covering my education, experiences, research activities, partnerships, teaching activities, students I supervised and publications I authored.

In the second chapter, the three first usages are illustrated with the help of the three main fields of applications I am working on: biomass thermochemical conversion, the study of the interaction between light and microalgae and gas separation using hollow fibers membrane contactors. Scale up applications are the point I am aiming at and are developed as perspectives. Furthermore, even though only the modeling parts of my investigations are highlighted, hints of experiments are glanced, as they are essential material for proper modeling activities.

In the third chapter, I try to have a critical overlook on the work I led and the use I have for modeling. Then, an attempt to draw what my work could be in a n horizon of one to ten years is made. From it, it is clear that I have a solid driver and an established plan to improve photobioreactors designs using modeling tools. The same cannot be stated for biomass thermochemical conversion, as I deviated from it towards packed beds characterization, with my own curiosity as sole guide. Nonetheless, it yielded fruitful results. Regarding hollow fibers membrane conctactors, I shall support its transfer to the industrial sector as part of this ambitious project of the Chair of Biotechnology of CentraleSupélec.

Keywords: Modeling, Simulation, CFD, Chemical & Biochemical engineering

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Nomenclature

Latin symbols

A	frequency factor, depends
a	specific area, m^2/m^3
C	concentration, mol/m^3
c_p	specific heat capacity, J/kg/K
D	diffusivity, m^2/s
d	diameter, m
Ea	activation energy, J/mol
g	gravity acceleration, m/s^2
$\mathcal{H}$	Henry's constant, -
H	volumetric heat transfer coefficient, $W/m^3/K$
h	convective heat transfer coefficient, $W/m^2/K$
I	light intensity, $\mu molPhoton/m^2/s$
j	mass transfer coefficient, m/s
Kn	Knudsen number, -
l	width, m
m	mass, kg
M	molar mass, g/mol
N	molar flux, $mol/m^2/s$
n	normal vector, -
P	pressure, Pa
Q	flow rate, m^3/s
q	relative permeability, -
$\Re$	ideal gas constant, J/mol/K
Re	Reynolds number, -
r	radius, m
S	surface, m^2
T	temperature, K
t	time, s
u	velocity, m/s
V	volume, m^3
X	cell concentration, g/l
Y	mass fraction, -
y	molar fraction, -
z	height, m

Greek symbols

α	absorptivity, -
β	separation factor, -
ΔH	reaction heat, J/mol
Δ	Laplacian operator, $1/m^2$
ϵ	emissivity, -
ζ	porosity, -
κ	permeability, m^2
λ	thermal conductivity, W/m/K
μ	dynamic viscosity, Pa.s
ν	stoechiometric coefficient, -
ξ	radiation penetration coefficient, -
Π	volumetric heat of reaction, W/m^3
ρ	density, kg/m^3
σ	Stefan-Boltzmann constant, $W/m^2/K^4$
τ	tortuosity, -
ϕ	incident heat flux, W/m^2
Ψ	radiative heat loss function, W/m^2
ω	reaction rate, $kg/m^3/s$

Superscripts

g	gas
l	liquid phase
in	inlet
M	total number of solid species
N	total number of gaseous species
O	total number of reactions
out	outlet
T	matrix transposition operator
$\hat{}$	ordinary least square estimator

Subscripts

0	initial
λ	at a given wavelength
A	specie A
B	specie B
bw	bound water
eff	effective
fi	fiber
g	gas phase
$gasi$	gasification
I	gaseous species index
i	insulation
ini	initial
inn	inner
J	solid species index
K	reactions index
Kn	Knudsen
lw	liquid water
mem	membrane
out	outer
s	solid phase
sur	surrounding
tot	total

Other symbols

.	scalar product
$\boldsymbol{A}$	vector and matrix notation
$\mathcal{U}$	uniform density law
∇	nabla operator, 1/m
$\times$	vector product
$\sum$	sum

CHAPTER 1

Curriculum vitae

1.1 Civil status

Name: Pozzobon
First name: Victor
Date of birth: 27 December 1989
City: Rethel
Zipcode: 08300
Country: France
Phone: +0033 (0) 623 641 698
E-mail: victor.pozzobon@centralesupelec.fr

1.2 Education

PhD - Energetics and transfer
Université de Toulouse, France, 2012 - 2015
PhD Thesis title: *"Biomass gasification under high solar heat flux"*

Master Degree - Heat and mass transfer
Université Paul Sabatier, France, 2012
Main subjects: Energetics, Heat and mass transfer, Radiative heat transfer
Thesis title: *"Biomass gasification under high solar heat flux: a focus on drying and pyrolysis"*

Engineering school - Hydraulics
ENSEEIHT, Engineering school - Hydraulics section, France, 2010 - 2012
Main subjects: Fluid dynamics, Multiphase flow, Turbulence, CFD
Thesis title: *"Biomass gasification under high solar heat flux: a focus on drying and pyrolysis"*

Engineering school - Chemical engineering
Mines Albi, Engineering school - Energetics section, France, 2008 - 2010
Main subjects: Chemical engineering, Energetics, Chemistry, Instrumentation

1.3 Experiences

Research Engineer - Modeling and simulation - CFD and bioprocesses
Chair of Biotechnology of CentraleSupélec, Pomacle, France
December 2015 - now

<u>Research activities:</u> *(detailed hereinafter)*
Bioreactor design
Lignocellulosic biomass upgrading

Numerical characterization

Secondary missions:

Designing communication media (logo, poster templates, ...) in collaboration with the Communication Department

Designing and maintaining the Chair of Biotechnology website

Managing the Chair of Biotechnology's IT assets

PhD Student
RAPSODEE Laboratory, Albi, France
September 2012 - November 2015
Study of the gasification of lignocellulosic biomass under concentrated solar heat flux

Main activities:

Design and construction from scratch of an experimental device
↦ Highlighting new behavior

Elaboration of numerical model under OpenFOAM
↦ Better understanding of the coupling at stake

Spinoff works:

Modeling of a porous medium combustion reactor

Modeling of a char gasification circulating bed reactor

Assistant Engineer in R&D
Tokheim UK LTD, Dundee, Scotland
June 2011 - September 2011
Design and supervision of the construction of a test bench for solenoid valves
Technology monitoring on the proportional solenoid valves
Frequent reporting

Intership in a reasearch laboratory
ENSIACET LGC, Toulouse, France
May 2010 - August 2010
Operation of PIV and shadowscopy experimental device
Image processing using Matlab

1.4 Research activities

1.4.1 Research subjects and methods

I have three main fields of application for my research: **bioreactor design**, **lignocellulosic biomass upgrading**, and **numerical characterization**. The methodology I use to tackle problem in those fields is, somewhat, cross disciplinary: **modeling** assisted experiments and **experiments** inspired modeling. Indeed, no matter the field in which a problem is faced, I deeply believe in the fact that the conceptualization associated with modeling makes the experiments better, while experiments help to feel the physical phenomena at stake, making the model better.

Bioreactor design

With the recent shift towards greener production, biotransformation (transformation by microorganisms) of raw materials is rising into power. These transformations are led in vessels called bioreactors. Bioreactors are a specific type of chemical reactors as they host life. Thanks to previous work led in the chemical engineering field, bioreactor design research does not start from nothing. Indeed, the delivery of liquid and gas substrates to microorganisms in efficient way is directly transferable. Still, working with living organisms induces additional constraints, e.g., shear stress, hydrostatic pressure (for high bioreactor), light delivery for photosynthetic microorganisms. With the help of PhD students, I am currently leading both experimental and numerical investigations on those aspects. Being more specific, my research activities have a clear focus on how to take advantage of the interaction between light and microalgae at the photobioreactor scale.

Lignocellulosic biomass upgrading

The global context for this study is the well-known fact that mankind is currently facing an increase in energy cost and a climate change problem. As a consequence humanity has to reduce its reliance on fossil fuel in favor of renewable energy sources. Among the candidates, biomass pyro-gasification is of note. This process allows to produce a carbon neutral gaseous energy vector from biomass. Yet the transformation of biomass into an energy rich gas is a succession of complex phenomena. My investigations focused on supplying the energy required by the process using solar power. Indeed, the integration of solar energy can be considered as a means to store it into chemical form. This was the topic of my PhD thesis. Afterwards, with the help of Mines-Albi and a cofunded PhD student, I focused on another part of the process, a pretreatment called torrefaction. This is a key step as it stabilizes biomass properties, still, torrefied biomass can be subject to self-heating. We were one of the first team to investigate this phenomenon for this substrate.

Numerical characterization

Sometimes physical parameters are very difficult, or even impossible, to measure using direct methods. It can be because of their too low or too high values, or because of their correlation with numerous interfering phenomena. In these few cases modeling can be a way to access these parameters indirectly. Depending on the situation, two wide kinds of approach may be available. Either one reproduces the system numerically and computes the properties of interested from known boundary conditions. Or one feeds the model with experimental data and uses it to decorrelate each phenomena yielding the value of the parameter of interest. I have led both approaches in order to acquire almost non-measurable quantities such as granular bed permeability, heat flux higher than (1 MW/m^2), microscale mass transfer coefficient. Currently, I work on packed bed heat transfer phenomena with IFPEN, Solaize.

1.4.2 Academic partnerships

RIBP - Reims - Since 2019

I initiated this partnership as part of my research activity involves a proper understanding of photosynthesis. RIBP laboratory is a recognized actor of this field, focusing on higher plants. Together, we teamed up to tackle the challenge of better understanding how growth conditions influence microalgae photosynthesis. This collaboration yielded recently a co-authored article.

LPQM - Gif-sur-Yvette - Since 2019

My research in photobioreactor design also required to be able to engineer proper lighting devices. To do so, I use numerical tools, still I needed reflective materials optical properties. Being experts in optics, I started a partnership with LPQM laboratory. The combination of their measurement know-how and our numerical design procedures yielded a light concentrator whose design as published in a research article.

EMIR laboratory, IPEIM, Monastir - Tunisia - Since 2019

Looking for OpenFOAM and HPC expertise, Pr. Marzouk Lajili from EMIR laboratory was directed to me. After discussing together, we found several scientific subjects our entities share an interest in, e.g. lignocellulosic biomass drying and pyrolysis. This interaction materializes into a 3-month scientific stay of one of Pr. Lajili PhD student (Saaida Khlifi) in our laboratory under my supervision.

IFPEN - Solaize - Since 2018

IFPEN contacted me after one of my talk in an OpenFOAM conference where I presented my work on a fully numerical workflow allowing to compute granular media properties. They were interested in sharing my know-how. In order to better know one another they invited me for a two-day visit of their facility, including a presentation of my work. Sharing common interest and point of views, we teamed up to tackle some of the challenges of heat and mass transfer in granular media. The first solid token of this collaboration is a co-supervised internship (Ruoyi Ma) dealing with heat transfer in packed spheres bed.

RAPSODEE - Albi - Since 2016

Together with RAPSODEE laboratory, we investigated the problematic of carbonaceous feedstock self-heating when exposed to air. This alliance comes from a shared interested in this research topic and complementary skills. Indeed, looking for high quality experiments, I naturally turned myself toward my former laboratory. While RAPSODEE was willing to enrich its methodology using modeling. For this partnership, a half-half funded PhD was started between our entities (Amina Bouzarour, with publication).

Maison de la Simulation & ROMEO cluster - Reims - Since 2016

This partnership is the first I initiated. It finds its origin in my need for computational power. Along with my interaction with ROMEO cluster, I built a close relationship with the people operating it. Sharing both scientific and human values, our partnership yielded fruits I am proud of. Among them I would like to quote: the organization of a 3-day OpenFOAM tutorial on a yearly basis, two public fundings obtained together and the subsequent internships.

1.4.3 Industrial partnerships

GRTGaz

GRTGaz is leading a project aiming at building up an industrial scale workflow powering a methanisor using microalgae, the *Algues4Biométhane* project. I share the lead of the involvement of the Chair of Biotechnology of CentraleSupélec in our partnership on this project. The Chair provides its expertise on two different stages of the project: microalgae production and biogas purification. For both stages, I have designed and quoted the studies. Regarding more specifically the microalgae production, a preliminary study has already been delivered as subcontractor.

1.4.4 Public fundings

This section presents the public funded research activities I am involved in.

Leading

↦ MALE ALFA project - 2018

I initiated and led the project dealing with flow cytometry results analysis using machine learning. I teamed up with Maison de la Simulation and ROMEO cluster. For this project, I got two master trainees funded by SFR Condorcet.

↦ MILCA project - 2016

As with MALE ALFA, I initiated and led the project on the effect of light on microalgal growth and its numerical reproduction. The partners were the same as MALE AFLA. For this project, I got one master trainee and few months of a research engineer funded by SFR Condorcet.

Involved

↦ VitrHydrogène - 2018 - 2021

The aim of this French government supported project is to produce, purify and distribute biosourced H_2. My contribution lies in the first purification step (separating H_2 from CO_2). I co-supervise the PhD student (Sayali Chavan) funded by this project.

↦ IDEA Interreg - 2017 - 2020

The objective of this European project is to growth microalgae in North West Europe to use them as food/feed and natural chemicals source. I am involved as support in the modeling steps of the strain growth.

1.4.5 Private fundings

This section presents the activities as paid subcontractor I have taking part in.

Leading

↦ GRTGaz - 2018 - 2019

I have designed, supervised and reported a study on the performances of a new photobioreactor the client was considering to acquire. This study was commissioned as a Go/No Go before a potential industrial scale deployment.

Involved

↦ Compagnie de Chauffage Intercommunale de l'Agglomération Grenobloise - 2017

I have been involved in the numerical design of a wood drying tank.

1.5 Teachings activities

Reported here are the hours in classrooms, in front of students. The amount of time needed to prepare these teaching is not reported.

1.5.1 CentraleSupélec

As a research engineer, I am not asked to take part in teaching activities. As I like this activity and some needs arose, I have been, and am, involved in several teachings within CentraleSupélec. Those activities are mainly practicals. Even though I helped designing the teaching material, I am not in charge of those activities. A point of note is that my office is located more than two hours away from the campus. This hinders my possible involvement in teaching activities.

Practicals

M2

CFD with OpenFOAM - 84h

Living organisms modeling - 12h

L3

Integration week on *Heat exchangers biofouling* - 70h

1.5.2 Mines-Albi

As a PhD student, I had to take part in teaching activities, around 64 hours (tutorials equivalent) per years. Deeply motivated by my love for this activity, I took advantage of the opportunity Mines Albi offered me. All in all, I gave more than 250 hours of teachings including lectures in amphitheaters.

Lectures

L3

Fluid dynamics: 17 h

Tutorials
L3
Fluid dynamics: 67 h
Heat and Mass transfer: 42 h

Practicals
M2
Renewable energies (solar, wind and hydraulic power): 38 h
Wood drying modeling with Comsol: 53 h

L3-M2
Scientific research initiation: 45 h

1.5.3 Others

Trainings
3-day OpenFOAM training, open to academics and corporates: 4 editions

Lectures
AgroParisTech, Paris - Valorization of lignocellulosic biomass: 6 h
Néoma Business School, Reims - Bioprocess modeling: 1 h

Private tuition
Middle and high school - Mathematics, physics, chemistry: 15 pupils over 7 years (2008 - 2015)

1.6 Community dedicated activities

FOAM-U association secretary
FOAM-U is an association gathering French speaking users of OpenFOAM. I am a member and one of the two secretaries (sitting in the general assembly) of this association since 2016. Furthermore, I am in charge of directing the maintenance of the association WebSite - and its development while it was under construction.

IT assets manager
Since my hire at the Chair of Biotechnology of CentraleSupélec, I am in charge of managing the collective IT assets. This mission covers a broad spectrum including buying and installing new materials, dealing with the subcontractor and, of course, being a helping hand.

Communication media
After my arrival at the Chair of Biotechnology of CentraleSupélec, I initiated and took the lead of the renovation of the communication media. I built from scratch the website, helped in designing the logo, brochures, visit cards, ...

AERES / HCERES examinations
Both as PhD student and research engineer I have been involved, at different levels - never leading -, in the preparation of the AERES / HCERES examinations. This covered presenting my works (on a stand and in-lab), helping agglomerating indicators, writing part of the report and preparing the examination day.

Scientific animation
During the three years of my PhD, I organized scientific presentations of the PhD students and trainees working in the laboratory. Those sessions were scheduled on the first Tuesday of each month, with four presentations each time. My missions covered the whole process, from elaborating the program, gathering the speakers and the audience to booking the room and preparing the buffet.

1.7 Scientific visibility

OpenFOAM related
The main part of my scientific visibility comes from my activities associated to OpenFOAM. It can be divided into two levels France-wide and worldwide:

↦ on a national scale, this visibility originates from the trainings and teachings I give, my position as secretary in FOAM-U association and my participation to conferences dealing with OpenFOAM. As a consequence, every year, several companies and students contact me to know more about OpenFOAM. Their questions may be technical as well as inquiring about the OpenFOAM community and its actors. For example, our partnership with Pr. Marzouk Lajili (EMIR laboratory, IPEIM, Monastir, Tunisia) began thanks to this visibility. Or, our partnership with IFPEN was initiated after my presentation during the third Journées OpenFOAM, in Valenciennes.

↦ on a worldwide scale, this visibility comes from the scientific articles I wrote and my OpenFOAM teaching materials I published on ResearchGate. Both beginner and advanced versions of these documents have been downloaded more than 50 000 times.

As a consequence, I am identified as an entry point of this community. This is how I have been invited to review two chapters of the book associated to the 11th OpenFOAM Workshop.

Lectures
I have been invited as guest speaker to give several lectures. Among them, three are of note:

↦ I gave a lecture about my PhD topic in a von Karman Institute Lectures Serie themed on *"Pyrolysis phenomena in porous media"*, April 2019

↦ I presented my work on microalgae tracking in photobioreactors in *"Journée microalgues"*, a one day event organized by the European Center for Biotechnology and Bioeconomy, which gathered all the main actors of the microalgae field in France, October 2018

↦ I have been invited by ENSEEIHT - my former engineering school - to talk about my career as a PhD research scientist, January 2017

Visibility as reviewer
Finally, I have reviewed articles for several journals: Solar Energy Engineering, Powder Technology, Applied Energy, Energy Conversion and Management, International Journal of Hydrogen Energy, Bioresource Technology, Open Chemical Engineering Journal, Energy & Fuel, Solar Energy, Fuel, Journal of Cancer Science and Clinical Oncology. In addition, I reviewed numerous proceedings for several conferences.

1.8 Supervision

I have supervised, and still supervise, several PhD students at different level on involvement (estimation in bold). Two of them defended, another one is finalizing her manuscript. I also supervised several trainees from L3 to M2 level.

1.8.1 PhD students

Sayali Chavan, 2018 - 2021 - **40 %**
Université Paris Scalay
Thesis (tentative) title: *"Development, modeling and optimization of* CO_2 *gas-liquid absorption, intensified with hollow fibers membrane contactors, as an eco-efficient technique for purification of bio-sourced hydrogen"*

Wendie Levasseur, 2017 - 2020 - **60 %**
Université Paris Scalay
Thesis (tentative) title: *"Study of light pattern on microalgal growth"*
One article published in *Algal Research*, one review in *Biotechnology Advances*

Amina Bouzarour, 2016 - 2019 - **60 %**
Université de Toulouse, defended on December 11th 2019
Thesis title: *"Etude de l'auto-échauffement de matière carbonée : application au bois torréfié"*
One article published in *Fuel*

Na Cui, 2016 - 2020 - **60 %**
Université Paris Scalay
Thesis (tentative) title: *"Scale-down of microorganisms culture and mini-bioreactors design"*
One article under review in *Applied Microbiology and Biotechnology*

Najib Chouikhi, 2016 - 2020 - **20 %**
Université Paris Scalay
Thesis (tentative) title: *"Modélisation multiéchelle de transport de masse et chaleur dans les étapes d'un procédé de production de méthane à partir de biogaz par*

technologie de séparation par adsorption"

Wenbiao Jiang, 2015 - 2018 - **60 %**
Université Paris Scalay, defended on December 5^{th} 2018
Thesis title: *"Simulation of bubbling in a photobioreactor"*
One article published in *Biotechnology and Applied Biochemistry*

1.8.2 Internships

Supervisor

Elise Viau, 2019
M1, Sup'Biotech - 4 months
Thesis title: *"Viability study of the microalga, Chlorella vulgaris, by flow cytometry assisted by Machine Learning"*
Results currently under review

Saaida Khlifi, 2019
PhD, EMIR laboratory, IPEIM, Monastir, Tunisia - 3 months
Research topic: *"Etude numérique de la combustion des gaz issus de la pyrolyse"*

Ruoyi Ma, 2019 - **20 %**
M2, Ecole Centrale de Lyon - 6 months
Thesis title: *"Heat transfer simulation in fixed beds using OpenFOAM"*
Located at IFPEN, Solaize

Marion Pointcheval, 2019
L3, Université Reims Champagne-Ardenne - 6 weeks
Dissertation title: *"Etude du potentiel d'une microalgue locale : profils lipidique et pigmentaire"*
Results published in *Bioresource Technology Reports*

Robin Lacombe, 2017
M1, Sup'Biotech - 4 months
Thesis title: *"Study of the growth of microalgae under different micro-periods. Realization of μPhotoBioreactor and first cultures"*
Results published in *Algal Research*

Academic tutor
Daniel Durall Lopez, 2018
M2, Master Génie des Procédés et Bioprocédés, Université Paris-Saclay - 6 months
Thesis title: *"Développement de modèles de bioréacteurs agités dans le logiciel USIM PAC pour des applications en scale-up des bioprocédés"*
Located at CASPEO, Orléans

Rachel Irkankunda, 2020
M2, Master Génie des Procédés et Bioprocédés, Université Paris-Saclay - 6 months
Thesis title: *"Production et étude de la composition des microalgues "*
Located at HuddleCorp, Cébazat

1.9 List of publications

1.9.1 Articles in peer reviewed scientific journals

All in all, I authored or co-authored 20 articles, 11 as first author, 6 as second author and 3 as last author. Three other articles are currently under review. Two as first author, one as second.

Levasseur, W., Perré, P. & **Pozzobon, V.** (2020). A review of high value-added molecules production by microalgae in light of the classification. Biotechnology Advances.

Pozzobon, V., Levasseur, W., Do, Guerin C., Gaveau-Vaillant N., Pointcheval M., & Perré, P. (2020). Desmodesmus sp. pigment and FAME profiles under different illuminations and nitrogen status. Bioresource Technology Reports.

Jiang, W., Levasseur, W., Casalinho, J., Martin, T., Puel, F., Perré, P., & **Pozzobon, V.** (2020). Shear stress computation in an millimeter thin flat panel photobioreactor: numerical design validated by experiments. Biotechnology and Applied Biochemistry.

Pozzobon, V., & Perré, P. (2020). Mass transfer in hollow fiber membrane contactor: computational fluid dynamics determination of the shell side resistance. Separation and Purification Technology, 116674.

Pozzobon, V., Levasseur, W., Do, K. V., Palpant, B., & Perré, P. (2020). Household aluminum foil matte and bright side reflectivity measurements: Application to a photobioreactor light concentrator design. Biotechnology Reports, 25, e00399.

Fougerit, V., **Pozzobon, V.**, Pareau, D., Théoleyre, M. A., & Stambouli, M. (2019). Experimental and numerical investigation binary mixture mass transfer in a gas–Liquid membrane contactor. Journal of Membrane Science, 572, 1-11.

Levasseur, W., Taidi, B., Lacombe, R., Perré, P., & **Pozzobon, V.** (2018). Impact of seconds to minutes photoperiods on Chlorella vulgaris growth rate and chlorophyll a and b content. Algal research, 36, 10-16.

