UNIVERSITE POLYTECHNIQUE
HAUTS-DE-FRANCE

HABILITATION A DIRIGER DES RECHERCHES

RAPPORT DE SOUTENANCE

<u>Thèse ou ensemble de travaux exposé le</u> : 13 novembre 2019

<u>Par</u> : Monsieur Talib DBOUK

<u>Sur le sujet</u> :

« Optimisation topologique des systèmes complexes thermofluidiques : Modélisation et design multi-physiques multi-échelles ».

« Topology Optimization of Complex Thermofluid Flows and Systems : MultiPhysics Multiscale Modeling and Design »

<u>Composition du jury :</u>

Monsieur Michel CABASSUD, Professeur à l'Université de Toulouse - GC-GP & LG – UMR CNRS 5503
Madame Lingai LUO, Professeur à l'Université de Nantes – LTN 6 UMR CNRS 6607
Monsieur Julien REVEILLON, Professeur à l'Université de Rouen – CORIA – UMR CNRS 6614
Madame Chérifa ABID, Maître de conférences-HDR- Aix Marseille Université – IUSTI – UMR CNRS 7343
Monsieur Elie HACHEM, Professeur à l'Université Côte d'Azur – Mines Paris Tech – CEMEF – UMR CNRS 7635
Monsieur Laurent KEIRSBULCK, Professeur à l'Université Polytechnique Hauts-de-France–LAMIH UMR CNRS 8201
Monsieur Philippe MARTY, Professeur à l'Université de Grenoble – CEA – LEGI – UMR CNRS 5519
Monsieur Didier SAURY, Professeur à l'Université de Poitiers – Institut P' – UPR CNRS 3346
Madame Elisabeth LEMAIRE, Directrice de Recherche CNRS-Université de Côte d'Azur –INPHYNI – UMR CNRS 7010, invitée
Monsieur Rainier HREIZ, Maître de conférences à l'Université de Lorraine – LRGP UMR CNRS 7274, Invité

T.S.V.P

RAPPORT DE SOUTENANCE:

Talib Dbouk a parfaitement présenté une synthèse de ses travaux sur la modélisation multi-échelle mutli-physique en particulier dans le cadre de l'optimisation topologique des systèmes thermofluidiques, avec enthousiasme et dynamique. Ses activités comportent une forte composante numérique et informatique en plus de la modélisation et de la mécanique numérique. M. Talib Dbouk a démontré qu'il maîtrise tous ces domaines comme l'attestent ses nombreuses contributions scientifiques. De plus, il possède une forte expérience d'encadrement et une bonne maîtrise des interactions avec les industriels par une valorisation prononcée. C'est un excellent pédagogue qui a répondu à toutes les questions de jury avec expertise et d'une manière passionnante. Pour toutes ces raisons, le jury unanime lui décerne l'habilitation à diriger des recherches.

Valenciennes, Le 13/11/19

Le Président et Les Membres du Jury,

Elie Hachem

Philippe Marty (visio)
Lingai Luo (visio)
Didier Saury (visio)

UNIVERSITÉ POLYTECHNIQUE HAUTS-DE-FRANCE

HABILITATION À DIRIGER DES RECHERCHES (HDR)

Topology Optimization of Complex Thermofluid Flows and Systems: MultiPhysics Multiscale Modeling and Design

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A manuscript thesis submitted in fulfillment of the requirements for the degree of Habilitation à Diriger des Recherches (HDR)

in ***Physics and Applied Sciences***

September 9, 2019

Université Polytechnique HAUTS-DE-FRANCE	**Demande d'inscription Habilitation à Diriger des Recherches**	UNIVERSITE POLYTECHNIQUE HAUTS-DE-FRANCE SCEVE – SERVICE SCOLARITÉ LE MONT HOUY 59313 VALENCIENNES CEDEX 9 ☎03 27 51 10 03

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TITRES UNIVERSITAIRES FRANÇAIS (préciser pour la thèse : titre – date – lieu de soutenance – Nom du Directeur de Thèse) **:** Diplome national de docteur de Physique – 14 Décembre 2011 – Université de Nice-Sophia Antipolis – Nom de Directeur de Thèse: Prof. Elisabeth LEMAIRE

DIPLÔMES (avec mentions éventuelles), **TITRES ÉTRANGERS :** Diplome national de Master (Recherche) – Le 12 Décembre 2008 – Université de Nantes (Ecole centrale de Nantes)