Pozzobon, V., Colin, J., & Perré, P. (2018). Hydrodynamics of a packed bed of non-spherical polydisperse particles: A fully virtual approach validated by experiments. Chemical Engineering Journal, 354, 126-136.

Pozzobon, V., Salvador, S., & Bézian, J. J. (2018). Biomass gasification under high solar heat flux: Advanced modeling. Fuel, 214, 300-313.

Pozzobon, V. (2018). 10% Loss of Incident Power through Solar Reactor Window: Myth or Good Rule of Thumb?. Applied Solar Energy, 54(2), 131-133.

Spiesser, C., **Pozzobon, V.**, Farges, O., & Bezian, J. J. (2018). Probabilistic modeling of coupled heat transfer: A step towards optimization based on multiphysics Monte Carlo simulations. International Journal of Thermal Sciences, 132, 387-397.

Bouzarour, A., **Pozzobon, V.**, Perre, P., & Salvador, S. (2018). Experimental study of torrefied wood fixed bed: thermal analysis and source term identification. Fuel, 234, 247-255.

Chastang, T., **Pozzobon, V.**, Taidi, B., Courot, E., Clément, C., & Pareau, D. (2018). Resveratrol production by grapevine cells in fed-batch bioreactor: Experiments and modeling. Biochemical engineering journal, 131, 9-16.

Pozzobon, V., & Perre, P. (2018). Han's model parameters for microalgae grown under intermittent illumination: Determined using particle swarm optimization. Journal of theoretical biology, 437, 29-35.

Pozzobon, V., Baud, G., Salvador, S., & Debenest, G. (2017). Darcy scale modeling of smoldering: impact of heat loss. Combustion Science and Technology, 189(2), 340-365.

Fougerit, V., **Pozzobon, V.**, Pareau, D., Théoleyre, M. A., & Stambouli, M. (2017). Gas-liquid absorption in industrial cross-flow membrane contactors: Experimental and numerical investigation of the influence of transmembrane pressure on partial wetting. Chemical Engineering Science, 170, 561-573.

Ephraim, A., **Pozzobon, V.**, Louisnard, O., Minh, D. P., Nzihou, A., & Sharrock, P. (2016). Simulation of biomass char gasification in a downdraft reactor for syngas production. AIChE Journal, 62(4), 1079-1091.

Pozzobon, V., Salvador, S., & Bézian, J. J. (2016). Biomass gasification under high solar heat flux: Experiments on thermally thick samples. Fuel, 174, 257-266.

Pozzobon, V., & Salvador, S. (2015). High heat flux mapping using infrared images processed by inverse methods: an application to solar concentrating systems. Solar Energy, 117, 29-35.

Pozzobon, V., Salvador, S., Bézian, J. J., El-Hafi, M., Le Maoult, Y., & Flamant, G. (2014). Radiative pyrolysis of wet wood under intermediate heat flux: Experiments and modeling. Fuel Processing Technology, 128, 319-330.

1.9.2 Invitations as guest speaker

Pozzobon, V. (2019). Biomass gasification under radiative heat flux. VKI lecture series *Pyrolysis phenomena in porous media*, Sint-Genesius-Rode, Belgium.

1.9.3 Conferences with proceedings

I have been involved, at various levels, in the redaction of 6 conference proceedings.

Jiang, W., **Pozzobon, V.**, Casalinho, J., Martin, T., Perre, P., & Puel, F. (2018, June). Bubble formation and detachment: an investigation by experiments and simulations. In 8th International Colloids Conference.

Fougerit V., **Pozzobon V.**, Pareau D., Théoleyre M-A., & Stambouli M. (2017, August). Modeling the absorption of a gas mixture in a cross-flow hollow-fiber membrane module. 13th International Conference on Gas–Liquid and Gas–Liquid–Solid Reactor Engineering (GLS13), Sint-Genesius-Rode, Belgium.

Ephraim A., **Pozzobon V.**, Minh DP., Nzihou A., & Sharrock P. (2016, May). Behaviour of chloride pollutants in syngas from wood waste pyro-gasification: a modeling approach. 6th International Conference on Energy from Biomass and Waste, Venice, Italy.

Ephraim A., **Pozzobon V.**, Louisnard O., Minh DP., Nzihou A., & Sharrock P. (2016, May). Simulation of biochar gasification in a downdraft reactor for syngas production. In WasteEng 2016-6th International Conference on Engineering for Waste and Biomass Valorisation.

Pozzobon, V., Salvador, S., Bézian, J. J., El-Hafi, M., & Flamant, G. (2014, August). Beech wood gasification under high radiative heat flux. In WasteEng 2014-5th International Conference on Engineering for Waste and Biomass Valorisation, Rio de Janeiro, Brazil.

Pozzobon, V., Salvador, S., Bézian, J. J., El-Hafi, M., & Le Maoult, Y. (2013, May) Gazéification de la biomasse lignocellulosique sous haute densité de flux solaire: séchage et pyrolyse. In SFT Conference 2013, Geradmer, France.

1.9.4 Conferences without proceedings

Poster presentations are not reported, only oral communications.

Pozzobon, V., & Perré P. (2019, June) Photobioreactor upscaling: a focus on perceived light frequencies. Journées FOAM-U 2019, Marseille, France.

Chavan S., **Pozzobon, V.**, Lemaire J., & Perré P. (2019, April) Binary gas mixture separation in a hollow fibers Membrane Contactor: towards predictive modeling. Journées jeunes chercheur, SFR Condorcet, 2019, Reims, France.

Pozzobon, V., & Fougerit V. (2019). Numerical investigation of biogas purification using hollow fibers membrane contactor. VKI lecture series *Pyrolysis phenomena in porous media*, Sint-Genesius-Rode, Belgium.

Pozzobon, V. (2018, June) Modélisation de la croissance de micro-algues en photobioréacteur : effet de la photopériode (projet MILCA). Journées Condorcet, Calais, France.

Pozzobon, V., Colin J., & Perré P. (2018, June) Caractérisation hydrodynamique d'un lits de plaquettes forestières à l'aide d'outils HPC. Journée scientifique ROMEO 2018, Reims, France.

Pozzobon, V., & Perré P. (2018, May) Granular media characterization: an application to wood chips bed. Journées FOAM-U 2018, Valenciennes, France.

Bouzarour A., Salvador S., Perré P., & **Pozzobon, V.** (2018, January) Auto-échauffement de la biomasse lignocellulosique dans un lit fixe de particules : Approche expérimentale. Journées jeunes chercheur, SFR Condorcet, 2018, Amiens, France.

Pozzobon, V., & Perré P. (2017, May) Suivi Lagrangien de microalgues en photobioréacteur. Journée scientifique ROMEO 2017, Reims, France.

Pozzobon, V., & Perré P. (2017, March) Microalgae Lagrangian tracking in photobioreactor. Journées FOAM-U 2017, Nevers, France.

Pozzobon, V., Bézian, J. J., & Salvador, S. (2016, May) Biomass gasification under high solar heat flux. Journées FOAM-U 2016, Rouen, France.

Pozzobon, V., J., Salvador, & Bézian, J. (2014, October) Modélisation de la gazéification de biomasse sous haute densité de flux solaire avec déformation du milieu. 12èmes Journées d'Etudes des Milieux Poreux, Toulouse, France.

Pozzobon, V., Bézian, J. J., Salvador, S., El-Hafi, M., & Flamant, G. (2013, December) Gazéification de biomasse sous haute densité de flux solaire. Journées FédéSol 2013, Dourdan, France.

Pozzobon, V., Bézian, J. J., Salvador, S., El-Hafi, M., & Flamant, G. (2012, November) Interaction entre la biomasse et le rayonnement solaire concentré. Journées FédéSol Junior 2012, Nantes, France.

CHAPTER 2

Modeling applications

Introduction

Modeling is a very general tool that can be used to tackle problems with varying levels of complexity over different length and time scales. Among the scope of all the applications possible, four broad domains can be drawn: the understanding, the characterization, the design and the scale up. All having their place at different stages of scientific and engineering works. Figure 2.1 describes their interconnection and the way they succeed to each other in the whole process of solving a problem in chemical engineering - either building a new process or identifying the pathology on an existing one.

Understanding lies on the ground of this scheme as it is related with the very first steps of knowledge building. It is often said that a proper mechanistic model can be used to assess for the impact of each of its components. This can be done by turning them on and off or changing the way they are described. This kind of approaches highlights the couplings at stake and weights the origins of observed phenomena.

Numerical characterization comes after understanding as it requires at least basic knowledge and description of the phenomena. This application of modeling helps in computing properties that are obtained only with difficulty, if at all, using conventional direct measurement approaches. Different indirect methods can be employed depending on the problem. One implies to model a system at a lower of level representation than the one of primary concern. Then, to run the model so that it yields quantities of interest at this low level and compute from these quantities parameters that are relevant at primary level of interest. Another option is to use inverse method. This approach requires to model the system, yet this time, it can be fed with experimental data to obtain the parameters of interest.

Virtual design can be set at the same level as characterization, or after as its direct succession. Its position depends on the accuracy with which parameters describing phenomena are known. It aims at lowering costs and development times by delivering valuable insights beforehand. It is today commonly used in numerous industries such as automotive or aerospace. Thus it is all the more natural to use it when designing experiments. On one hand pitfalls can be avoided when building up our research prototypes. On the other hand, it also helps in delivering better experimental apparatus, better answering one's questioning.

Scaling up a system is usually associated with its last step towards commercial deployment. Indeed going from the labscale proof of concept to the economically viable industrial unit requires most of the time to increase the fluxes that can be processed by the system. This is not an easy task as several phenomena may not scale with the system size, e.g. gravity, fluid physical properties, ... In this process, modeling is a guide that allows potential misadventures to be avoided.

The three first applications of modeling will be illustrated hereinafter, as I have used them to tackle various problems. Scale up applications are the point I am

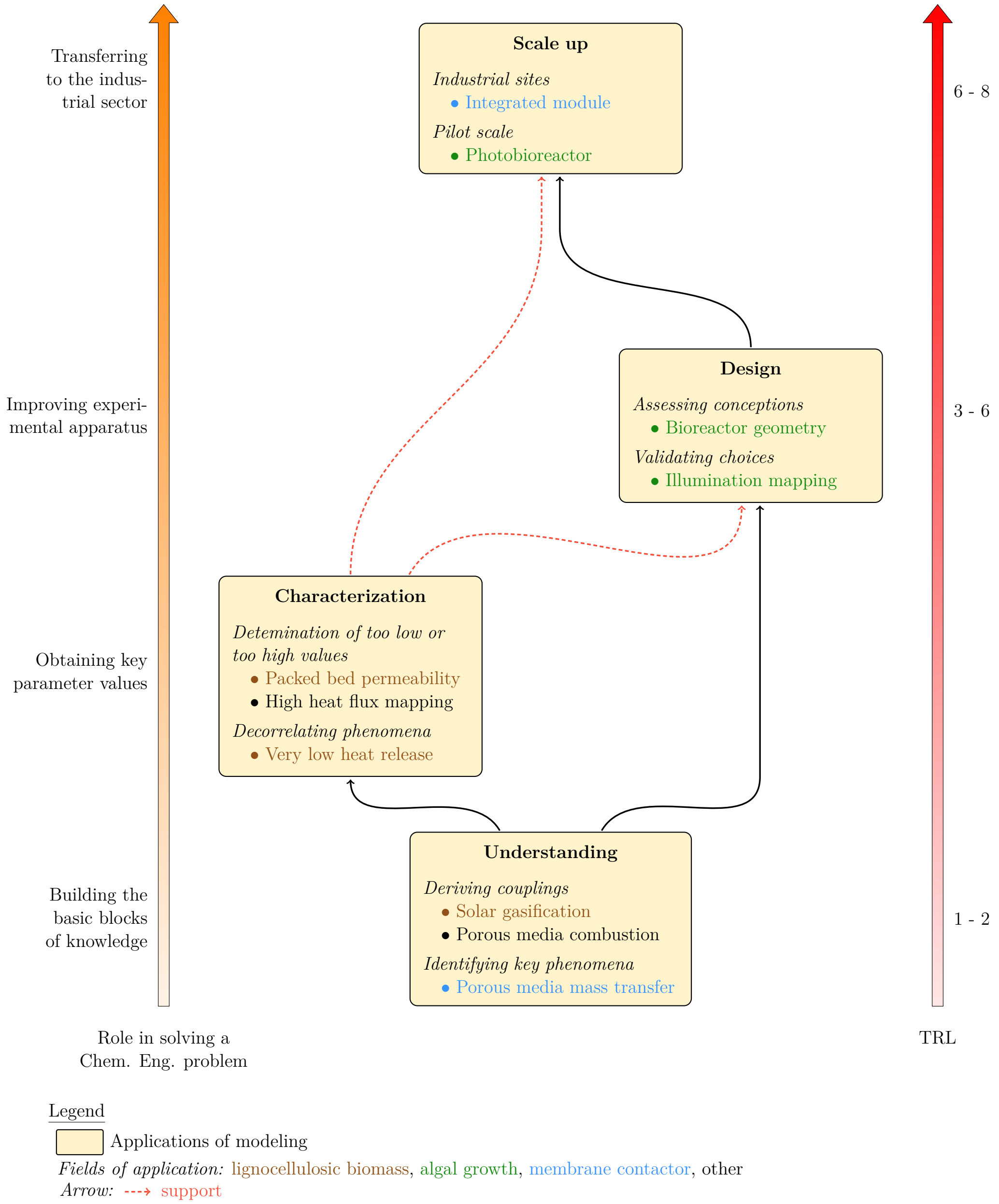


FIGURE 2.1: Illustration of the different applications of modeling and their interaction in the solving of a chemical engineering problem. Square: application of modeling and examples detailed hereinafter

aiming at and will be further developed in the next chapter. Before spotlighting some of my investigations, the fields of application I am focusing on will be introduced. Indeed they are the backbone which supports my day-to-day work. Finally, I would like to point out that even though I will highlight the modeling parts of my investigations, high quality experiments are essential material for proper modeling activities.

2.1 Fields of application

In order to introduce the background withstanding my work, the technical fields I am applying modeling to will be presented. They can be classify into three main categories:

- bioreactor design, more specifically microalgal growth with a focus on the influence of lighting conditions,
- lignocellulosic biomass thermochemical conversion, and more generally heat and mass transfer in reactive porous media,
- spin-off works for which, even though I may lead part of the investigations associated to them, they are not the core of my research activity, e.g. biogas purification.

2.1.1 Microalgae and lighting conditions

Microalgae are receiving increasing attention because of thier potential application in numerous domains such as high added value molecules production, wastewater treatment or atmospheric CO_2 fixation [1–4]. Two different cultivation approaches coexist: open ponds and closed photobioreactors. The first ones deliver a cost effective high scale solution, at the price of low control over the growth conditions and a very high risk of contamination [5]. The second allows for a very tight control of operating conditions, while being expensive and scalable only with difficulty.

As a consequence, open raceway ponds are used for mass production of cheap commodities such as feed, or low added-value applications like wastewater treatment. Closed photobioreactors are employed to produce high added-value biosourced compounds intended for pharmaceutical or nutraceutical use. These last two industrial sectors can cope with high costs and a substantial amount of engineering in designing new production vessels and operating protocols.

Our focus will be on closed photobioreactor as several challenges still need to be faced in their design. Because of their very controlled nature, photobioreactors are reasonably assumed to be perfectly stirred reactors regarding nutrients and dissolved gases concentrations. Regarding illumination inside of the reactor, it is well known that such an assumption cannot be drawn because of light attenuation [6]. Yet light is key to microalgae growth. It is therefore a critical parameter when designing a photobioreactor. At the Chair of Biotechnology of CentraleSupélec, we have chosen to tackle this problem with the help of numerical modeling and original experiments.

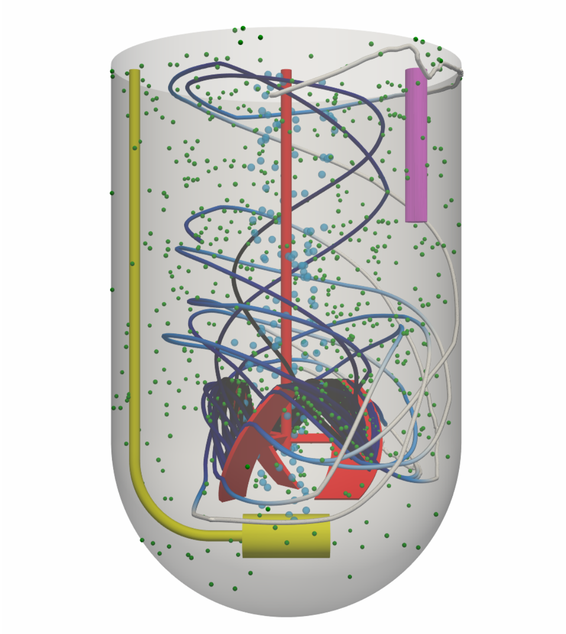
Being the principal investigator of behalf of the Chair, an important part of my work is dedicated to this topic.

The existing models describing the impact of light on algal growth can be sorted out into three different categories [7]:

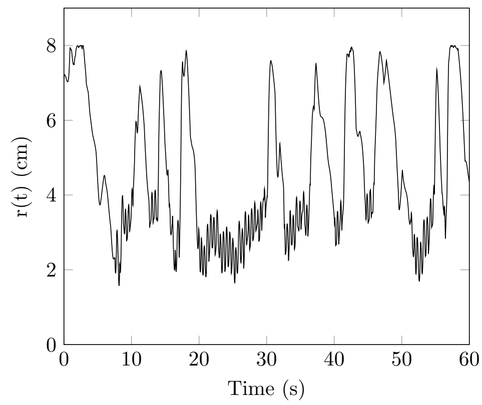
- black boxes: they predict the total photosynthetic yield of a culture as a function of the total or averaged light intensity reaching the culture [8]. These models are very easy to handle. In addition, they allow for a simple 0D modeling approach. Nevertheless, their shortcomings are numerous, the most dramatic one is that they critically depend on the experimental data that have been used to calibrate them. Obviously, they can not be of much help when designing a new photobioreactor,
- local light intensity models: they describe the attenuation of light throughout the reactor. Thus they allow for spatial integration of light and related growth rate distribution over the reactor volume. Usually, they can account for light attenuation based on cell density and cells pigment content [9]. They yield significantly better results than black boxes models. Nevertheless, they assume that microalgae response to light is always in steady state. Thus, they are not able to take into account dynamic temporal effects (light/dark cycle) inside of the reactor which are today known to have an important impact on microalgae behavior [10],
- mechanistic models: they describe the microalgae response to light in term of activation of the key proteins at stake in the photosynthetic process. Among them, PhotoSynthetic Units (PSU) model [11] is nowadays widely used in the community. It is an improvement of the firstly proposed model [12] which take into account photodamages due to light overexposure. This model can therefore account for the impact of light history on microalgal growth. Yet it is not necessary as simple to handle as the previous ones.

PSU models are particularly well suited for photobioreactor numerical design. Indeed, inside of those vessels, microlagae are shuttled from light to dark zones, induced by mutual shading. Hence, cells experience dynamic illumination variations. Yet these models require to know the position of the microalgae inside of the reactor, and the corresponding illumination, to yield the full-extend of their power. Luckily, using CFD capabilities, it is nowadays possible to access positions, hence light patterns, experienced by tracers reproducing microalgae. Figure 2.2 illustrates this approach. The visualization on the left presents the simulation of a 5 liter photobioreactor with sparged bubbles, a mechanical stirrer and tracked microalgae. The figure on the right is the corresponding radial position of the tracer trajectory drawn on the left.

The aim of my work is to bridge this gap by developing and validating a fully coupled numerical model linking photobioreator design and microalgal growth. This tool would be used to assess the capability of a new design without producing it, paving the way to fully in silico design and optimization. Yet the road is still long and various challenges have to be faced before achieving this ambitious goal. Among them, the understanding of the intrinsic behavior of microalgae with respect to



(A) Reactor visualization after 2 minutes



(B) Tracer radial position

FIGURE 2.2: Numerical simulation of a 5 liter photobioreactor. Aeration: 0.1 vvm, stirring: 100 rpm. Lagrangian tracers: 10 000, only 500 represented (randomly drawn). Total runtime: 11 minutes. Color legend: blue - bubbles, green - tracers, red - stirrer, yellow - sparger, purple - pH probe. Tube: one tracer trajectory over 1 minute, color: radial position

lighting conditions is a first step (current work of Wendie Levasseur). It will have to be followed by the modeling of microalgal response before being coupled with a CFD code that would not only predict fluid (PhD of Wenbiao Jiang) flow but also illumination inside of the reactor.

2.1.2 Lignocellullosic biomass thermochemical conversion

My interest for this research topic lies in the beginning of my research and engineering career. Being keen on fluid dynamics as well as heat and mass transfer, I chose a PhD topic dealing with both, *i.e.*, the study of lignocellulosic biomass gasification under high solar heat flux. The global context for this study was the well-known fact that mankind is currently facing an increase in energy cost and a climate change problem [13, 14].

As a consequence humanity has to reduce its reliance on fossil fuel in favor of renewable energy sources. Among the candidates, biomass pyro-gasification is of note. This process allows to produce a carbon neutral gaseous energy vector from biomass. Yet the transformation of biomass into an energy rich gas is a succession of complex phenomena (Fig. 2.3). It starts with the drying of biomass [15] around 100 °C, where water evaporates from the biomass. Then, pyrolysis takes place around 400 °C. This complex stage turns dry biomass into three main products: light gases (from H_2 to C_3H_8), tars (a mixture of more than 300 hydrocarbon molecules [16]) and char (a solid residue mainly made of carbon and trace elements [17]). Finally, around 800 °C, steam - and to a lesser extend CO_2 - can oxidize char and transform it into syngas (H_2 and CO). Higher levels of temperature - around 1200 °C - also enable tar thermal cracking [18] and tar steam reforming [19]. The produced gas, referred to as *producer gas*, is therefore a combination of pyrolysis gas, syngas and thermally cracked and steam reformed tars. Once upgraded, this gas can be used in a wide variety of processes: fuel cells, gas turbines, combustion for heat, Fisher Tropsch synthesis. Being a highly endothermic transformation, the required heat is classically supplied by burning a fraction of the biomass feed. Two main drawbacks come with this technique: the efficiency with respect to the biomass is lowered and the produced syngas is diluted by N_2 and fumes coming from air combustion [20, 21].

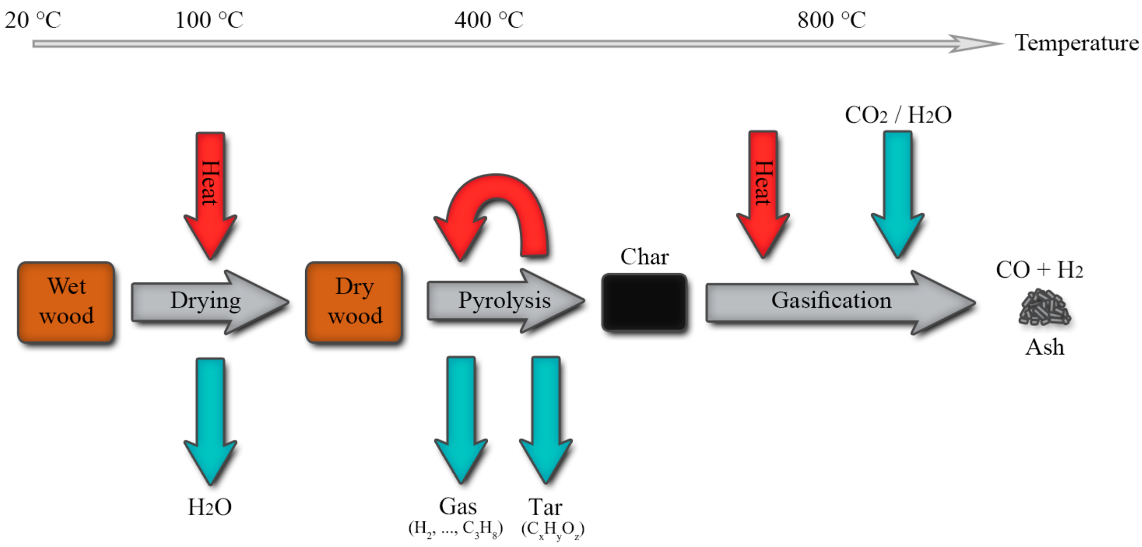


FIGURE 2.3: The different steps leading to biomass gasification

Supplying the required heat using solar energy would avoid these drawbacks. Indeed, on large scale, solar concentrated power plants can achieve incident heat flux higher than 1000 kW/m^2. Hence, it would be possible to reach a temperature of 1200 °C or higher and therefore to lead pyrolysis and gasification reactions.