AVIS ARGUMENTÉ DU DIRECTEUR DE RECHERCHE

À défaut d'une personnalité scientifique compétente dans le domaine du candidat

Je collabore depuis quelques années avec Mr Talib Dbouk au travers la thématique du transport de particules. Je suis donc de ce fait les activités qu'il développe au département d'Energétique Industrielle de l'IMT Lille Douai où il est Maître-Assistant. Ses travaux numériques autour des phénomènes de transport dans les suspensions concentrées (transfert thermique et migration de particules induite par un écoulement) sont de très grande qualité. Il a développé des méthodes originales pour traiter ces problèmes complexes et a obtenu des résultats de tout premier plan qu'il a publiés dans de très bonnes revues internationales. Il a par ailleurs une bonne activité d'encadrement de jeunes chercheurs (post-doctorants, doctorants et Master 2). Compte tenu de la grande qualité de ses travaux de recherche et du dynamisme dont il fait preuve pour développer des projets originaux et ambitieux, je donne un avis très favorable à son inscription en HDR.

Fait à Valenciennes, le 28/02/2019

Keirsbulck Laurent, professeur

AVIS ARGUMENTÉ DU DIRECTEUR DE LABORATOIRE

Joindre l'avis du comité des thèses du laboratoire si existant

Avis très favorable. Le comité des thèses et HDR a statué dans ce sens également.

Fait à Valenciennes le 28 / 02 / 2019 **NOM et SIGNATURE :** Thierry Marie GUERRA

Thierry Marie GUERRA
Directeur du LAMIH

PIÈCES À JOINDRE :

- Un curriculum vitae détaillé de vos activités pédagogiques et scientifiques (publications, ouvrage, travaux) de 2 pages MAXIMUM. (1 page pour les activités pédagogiques et 1 page pour activités de recherche)

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DIPLÔMES (avec mentions éventuelles, TITRES ÉTRANGERS : Le Diplome national de Master (Recherche) – Le 12 Décemebre 2008 – Université de Nantes (Ecole centrale de Nantes)

AVIS ARGUMENTÉ DU DIRECTEUR DE LABORATOIRE

Joindre l'avis du comité des thèses du laboratoire si existant

M. Talib DBOUK est Maître-Assistant au Département Energétique Industrielle de l'IMT Lille Douai depuis septembre 2014. Il a développé au sein du département des activités de recherche très soutenues dans les domaines de l'optimisation des transferts thermo fluidiques avec notamment le développement d'une plateforme logicielle d'optimisation topologique totalement innovantes et dans la simulation des phénomènes de transport dans les suspensions non colloïdales. Ces travaux de recherche ont fait l'objet d'une production scientifique tout à fait remarquable avec un grand nombre de publications dans de grandes revues internationales ainsi que l'élaboration de plusieurs codes de calculs d'un intérêt très important pour le rayonnement du laboratoire et le développement de collaborations scientifiques avec des partenaires académiques et industriels. En outre, Monsieur Talib DBOUK a une activité d'encadrement de chercheur conséquente avec quatre thèses encadrées, un postdocdorant, un ingénieur de recherche et deux étudiants de Master. Par la qualité des développements scientifiques de son parcours, par les encadrements de thèses assurés et les activités mentionnés ci-dessus, M. Talib DBOUK a selon moi pleinement les compétences nécessaires à la direction de thèses.

J'émets donc un avis très favorable à la préparation par M. Talib DBOUK d'une Habilitation à Diriger des Recherches.

Fait à Douai**, le** 03/12/2018 **NOM et SIGNATURE**

PIÈCES À JOINDRE :

- **Un curriculum vitae détaillé de vos activités pédagogiques et scientifiques (publications, ouvrage, travaux) de 2 pages MAXIMUM. (1 page pour les activités pédagogiques et 1 page pour les activités de recherche)**

Université Polytechnique HAUTS-DE-FRANCE

Délibération 2019-03-COR R

Séance du 21 mars 2019

Extrait du recueil des actes de la Commission de la Recherche du Conseil Académique réunie en formation restreinte aux représentants des Enseignants-Chercheurs

Avis sur la demande d'inscription à l'Habilitation à Diriger des Recherches (HDR) de M. DBOUK Talib

La Commission de la Recherche du Conseil Académique de l'UPHF s'est réunie en séance restreinte dans la salle du conseil - Maison des Services à l'Etudiant le jeudi 21 mars 2019, sur la convocation de Monsieur Abdelhakim ARTIBA, Président de l'Université et, en application de l'article 12 des statuts de l'Université Polytechnique Hauts-de-France, sous la présidence de Monsieur Eric MARKIEWICZ, Vice-Président de la Commission de la Recherche ;

Le quorum étant atteint,

Vu l'arrêté du 23 novembre 1988 relatif à l'Habilitation à Diriger des Recherches ;

Monsieur le Vice-Président de la Commission de la Recherche du Conseil Académique en formation restreinte aux représentants des enseignants-chercheurs titulaires d'une Habilitation à Diriger des Recherches (HDR), présente la demande d'inscription à l'Habilitation à Diriger des Recherches (HDR) formulée par Monsieur DBOUK Talib afin d'encadrer des doctorants et poursuivre des projets de recherche.

Après en avoir délibéré,

La Commission de la Recherche du Conseil Académique rend un avis favorable à l'unanimité des membres, titulaires d'une Habilitation à Diriger des Recherches (HDR), sur la demande d'inscription à l'Habilitation à Diriger des Recherches de Monsieur DBOUK Talib.

Valenciennes, le 22 mars 2019

Le Président de
l'Université Polytechnique Hauts-de-France
Professeur Abdelhakim ARTIBA

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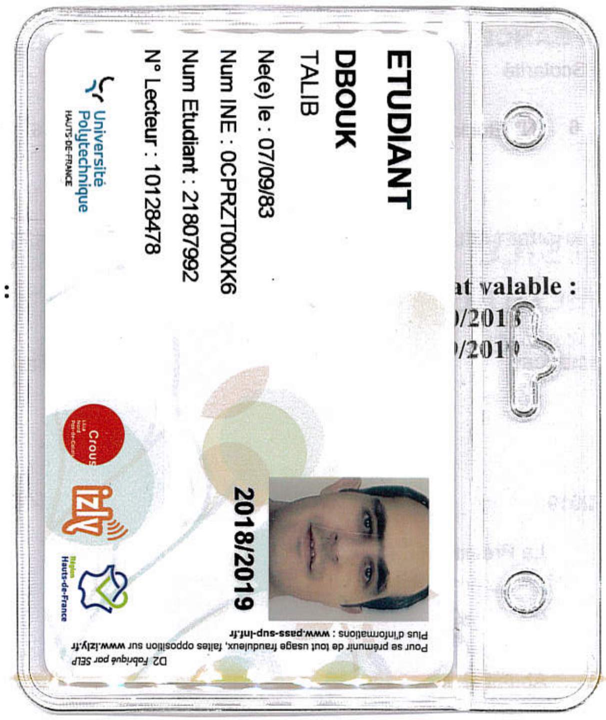

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Lundi, Mardi, Mercredi Jeudi, Vendredi	8h00 - 19h00
Samedi	8h00 - 13h00

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Douai, 10 décembre 2018

Attestation

Je soussigné, Jean-Luc HARION, Professeur à l'IMT Lille Douai et Directeur de la Thèse de M. Vignaesh SUBRAMANIAM intitulée « *Topology Optimization of Conjugated Heat Transfer Devices: Experimental and Numerical Investigation* », débutée le 4 janvier 2016 au Département Energétique Industrielle de l'IMT Lille Douai, atteste que cette thèse a été encadrée à 100% par M. Talib DBOUK.
La de thèse de M. Vignaesh SUBRAMANIAM a été soutenue avec succès le 7 décembre 2018.
Durant tout le déroulement de cette thèse, M. Talib DBOUK a assuré avec une grande efficacité et une attention constante l'encadrement de de ce travail.
Il a de plus pour très large part, et avec une très grande acuité et maturité scientifiques, défini et planifié le contenu et le déroulement de cette thèse qui s'intègre parfaitement dans la stratégie de développement de son axe de recherche.
La Direction de thèse que j'ai assurée s'est limitée au suivi régulier de l'avancement, aux échanges réguliers avec l'encadrant et le doctorant, ainsi qu'aux relectures de mémoire de thèse et articles.
Au vu de ces éléments, je considère sans aucune réserve que l'encadrement de cette thèse est entièrement sien et que M. Talib DBOUK a toutes les capacités d'encadrement, d'attention à l'avancement et au suivi, ainsi qu'à la définition stratégique de sujets de thèse et de partenariats pertinents. Il a ainsi, à mon sens, toutes capacités à diriger des thèses.

Pour faire valoir ce que de droit.

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In

memory

of

my

father

Ahmad DBOUK (1950 - 2009)

Abstract

Complex thermofluid flows like concentrated non-colloidal suspensions and fluid flows in porous media are present in many mechanical, chemical, geological, civil, biological, industrial and process engineering applications (e.g. blood, concrete, oil and fuels, cosmetics, detergents, drilling muds, rivers, food processing, cpu coolers, heat exchangers, etc).

Developing advanced numerical methods and robust, reliable and sustainable Computational Fluid Dynamics (CFD) tools is very important. These numerical tools, thanks to the High Performance Computing (HPC) resources today (I.e. affordable clusters, cloud and parallel computing) permit scientists to deeply analyze different complex multiscale multiphysics phenomena. They allow deep analysis, understanding and knowledge of the different phenomena (multiphase fluid flow dynamics, heat and mass transfer) while reducing both time and money costs compared to mounting of expensive experimental setups.