The investigation, at labscale, of this potential synergy has been the work of my PhD. It has been the topic of several publications and a lecture at the von Karman Institute, Belgium, in 2019. Furthermore, the know-how I built during these years has paved the way to other lignocellulosic biomass studies I directed. The mains ones being the self-heating phenomena that may occur in torrefied wood chips beds (PhD of Amina Bouzaour) or the characterization of packed beds.

2.1.3 Biogas purification

As aforementioned, this topic does not lies in the core of my expertise and will be kept short for the sake of readability. My implication in this matter originates from the need of a PhD student (Valentin Fougerit) working on biogas purification to better understand the phenomena at stake in a hollow fibers membrane contactor

(Fig. 2.4). Indeed these mass exchangers offer a low-cost and modular solution to purify gases with different solubility into a liquid. Here they were applied the separation of the methane and carbon dioxide composing biogas. The PhD student solicited my support to produce a model describing mass transfer at local scale inside of the mass exchanger.

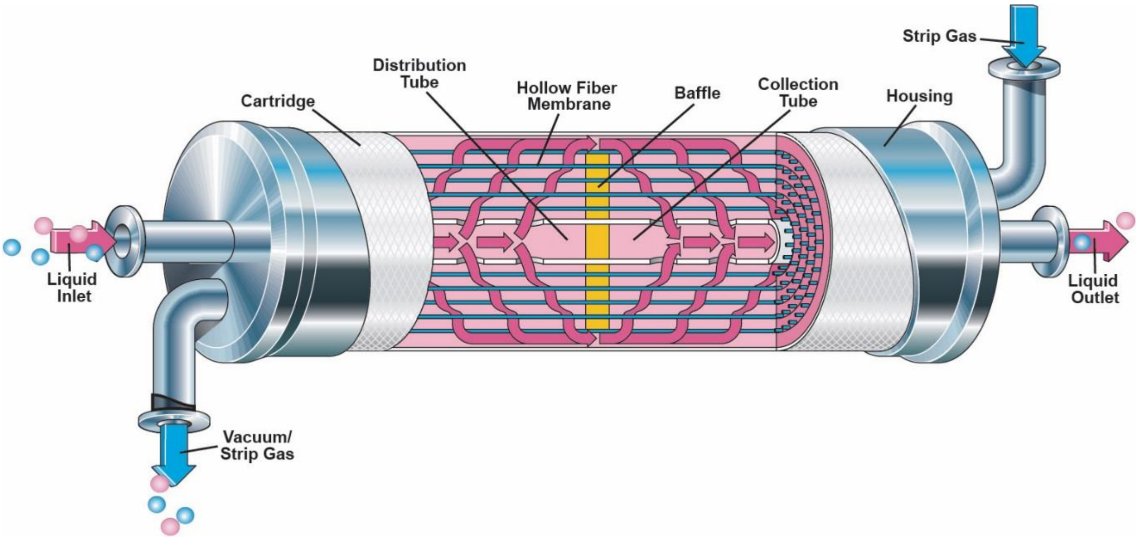


FIGURE 2.4: Schematic of a hollow fibers membrane contactor. Gas is entering on one side of the contactor and is distributed inside of the lumen of the fibers. Water is flown in the openness in-between fibers in a counter current manner. Gas can diffuse into the porosity of the fiber material and dissolve into liquid. The internal geometry features a baffle to effectively enhance mass transfer [22]

Even though this PhD student left the laboratory, thanks to his work on biogas purification, the Chair of Biotechnology has published several articles and patented some of his work. We are now working on transferring this technology to the industrial sector, as it would be an economically viable solution for small scale biomethane production. This is especially true for less than 100 livestock units farms that cannot afford water scrubbing tower, for example. In addition to that, we are currently supervising a PhD student (Sayali Chavan) working on the application of this technology to syngas.

2.2 Simulation and visualization

The modeling work I underwent is to be presented in the coming sections. Beforehand, I would like to mention the simulation and visualization tools I use to lead it.

The simulation approach depends mainly on the geometry the model is to be simulated on. As much as possible, I try to simplify computational domains. This can be done by drawing assumptions, e.g. a perfectly stirred reactor can be considered as 0D, or taking advantages of symmetry plans and axis. Depending on the resulting case geometry, I choose either OpenFOAM or a homemade code.

OpenFOAM is a C++ CFD framework that is very versatile. Its main advantages are: being open-source and already well-developed and being able to handle complex 3D geometries. I use it when the computational domain cannot be reduced to at least transient 1D. When dealing with a 1D case, I implement the model under Python, a high level programming language. The computational power delivered by this language is hindered by its user-friendliness. When I need a high amount of power, I rely on C++. Yet whenever the code architecture allows it, I use hybrid Python-C++ codes. In these cases, the codes bottlenecks are coded in C++ while input/output and thread management can be efficiently handle by Python.

Regarding numerical methods, I use an incremental approach. I start with first order centred explicit schemes most of the time. Then, according to the needs, I turn towards more complex methods. When facing time integration instability, I prefer to switch to implicit schemes than to increase grid refinement, as it is more efficient in terms of computational power. The same is true for spatial schemes. When higher accuracy is needed, I rely on second order schemes, or when fronts are to be transported, I use off-centred or limited schemes.

Disregarding the implementation and numerical methods, the simulation process always follows the same methodology. First, the model is implemented. A very basic test case is used to troubleshoot the problems arising from implementation. Then, numerical parameters (e.g. grid and time step) convergence is carried out. Afterwards, the model predictions are compared to analytical solution in specific case. Once the model has passed all of those safeguards, it can be run to produce results.

The next step is the visualization of the results. The tools I use are common among the community and I am only an end-user of them. In the case of complex geometries, I rely on Paraview, an open-source visualization dedicated software. Even though those visualizations are useful to have an overview of complex systems, they are rarely quantitative. Quantitative results (2D maps, cut lines, point time evolution) are processed and visualized using Python modules: Numpy for results processing and Matplotlib for graph drawing.

2.3 Understanding

Chemical engineering aims at transforming matter and energy with the help of human controlled physical and chemical phenomena. Hence the knowledge of these phenomena and their couplings is key. In this context, modeling can be a valuable tool when building the basic blocks of knowledge surrounding a new process.

By joining individual description of the building blocks of a process, one can construct a sophisticated model that will allow the prediction of complex behavior and even to bring to light new ones. When such a model is delivering good agreement with experiments, it can be used to assess for the different contribution of each physical phenomena to the resulting system. This will be illustrated with the two first examples. In more dire cases, the sole fact of being able to reproduce faithfully experimental observations is the validation of a foreseen explanation. This second way of getting better understanding from modeling will be our last example.

2.3.1 Solar char gasification

During my PhD, the question of the interaction between concentrated radiative heat flux (higher than 1 MW/m^2) and lignocellulosic biomass arose. Indeed, the potential interactions between those two substrates could be numerous as they encompass heat and mass transfer, phase change, biomass thermochemical degradation. Figure 2.5 presents a schematic view of the foreseen phenomena.

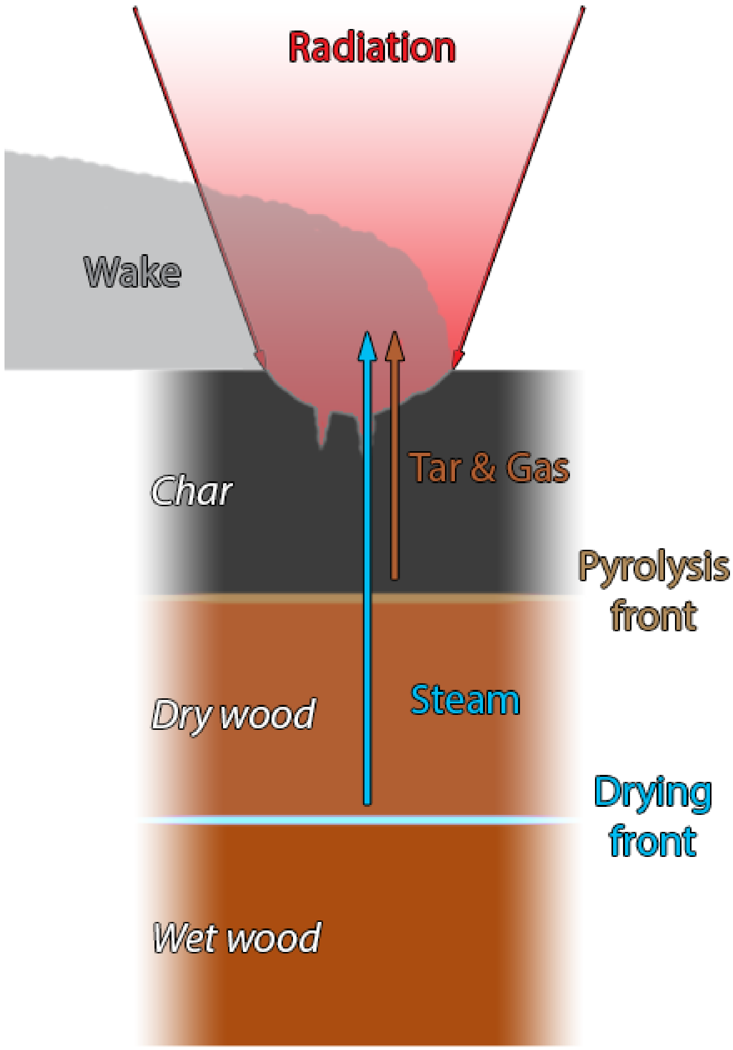
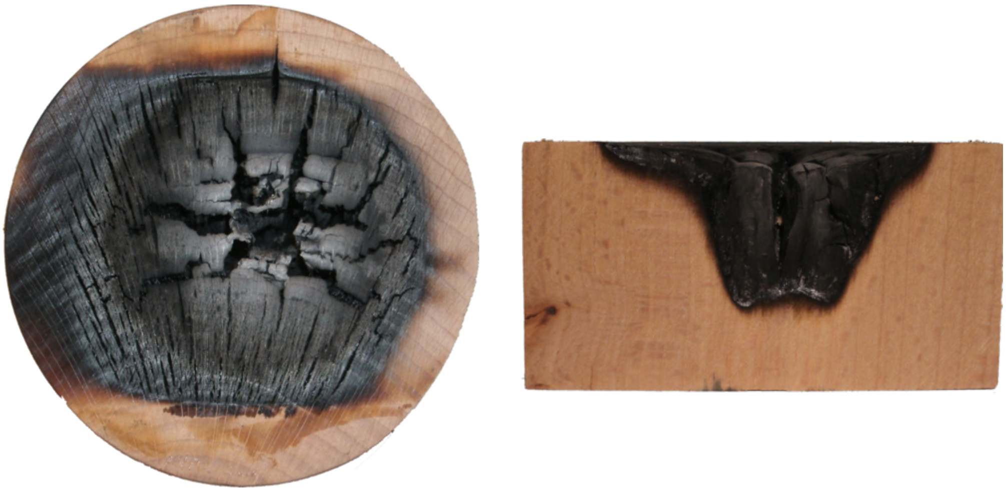


FIGURE 2.5: Schematic representation of the phenomena at stake during biomass radiative pyrolysis

The investigations started with experiments. I exposed cylinders (10 cm diameter, 5 cm high) of beech wood to concentrated radiative heat flux. As a result, pyrolysis of the wood occurred. Yet a particular phenomena was brought to light: a char crater was formed at the center of the samples where the high heat flux reached the sample. Figure 2.6 shows this crater from top and cut views. This crater was filled with char rods for low initial moisture content wood while it was empty for high initial moisture content samples. Given the levels of temperature reached, char steam gasification was a possible explanation, yet the magnitude of its contribution remained to be assessed. Indeed, flash pyrolysis is known to yield only very little amount of char, in addition, even for dried samples, water originating from pyrolysis could contribute to char gasification. Modeling was used to uncorrelate those phenomena and answer these questions [23].



(A) Top view (B) Cut view

FIGURE 2.6: Beech wood sample after 5 min exposure, orientation with the grain, initial moisture content 9 %wb, total radiative power: 655 W, peak heat flux: 1335 kW/m^2

2.3.1.1 Phenomena at stake

In these biomass pyro-gasification experiments, several phenomena occur. Dimensionless number analysis revealed that given the thermally thick configuration, drying, pyrolysis and gasification took place at the same time inside of the sample. These transformations release gaseous reactive species that move throughout the medium (Fig. 2.5). In addition, they have an impact on the medium temperature, which in turn has an impact on reaction rates. This configuration leads to numerous potential couplings. The individual phenomena and their associated components are:

- incident radiative heat flux: heat flux distribution (see Sec. 2.4.2), radiation interaction with the flue gas, radiation penetration into the medium,
- heat and mass transfer inside of the sample: conductive, convective and radiative heat transfer as well as mass convection and diffusion,
- heat and mass transfer outside of the sample: convective heat and mass transfer,
- thermochemical conversion: wood pyrolysis, tar thermal cracking, tar steam reforming, char gasification,

- phase change: drying,
- geometry modification: wood shrinkage, char rod formation, char consumption by gasification.

Among the listed phenomena, tar steam reforming was not taken into account. Indeed, no kinetic model of intra-particular tar steam reforming was available. In addition, wood shrinkage resulting from drying or pyrolysis was not taken into account as it is of negligeable magnitude in this particular case [24, 25]. All the remaining physical phenomena were taken into account in the model.

2.3.1.2 Mathematical model

Taking into account the aforementioned physical phenomena led to a complex model whose key equations are detailed hereinafter. The first ones are the mass balances for both solid (Eq. 2.1) and gaseous (Eq. 2.2) phases, which account for source and sink terms coming from chemistry (ω_K) as well as anisotropic convective and diffusive transport:

$$\frac{\partial \rho_J}{\partial t} = \sum_{K=1}^{O} \nu_{J,K}\omega_K \tag{2.1}$$

$$\frac{\partial \zeta \rho_g Y_I}{\partial t} + \nabla.(\rho_g \vec{u_g} Y_I) = -\nabla.(-\rho_g \boldsymbol{D_s} \boldsymbol{q_g} \nabla Y_I) + \sum_{K=1}^{O} \nu_{I,K}\omega_K \tag{2.2}$$

Then, by combining these equations, mass conservation, ideal gas assumption and Darcy's law, momentum conservation for the gaseous phase can be written:

$$\frac{\zeta M_g}{\Re T}\frac{\partial P}{\partial t} - \nabla.(\rho_g \frac{\boldsymbol{\kappa_g} \boldsymbol{q_g}}{\zeta \mu_g}(\nabla P - \rho_g \vec{g})) = \sum_{K=1}^{O} \omega_K \tag{2.3}$$

The heat balance is the last key equation (Eq. 2.4). It features, in order of appearance, thermal inertia, heat transport resulting from liquid water motion, heat transport resulting from gaseous motion, heat conduction, heat release and consumption from chemical reactions and phase changes, heat transport resulting from gaseous diffusion, heat transport resulting from bounded water diffusion and radiation penetration into the porous medium (described using volumetric approach):

$$\begin{gathered}(c_{p_s}\rho_s + \zeta c_{p_g}\rho_g + c_{p_{lw}}(\rho_{lw} + \rho_{bw}))\frac{\partial T}{\partial t} + c_{p_{lw}}\rho_{lw}\nabla.(\vec{u_{lw}}T) + c_{p_g}\rho_g\nabla.(\vec{u_g}T) = \\ -\nabla.(-\boldsymbol{\lambda_{eff}}\nabla T) + \sum_{K=1}^{O}\omega_K \Delta h_K + \sum_{I=1}^{N} c_{p_g}\rho_g \boldsymbol{D_s}\boldsymbol{q_g}\Delta Y_I + c_{p_{lw}}\boldsymbol{D_{bw}}\Delta\rho_{bw} + Q_{pen}\end{gathered} \tag{2.4}$$

Wood anisotropy is taken into account through tensors such as $\boldsymbol{D_s}$ for gas diffusivity, $\boldsymbol{\kappa_g}$ for permeability or $\boldsymbol{\lambda_{eff}}$ for heat conduction. While the presence liquid water into the pores is described using $\boldsymbol{q_g}$, the relative permeability tensor, a function of liquid water density field. The presented equations were implemented in an OpenFOAM homemade code where the 11 scalar and 2 vector variables were solved.

Taking advantage of the fact that during experiments the wood fibers were aligned vertically and assuming radial and azimuthal directions of the material have similar physical properties, the case setup can be drawn as axysymmetrical. Figure 2.7 presents this case setup with key initial and boundary conditions.

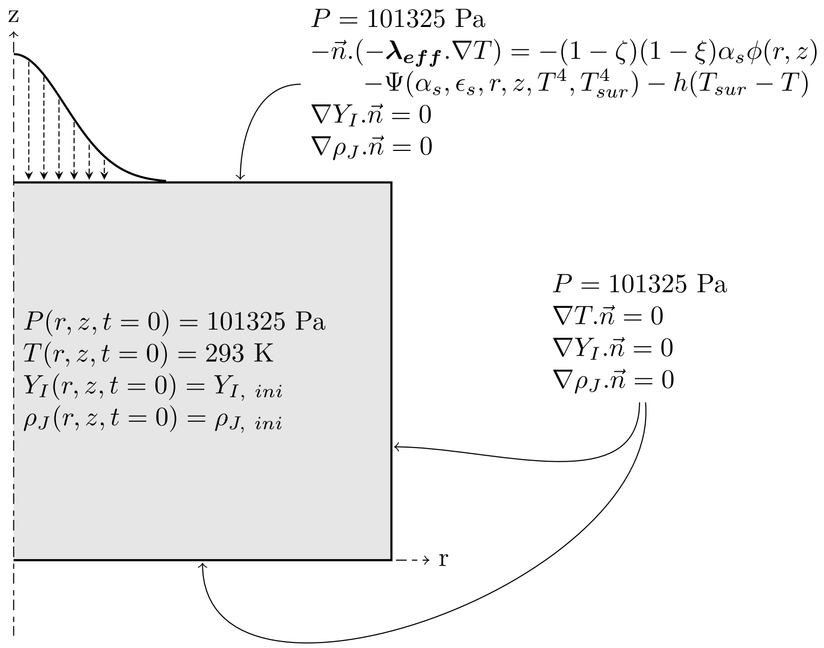


FIGURE 2.7: Computational domain and associated boundary and initial conditions. $\Psi(\alpha_s, \epsilon_s, r, z, T^4, T_{sur}^4)$ being a view factor of the char crater with itself

A first validation against experimental results was carried out by comparing qualitatively crater shapes. Figure 2.8 presents cuts views of both experimental and numerical samples after 5 minutes exposure to concentrated radiative heat flux. For the three initial moisture contents, the predicted char fields are coherent and in agreement with experimental observations in terms of char layer thickness and position.

More quantitatively, the different product yields for different initial moisture contents (0, 9 and 55 %wb) were also confronted (Fig. 2.9). Model results are in close agreement with experimental observations for wood consumption and char production for the three different initial moisture contents. The model underpredicts gas production while overpredicting tar yield. This was explained by the fact that tar cracking could occur experimentally in the hot gas stream escaping the sample, before reaching the measurement point. This phenomenon not being implemented, the model cannot properly account for it. Finally, water consumption is consistently under predicted by the model. This could be explained by the simplistic boundary condition (free escape) that was used on the steam field.

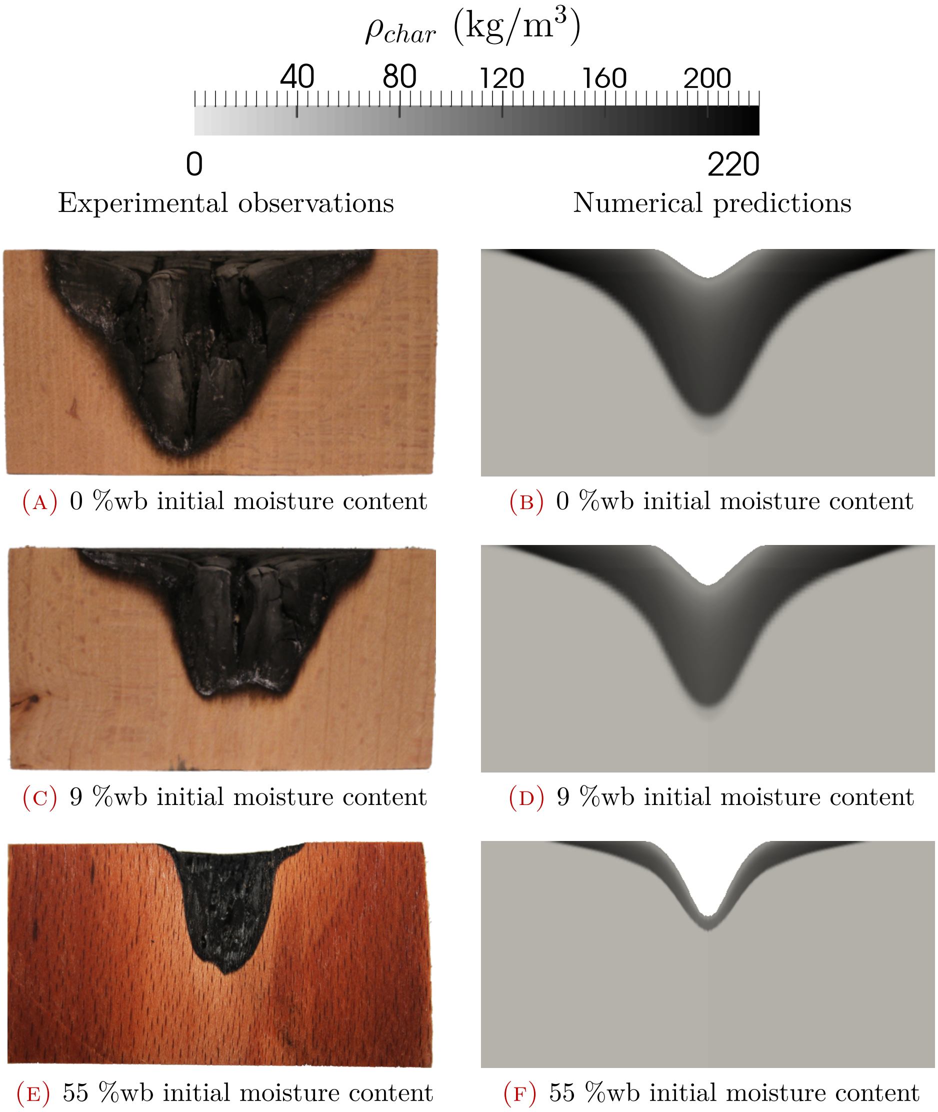


FIGURE 2.8: Experimental and numerical crater cut views after 5 minutes exposure. Colormap: char density

Once confident in the model predictions, it was used to get insights about the couplings occurring in the sample.