Topology Optimization of complex thermofluid flows and systems allow designing unpredictable artificially intelligent optimal components at different scales such as optimal heat exchangers, static and dynamic mixers, coolers, separators, heaters, air pollution filters, biogaz separators, etc. Topology optimization is known to produce optimal designs of complex geometries where the fabrication is not a big issue today ! This is thanks to the technology of additive manufacturing or 3D printing. The optimal component design produced by topology optimization can ensure different important features based on the user's desired options such as: a maximum energy efficiency, a minimum weight, a maximum rigidity and a minimum pressure drop, all for predefined objective functions and at different industrial constraints.

My research, development and innovation activities and scientific contributions during the last decade have been developing in this context. They are grouped into three major research axes or themes: **Axis no.1** - Complex-fluid flows of non-colloidal suspensions, **Axis no.2** - Topology optimization and design of complex thermofluid flow systems, and **Axis no.3** - Multi-component fluid flows in adsorbent porous media. These three research axes have been contributing importantly to the scientific reputation of all my host research units during the last decade. They constitute a solid academic database and a huge potential for future scientific reputation. This is due to multiple undergoing scientific collaborations with different national and international universities, institutions and industrial partners.

My research activities have been always developed trying to propose future solutions strategies in attempts to overcome some of the coming socioeconomic and industrial challenges (i.e. optimization and design of innovative components and materials, pollution reduction, energy savings and energy efficient new technologies).

Keywords: Topology optimization, adjoint methods, non-linear programming, optimization algorithms, constrained optimization, conjugated heat and mass transfer, non-colloidal suspensions, granular media, computational physics, computational fluid dynamics (CFD), high performance computing (HPC), parallel computing, numerical analysis, open-source code, C++, multiphase complex fluids, flow in porous media, multi-component adsorption, fluid structure interaction, Finite Volume Method, Immersed Boundary Method

Résumé

Les écoulements thermofluidiques complexes, tels que les suspensions concentrées des particules non-colloïdales, et les fluides dans des milieux poreux, sont présents dans de nombreuses applications en génie mécanique, chimique, géologique, civile, biologique, industrielle et de procédés (e.g. sang, béton, huiles et combustibles, cosmétiques, détergents, boues, rivières, aliments, refroidisseurs de processeurs, échangeurs de chaleur, etc).

Développer des methodes numériques avancées et des outils de CFD (Computational Fluid Dynamics) robustes, fiables et durables est très important. Aujourd'hui, grâce aux ressources HPC (High Performance Computing) et les grands centres de calculs abordables, les clouds et calculs parallèles, ces outils numériques permettent aux scientifiques d'analyser en profondeur différents phénomènes complexes multi-échelles multi-physiques. Ils permettent une analyse approfondie, la compréhension et la connaissance des différents phénomènes (dynamique des fluides multiphasiques, transfert de chaleur et de masse) tout en réduisant les coûts en temps et en argent par rapport à des montages expérimentaux coûteux.

L'optimisation Topologique des systèmes thermofluidiques complexes permet de concevoir des composants optimaux imprévisibles intelligents artificiellement à différentes échelles, tels que des échangeurs de chaleur optimaux, des mélangeurs statiques et dynamiques, des refroidisseurs, des séparateurs, des réservoirs de stockage de la chaleur, des ballons d'eau chaude sanitaires, des filtres de pollution atmosphérique, des séparateurs de biogaz, etc. L'optimisation topologique est bien connue pour produire des conceptions ou designs optimales de géométries complexes où la fabrication n'est plus un gros problème aujourd'hui grâce à la technologie de fabrication additive ou l'impression 3D. La conception optimale des composants produite par l'optimisation topologique peut assurer différentes caractéristiques importantes en fonction des options souhaitées par l'utilisateur, telles que: une efficacité énergétique maximale, un poids minimal, une rigidité maximale et une perte de charge minimale, tout pour des fonctions objectives prédéfinies et pour des différentes contraintes industrielles.

Mes activités de recherche, de développement et d'innovation et mes contributions scientifiques au cours de la dernière décennie se sont développées dans ce contexte. Ils sont regroupés en trois grands axes ou thèmes de recherche: **Axe n.1** – Écoulement complexe de suspensions non-colloïdales, **Axe n.2** – Optimisation topologique et conception optimale de systèmes complexes thermofluidiques et **Axe n.3** – Écoulement aux composants multiples dans des milieux poreux adsorbants. Ces trois axes de recherche ont largement contribué à la réputation scientifique de toutes mes unités de recherche hôtes au cours de la dernière décennie. Ils constituent une base de données universitaire solide et un énorme potentiel pour une réputation scientifique au future. Cela est dû à de multiples collaborations scientifiques en cours avec différentes universités, institutions et partenaires industriels, nationaux et internationaux.

Mes activités de recherche ont toujours été développées en essayant de proposer des stratégies de solutions futures pour tenter de surmonter certains défis socio-économiques et industriels (optimisation et conception de composants et matériaux innovants, réduction de la pollution, nouvelles technologies avec une basse consommation ou maximum éfficacité énergétique).

Mot clés: Optimization topologique, méthode d'adjoints, programmation non-linéaire, algorithmes d'optimisation, optimisation sous contraintes, transfert de chaleur et du masse, suspensions non-colloïdales, milieux granulaires, physique numériques, CFD, calcul haute

performance, calcul parallèle, analyses numériques, code open-source, C++, fluides complexes multiphasiques, écoulement en milieux poreux, adsorption multi-composants, interaction fluide structure, Méthode des Volumes Finis, Méthode des frontières immergées

Acknowledgements

First, I would like to express my sincere gratitude and thanks to my family: my mother Loubna, my brother Bilal and my sisters Houda and Nada for their continuous support and sacrifices.

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I would like to express my sincere gratitude and thanks to the 3 Professors reporters and all the jury members who accepted the invitation to report and review this HDR manuscript.

I owe my deep gratitude to: Institut Mines-Télécom (IMT), Mines-Douai, IMT Lille Douai, IMT Atlantique, University of Haut-de-France, University of Lille, University of Nantes, University of Côte d'Azur, CEMEF Mines-ParisTech, University of Nice-Sophia Antipolis, Lebanese University, American University of Beirut, Lebanese International University, French CNRS, Lebanese CNRS, CEA-Cadarache, IRSN®, CEDRE France-Liban, Région Haut-de-France, ArcelorMittal®, Valeo®, EcoTech-CERAM®, Boet-Stopson®, for supporting and funding my different research projects.

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Many thanks to my colleagues and friends at the internal research unit (Amir, Caroline, Chrystèle, Daniel, François, Jean-Philippe, Jules, Julien, Mélanie, Mohammed, Nadine, Odin, Patrice, Pascale, Rémi, Serge, Souria).

A special thanks to Dr. J.-P. VERMEULEN for his continuous listening and his useful discussions.

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A special thanks to "Thérèse" for her listening, friendship and discussions.

I would like to express my sincere gratitude and special thanks to Prof. Jean-Luc HARION (at IMT Lille Douai), for his continuous support, scientific collaborations and discussions, his kindness and continuous encouragement.

[1]Institut Mines-Télécom Lille-Douai

[2]Centre d'Enseignement, de Recherche et d'Innovation Énergie et Environement

[3]Efficacité Énergétique des Composants, Systèmes et Procédés

A special thanks to Prof. Pascaline PRÉ (at IMT Atlantique, University of Nantes), for her useful discussions and scientific collaboration.

Thanks to Prof. Vincent THOMY (at IEMN, University of Lille), for his useful discussions and scientific collaboration.

I would like to express my sincere gratitude and special thanks to Prof. Elisabeth LEMAIRE (at INPHYNI, Nice), for her continuous support, kindness and encouragement. I mention also Laurent and François.

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Thanks to all my friends outside the research unit (Abbas, Abir, Ahmad, Ali, Ayman, Bachar, Bilal, Charbel, David, Dmytro, Elias, Elie, Fadi, Fadl, Frédéric, George, Habib, Harry, Hassan, Hussein, Ibrahim, Jean, Jean-Marie, Julien, Kader, Kamal, Lala, Laurent, Lilla, Moamar, Mohammad, Moussa, Nacho, Omar, Patrick, Pavel, Pierre, Prashantha, Rafic, Salim, Samer, Sami, Sébastien, Tammam, Tarik, Thérèse, Toufic, Valerie, Yan).

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A special thanks to all my PhD students that i have been supervising and collaborating with during the last years: Vignaesh SUBRAMANIAM, Hatim BELKHOU, Charlène OCTAU, Hassan KARKABA and Masoud MOAZZEN, for their patience, valuable efforts and scientific discussions and collaboration.

Finally, very much thanks to all our junior researchers for whom I shared with great moments the last five years, and for whom we believe in to follow and continue the different research missions and path. I mention: PhD students (Assadour, Bineet, Charlène, Hatim, Hassan, Joseph, Mohammed, Mohammed-Amine, Masoud, Samer and Vignaesh), Masters students (Amine, Chinh, Victor), Research Engineers (Mahdi), and all the post-Graduate and under-graduate students for their hard work efforts and scientific contributions to our IMT institution and our research unit overall development and reputation, and each person who contributed in one way or another to my personal R&D&I works which made this manuscript possible.