2.3.1.3 Monitoring char production and gasification

First of all, using the model, it is possible to track char production and disappearance over time. Something only possible with modeling is to account for the exact amount of produced char by creating a dummy species that would not undergo gasification. This first step revealed that on the upper part of the sample, where the heating rate is at its maximum, char production is minimal, but not critically low (porosity lower than 0.975). Hence, heating alone was not responsible for medium ablation. Yet given the small amount of char produced, a very low amount of steam should be enough to induce an important sample deformation through gasification. This could

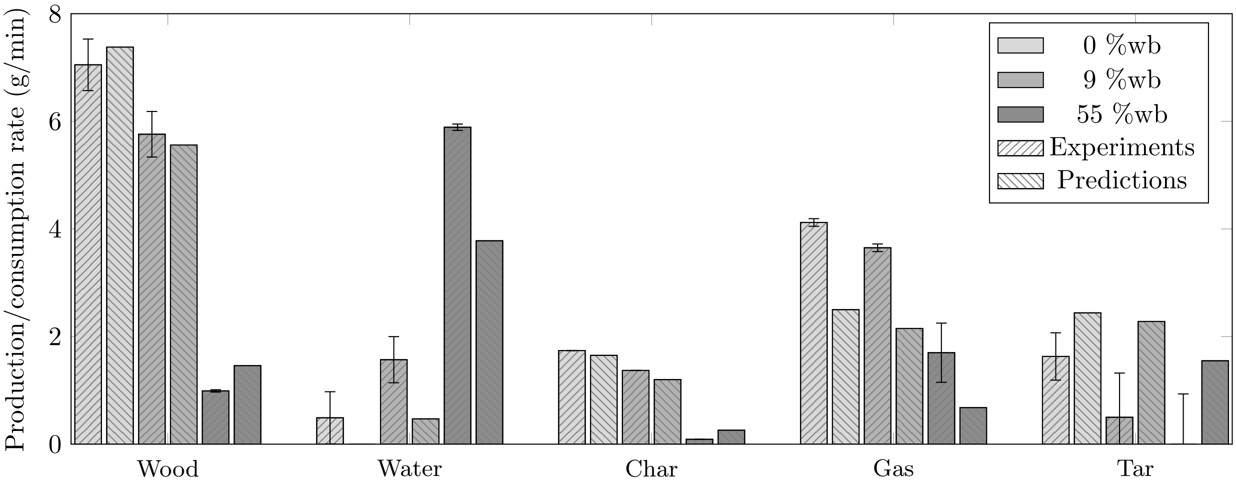


FIGURE 2.9: Experimental and numerical time averaged production/consumption rates over 5 minutes exposure

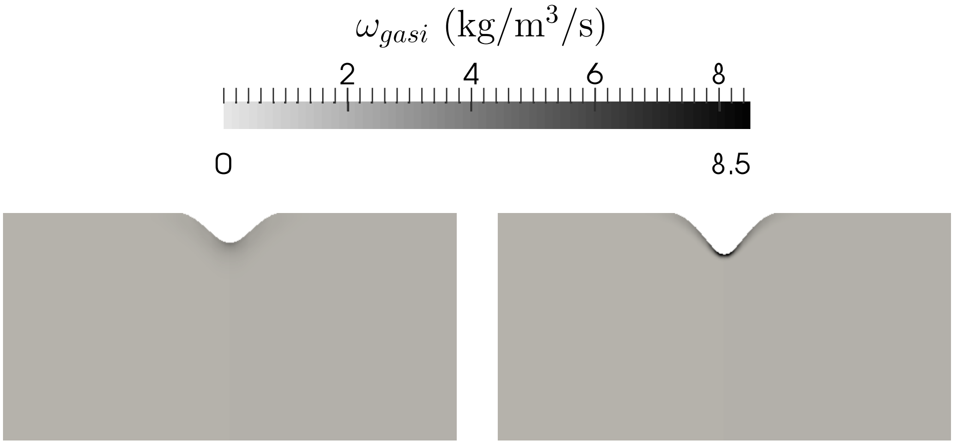
be confirmed by monitoring water under all of its forms. It turned out that the sum of free water, bounded water and pyrolysis water could be sufficient to release enough steam to gasify part of the sample, provided this steam encounters char at a high enough temperature.

Once the coupling had been understood, a second step was to dissect it further and explain why in 9 %wb initial moisture samples were exhibiting char rods, while 55 %wb samples had none. Numerically it is easy to assess the extend of phenomena almost impossible to quantify experimentally, in this case the local intensity of gasification reactions. Figure 2.10 reports gasification reaction rates for both 9 and 55 %wb initial moisture content samples. Char steam gasification was much more intense for high initial moisture content samples, with a maximum rate of 8.5 kg/m^3/s, while it peaks at 2.5 kg/m^3/s for 9 %wb initial moisture content samples. With the combined knowledge of steam, char and temperature fields inside of the sample, this procedure allowed to find out the underlying mechanisms. For high initial moisture content samples, char rods gasification is limited by heat supply, as gasification endothermicity limits sample upper boundary temperature. Thus all the char is consumed and excess steam escapes the sample. For low initial moisture content samples, gasification is limited by water availability, hence not fully gasified char is left to stand.

In the context of this PhD thesis, modeling allowed to weight the contributions of individual phenomena to the behavior of the system as a whole. It delivered explanation of the observed differences between high and low initial moisture content samples.

2.3.2 Shape of smoldering fronts

During my PhD, I also tackled another challenge involving heat and mass transfer in reactive porous media: the description of the evolution of a smoldering front in a



(A) 9 %wb initial moisture content (B) 55 %wb initial moisture content

FIGURE 2.10: Gasification reaction rate fields for 9 and 55 %wb initial moisture content cases, after 2 minutes and 30 seconds. Colormap: gasification reaction rate

cylindrical packed bed made of low carbon content porous alumina spheres. Smoldering is a process in which a combustion wave propagates through a porous medium. It is involved in many situations appearing both naturally and in man-controlled processes. Energy applications [26, 27] but also environment science [28, 29] and forest management [30, 31] are classical areas of application. Its control remains a challenge and labscale studies are still required to get a firmer grasps at this phenomenon.

In this context Mines Albi developed an experimental apparatus (Fig. 2.11) made of a fully instrumented cylindrical shape packed bed surrounded by insulation. The bed is filled with low carbon content alumina porous spheres and vented with air. Ignition starts at the top of the bed and a combustion front travels downwards being monitored by thermocouples and gas analyzers.

Over the course of the experimental run, a bending of the combustion front was observed near the walls of the bed. Yet this bending was case dependent. Understanding why a front is not flat is interesting for man-controlled applications because it underlies the front stability question. Assumptions were drawn regarding its origin. Wall heat losses induce a cooling of the gas, lowering its viscosity hence driving the gas towards from the walls. Furthermore, gas density is also increased leading to a higher supply of oxygen, the limiting reactant, favoring a higher front velocity at the walls. Finally packing near the wall would have been a possible explanation. Yet this last possibility was discarded because of its low magnitude compared to the bending amplitude. The two remaingin mechanisms were in favor of a faster front near the walls, which is not always the case. Modeling was used to investigate [32].

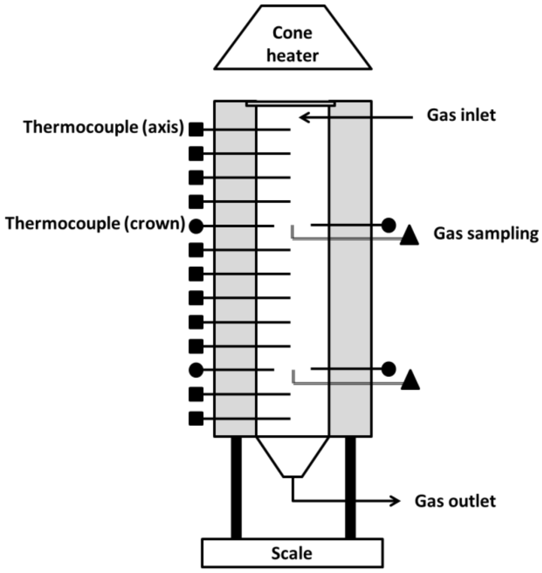


FIGURE 2.11: Schematic of the experimental apparatus [33]. Bed diameter: 9.1 cm, bed height: 60 cm. The smoldering front traveling from top to bottom

2.3.2.1 Reactor modeling

In order to model the smoldering reactor, it was divided into two parts: the reaction medium and the surrounding insulating material. The reacting porous medium was described as a homogeneous domain governed by mass (Eq. 2.5, for gas), heat (Eq. 2.6 for solid, and Eq. 2.7 for gas) and momentum (Eq. 2.8, $\boldsymbol{D_k^*}$ accounting for dispersion effects) conservation laws. Properly describing carbon oxidation (ω) in porous media is a challenging task [34–37]. In this case, we relied on an imperfect Arrhenius law equation. Even though limited, it allowed to account for the thermal dependence of the oxidation reactions.

$$\frac{\zeta\rho_g\partial Y_I}{\partial t} + \nabla.(\rho_g\vec{u_g}Y_k) = \nabla.(\zeta\rho_g\boldsymbol{D_k^*}\nabla Y_I) + \omega_K \tag{2.5}$$

$$\frac{\partial(1-\zeta)\rho_s c_{p_s}T_s}{\partial t} = -\nabla.(-(1-\zeta)\boldsymbol{\lambda_s}\nabla T_s) + HS(T_g - T_s) + \alpha\Pi\omega \tag{2.6}$$

$$\frac{\partial\zeta\rho_g c_{p_g}T_g}{\partial t} + \rho_g c_{p_g}\nabla.(\vec{u_g}T_g) = -\nabla.(-\zeta\boldsymbol{\lambda_g}\nabla T_g) - HS(T_g - T_s) + (1-\alpha)\Pi\omega \tag{2.7}$$

$$\frac{\partial\frac{\zeta M_g}{\Re T_g}P}{\partial t} - \nabla.(\rho_g\frac{\kappa}{(1+\gamma\sqrt{Re_p})\zeta\mu_g}\nabla(P - \rho_g\vec{g})) = \omega \tag{2.8}$$

The insulating shell was ruled by a heat transport equation.

$$\frac{\partial\rho_i c_{p_i}T_i}{\partial t} = -\nabla.(-\lambda_i\nabla T_i) \tag{2.9}$$

The coupling between the reacting region and the insulating shell was modeled as a perfect contact ($T_s = T_i$ and $-\lambda_s \nabla T_s = -\lambda_i \nabla T_i$ on the surface between reacting medium and the insulating material).

The case setup was taken as a 2D transient axisymmetrical case (Fig. 2.12). A special care was taken in choosing the boundary conditions which best described experimental operating conditions in order to faithfully reproduce heat losses. Given the wide range of temperatures across the reactor, physical properties dependencies over temperature were taken into account. Finally, gas phase was described as an ideal gas and ideal mixture.

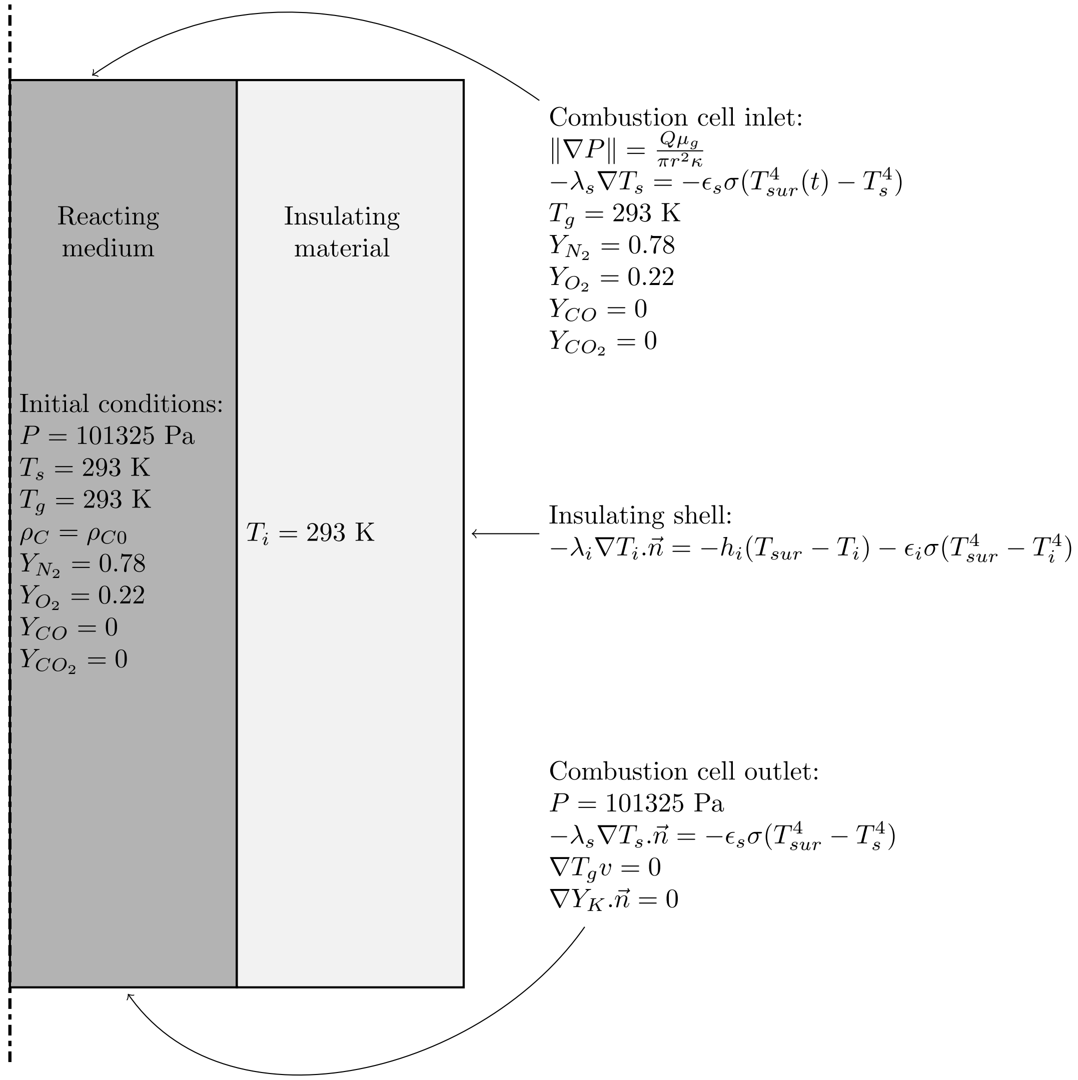


FIGURE 2.12: Numerical domain schematic with boundary conditions

All in all, the model featured 7 scalar and 1 vector variables. It was implemented under OpenFOAM and validated against five experimental configurations, three with different initial carbon contents and three with different air flow rates (one being common to the two sets). The model predictions were in satisfactory agreement with experimental results. Despite the fact that absolute values may not have always been accurately captured by the model, trends were properly reproduced.

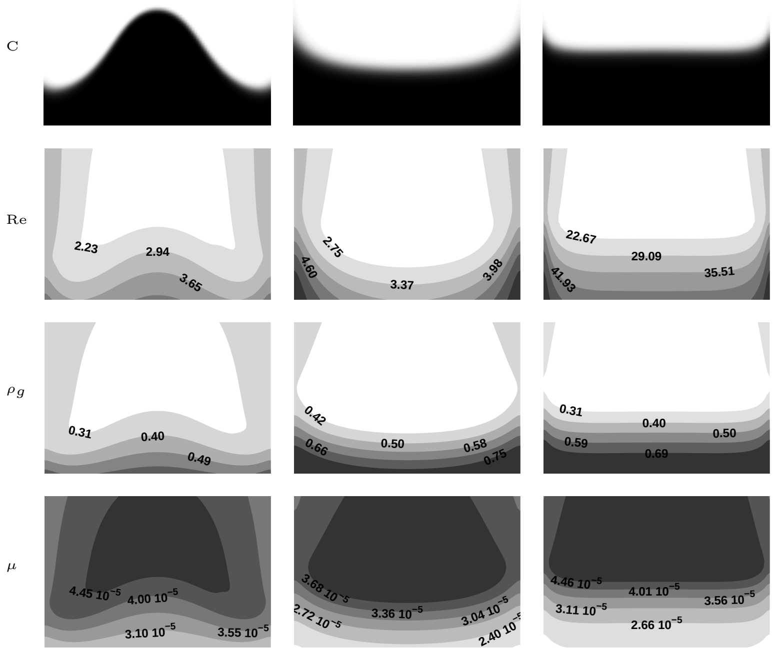


FIGURE 2.13: Different front shapes, viscosity, density and Reynolds number maps observed in the reference case (center), with high carbon content (left) and with high gas velocity (right). Position: 20 cm away from the ignition zone. Color legend: the darker, the higher

2.3.2.2 Front bending near the walls

Figure 2.13 reports the front shapes for three different cases: reference carbon content and velocity, high carbon content and reference velocity, reference carbon content and high velocity. In addition to predicting the carbon front shape (upper row), the model also allows to access gas composition density, viscosity and Reynolds number. As one can see the model was capable to predict different configurations: a stable front curved upward (middle and left column) and an unstable front curved downward (left column).

Analyzing the model results, it turned out that front curvature originated from the coupling between the oxidation reaction rate and the temperature. In the case of high initial carbon content, the front temperature is high, around 1200 °C, allowing to combust the major fraction of inlet oxygen. In this case, oxygen supply is what limits the front progress. Thus the fact that the heat losses drive more oxygen towards the walls favors front wall creeping.

For the lower initial carbon content cases, the front temperature in much lower, around 750 °C. This low temperature leads to the percolation of about 5 % of the supply oxygen thought the front. In this second case, the front progress is limited by the chemical kinetic. Hence the additional supply of oxygen near the wall does not favor its progress. The front is even bend upward because heat losses induce a lower reaction rate. The same can be concluded for the high gas flow rate case, with a much higher oxygen percolation, around 10 %.

In addition to explaining the origin of the front curvature, modeling was used to quantify the relative magnitude of the two effects increasing the front velocity near the walls: higher gas density and lower viscosity. The method used to obtain this information was inhibiting turn by turn density and then viscosity temperature dependence. As a result, the model showed that the higher density at the walls was responsible for three quarters of the front deformation. While the smaller gas viscosity and induced higher local gas velocity were responsible for the remaining quarter.

2.3.3 Mass transfer inside a hollow fibers membrane contactor

As aforementioned, hollow fibers membrane contactors may be an attractive way to purify biogas into biomethane at small scale. Their understanding and packaging into a streamlined gas separation solution could be the key to unlock an important part of France biomethane production potential. This was the work of a former PhD student at the Chair of Biotechnology. His aim was to develop a well-characterized pilot scale unit before upscaling it to on field dimensions. Yet given the complex internal geometry of contactor (Fig. 2.4), upscaling is not straightforward. Even though industrial scale modules exhibit similarities with labscale ones, predicting their performances has been shown to be challenging because of the differences of their internal hydrodynamics. Hence the PhD student decided to rely on numerical modeling to lead his upscaling procedure.

Looking for help, he came to me and we teamed up to tackle this challenge. Together we designed a model describing the contactor as an anisotropic porous medium. Both liquid and gas could flow into this contactor and gaseous species were capable of going from the gas phase into the liquid phase (or vice versa). Our first step was to validate the model in a configuration where the gas was pure carbon dioxide. Indeed it allows to neglect gas phase and membrane mass transfer resistances. After fitting the parameters of a correlation linking local Sherwood, Reynolds and Schmidt numbers, the model yielded predictions in close agreement with experiments [38].

The next step was to tackle gas mixture (methane and carbon dioxide) separation using this model. It turned out to be far more complicated than expected [39].

2.3.3.1 Conventional models and their limits

When aiming at describing binary gas mixture absorption, we relied on two elements: our model working well with pure gas and guidance from literature. Other authors classically used the same methodology, obtaining mixed results.

Given the long operation duration and the experimentally reported briefness of the transient state, the model was derived in steady state. It features mass balance for carbon dioxide and methane (dummy variable A in the following equations), in liquid (Eq. 2.10) and gas (Eq. 2.11). The last term of those equations is the mass exchange term between liquid and gas phases. The contactor is considered to be a porous medium, thus gas and liquid velocities are computed using Darcy's law (Re < 1). Gas phase momentum equation is the combination of mass continuity, Darcy's law and ideal gas assumption. In addition, given the orientation of fibers, the medium properties are anisotropic and taken into account via tensor of permeability and diffusivity.

$$\nabla.(\vec{u_l}C_A^l) = \frac{\zeta_l}{\tau_l}\boldsymbol{D_A^l}\Delta C_A^l + j_{A,tot}a(\mathcal{H}_A C_{tot}^g y_A - C_A^l) \tag{2.10}$$

$$\nabla.(\vec{u_g}C_{tot}^g y_A) = \frac{\zeta_g}{\tau_g}\boldsymbol{D_A^g}\Delta C_{tot}^g y_A - j_{A,tot}a(\mathcal{H}_A c_{tot}^g y_A - C_A^l) \tag{2.11}$$

Figure 2.14 provides a view of the geometry and the case setup. The particularity of this code is the use of different meshes for liquid and gas phases as the central baffle deflect liquid while it is crossed by hollow fibers, hence gas flow.

The key parameter in this model is the mass transfer coefficient from gas to liquid ($j_{A,tot}$). Using a resistance in series approach it encompasses gas phase, membrane and liquid phase resistance contribution (Eq. 2.12). The more challenging term being the contribution of the membrane ($j_{A,mem}$). Literature pointed out that given the small diameter of the pores of the fibers (around 30 nm) part of the diffusion may occur in the Knudsen regime (Kn = 0.34, for CO_2). As a consequence, they advise to correct mass transfer coefficient across the membrane in the following manner (Eq. 2.13):

$$\frac{1}{j_{A,tot}d_{fi,out}} = \frac{1}{j_{lw}d_{fi,out}} + \frac{\mathcal{H}_A}{j_{A,mem}l_{mem}} + \frac{\mathcal{H}_A}{j_g d_{fi,inn}} \tag{2.12}$$

$$j_{A,mem} = \frac{\zeta_{mem}}{\tau_{mem}l_{mem}}\left(\frac{1}{D_{AB}} + \frac{1}{D_{A,Kn}}\right)^{-1} \tag{2.13}$$

Where ζ_{mem} is the membrane porosity, τ_{mem} its tortuosity and l_{mem} its thickness.

We implemented this correction and ran the model in order to compare its predictions to data the PhD student had produced over different operating conditions (varying liquid and gas flow rates as well as gas composition). Sadly the model predictions were far from experimental observations (Fig. 2.15). Both in terms of

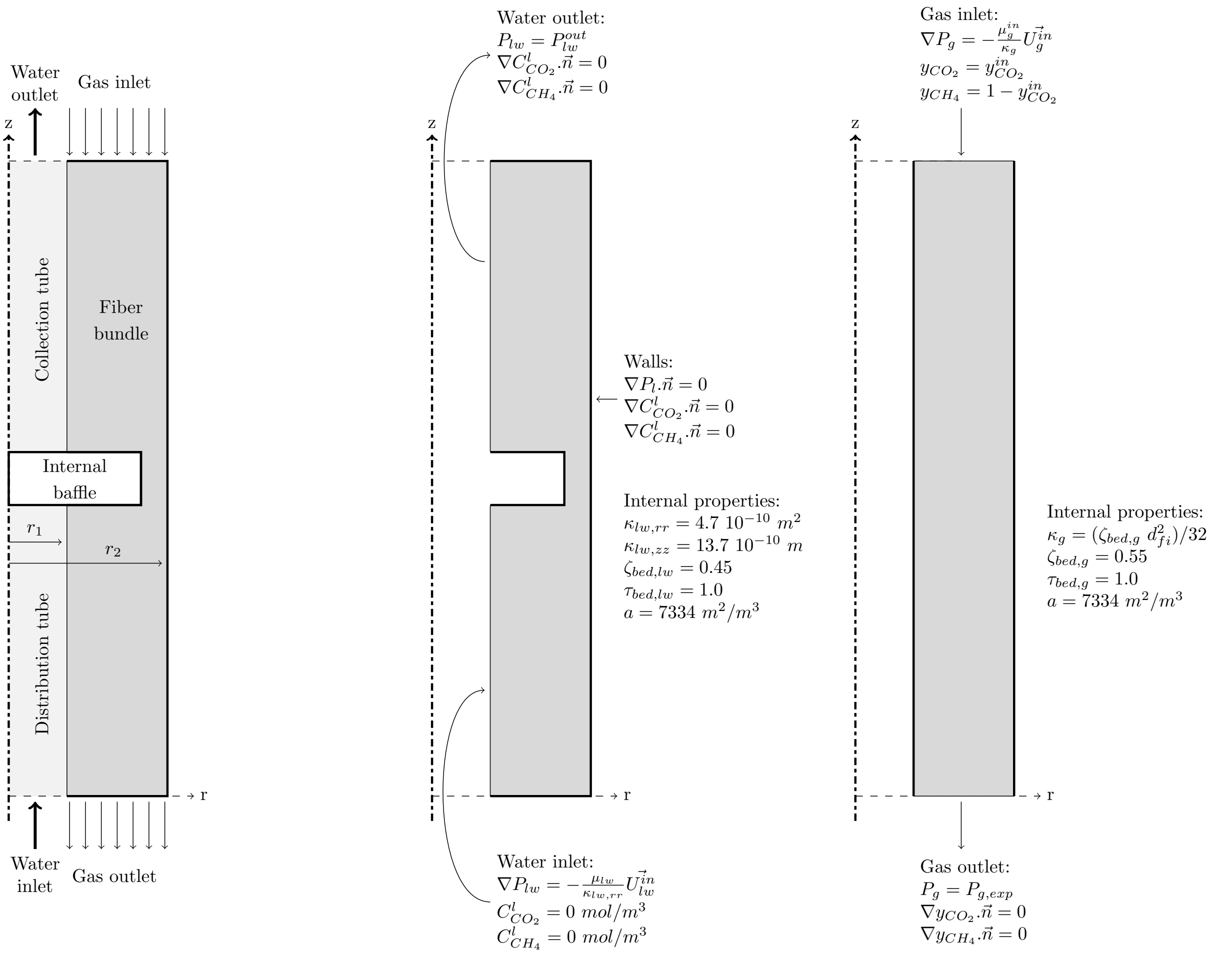


FIGURE 2.14: From left to right, schematic of the inner geometry of a hollow fibers membrane contactor, liquid phase setup, gas phase setup

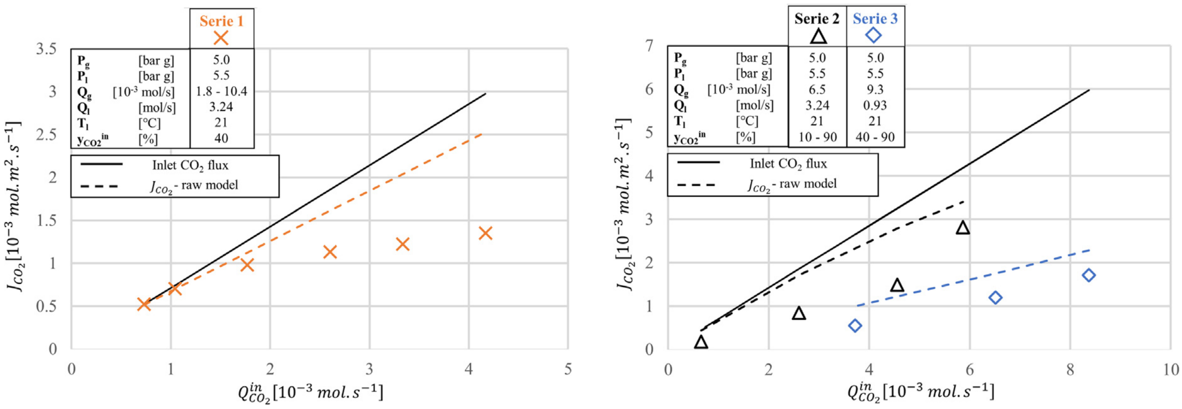
trends and absolute values, the model failed to reproduce experimental data.

As a consequence, we carefully checked the model numerous times. Everything seemed well implemented. Diving further into the problem and tuning the model, we were able to identify that discrepancies originated from membrane mass transfer coefficient.

2.3.3.2 Mass transfer in rarefied gas

Despite this misadventure and the student departure, we were still keen on understanding the phenomena at stake in the membrane. Thus we led several attempts to enhance mass transfer description: accounting for hypothetical pressure effect on diffusion in binary mixture, describing a potential viscous component of the flow inside the membrane, ... None of them worked, meaning that the proposed phenomena were not valid explanations.

Finally, we decided to go back to the fundamental of binary mixture diffusion



(A) Varying gas inlet flow rate

(B) Varying gas composition pour two different gas flow rates

FIGURE 2.15: Absorbed CO_2 flux versus inlet CO_2 flux. Model predictions versus experimental observations. Marks: experiments, dashed line: model predictions, solid line: first bisector. Credit: Valentin Fougerit

in transition regime (0.01 < Kn < 1) [40]. We luckily found an article deriving the equations governing this phenomenon [41]. From this article, we were able to obtain a proper way to describe the diffusion into the membrane of the contactor. As we had guessed, the governing equation indeed features a dependence on gas composition, molecular and Knudsen diffusivities (Eq. 2.14):

$$\vec{N_A} = y_A \frac{D_{A,Kn}}{D_{A,Kn} + \frac{\zeta_{mem}}{\tau_{mem}} D_{AB}} (\vec{N_A} + \vec{N_B}) - (\frac{1}{\frac{\zeta_{mem}}{\tau_{mem}} D_{AB}} + \frac{1}{D_{A,Kn}})^{-1} C_{tot}^{g} \nabla y_A \quad (2.14)$$

Which lead to Eq. 2.15 after integration with $\beta = \sqrt{M_A/M_B}$.

$$\|N_{A,mem}^{\rightarrow}\| = \frac{\frac{\zeta_{mem}}{\tau_{mem}} D_{AB} C_g^{tot}}{(1+\beta) l_{mem}} ln(\frac{1 - y_A^{out}(1+\beta) + \frac{\zeta_{mem}}{\tau_{mem}} D_{AB}/D_{Kn,A}}{1 - y_A^{in}(1+\beta) + \frac{\zeta_{mem}}{\tau_{mem}} D_{AB}/D_{Kn,A}}) \quad (2.15)$$

The next step was to implement this equation and run the code again. The predictions of this improved version of the model were compared to the experimental data (Fig. 2.16). This time model properly predicted experimental results. Both trends and values were captured. To achieve this, no tuning parameter was used, only the relevant physical and geometrical properties at stake in the system. The quality of the agreement was a token of the fact the phenomenon underlying the chosen model was the one dominating mass transfer across the membrane. Hence from building this model, further understanding of the working principle of the hollow fibers membrane contactor was derived.

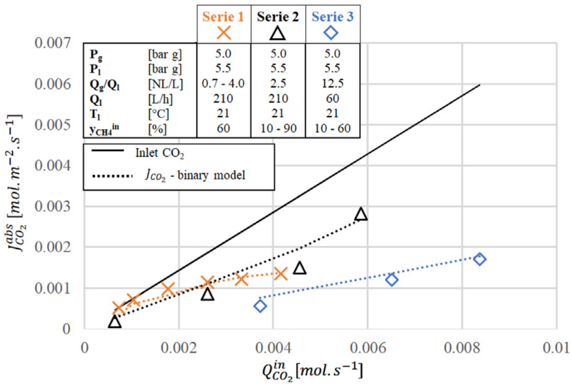


FIGURE 2.16: Absorbed CO_2 flux versus inlet CO_2 flux. Model predictions versus experimental observations with improved mass flux description across the membrane. Marks: experiments, dashed line: model predictions, solid line: first bisector. Credit: Valentin Fougerit

2.3.4 Closing thoughts

These three works presented how modeling can be used to develop a better understanding of coupled phenomena. With this tool, it is possible to better envision for the role of each component that comes into action in a complex system. There are two main ways of deriving insights. The first one is by relying on a thoroughly validated model. Being highly confident that the proper physical phenomena are described, the model can dive into the intimacy of their interaction and help to better understand them.

The second way is more of a trial and error process. While building a model some phenomena are accounted for, others discarded. For a model to properly reproduce experimental observations, all the phenomena at stake have to be described in a rightful manner. Hence, adding or removing a part of a model allows to weight the contribution of the phenomenon it is associated to, ultimately pointing out the most relevant ones.

2.4 Characterizing

After deriving a proper understanding of the phenomena of interest, their simulation requires well-characterized sets of parameters and boundary conditions. Sometimes physical parameters are very difficult, or even impossible, to measure using direct methods. It can be because of their too low or too high values, or because of their correlation with numerous interfering phenomena. In these few cases modeling can be a way to access these parameters indirectly. Depending on the situation, two wide kinds of approach may be available. Either one reproduces the system numerically and computes the properties of interested from known boundary conditions, this will be our first example. Or one feeds the model with experimental data and uses it to decorrelate each phenomena yielding the value of the parameter of interest. Inverse methods will be our two other examples.

2.4.1 Wood chips bed permeability

Biomass thermochemical conversion, like other fields of chemical engineering, heavily relies on packed bed reactors. Most of the time, these beds are made of particles poured into a container which is then crossed by a temperature controlled flow. It is widely admitted that the hydrodynamic properties - permeability, tortuosity, dispersion coefficients, ... - of such devices are key to properly operate them [42–47]. Yet they can be quite hard to determine. Among them, permeability is of note as it directly influences the pressure drop across the bed, hence the pumping cost.

2.4.1.1 Obtaining permeability

Three different approaches are available to determine this parameter. The first one is to use correlations coming from the literature such as Ergun [48] or Kozeny-Carman expression [49]. These semi-empirical correlations are widespread. They were derived, most of the time, for packed bed made of monodisperse spheres. Even though, they can present refinements taking into account media made of non-spherical particles, polydispersed media or inertial effects, they usually only yield an estimation of the permeability.

The second method consists in experimentally measuring the permeability value. Yet these measurements are not always easily conducted. Indeed, the flow has to reach steady state, which may take a tremendous amount of time for almost not permeable media, such as rocks [50] or tropical wood species [51]. The other extreme is very permeable media, that would induce only a minor pressure drop. This is the case for industrial scale wood chips packed beds. In this case, the experimental apparatus has to be long enough so that a pressure drop can be precisely measured. Another technique is to use liquids instead of gases [52], as they have a higher viscosity. The drawback is that liquids are less convenient to use than gas mainly because it is very difficult to ensure full saturation of the sample and to avoid degasing during measurement.

A last approach consists in using a numerical tool to compute steady state flows inside of a numerical reproduction of the bed. Such simulations yield pressure drops associated to given flow rates. From them, it is possible to obtain the permeability value, as they are linked by the Darcy's law for low Reynolds numbers (Eq. 2.16).

$$\frac{Q}{S} = \frac{\kappa}{\mu} \frac{\Delta P}{z} \tag{2.16}$$

To successfully lead this approach the bed geometry has to be acquired. An option is to scan the bed. Yet it requires high end apparatus and skilled technician. An alternative is to numerically recreate the bed. In our case, we relied on the numerical generation of the bed using a DEM code, LMGC90 [53, 54]. This code was fed with the geometry of 536 wood chips (measured in 3D with a caliper) that were bootstrapped until 15 000 elements had been generated. The pouring of these thousands of chips was then simulated. This numerical generation procedure was repeated several times in order to acquire different bed morphologies (Fig. 2.17).

FIGURE 2.17: Example of a wood chips bed generated using LMGC90. Tube diameter: 8.0 cm. Number of chips: 15 000. Brown: wood chips, dark gray: tube

The second step is to lead CFD computation inside of the bed in order to acquire the pressure drop for given flow rates. This approach uses conventional CFD tools, in our case OpenFOAM. Even though this is rather basic, difficulty emerges from the need to ensure grid independence and properties convergence. To do so, the numerical parameters allowing for the meshing of the bed geometry have to be screened until having no more effect. Furthermore, to ensure proper representativeness of the obtained value, the procedure was conducted over different beds and at different locations inside of a same bed. Only once completed, it is possible consider that a proper value of the permeability has been computed. A drawback of this approach is that no desktop computer can currently run this case as the required RAM amount is too high. In our case, we relied on ROMEO cluster, from Université Reims Champagne Ardennes

2.4.1.2 Validation & Results

In parallel to the numerical work, experimental validation was undergone. The experimental apparatus developed for permeability measurement was quite simple. Basically, it boils down to a 5.0 meter high, 8.0 cm diameter tube with a grid 5.0 cm above its lower extremity. The tube was filled with wood chips and two pressure sensors were set with a height difference of 4.65 m. The highest height available was chosen as the highest available in order to maximize pressure drop, hence pressure signal. The diameter was chosen in order to minimize wall-particle packing effects. These effects range from up to 2 diameters for spheres [55] to less than 1 diameter for anisotropic solids [56], such as our wood chips. The fraction of cross sectional area impacted by these wall effects is estimated to be lower than 5 %. Air tightness of the tubing was verified before and after the experimental measurements. Furthermore, even under load no deformation of the tube due to bed static pressure was measured.

Pressure drops were measured over flow rates ranging from 1.5 to 15 Nl/min. As a consequence, Reynolds numbers range from 1 to 10. Inertial effects were found to appear for the highest Reynolds numbers. They induced a decrease of the apparent bed permeability. Nevertheless, the measurements over the linear range were repeatable enough to properly determine the value of the bed permeability.

In addition, in order to assess for experimental repeatability, experiments were conducted on two different beds. The tube was unloaded, chips were mixed, then the tube was reloaded. Both beds yielded the same value of permeability: $1.63 \pm 0.04 \times 10^{-8}$ m^2.

Meanwhile, numerical simulations were run for Reynolds number ranging from 10^{-2} to 0.1 (illustration on Fig. 2.18, convergence over 3 beds and 2 positions in one bed reported on Fig. 2.19). The predicted permeability value was $1.89 \pm 0.10 \times 10^{-8}$ m^2. With a deviation of 16.0 % - with reference to the experimental measurements - and a variation coefficient of 5.04 %, this result was close to reality. In addition, it represents a subsequent improvement over Kozeny-Carman estimation - which gave a 115 % deviation -.

Confident in our results, we went one step further and computed pressure drop in the inertial regime. Indeed, most of the time industrial wood chips bed are operated in this flow regime. Simulations with a Reynolds number increasing from 0.1 to 1000 were carried out (Fig. 2.20). Once again, even in the inertial regime, the predicted pressure drop was in agreement with our measurements. Hence, we have been able to compute the parameters for both Ergun and Forshheimer equations - two equations improving the Darcy's law in the sense that they account for inertial effects on the pressure drop.

Taking a step back, we can consider that we produced a numerical worklflow allowing to compute the permeability of a granular packed bed made of non-spherical polydisperse particles. This workflow required only the particle size distribution as input data. This tool allowed to reproduce faithfully experimental measurements and to obtain a parameter challenging to measure because of its low value. In addition, it even permitted to broaden investigation range by exploring otherwise inaccessible experimental conditions.

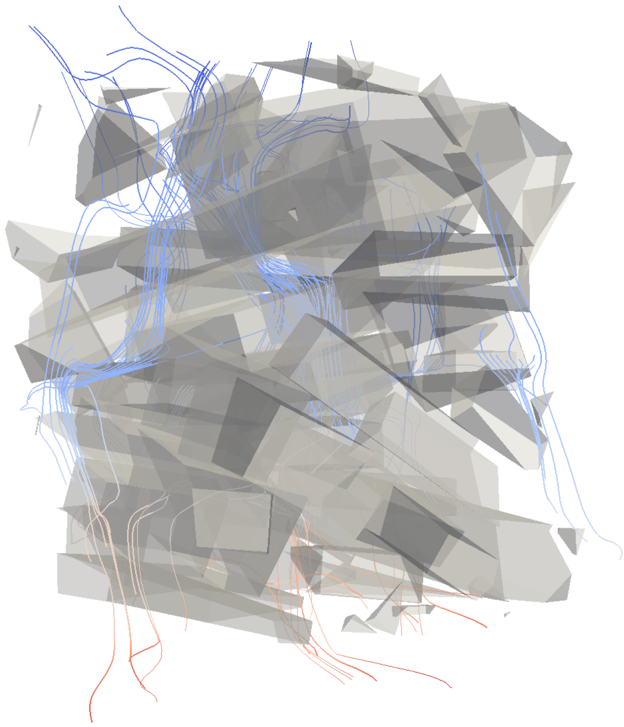


Figure 2.18: Upright flow visualization. Reynolds number of 0.1. Domain size: 12 averaged sphere equivalent diameters of the chips. Translucent gray: wood chips, colored lines: streamlines colored by pressure field values (seeds, two perpendicular horizontal lines crossing at the center of the sample)

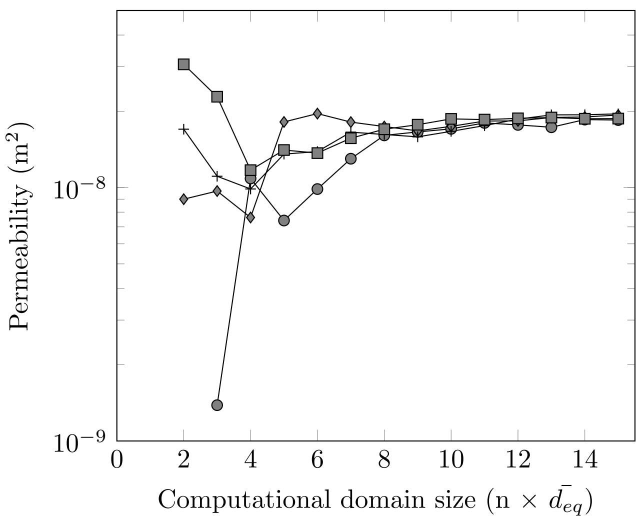


Figure 2.19: Permeability convergence with increasing computational domain size. Squares: bed 1 at position 1, diamonds: bed 1 at position 2, circles: bed 2, crosses: bed 3.

2.4.2 High heat flux mapping

Values too low to be directly obtained have been illustrated above. In the following section, our topic will be to acquire very high parameters value through indirect method.

My PhD topic dealt with concentrated radiative heat flux. In my case, the

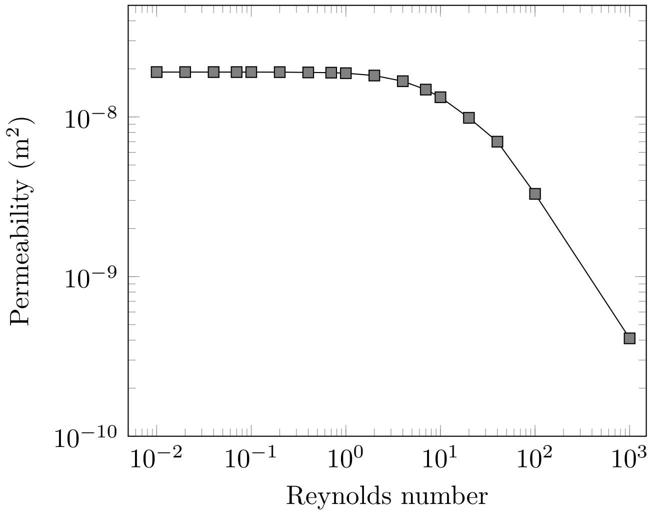


Figure 2.20: Computed effective permeability evolution with increasing Reynolds number

radiation source was a 2 kWe Xenon arc lamp enclosed in a optical system focusing the beams toward a focal spot. As my samples were exposed to this intense heat source, the proper determination of both radiation intensity and spatial distribution at their surface was an important parameter to know.

The problem of high heat flux mapping has been approached using various methods. In some moderate heat flux cases (less than 100 kW/m^2) a radiometer [57] or equivalent [58] is used to map the focal spot. Using this method is time consuming and offers a low spatial resolution map. Yet it yields an absolute value of the incident heat flux and requires no external scaling factor.

In other cases a CCD camera is used to record a grey value image of a water-cooled target [59, 60]. Then using an external measurement, often a radiometer reading, a scaling factor is applied to the recorded image. This method allows for a high resolution but relies entirely on the external scaling factor and the use of a high-end (and incidentally unaffordable) water-cooled target. Still this technique was the only available to measure high intensity heat flux, which could not be withstood by conventional measurement apparatuses.

One last way of mapping the heat flux distribution is to run the device at minimal power, for example using the moon instead of the sun [61]. Pictures can be taken and processed to yield high resolution incident heat flux map. Then, the actual map can be computed using the ratio of the two source powers. Sadly, this is not possible for certain devices such as Xenon arc lamps because their minimal power is very close to their nominal operating condition. As a consequence, we had to develop a new method.

To measure the incident heat flux at the focal we chose to monitor the transient thermal behavior of a thermally thin metal plate of known emissivity using an IR camera (Fig. 2.21). With this approach, we could follow the back face (as the front face reflection would have blinded the camera) temperature rise of the plate until it eventually melt. Sadly, the processing of the IR images sequence is not straightforward. Indeed, the back face temperature is the combination of two effects: the incident heat flux reaching the surface and the lateral heat conduction. These effects were decorrelated using modeling [62].

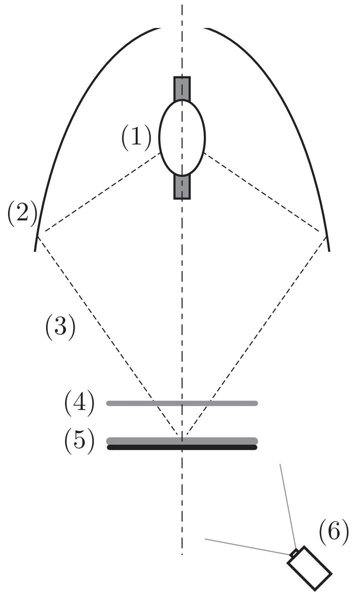


FIGURE 2.21: Image furnace schematic mounted with measurement device. 1: 2 kWe xenon arc lamp, 2: elliptical mirror, 3: a light ray, 4: shutter, 5: screen, 6: camera, black line: paint

2.4.2.1 Modeling the plate thermal response

In order to accurately describe the plate temperature evolution, the model has to account for interception of the incident heat flux, conduction inside of the screen, convective and radiative heat loss on the two faces. In this case, the temperature of the screen is governed by a classic 3D transient heat conduction model (Eq. 2.17):

$$\rho c_p \frac{\partial T}{\partial t} = \lambda \Delta T \tag{2.17}$$

The set of boundary conditions is based on the heat flux continuity. On the upper surface of the plate, incident heat flux, convective and radiative heat losses contribute to the net heat flux (Eq. 2.18):

$$-\lambda \nabla T = -\alpha \phi + h(T - T_{sur}) + \epsilon \sigma (T^4 - T_{sur}^4) \tag{2.18}$$

On the lower surface of the screen, convective and radiative heat losses govern the net heat flux (Eq. 2.19):

$$-\lambda \nabla T = h(T - T_{sur}) + \epsilon\sigma(T^4 - T_{sur}^4) \tag{2.19}$$

In order to simplify this model into a 2D model, we chose a highly conductive material and a very thin plate - 0.8 mm of stainless steel 304L -. This way the plate Biot number fell below 0.1 in its thickness. Thus the 3D model could be turned into a simple 2D model (Eq. 2.20):

$$\rho c_p \frac{\partial T}{\partial t} = -\lambda \Delta T + \frac{\alpha\phi}{l} - \frac{2h}{l}(T - T_{sur}) - \frac{2\epsilon\sigma}{l}(T^4 - T_{sur}^4) \tag{2.20}$$

Knowing the experimental evolution in time and space of the temperature field (T in E. 2.20) and the plate physical properties, it is possible to derive for each and every pixel the incident heat flux (ϕ) and the convective heat transfer coefficient (h).