*"If i forgot to mention your name, and you are reading this: please forgive me **:-)** "*

The Future ? : From *Real-Physics* to *Digital-Physics* :

Research and development in Physics, Applied Sciences and Engineering induce a constant flow of innovations and breakthroughs that vitalize the future of industry and society where academic research (Public Institutions and Universities) is complementary to the applied R&D conducted by industry (NAE, 2003). "We are today in a world of "bits" and bytes" ("0" and "1") and no more in a world of atoms. We are in the era of digital sociology, digital media, computing and society where computational science is becoming in fact a new "science of society". A very good example is AI (Artificial Intelligence) where machines are expected to mimic humans in the near future.

"As a *numerical* Physicist, I still believe in the huge potential behind the "C++ programming language"(Stroustrup, 2013) applied to: "Physics", "Mathematics", "Engineering" Sciences and "Algorithms coding". Moreover, I believe in the open source codes (opensource.com, 2018) philosophy and their use in research and engineering, linear and nonlinear programming, and in code development communities that try to make our world better and propose more efficient and robust solutions and correct predictions for the coming socioeconomic challenges in the context of Numerical and Ecological Transitions of Societies (i.e. Pollution and Environmental Climate Change Challenges, see Climate Extremes and Society by Diaz and Murnane, 2008, Energy Efficient, Connected and Artificial Intelligent Systems)."

Manuscript structure

This manuscript is divided into 6 chapters grouped under 3 parts and one appendix as the following:

Part I (Chapters 1 and 2) shows my Curriculum Vitae and general introduction including a statistical list for my: research and pedagogic activities, scientific publications, communications, scientific awards and prizes and the different research projects that i have been enrolled in during the last decade.

Part II (Chapters 3, 4 and 5) present a summary with some discussions of my Research, Development and Innovation activities that i have been developing under **3 major research axes**: **Axis no.1 - Complex-fluid flows of non-colloidal suspensions**, **Axis no.2 - Topology optimization and design of complex thermofluid flow systems**, and **Axis no.3 - Multi-component fluid flows in adsorbent porous media**. Through these 3 research axes, I have been contributing majorly to the new infrastructure or "chassis" building of our research unit structure during the last 5 years at: the ex-DEI[1] (named now ECSP[2]) at the IMT-LD[3]. These 3 axes constitute a solid background and huge potential for future scientific national and international reputation due to multi-interactions with both internal and external research units. They integrate very well the research themes of our IMT institution and our new research center named CERI-EE[4].

Part III (Chapter 6) introduces my research and development project-plan and perspectives for the next decade, and their position in the new CERI-EE[4] at the IMT-LD[3]. In this Chapter future research and development activities to be developed are proposed that might contribute well to our research unit development activities and reputation, and to the overall scientific community (i.e. future scientific collaborations opportunities, research projects and funding plans, industrial sectors targeting, etc). This part III is in the context of trying to propose future solutions strategies to try to overcome some of the coming socioeconomic challenges in different research axes/topics (i.e. optimization and design, innovative materials, pollution reduction, energy savings technology, renewable energy resources, etc).

The attached **Appendix** groups all author's scientific publications.

[1] Département Énergétique Industrielle
[2] Efficacité Énergétique des Composants, Systèmes et Procédés
[3] Institut Mines-Télécom Lille-Douai
[4] Centre d'Enseignement, de Recherche et d'Innovation - Énérgie et Environnement

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Part I

My Curriculum Vitae

1 My Curriculum Vitae

Dr. Talib DBOUK

Date of birth:

07/09/1983

Attachment (Research Host), September 2014 - Present :

IMT Lille-Douai, i-Site member, University of Lille, North of Europe

Research Center, 764 Blvd. Lahure, 59500, Douai - FRANCE

CERI-EE, ECSP Research Unit (ex-Département Énergétique Industrielle)

Qualifications MCF: CNU section 60

Mâitre-assistant: September 2014 (Status: Armines Contract)

Nomination: July 2016

Titularisation (*fonctionnaire*): October 2017

E-mail: talib.dbouk@imt-lille-douai.fr

Some Online Research Production Profiles:

Google Scholar: Talib Dbouk

ResearchgGate ID: Talib Dbouk

ORCID ID: 0000-0002-9710-4978

Personal Webpage:

http://www.talibdbouk.com

Member in social and professional organizations:

Order of Engineers and Architectures (OEA), Beirut, Lebanon

La Société Française de Thermique (SFT)

La Société Française de Génie des Procédés (SFGP)

L'Association Française des Utilisateurs et Utilisatrices d'Openfoam (FOAM-U)

1.1 Scientific Influence

Table 1.1 shows my statistical data for the number of supervised (and co-supervised) Postdoc, PhD, Masters (MSc) and Research Engineers (RE) students that I have been supervising since 2014/2015. For more details about my percentage supervision per student (in French: *"taux d'encadrement"*), see section 1.4.2.