2.4.2.2 Validation & Results

As always, before being used, the method had to be validated. To do so a plate was positioned 100 cm away from the focal spot. At such a distance, the incident heat flux density is reasonably low so that it can be measured with a Gardon (water cooled) radiometer. On one hand, the plate transient heating was followed by the IR camera, the images were processed and a heat flux map was obtained. On the other hand, the radiometer was positioned at numerous places across the plate so that a reference map could be hand drawn.

The measurements yielded by these two different methods were later compared (Fig. 2.22). As one can see, the model reconstruction captures faithfully both trend and absolute value of the incident heat flux.

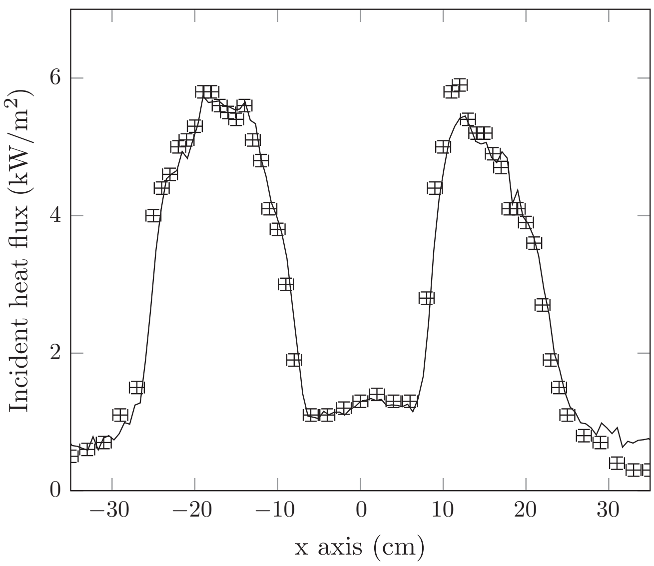


FIGURE 2.22: Heat flux 100 cm away from the focal spot on the x axis. Continuous line: model reconstructed heat flux, crosses with error bars: Gardon radiometer

Two points have to be raised before applying the method to the indirect measurement of high heat flux. First of all, even though the Biot number is below 0.1, it does not mean that the two faces of the screen have the same temperatures. Indeed, this criterion applies to steady state. In our case, a small lag time was induced by heat conduction in the screen thickness. To prevent this bias, the first few pictures recorded by the camera were discarded. Second of all, the Biot number of the two configurations is not the same. Thus we cannot claim to work under the scale-similarity hypothesis. We can only claim to be in the same regime, *i.e.* Biot number below 0.1.

Nonetheless, confident in our method, we have applied it the determination of the heat flux map at the focal spot. Figure 2.23 reports the 2D heat flux map yielded by the model. The spatial distribution has a maximum of 1335 kW/m^2 and a half width diameter of about 3 cm. Cuts along x and y axis both exhibit a very similar Gaussian shapes, which is congruent with literature [57, 59, 60].

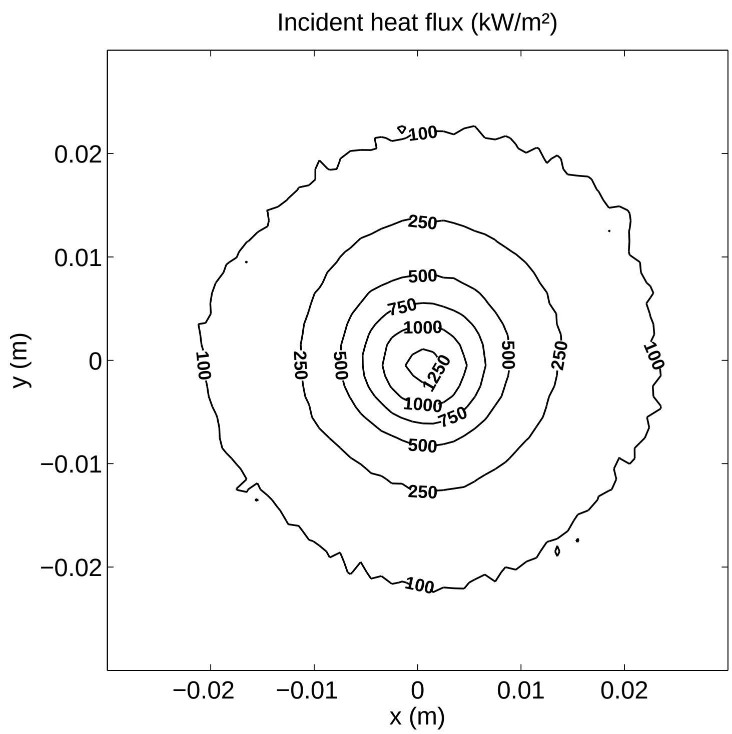


FIGURE 2.23: Heat flux map at the focal spot

2.4.3 Torrefied beech wood self heating

The former examples featured how simple models (even *out of the box* CFD for the first case) can help in accessing too low or too high values. In the coming example, we will see that it is possible to access parameters values in a more complex situation by designing hand in hand experiments and model. In this case, inverse methods helped to alleviate one of the drawbacks of direct measurement: the fine control over boundary conditions.

Torrefaction is a common pretreatment of lignocellulosic biomass as it substantially improves its properties, namely hydrophobiciy, grindability, reactivity and energy density. It is also referred to as *mild* pyrolysis as it is its very early stage, from 250 to 300 °C under inert atmosphere. Yet when this treatment is not immediately followed by pyrolysis, the substrate needs to be cooled down before storage. Industrially this cooling stage is expensive. Indeed the torrefied biomass is more reactive than the virgin one and should not be exposed to oxygen while hot, otherwise self-heating may appear.

Torrefied biomass self-heating is a complex and long-running phenomenon. Indeed, it is believed to originate from low temperature oxidation reactions. Yet these reactions being weakly exothermic, they are difficult to characterize in labscale devices. While, on industrial scale plants, in combination with a large stockpile dimensions, preventing ventilation, they can lead to uncontrollable thermal runaways. This dire case leads to the loss of the substrate and may induce severe damages to the torrefaction reactor.

To tackle this problem, together with Mines Albi (PhD of Amina Bouzarour), a new strategy was adopted. Instead of trying to measure very low heat release in small scale devices, such as TGA coupled with DSC, a pilot scale approach was chosen. Indeed at small scale, the combination of both low intensity heat release and high specific area does not favor high temperature rises. It makes the direct consequence of self-heating hard to measure with conventional devices. By increasing the reactor size, specific surface area decreases, lowering relative heat losses proportion. In this way, temperatures elevations can be monitored with standard thermocouples. Furthermore, this last configuration is much closer to industrial one than TG-DSC analyzers. For example, the gas is flown throught the chips bed and not around a crucible full of powder.

Experimentally substrate cooldown under oxidative atmosphere is reproduced as follows. First, a large quantity of wood chips is torrefied in a fully monitored 4-liter vented packed bed reactor (Fig. 2.24). Then chips temperature is stabilized at 150 °C. Finally they are exposed to various flow rates and compositions of an oxygen nitrogen mixture. The resulting thermal behavior is a combination of thermal inertia, heat convection, heat diffusion and heat coming from oxidation reactions. Over the course of experiments, some of these configurations led to a moderate self-heating, others to thermal runaways. All in all, this approach yielded a rich dataset to compare to.

2.4.3.1 Obtaining the source term

The first step is to propose a model of the thermal behavior of the packed bed. The reactor can be considered as porous medium under constant forced convection. Local heat balance can be classically derived by accounting for three main phenomena: heat convection, heat diffusion and heat production/consumption by the medium.

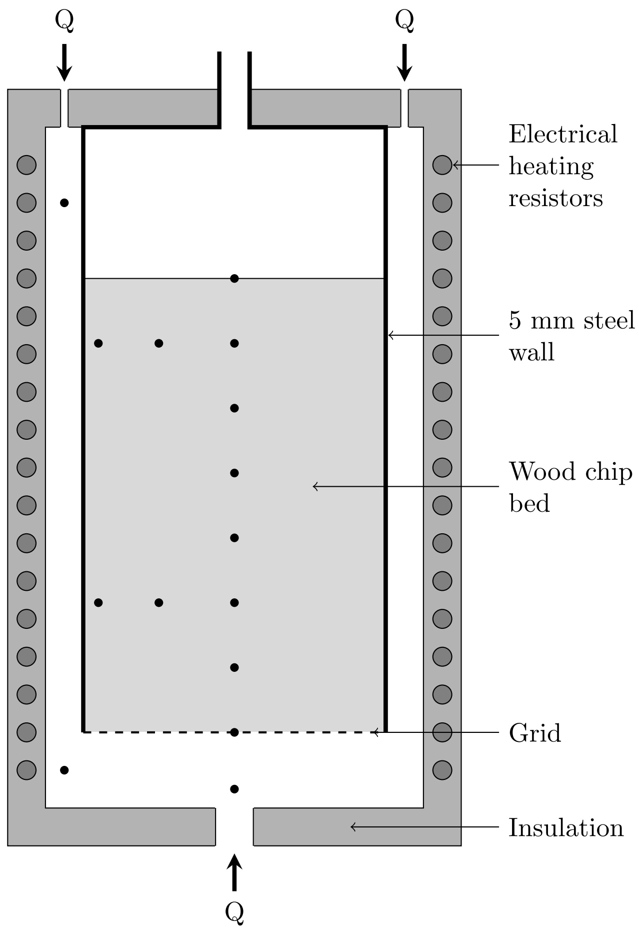


FIGURE 2.24: Schematic of the 4 liter wood chip packed, featuring electrical heating, three point air injection (Q, total flow rate 20 Nl/min), thermocouple temperature monitoring (black dots)

This balance can be written as Eq. 2.21:

$$\frac{\partial(\zeta c_{pg}\rho_g + (1-\zeta)c_{ps}\rho_s)T}{\partial t} + \nabla.(\rho_g c_{pg} T\vec{u}) = \lambda_{eff}\nabla^2 T + \Pi \tag{2.21}$$

This model, provided it is supplied with the right physical properties and source term expression, should be capable of reproducing the thermal behavior of the reactor. It would predict the temperature evolution with time across the reactor. Yet in our case, supplying the proper the source term is the challenging task. In addition, given the reactor complexity - radiative electrical heating, three point air injection - a proper description of the boundary conditions is out of reach. Even though the inlet can be characterized using thermocouples monitoring, the other boundary conditions feature heat conduction, convection and radiation in an intricated way. Therefore, we chose to reverse this model so that it would yield the source term using experimental observations as input. In this particular case, this reversal is quite simple. Indeed, it just requires to isolate the source term in Eq. 2.21 to yield Eq. 2.22:

$$\Pi = \lambda_{eff}\nabla^2 T - \frac{\partial(\zeta c_{pg}\rho_g + (1-\zeta)c_{ps}\rho_s)T}{\partial t} - \nabla.(\rho_g c_{pg} T\vec{u}) \tag{2.22}$$

In a common configuration, the equations system should be closed using initial and boundary conditions, this is not the case here. The source term can be determined using temperature evolution recorded experimentally from the numerous thermocouples monitoring the bed. Then $\frac{\partial T}{\partial t}$, ∇T and $\nabla^2 T$ can easily be reconstructed using experimental readings and finite difference method. This procedure alleviates the problem of the proper description of heat losses in the reactive packed beds as faced in Section 2.3.2. In addition, it also solves the problem of a proper description of the initial condition which would require to be able to evaluate the temperature field inside of the bed.

2.4.3.2 Validation & Results

In order to assess the reliability of this method, a validation procedure was undergone. We filled the reactor with alumina spheres and exposed them to the same temperature and flow rate variations as the treated biomass. Temperature histories and flow rate values were recorded as if it was a regular run. Then, those readings were supplied to the processing algorithm.

As the spheres constituting the medium are inert, if working properly, the reverse model should yield a source term null and constant. This, even though, flow rate and oven temperature change with time. Model results showed that accumulation, convection and diffusion terms calculated compensated one another. Thus, the reconstituted source term was null (Gaussian noise centered around 0 W/m^3) throughout the bed. The fact that this approach computes an almost zero source term for inert material is a token of its quality and allowed us to be confident in the results it will yield when applied to the other runs.

As a result, the source term at the origin of torrefied biomass self-heating under oxygen was computed for different oxygen contents and temperatures. Those results were shown to follow an exponential trend (Fig. 2.25). The final step was to propose a correlation linking heat release, temperature and oxygen contents (Eq. 2.23) [63]:

$$\Pi = \Delta H \times \zeta \times Aexp(-\frac{Ea}{\Re T})\rho_{O_2}^n \tag{2.23}$$

With ΔH = 14.062 MJ/kg$_{O_2}$, A = 2.50 × 10^{-9} s$^{-1}(\frac{kg}{m^3})^{n-1}$, Ea = 99.8 kJ/mol and n = 0.734.

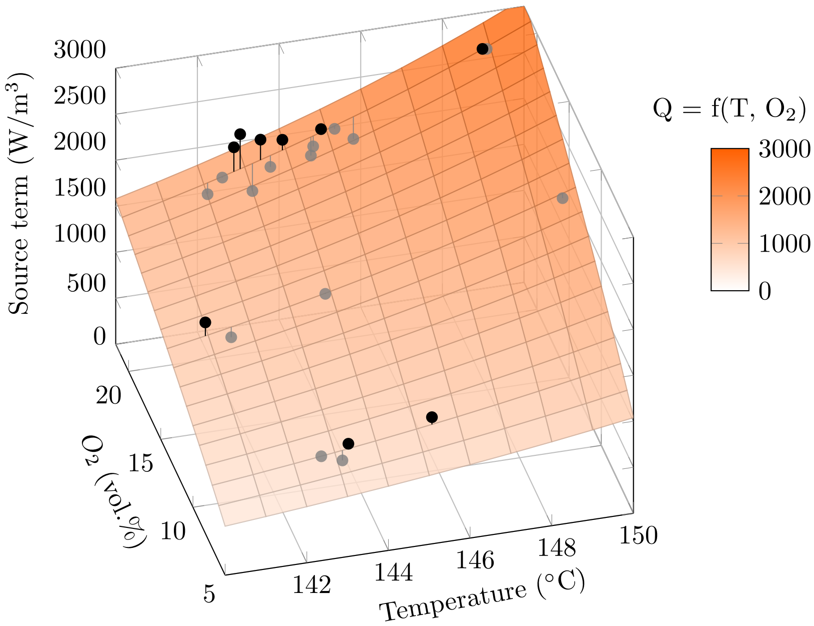


FIGURE 2.25: Experimentally obtained heat release (points) and subsequent analytical expression (colormap) for temperatures ranging from 141 to 149 °C and oxygen contents of 7, 14 and 21 %vol

2.4.4 Closing thoughts

These three examples illustrated how one can rely on modeling when he cannot measure a quantity of interest directly. Indeed, most of the measurements methods are straightforward in a sense that they deliver directly the desired value. Sadly this approach can be limited when values of interest are too low or too high to be easily accessible. When facing such cases, modeling is of help through inverse methods, especially to uncouple phenomena or tolerate uncertainty over initial and boundary conditions. In addition, given the fact that the obtained values are no end *per se* and will be used for other purposes, confidence in them is mandatory. This confidence is always built by confronting the decorellation results with experimental measurements gathered over validation cases.

2.5 Design

As in most of activities, when facing a design problem, two factors are key: time and cost. Industrially, they are strongly tied together, as one has to pay for both manpower and material expenses. In the highly competitive academic world, time is, usually, what matters the most. In these conditions, modeling is a valuable tool as it can shorten the development time and cut the costs.

Designing usually means making choices beforehand. Most of them are luckily trivial, some require expertise and few can only be arbitrated by trial and error. These last ones can lead into dramatic pitfalls inducing loss of time and effort. To address these key questions in an early stage of the process modeling can be a relevant tool. We have already seen how it can reveal insights about the behavior of the foreseen system, allowing to better understand and characterize it. In this section, we will see how it can help designing it.

These words are going to be illustrated through the design of a new flat panel ultra-thin photobioreactor with the aim of studying the influence of lighting conditions on microalgae growth.

2.5.1 The foreseen design

When studying the impact of lighting conditions on microalgal growth uniform illumination inside of the culture vessel is mandatory. Hence the design of the reactor aims at offering homogeneous lighting to the culture.

As microalgae absorb light, an illumination gradient naturally sets up in reactors. This gradient becomes all the stronger as the culture grow. In dense biomass production vessels, despite intense external lighting, only the few first centimeters of the culture are actually lit. To prevent illumination heterogeneity, research photobioreactors are often operated as turbidostats. The optical density ($OD = -log(I_z/I_0)$) is set around 0.2 [64], ensuring that, even though light is attenuated through the reactor, the cells grow under 63 to 100 % of incident light. Yet as light attenuation, concentration and thickness correlate (as in Beer-Lambert law, Eq. 2.24), thickness is the key design parameter of this kind of reactor. Hence the lower the thickness, the higher the cell concentration for a given optical density.

$$I_z = I_0 exp(-\alpha_\lambda X z) \tag{2.24}$$

The foreseen design is high, narrow, with a V-shaped bottom part. A nozzle can be found at the lower end of the V-shaped part (Fig. 2.26). This nozzle bubbles air, or CO_2-enriched air, and ensures culture mixing and carbon supply. In order to allow several tests to be run in parallel, the total volume of the reactor is quite low, around 30 ml, with a height of 15 cm and a width of 6 cm. Furthermore, this design could allow for a fast deployment using plastic or metal 3D printers.

In our case, in addition to running the photobioreactors as turbidostats we would also like to operate them in batch mode. In this case, to broaden the time lap during which culture growth can be considered optically homogeneous, we reduced the thickness of the reactor down to 6 mm. For this study, the model microalga *Chlorella vulgaris* was chosen. Even though this strain is somewhat tolerant to mechanical stress (threshold shear stress around 0.9 Pa [65]), this thickness reduction gave rise to some concerns about internal shear stress intensity.

2.5.2 Shear stress level

To assess for the shear stress level in the foreseen reactor, CFD was used. As it is an efficient and practical tool for predicting flows, it is the most straightforward way to

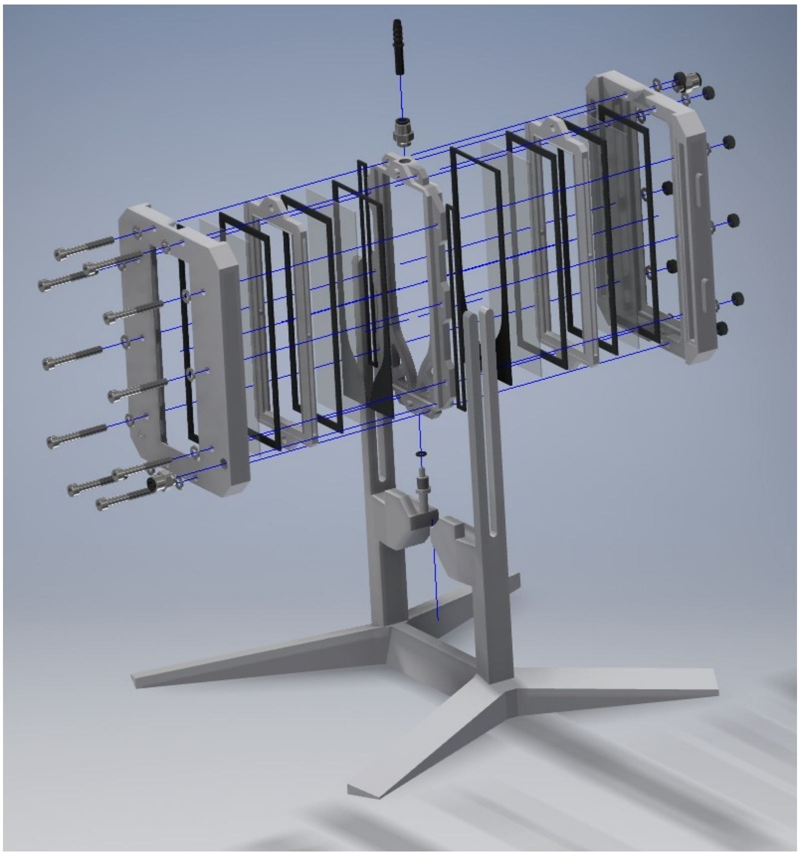


FIGURE 2.26: Technical view of the foreseen photobioreactor, with its feet, sealants and bolts

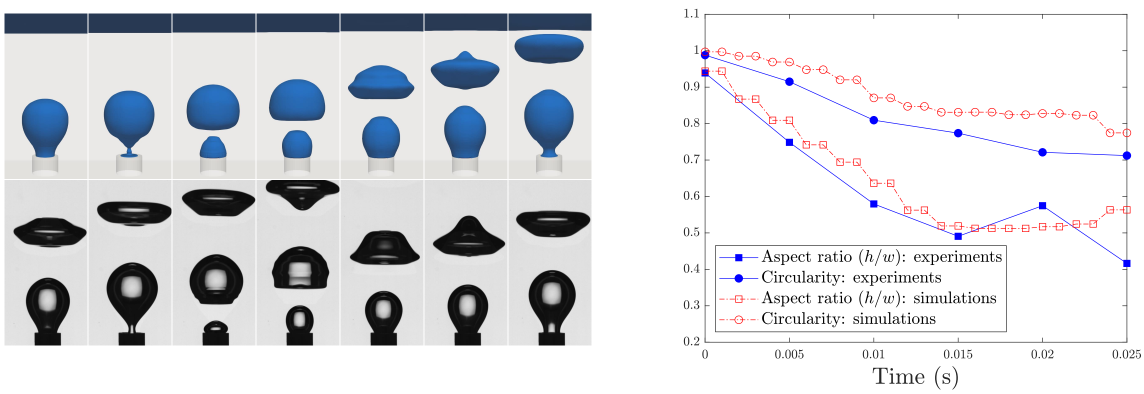
compute the shear stress.

In our case, the photobioreactor is the place of a bubbly flow. Thus it is important to properly describe bubble behavior in order to accurately predict the velocity, hence the shear stress. To simulate gas-liquid flows, the main methods are Eulerian-Lagrangian, Eulerian-Eulerian and Volume of Fluid (VoF). Eulerian-Lagrangian method considers the liquid as a continuum phase and gas as a discrete phase. One disadvantage of this method is that it requires the bubble size distribution from experiments [66, 67]. The Eulerian-Eulerian method describes both phases as continuous [68–70], therefore it is difficult to study the bubble behaviors using this method. VoF is a method that allows for the tracking of the gas-liquid interface by the calculation of a phase indicator field in every the cell of the mesh. Consequently, the bubble shape and motion could be well represented by this method, yielding a faithfull representation of the shear stress inside of the reactor. Nevertheless, this method requires sizable computational resources [71–76]. Luckily with the global increase in available computational power, the VoF approach is now accessible. This latter method was adopted in this design procedure.

2.5.2.1 Model and validation

VoF simultations were led with OpenFOAM, as it was already successfully applied to the simulation of bubbles [77, 78] and droplets [79–81].

In order to validate the OpenFOAM solver for our application, we decided to confront it to experimental results. This work was led by Wenbiao Jiang (PhD student). To do so, a whole new experimental setup was built. With this bench, bubbly flows features were measured in a lab-scale photobioreactor under different bubbling conditions. These results were produced by using shadowgraphy technique. Those features were latter compared to numerical predictions in actual 3D geometries.



(A) Simulation predictions (top) and shadowgraphy observations (bottom)

(B) Shape factors

FIGURE 2.27: Visual and qualitative comparison of a bubble formation. Gas flow rate of 45 Nml/min. Circular marks: circularity, square marks: aspect ratio. Blue: experiments, red: model predictions. Credit: Wenbiao Jiang

Figure 2.27 presents qualitative and quantitative comparisons of experimental and numerical bubbles, for the flow rate that is anticipated to be used in the photobioreactor. Bubble shape deformation is visually well predicted (Fig. 2.27 (A)). More quantitatively, the PhD student has shown that the volume of numerical bubbles agrees well with experiments, both in terms of temporal evolution and value. In addition, the evolutions of two shape factors of bubbles were investigated: aspect ratio (ratio of height over width) and circularity (ratio of the perimeter square and the projected area). These indicators were applied to arbitrarily chosen numerical bubbles. As one can see, the simulation correctly represents the trends observed by the video camera for both factors, with a relative difference of about 10%, absolute (Fig. 2.27 (B)). The code is even capable to accurately describe bubble merging at high flow rate (not reported here). These results show that OpenFOAM is both appropriate and efficient in representing the dynamic of the bubble shape evolution. Confident in those results, the code was applied to derive the shear stress imposed over microalgae in the foreseen photobioreactor design.

2.5.2.2 Reactor scale validation

The envisioned designs were reproduced numerically before being simulated. A few precautions were taken before assessing for the quality of the designs.

The first one was to remove numerical transient regime. Indeed, before the injection of gas, the liquid in the numerical photobioreactor is still. However, this initial state will be broken from the moment the gas is injected, since the bubbles will start to stir the liquid. Nevertheless, after a certain time of bubbling, the two-phase flow will reach a quasi-steady state, which implies that some physical quantities are almost time-independent. We used the evolution volume-averaged momentum as indicator of the time required for the reactor to enter the quasi-steady state. This time lap, around 2 seconds, was discarded for all runs. Indeed, given microalgal growth rate, experiments would last days, making the contribution of the transient regime irrelevant.

Once the reactor enters into a quasi-steady state, it is possible to validate the description of the mini bioreactor hydrodynamics by comparing with test case experiments. To do so, mixing time was used as a point of comparison. Experimentally a drop of methylene blue was injected in a 3D printed plastic reactor, initially filled with water. Using a portable spectrophotometer, the absorbance was monitored [82]. The experiment was repeated twice.

The exact same setup was reproduced using OpenFOAM. A passive scalar transport equation, restricted to liquid phase was added. The turbulent Schmidt number associated with this scalar transport is a very important parameter, tremendously difficult to obtain. In our case, we used a value of 0.66, a value used in literature for similar cases [83, 84]. Like for experiments, two different numerical trials were led with two different initial states.

Both experimental and numerical mixing times are close. This second validation, at the photobioreactor scale, can be taken as a token of the faithfulness of the numerical predictions.

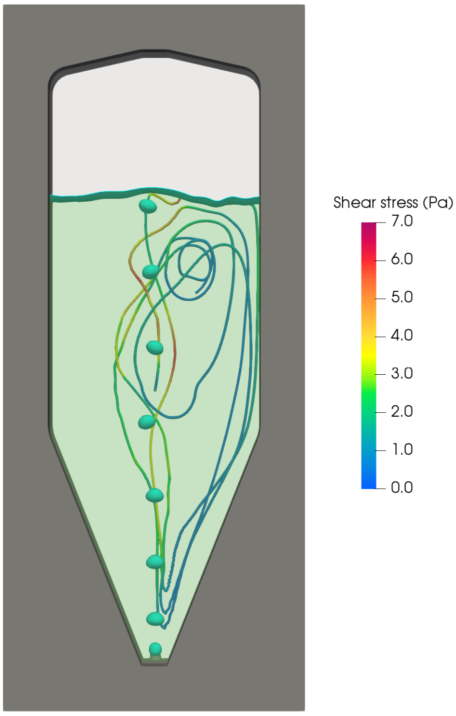
2.5.2.3 Design investigations

Upon entering quasi-steady state, the reactor was uniformly filled with 1000 Lagrangian tracers emulating microalgae. Those tracers were followed for 10 seconds. This tracking time was chosen as it ensured population value convergence. An evaluation of the shear stress experienced by the tracer was computed using the maximum eigenvalue of the shear stress tensor [85] (Eq. 2.25, the left term being viscous stress for a Newtonian fluid, the right term being an estimation of the turbulent stress).

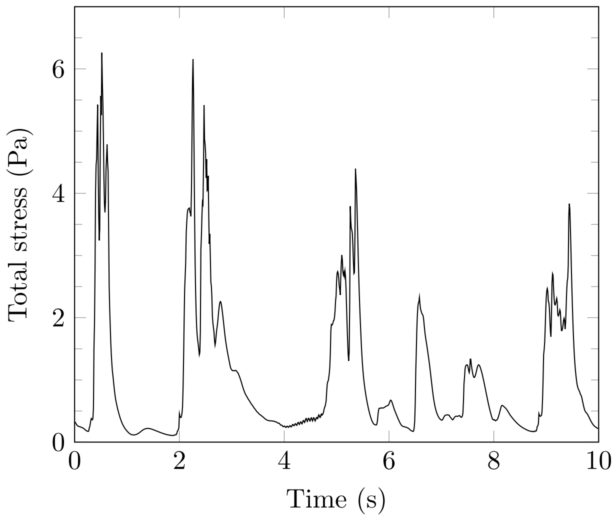
$$\bar{\bar{\tau}} = \frac{1}{2}\mu(\nabla\vec{u} + \nabla\vec{u}^T) - \rho\overline{v_i'v_j'} \simeq \frac{1}{2}\mu(\nabla\vec{u} + \nabla\vec{u}^T) + \rho\frac{2}{3}k \tag{2.25}$$

Figure 2.28 presents the path of a tracer and the shear stress it is submitted to over the course of the simulation. The highest amount of shear is experienced near the center of the reactor, when the tracer is lifted up by a bubble. During these rising stages the tracer is submitted to shear stresses that are around 10 fold higher than the downcoming ones. In order to compared with experimentally measured critical shear stress value, the average shear stress at the population level was computed. The population exhibits a Gaussian shape with a mean of 0.76 Pa (standard deviation 0.17 Pa).

From a design perspective, it is important to explore the impact of reducing the reactor thickness even further. Indeed, it would provide an even shorter optical pathway, allowing a higher cell concentration for the same optical density. 4 mm and 2 mm thick designs were investigated. As one could have expected, lowering the thickness increased the average shear stress to 0.86 and 1.09 Pa respectively (standard deviation 0.28 Pa and 0.66). Given the inherent uncertainties associated with numerical design, the 4 mm thick configuration was dimmed to close the strain critical shear stress (0.9 Pa) to be a safe choice. Hence we choose to design a 6 mm thick photobioreactor.



(A) Visualization of the trajectory of a tracer history throughout the reactor over 10 seconds



(B) Shear stress experienced by the tracer

FIGURE 2.28: Tracer trajectory and experienced shear stress. Flow rate: 50 Nml/min.

2.5.3 Illumination

The second key condition for light homogeneity at the photobioreactor scale is the uniformity of the incident light field. From a technical perspective, in addition to being uniform, the light source should also be flexible in terms of power and light / dark cycles. Hence, we chose a dimmable LEDs panel as light source. Given LED small size compared to the photobioreactor one, the question of obtaining an uniform and high light intensity at the surface of the reactor was risen.

2.5.3.1 Strategy to obtain an uniform illumination

There are two ways of obtaining an uniform light field on the surface of the reactor:

- place the LEDs panel in contact with the reactor. It would be very simple and yield a high luminous flux on the reactor surface. Sadly, it would lead to an overheating of the photobioreactor and the potential loss of the culture,
- place the LEDs panel further away from the reactor and use a light concentrator.

The second option was chosen. The foreseen design is pictured in Figure 2.29. The LEDs panel would be placed at one end of a rectangular shaped concentrator, while the photobioreactor would be at the other end, 9 cm away from the outlet. Due to geometrical constraints, the concentrator could be 70 cm long while 22.5 cm high and 13 cm wide at maximum. We chose to work with the maximal dimensions. Indeed the longer the concentrator, the higher the reflected amount of LEDs emitted light. Furthermore, a wide cross sectional area would increase the chance to have a large enough uniform area at the center of the lighted zone into which the photobioreactor could be placed. The inner faces of the concentrator were to be coated with aluminum foil as it is an unexpensive way to obtain a high reflectivity surface.

Before constructing the concentrator, we were willing to validate that it would offer the expected performances. To do so, we decided to use modelling to predict the induced lighting conditions over the photobioreactor. Hence we downloaded Soltrace, an open source raytracing software, developed by the NREL [86]. Soltrace is a C++ coded tool combining a raytracing core and a GUI. It is originally intended to help designing concentrated solar power systems. As it is open source, it was possible to modify it so that a LEDs panel could be modeled as light source. It allowed to describe LEDs positions and orientation, as well as emitted light angular distribution. Soltrace also offers the possibility to take into account reflectivity dependence on incidence angle as well as slope error and diffuse reflection. Finally, benchmarks have shown that its computing capabilities allow it to compete even with commercial codes [87].

2.5.3.2 In silico analysis

The foreseen setup was reproduced into our modified version of Soltrace. This configuration were simulated using aluminum foils properties deduced from integrating sphere measurements - obtained with the help of our colleagues from LPQM,

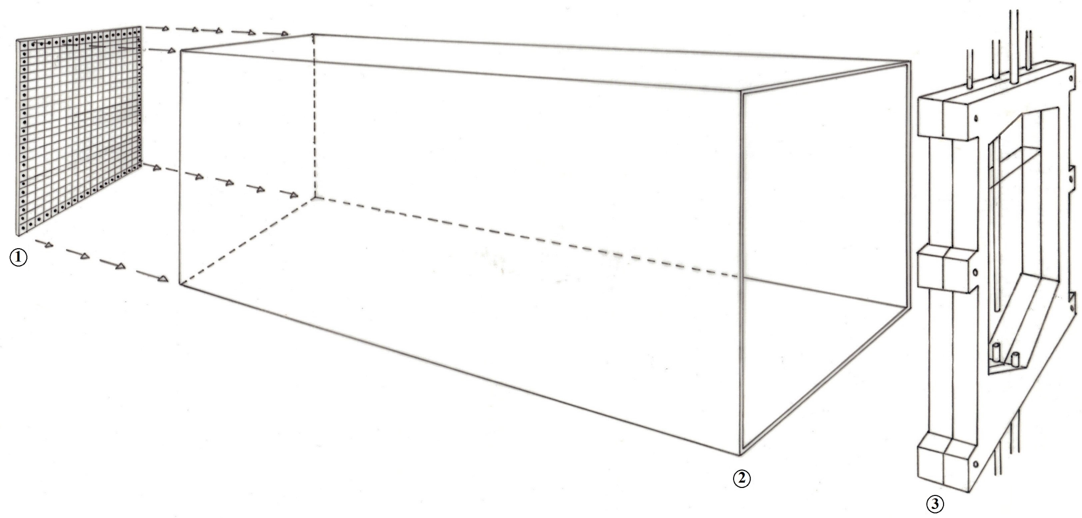


Figure 2.29: Scheme of the photobioreactor and its lighting system. (1) LEDs panel; (2) aluminum coated concentrator; (3) flat panel photobioreactor. Credit: Wendie Levasseur

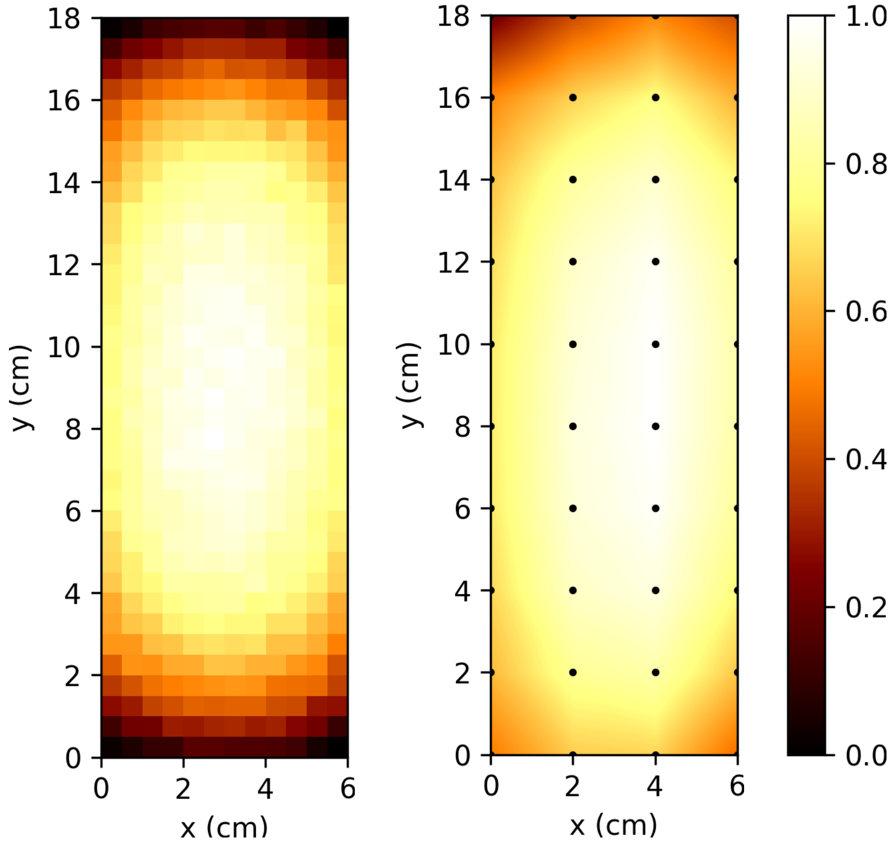
CentraleSupélec, laboratory -. Given the fact that photosynthesis is only triggered by 400 to 800 nm radiation, the measured spectra were integrated over this range only before being incorporated into the code. In addition to providing reflectivity values, measurements also were used to derive the variance of the Gaussian distribution describing the reflection errors. Finally, reflectivity dependence on incidence angle was not taken into account, as we had no data that could be used to describe it.

In order to compute the lighting over the photobioreactor available area, rays were emitted from the LEDs panel and traced until they reached the targeted zone or escaped the numerical scene. Soltrace using a Monte Carlo approach, a large number of rays have to be traced in order to achieve results convergence. Here, 352 millions hits on the targeted area were required to achieve light map convergence.

Relative incident light intensity over the photobioreactor is plotted in Figure 2.30 (A). This type of plot allows to visualize spatial uniformity of the incident light field. In this case, an uniform area exists at the center of the foreseen position. This zone is large enough to host our photobioreactor. In this zone, the reactor would not be subjected to a core to edge difference higher than 10 % of the averaged incident light intensity.

As a result of this work, the suggested design was used to build the concentrator. Once finished, in order to validate the predicted incident light map, we used a biology oriented photometer (LICOR LI-250A) to acquire the incident light map on the available area. These measurements and the reproduced map are available in Figure 2.30 (B). From a qualitative point of view, one can see that the light field predicted by our modified version of Soltrace is in very good agreement with the measurements.

From a more pragmatic perspective, the lighting over the photobioreactor can be considered uniform.



(A) Predicted map (B) Measured map

FIGURE 2.30: Relative intensity map over the reactor. On the left, black dot: measurement position. Colormap reconstituted via Delaunay triangulation

2.5.4 Closing thoughts

Numerical tools capabilities have been illustrated to be of great help when facing questions regarding the design of a new photobioreactor. The main objective was to create a growth environment within which light would be as homogeneous as possible. Yet getting intuitive on light distribution is not easy.

One can say that the lower the thickness, the more uniform the light over the photobioreactor depth, at the price of a higher shear stress. Using CFD, shear stress inside of the reactor has been assessed. It allowed to guide our choice regarding the lowest thickness that would not hinder the microalgae growth.

The second key parameter was uniformity of the incident light field. Here again, a solution was suggested, tested in silico and validated before being actually build.

As a closing word on numerical design, one could argue that the deployment of such numerical workflow takes time, and it is indeed true. On the short run, designing two to three light concentrators would surely have been faster than getting to know how to use Soltrace. On the long run, the second option remains the most efficient one. Indeed, Soltrace is now used to produce lighting maps of several different photobioreactors and lighting devices. The process was obviously more profitable when assessing the shear stress intensity. Indeed, producing on demand photobioreactors is an expensive process with several months lead time associated to it. A trial and error approach was therefore out of the scope.

Conclusion

This chapter presented the different applications for the tool that is modeling. Among the four main purposes this tool can be used for, I worked with three until now.

In the first stage of building basic knowledge blocks in chemical engineering, modeling can be used to derive a better understanding. There are two main ways of getting new insights: either by using the model to dissect the couplings, or by turning on and off part of the model and evaluate the contribution of phenomena represented. Even if very valuable, this approach cannot be led alone. Indeed among the various applications of modeling, this is the one depending the most on experimental measurements.

Once a good understanding has been derived, numerical characterization can be used to acquire values either too low, or too high, to be measured. Indeed, when direct measurement are out of the scope, accessing the values indirectly through modeling is a convenient way. It may require to transform the experimental device to monitor consequences of the phenomena before reconstructing them using the model. Given the complexity of the process and the intended use of the value, extensive experimental validation over toy cases is mandatory to ensure the reliability of the obtained values. Yet once validated, inverse methods can be trustfully used with greater ease than direct one (e.g. low control over boundary conditions).

When basic components of a system are well understood and characterized numerical design can be used to improve the conception of new experimental apparatuses. In this way, it is possible to produce more reliable and versatile experiments and reduce the number of design iterations at the same time. Nevertheless this approach applied to modern research usually requires to couple several fields of science, e.g. CFD and radiation modeling. As a consequence, the learning curve is quite steep. Still acquired skills can later be reused with greater ease, making the overall process beneficial.

Scale up is the topic I have not much experience with and has therefore not been illustrated here. It can be seen as the next step of the current stage of my research and will be addressed in the next chapter.

Finally, even though they were not featured in this chapter, experiments are always in close interaction with modeling. Whether as a direct aim, for example, by improving the design of a new experiment, such as the photobioreactor, or to feed the model with high quality inputs, like the determination of a radiative boundary condition during my PhD. Finally, model predictions always have to be confronted to validation case experimental results. This last point bears a tremendous importance as it is both the safeguard and the judge of proper modeling work.

CHAPTER 3

Critical overlook and perspectives

Introduction

In this third chapter, coming years perspectives for the three fields of my research are drawn. My projections in the chemical engineering field will be presented first, followed by the one in biochemical engineering. As they are of different importance, the level maturity of my reflection on them varies.

My contribution to chemical engineering community lies in two domains: biomass thermochemical conversion and gas separation using hollow fibers membrane contactors. The first is a field I somewhat left after the completion of my PhD. My thinking and criticism on this topic is, I hope, accurate. Yet I do not actually know where the community is and what it is aiming at. Therefore the positioning of my work is limited. The self-awareness I have regarding second topic is quite low. This is mainly due to the fact that this topic lies outside of my core of expertise and outside of my initial research prerogatives. Still I will be involved in the coming actions of the Chair of Biotechnology of CentraleSupélec with this technology. Hence it is mandatory for me to take the time to think about where I should stand.

Being the core of my research activity and the project I spend the most time working on, the study of microalgal growth under different lighting conditions is the most developed. The aims of this research project are clear and the steps to reach them can be drawn. This is also the project for which the criticism is the most mature.

This chapter is structured as the mirror to the previous one. In the former, the emphasis was put on the uses the tool that is modeling can have, casting aside the research context. Here, as a critical overlook upon my past work, a general comment of my work with modeling is proposed first. Then, more detailed analyses are undergone on my main research projects. These analyses are divided into four parts: a look back over what was done, and short (1 to 3 years), medium (3 to 5 years) and long (more than 6 years) term perspectives.

3.1 General comment about modeling

Among the two kinds of modeling that are cognitive and non-cognitive modelings, I presented illustrations featuring only the first one. Both having their own advantages and drawbacks, one has to see them as two different tools, fitted for two different applications.

Cognitive modeling is the approach that makes the most in sense in a long term perspective. It finds its foundation in the deep understanding of the physical phenomena and their representation. As a consequence, it can be used, as we have seen, to derive further understanding. In that way it helps in agglomerating new basic blocks of knowledge. All in all, it broadens knowledge foundation of both individuals researcher and mankind. Its main limitation comes from its human origin.

Hence, when one is overwhelmed by complexity, cannot draw clear cause-consequence schemes, cannot accurately enough characterize the system of interest, cognitive modeling deployment is severely hindered.

Non-cognitive modeling can be seen as a way to solve a problem at the price of sacrificing the deep understanding provided by its cognitive counterpart. It is nonetheless a very valuable approach. Especially in the case of problems that are far too complex for one to envision all the inputs and outputs. In these conditions a machine learning algorithm can be of great help.

From my own perspectives, I mainly used the first one until now. To be even more specific, I deployed cognitive modeling with deterministic resolution procedures. It can be seen as a direct consequence of my education as a fluid mechanics engineer. This field of science relied heavily on this approach. Hence I was taught its methods and I therefore feel more at ease using them. Nevertheless, I have a keen interest in non-cognitive modeling as I have been made aware of the power. I am now also trying to acquire some skills in this field. To this regard, I have acknowledged the importance of people I have worked around. The most prevailing one being the PhD student (Christophe Spiesser) I shared my office with during my own PhD. He was working on stochastic modeling and statistical approaches to solve heat transfer equation using Monte Carlo method. This was stochastic resolution of a cognitive model. Yet our numerous discussions helped a lot in demystifying the statistic based approaches which paves to non-cognitive modeling. It even led to me contribuing to one of his article [88].

In terms of solid actions, my interest for non-cognitive modeling is materialized by the fact that I learned how to use Particle Swarm Optimizer. This general tool turned out to be highly effective to search wide candidate space and highly non linear functions [89]. From a more biologically oriented perspective, I also passed a project aiming at using clustering and classification algorithms to process flow cytometry results. Indeed, this kind of analysis yields four or five variables over millions of cells in a few minutes when screening a microalgal culture. As a consequence, flow cytometry readings are difficult for a human to interpret. Nevertheless, this make them proper candidates for data driven problem solving.

Over the past years, I have also made progress in the way modeling work can be shared with the community. I looked at the number times some of my published articles were downloaded and cited. This analysis made me realize something I feared: too complex models are not picked up by the community. Even though it acknowledges their capabilities, only few other authors actually try to implement them. On one side, it increases one notoriety. On the other, it slows down the diffusion of scientific work. Since this observation, I tend to propose more gradual articles with clearer take-home points.

3.2 Chemical engineering

As aforementioned, my contributions to chemical engineering field belong to two domains: biomass thermochemical conversion and gas separation using hollow fibers membrane contactors.

3.2.1 Progress review

My involvement in the biomass thermochemical conversion started with my PhD. As a consequence, I dedicated a few years of my life to this topic. Like every PhD student, I have a solid background in the domains at the core of my PhD. Without claiming to be an expert in those fields, I have an advanced scientific knowledge of pyrolysis and gasification. Given the fact that my PhD was not intended to be directly applied to an industrial process, I do have only partial awareness of how those fields are transposed to the industrial sector. Nevertheless, this background, completed by literature elements, allows me to confidently give lectures to master students on this topic.