Supervised Students	Postdoc	PhD	MSc	RE
Finished	1	2	3	1
Running	0	3	0	0
Total	1	5	3	1

TABLE 1.1: Number of Postdoc, PhD, Master (MSc) and Research Engineers (RE) that I have been supervising since 2014/2015. More detailed information about the percentages of supervision per student are provided in section 1.4.2.

Table 1.2 shows my scientific influence through the production of scientific articles published after my PhD (defended on 14^{th} of December 2011). For more details, see section 1.4.3.

Type	Quantity	*Status*
Article in peer-review journal (*ACL**)	16	*Published*
	6	*Under Review*
Article in conference proceeding (*PCL***)	8	*Published*
Total	30	

TABLE 1.2: Production of scientific articles (see section 1.4.3).
**Article dans un journal scientifique avec comité de lecture.*
**Proceeding dans une conférence internationale avec comité de lecture.*

Table 1.3 shows my scientific communications in many international and national conferences. For more details, see section 1.4.4.

Type	Quantity
Oral presentation	20
Poster	14

TABLE 1.3: Scientific communications in international and national conferences (see section 1.4.4).

International scientific prizes/awards are shown in table 1.4 (for more details, see section 1.4.11).

Award	Year	Organization
PhD Grant Award	2008	French Ministry of Higher Education
Best PhD thesis in France	2017	Foam-U Association
Best Paper	2018	Proceeding ENFHT-2018-Conference
Best Poster	2017	JJC-GEPROC-UGEPE

TABLE 1.4: Scientific awards and prizes (see section 1.4.11).

Over the last decade 6 huge new CFD scientific codes have been developed and maintained by the author inside the open-source OpenFOAM® C++ library as shown in table 1.5 (for more details, see section 1.4.8). These advanced new CFD solvers (or codes) have produced several R&D activities enriching the numerical CFD scientific community by the modeling and simulation of different complex thermofluid and topology optimization applications.

Developped CFD codes	**Quantity**	Numerical Platform
New Solvers (codes)	6	OpenFOAM®

TABLE 1.5: Developped Open-Source CFD solvers (codes) for different thermofluid and optimization applications (for more details, see section 1.4.8).

1.1.1 Reporter - reviewer for:

- Structural and Multidisciplinary Optimization
- Journal of Fluid Mechanics
- Journal of Non-Newtonian Fluid Mechanics
- Physics of Fluids
- International Journal of Heat and Fluid Flow
- International Journal of Heat and Mass Transfer
- International Communications in Heat and Mass Transfer
- Mathematics and Computers in Simulation
- Applied Thermal Engineering
- Chemical Engineering and Processing
- Chemical Engineering Communications
- Chemical Engineering Research and Design
- Chemical Engineering Science
- Energy
- International Journal of Thermal Sciences
- Modern Physics Letters B
- Engineering Applications of Computational Fluid Mechanics
- Journal of Mechanical Engineering Science
- Frontiers in Heat and Mass Transfer
- Transactions of FAMENA
- Mechanics and Industry
- Materials
- EuroTherm Seminars
- SFT Conferences

1.1.2 Academic Member Editorial Board of:

- International Journal of Hydromechatronics
- Viser Technology - Viser Journal Publishing

1.2 Academic and professional backgrounds

September 2014 – Present: Maître-Assistant (*Associate Professor*)

- (Maître-Assistant): IMT-LD[3], ECSP[2], CERI-EE[4], Douai, France.

  Research Axes:

- **Axis no. 1:** Complex-fluid flows of non-colloidal suspensions
- **Axis no. 2:** Topology optimization and design of complex thermofluid flow systems
- **Axis no. 3:** Multi-component fluid flows in adsorbent porous media

September 2013 – August 2014: Post-Doc.

- CEA-Cadarache IRSN (Radioprotection and Nuclear Safety Institution) - Saint-Paul-Lez-Durance, France.
- *Research topic: Rheology of immersed granular materials in presence of Hydrodynamic interactions.*

January 2012 – June 2013: Post-Doc.