Apart from a background, these investigations allowed me to further my skills in modeling of heat and mass transfers in reactive porous media. I have had the time to develop a numerical model of biomass gasification involving state of the art features (moving mesh, liquid-vapor equilibrium). These capabilities were considered at the time as the next step for this community. The quality of this model has been acknowledged by the peers, as shown by my invitation as lecturer to a von Karman Institute lecture series in 2019.

I stopped actively contributing to this field of science after the completion of my PhD degree. Nevertheless, the skills I have acquired paved the way to a broadening of my scientific horizon. Indeed, heat and mass transfers in porous media applications are not restricted to biomass thermochemical conversion. I have applied them to combustion in low carbon content porous media as well as torrefaction. My experience also challenged my curiosity. For example, knowing how complicated some porous media properties are to measure, I tried to acquire them numerically. This was my main motivation to lead the study on granular bed permeability. Even though motivated by the sole academic interest, this study initiated my collaboration with IFPEN on packed beds characterization.

Neither active research on biomass thermochemical conversion or packed beds characterization lie at the heart of my research prerogatives at the Chair of Biotechnology of CentraleSupélec. Luckily, my management allows this involvement as long as it does not hinder my core research subject.

Taking a step back, I would say that, coming from biomass thermochemical conversion, this field of application evolved into packed beds numerical characterization. In any case, the underlying skill is the modeling of heat and mass transfer in reactive porous media. This skill allowed me to tackle gas separation using hollow fibers membrane contactors. As aforementioned, my involvement in this topic originates from the needs of a former PhD student of the Chair of Biotechnology. As he asked me for support on the modeling aspects of his work, I restricted my participation to those aspects. Indeed, he was already supervised. I intentionally limited my involvement to modeling in order to avoid potential conflicts that could have been created by my implication on other parts of his work. This choice has had a dire consequence. I only have a scientific understanding of the phenomena at stake in the process. Even though technical and economical sides are known to me, I am far from mastering them.

At the Chair of Biotechnology level, we are pushing to transfer to the industrial sector the very promising results this PhD student had. I am taking part in this process as scientific support. This project materializes itself into three different actions: the active advertising of the technology toward potential industrial partners - led by the Chair business developer -, the involvement of the Chair of Biotechnology in an industrial project aiming at producing biomethane (from biogas) and the current PhD thesis dealing with syngas separation using hollow fibers membrane contactors.

3.2.2 Short term

Short term projections are the direct continuation of my current work. On the packed beds side, my collaboration with IFPEN should provide me with both research objectives and partners to tackle them. Our joined goal is to be able to numerically reproduce heat transfer in gas vented packed beds. Provided everything works well, we may be able to produce geometry specific correlations that would be of interest for both engineers and researchers. In addition, we could provide not only parameters unique value, but also their distributions inside of the bed, for tortuosity for example.

Until now, I have only used numerically generated media. This limits the possible applications to simple geometries such as packing of spheres, cylinders, or somewhat more complex shapes. Applying this approach to actual media that would have been 3D scanned, is a direction I intend to follow. Indeed, it would widen the scope of the applications, hence increase the number of potential industrial or academic partners. To this regard, the Chair of Biotechnology of CentraleSupélec possesses a 3D tomograph with down to 700 nm resolution. Having this high-end equipment at hand will facilitate our coming investigations on real morphologies.

On the gas separation side, the goals of the current PhD student are quite high. We aim at achieving 99.97 % H_2 purity at pilot scale level. This will be done not only by understanding the phenomena at stake inside of the contactor, but also by bench architecture optimization. To do so, our first step will be to transform our current 3D CFD model into a much simpler one. By doing so, we will be able to integrate it into an optimization loop at the rig scale, guiding our pilot unit design.

The initiation of industrial partnerships can be envisioned in the coming years.

The most likely field of application would be biogas purification, as solid results have already been published and the Chair is involved in key projects. The application of the technology to other gas mixtures separation processes can also be an option. It would need further development and the achievement of proof-of-concept for those new mixtures. Even though those partnerships could start on a short term horizon, the delivery of pilot scale units for those new mixtures cannot be foreseen in a coming future.

Finally, I take part at a low level in several projects (industrial contracts or PhD supervision) where I intend apply the tools I developed. For example, biogas purification using pressure swing adsorption (with Air Liquide) is of note as it combines both packed beds and biogas knowledge I have. The value of this kind of involvements is not the reinforcement of my skills, but keeping them well trained and paving the way to new collaborations with existing or new partners.

3.2.3 Mid term

Projections in a somewhat more distant future are blurry for packed beds characterization. From the current interest of both industrial and academic actors I could be involved as subcontractor for industrial, or member of a research project for academics. From this perspective, industrial partners could be looking for process problem diagnosis and remediation, while academic one would be more interested in new media characterization. Still leading a major project seems out of the scope. These two kinds of involvement would only be possible if at least some of my short term objectives are fulfilled.

Perspectives are much clearer for my effort on hollow fibers membrane contactors. The natural continuation of producing and validating simple 1D or 0D models is to transfer them to engineers for process design purposes. The models would have to be validated for different gas mixtures and shown to work at process scale. This will get along with the mentioned industrial interactions in the former section. R&D teams could learn by working with us or hiring PhD students who completed their PhD degree in our laboratory.

3.2.4 Long term

As aforementioned, curiosity is my sole driver for my packed beds investigations. Having no clear objectives, accurate long term projection is out the scope. From a general perspective, my skills in modeling of heat and mass transfer in reactive porous media will keep getting applied to various problems, driven by needs of academic or industrial partners. Only time will tell how and with who.

Regarding hollow fibers membrane contactors, two different pathways draw themselves. Either industrial partners face challenges and come to us for help. In this case, we would have both research and financial inputs to lead new scientific investigations. Otherwise, the scientific interest will dwindle. In this second case, our involvement in this field will be limited to high-end technical support.

3.3 Microalgae and lighting conditions

3.3.1 Progress review

Almost four years ago, I have been hired at the Chair of Biotechnology of CentraleSupélec to work the Lagrangian on tracking of microalgae inside of photobioreactors. This subject was part of a larger project envisioned by our director: enhancing the prediction of photobioreactors performances. In his vision, and I fully agree with him, it can be done by tracking them with CFD before coupling the results with a biological model. This would allow to obtain insights at the photobioreactor scale. Those could then be used for easing scale up and propose new designs. It would represent a major step forward for the biotechnology community as scale up procedures are mostly based on a trial and error approach with the associated hurdles.

3.3.1.1 Personal perspective

My legitimacy to work on this topic came from my education in fluid dynamics and my modeling oriented PhD. My current role as principal investigator originates from the combination of three external factors: my arrival at the early beginning of the project, the available funding of the Chair, the lack of direct competition within my entity. All in all, and with both honesty and humility, it boils down to mere luck.

The first factor allowed to me to take part in the shaping of this project, with two consequences: pushing my involvement even further and making me a key part of it. The second factor translates into a long term - three years, renewable and renewed - contract allowing me to plan this project over several years. In addition, it gave the Chair the flexibility to hire one PhD student on internal funding to work full time on this project under my supervision. The third factor was the most critical one. Having a background in biomass thermochemical conversion and fluid dynamics, I needed time to update on biology and bioprocess. This updating required the reading of numerous articles, the assimilation of basic biology skills and a total time of three years. I do not claim to be biologist today, yet I can discuss with one and manipulate more than the most basic concepts.

Finally, as a general comment on this field of application, I would say that, with the help of my director, I learned a lot in the way of structuring research activity on the long run. I had luck, I made mistake, yet I now have a clear road-map I am entitled to follow.

3.3.1.2 Research perspective

Being the core of my research activity, the key steps to facilitate photobioreactors upscaling are easily identifiable (Fig. 3.1).

The very first step of this project was to survey the literature in order to identify which were the bottlenecks preventing proper upscaling of photobioreactors. It revealed a consensus on this question: illumination inside of the reactor is an actual challenge for scale up. In addition, the realization of microalgae full industrial potential is hindered by numerous other factors. Among them, one can quote the harvest of the microalgae themselves [90] and the extraction of the targeted metabolites. Nevertheless, economical viability of the whole chain of value requires productive and affordable photobioreactors, our objective here.

The current consensus is that light perceived by a microalgal cell is a combination of the illumination field inside the photobioreactor and the position history of the cell. Yet experimentally capturing those patterns is not possible in complex geometries. Therefore predicting those patterns numerically was the first building block of this project. It was led by a PhD student (Wenbiao Jiang). As a result, a code using either Volume Of Fluid or Lagrangian approach for bubbles tracking has been produced. Its extensive validation could be the work of a master student over an internship.

With the confidence in the fact that microalgae could be tracked in complex geometries, experimental characterization of their response to different light patterns was undergone. Indeed, currently most of the photobioreactors geometries are simple: flat panels, tubes, ... In these configurations, Beer-Lambert law can be used to easily derive knowledge of the illumination field, even though my research group does not have the skills to compute complex illumination fields yet. Combined with microalgae position, light field knowledge yields light history of each tracer. The first investigation of light patterns influence was carried out by a master trainee (Robin Lacombe). I acquired an external source of funding for this internship. The set of experiments was realized in optically thin configurations on an improvised test bench. In order to be able to compare our results with literature, we chose a model microalga *Chlorella vulgaris*. This strain will be kept throughout all of our development, as it is a reference among the community. The student results were promising and the Chair of Biotechnology accepted to fund a PhD student (Wendie Levasseur) to investigate further. The internship results have been published by the PhD student.

The next stage is where the project currently is. On the experimental side, it went from improvised test bench to engineered 3D printed photobioreactor prototypes. Those prototypes validated, steel machined counterparts are now being deployed. The PhD student is actively working on producing microalgae growth rates results to serve as input for PSU model calibration, as this type of model is the most suited one for deriving population behavior based on individual cell tracking. On the numerical side, CFD codes have been coupled with Han's model - parameter extracted from literature [89] -. They allow to compute to population response at

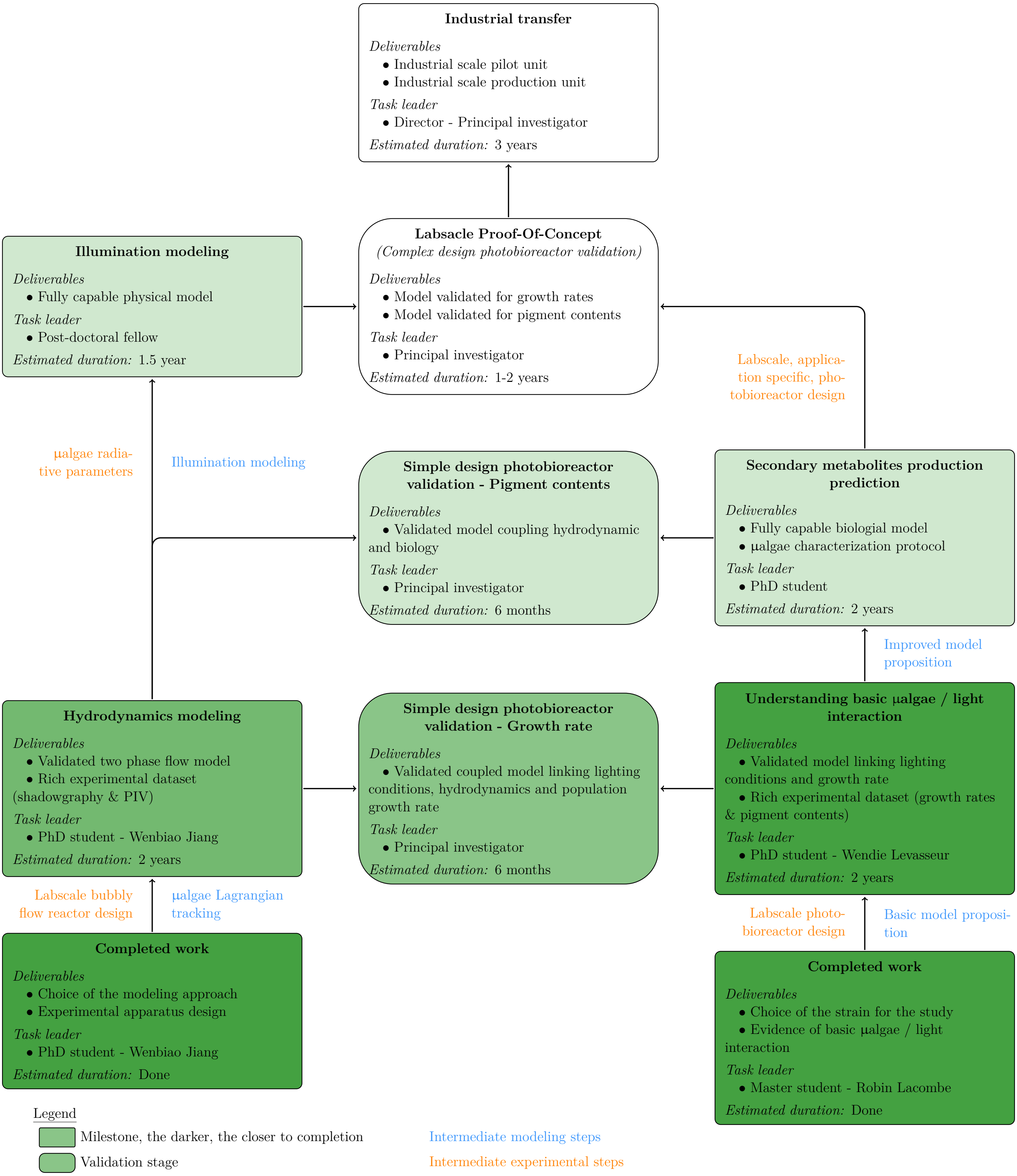


Figure 3.1: Photobioreactor upscaling project flow diagram

the photobioreactor scale. Yet validation remains to be achieved. Indeed, we lack an experimental reference point to compared to. This point would be the extraction of PSU model parameters for a given strain (*Chlorella vulgaris*, in our case). Then growing this strain in a simple shaped photobioreactor (e.g. a bubble column) and monitoring growth rates under different lighting conditions and cell concentrations. Finally comparing the CFD-PSU model predictions when applied to a numerical reproduction of the photobioreactor.

3.3.2 Short term

On the very short term, we aim at reaching the validation point presented above. Nevertheless some words of caution have to be drawn. Even though we are going to use PSU model, we know that it would probably not describe the proper biological phenomena. Indeed, these models are built considering microalgae photosystems which take a few milliseconds to react. Yet, because no dataset has been produced at those timescales, these models are usually calibrated with data featuring light variations of the order of magnitude of the second [91]. It reveals that even if the mathematical shape may be suited for the intended application, there is a need for a new data, pinpointing the proper biological phenomena. We intend to produce this dataset. This should be done by the end of the current PhD.

Growth rate validation is only the first of the model construction. Once achieved, we will tackle the question of secondary metabolites - such as pigment or lipids. Their production is triggered by nitrogen deficiency and light stress. Here, we intend to enhance the formerly proposed model, calibrate it at small scale, before coupling it with CFD and validating it at reactor scale. Provided things go well, this is as far as the current PhD could go. In a more realistic projection, the continuation of her work by a postdoctoral fellowship is more likely. This consideration rises the very relevant question of who is carrying research actions and skill stability at the team level.

For both growth rate and secondary metabolites production, the methods developed during the former tasks would have to be streamlined into a protocol. This protocol could later be used with other microalgal strains than *Chlorella vulgaris*. Thus, in the case of an industrial application problem, we could obtain the parameters required to power our model from the desired strain. It would pave the way to on demand photobioreactor tailoring. These actions could be led with the help of master students. From a scientific perspective, these actions would also rise the question the metabolic difference between microalgal strains. Indeed, if important discrepancies emerge, enhancement of the model could be required.

On the numerical side, the next step is to be capable of predicting illumination field across complex geometries. Several approaches exist. Two broad choices are possible: stochastic methods such as Monte Carlo Method [92] or deterministic ones such as Discrete Ordinates Methods (DOM) [93]. The first one could be very efficient only if a limited number of particles has to be tracked. Nevertheless, the number of particles to be traced has to be high to ensure growth rate and secondary metabolites production convergence at the population level. Sadly, applied to a large number of tracers, Monte Carlo Method would become prohibitive. In this last case, DOM would yield an illumination field among which the tracers would evolve. This second approach takes far more time to compute than few Monte Carlo evaluations and becomes cpu-competitive only if the number of tracers is to be high. The choice between those two methods will depend on the application and emerge from CFD-PSU codes results. Illumination computation and codes coupling requiring high end skills, this work can only be carried out by a post-doctoral fellow, or the principal investigator. Another option is to team up with a research group which already acquired those methods.

With all of these tools, it will be possible in the coming future to share our expertise with the industrial sector. Without offering application specific design, we should be able to pin-point problems in existing photobioreactors and help in their alleviation. These interactions could be as subcontractor or academic partners depending on the task at hand and the available incentives.

3.3.3 Mid term

The former tasks could be completed under three years if no major hitch appears. At this point, our research team would have the possibility to characterize microalgae specific response to light and to compute perceived illumination inside of a custom photobioreactor design. Hence we could tackle the challenge of photobioreactor design with two constraints: a given strain and a targeted production objective (biomass and/or secondary metabolites).

The next step would be to develop a proof-of-concept of this procedure. It could be delivered in two ways. Either by enhancing the volumetric productivity of a given, well-established, strain in the industrial sector. We could aim at pigments or lipid production, as raw biomass production may not be a powerful enough driver. The message would be clear: new photobioreactor designs allow to enhance productivity. The second option is picking up a new, unknown, strain, express some secondary metabolites that could be of value. Then we would design a photobioreactor that would substantially increase the production of this metabolite. The message would be: new application of unknown strains can be unlock by proper photobioreactor design. In any case, it would have to be an in-house project, maybe partially public funded. Indeed no industrial partner would be willing to take the financial risk associated with such a project.

3.3.4 Long term

The most evident follow-up to the delivery of this proof-of-concept is to apply it to industrial design. Two kinds of industrial partnerships would be possible: either team-up with a small company aiming at delivering a new product to the market, or with an established company willing to change part of one of its process into a bioprocess.

In the first case, the company would have a given strain and a protocol to product the secondary metabolite of interest. We would help them in proposing a design, building it at labscale pilot unit. This unit would be tested in a laboratory before being shipped on a test industrial site. Finally, provided the former stages are conclusive, the design would be scaled up. The emergence of this new prototype and the acquisition of the skills by the company would need time and efforts. In terms of manpower it could translate into a PhD student later hired by the company. Public funding would certainly have to be acquired to lead this project.

In the second case, the company may rely on us for transforming one of its process. Under such conditions, it would be able to produce specifications the bioprocess would have to meet to replace the conventional one. Photobioreactor design would be only part of this task. Indeed, before designing a reactor, the transformation of the process would also require purely biologist skills. Hence, we may have to team up with another research group. Here again the project would be on the long run with external public funding.

Prospecting for industrial partnerships would be done with the guidance of the business developer of the Chair of Biotechnology.

Conclusion

Over the course of this exercise, I took a step back and considered the work I led over these last seven years. It started with an extended formal curriculum vitae covering my profile from eduction to valorized research activities. Then, it carried on with a critical thinking about modeling, a tool my work revolves around. I could draw four main applications: 1. understanding - aiming at the delivery of basic blocks of knowledge -, 2. characterization - providing hard to obtain parameters to later run models -, 3. design - guiding through the difficult process of new conception - and 4. scale up - transferring the most promising designs to the industrial sector -.

The second chapter was dedicated to presenting how I deploy modeling approaches in my research. This usage was illustrated with the help of the three main fields of applications I am working on. To serve as examples, I invoke my first domain of expertise: biomass thermochemical conversion, which would now better be described as heat and transfer in reactive porous media. I also pictured what is at the core of my current research activity: the study of the interaction between light and microalgae with a clear aim at photobioreactor upscaling. To a lesser extend, I illustrated modeling applications with works I took part in, such as gas separation using hollow fibers membrane contactors.

In the third chapter, I tried to have a critical look over the work I led and to draw what it could be done in a timescale of one to ten years. It is clear that I have a solid driver and an established plan to improve photobioreactors designs using modeling tools. The same cannot be stated for biomass thermochemical conversion, as I deviated from it towards packed beds characterization, with my own curiosity as sole guide. Nonetheless, it yielded fruitful results. Hollow fibers membrane conctactors are the third field of applications I am projecting myself into. In this last case, I know where I stand. I am contented with my role of support and pleased to be part of, but definitely not leading, this ambitious project of the Chair of Biotechnology.

Finally, this analysis rose the questions of who I am, where I intend to go and how. To put it in a nutshell, it could be turned into a SWOT matrix (Fig. 3.2). I leave time to tell me how mistaken my conception of modeling is and how wrong I was when I forecast what could be my coming years as a researcher.

	POSITIVE	**NEGATIVE**
INTERNAL	Strenghts (S) • Generality of mechanistic modeling • OpenFOAM visibility • Strong background • High quality model of biomass thermochemical conversion • Clear driver • Understaning of the physical phenomena • Heat and mass transfer background	Weaknesses (W) • Low delegation capacity • Need for computationnal power • Never ran long term projects • No clear driver • Partial background • Lack of technical skill • Weak technical background
EXTERNAL	Opportun. (O) • Technical and financial means offered by my lab • Available resources to learn stochastic modeling • Agglomerate a research team • Scientific community interest • General interest of the industry • Scientific aim of my entity • Lack of high quality models • Industrial demand • Topic driven by an in-house PhD students	Threats (T) • Laboratory internal competition • Lack of domestic visibility • Fierce worldwide competition • Low financial means of the targeted customers • Industrial resistance to change

Fields of application: general, lignocellulosic biomass, algal growth, membrane contactor

FIGURE 3.2: SWOT analysis of my profile as a researcher

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List of Figures

Modeling as a tool for chemical and biochemical engineering

Abstract: In this exercise, I take a step back and consider the work I led as a researcher over the last seven years. I introduce some of my works in order to illustrate the possible uses for the tool that is modeling. These illustrations are focused on the application of modeling to chemical and biochemical engineering. Four main applications are drawn: 1. understanding - aiming at the delivery of basic blocks of knowledge -, 2. characterization - providing hard to obtain parameters -, 3. design - guiding through the difficult process of new conception - and 4. scale up - transferring the most promising designs to the industrial sector -.

The first chapter is an extended formal curriculum vitae covering my education, experiences, research activities, partnerships, teaching activities, students I supervised and publications I authored.

In the second chapter, the three first usages are illustrated with the help of the three main fields of applications I am working on: biomass thermochemical conversion, the study of the interaction between light and microalgae and gas separation using hollow fibers membrane contactors. Scale up applications are the point I am aiming at and are developed as perspectives. Furthermore, even though only the modeling parts of my investigations are highlighted, hints of experiments are glanced, as they are essential material for proper modeling activities.

In the third chapter, I try to have a critical overlook on the work I led and the use I have for modeling. Then, an attempt to draw what my work could be in a n horizon of one to ten years is made. From it, it is clear that I have a solid driver and an established plan to improve photobioreactors designs using modeling tools. The same cannot be stated for biomass thermochemical conversion, as I deviated from it towards packed beds characterization, with my own curiosity as sole guide. Nonetheless, it yielded fruitful results. Regarding hollow fibers membrane conctactors, I shall support its transfer to the industrial sector as part of this ambitious project of the Chair of Biotechnology of CentraleSupélec.

Keywords: Modeling, Simulation, CFD, Chemical & Biochemical engineering