- Centre de Mise en Forme des Matériaux, CEMEF - Mines-ParisTech <> Arcelormittal Research, Sophia Antipolis Research Campus, Sophia Antipolis, France.
- *Research topic: Study and Development of scientific calculation codes (Fast-Models) for industrial strip rolling processes with thin film lubrication.*

October 2008 – December 2011: PhD

- L'Institut de Physique de Nice (l'INPHYNI CNRS UMR 7010) (previously LPMC Nice), University of Côte d'Azur, Nice, France.
- ***PhD topic:*** *Rheology of concentrated suspensions and shear-induced particles migration.*
- ***Defended on*** *18 December 2011 at LPMC, CNRS UMR 7010, Nice.*
- ***Mention****: Très Honorable avec les Félicitations du jury.*
- ***Jury Members:***
  M. Georges BOSSIS, ***Président***, *DR CNRS, Inst. de Physique de Nice, Univ. Côte d'Azur*
  Mme. Elisabeth GUAZZELLI, ***Rapporteur***, *DR CNRS, IUSTI, Univ. Aix-Marseille*
  M. Fadl MOUKALLED, ***Rapporteur***, *DR, CFD Department, American University of Beirut*
  M. Laurent LOBRY, ***Co-Directeur***, *CR CNRS, Inst. de Physique de Nice, Univ. Côte d'Azur*
  Mme. Elisabeth LEMAIRE, ***Directeur***, *DR CNRS, Inst. de Physique de Nice, Univ. Côte d'Azur*
  M. Georges GAUTHIER, ***Examinateur***, *MCF CNRS, Labo. FAST, Univ. de Paris-Sud 11*

Mars 2008 – September 2008: Master II-R

- Laboratoire de Thermique et Energie de Nantes LTEN - CNRS UMR 6607 - Ecole Polytechnique de Nantes, Ecole Centrale de Nantes, University of Nantes, Nantes, France.
- *Research Topic: Liquid-Liquid Dispersion and Chaotic Advection in Heat Exchangers (Modeling and simulation).*

September 2002 – September 2008: Diploma in Mechanical Engineering

- Lebanese University, Faculty of Engineering -III, Al Hadath, Beirut, Lebanon.

1.3 Varying Skills: Keywords

1.3.1 Theory

Applied Physics: Topology Optimization; Rheology of Fluids and Complex Materials; Non-colloidal suspension flows; Conjugated Heat Transfer; Mass Transfer; Mixing and Separation; Adsorption; Fluid Structure Interaction (FSI); Suspension Structure Interaction (SSI); Heating and Cooling Techniques; Pinch analysis and Process integration; Tribology; Porous media; micro-fluidics.

1.3.2 Numerics

Algorithms; Numerical Modeling; Numerical Analysis; Computational Fluid Dynamics (CFD); Numerical Methods: Topology Optimization, Immersed Boundary Method (IBM), Finite Volumes Method (FVM), Discrete Elements Method (DEM), Programming-and-Development of scientific computation codes; user-machine Interfaces, High Performance and Cloud Computing (HPC).

Linux/Unix® operating systems; open source CFD tools (OpenFOAM®) and CAD tools (FreeCAD®); open source mesh generation tools (GMSH®; SALOME®, etc); programming languages (C++®, Fortran®); Latex®; Open-Office®.

1.3.3 Experiments

Microscopy, Rheometry, Normal Stresses quantification, Suspensions of Particles, Shear-Induced Migration and Infrared Thermography.

1.3.4 Communications

Coordination and management of R&D studies; Research projects developments and writing according to the French and International European Systems; National and International scientific collaborations; Bibliographical Research and deep literature review; Writing technical and progress reports; Evaluation and valuation of results; National and International Conferences; Scientific publications in high-impact peer-reviewed journals; Reviewer and reporter of several scientific peer-reviewed journals

1.4 Research Activities and Responsibilities (2014 – Present)

1.4.1 Scientific Skills : Research, Development and Innovation

- Applied Physics (Theory, Modeling and Simulation, CFD)
- Condensed matter behavior (Complex-fluids flows : Suspensions, Micro-fluidics, Porous Materials)
- Opimization and Design Techniques : Topology Optimization
- Rheology of complex fluids (Theory and Measurements)
- Conjugate Heat Transfer (Heating and Cooling Technologies)
- Fluid Structure Interaction (FSI)
- Suspension Structure Interaction (SSI)
- Multi-component fluid flows in adsorbent porous materials
- Scientific Code Developments (Programming & Debug in C++® language)
- High performance parallel and Cloud Computing (HPC)

1.4.2 Some Research Projects (including funding and role as supervisor in %)

Funding Total Mass enrolled in research projects ≈ 1.07 M€

- **Postdoc project no.1** (April 2015 – April 2016)
  Postdoc's Name: Dr. Rémi GAUTIER
  Host Institution: IMT Lille-Douai
  Research Topic: Pressure-swing adsorption of gaseous mixture in isotropic porous medium: Transient 3D Modeling and Validation
  Supervisors: T. DBOUK **(100%)**
  Partners: Prof. Jean-Luc HARION (IMT Lille-Douai), Prof. Pascaline PRÉ (IMT Atlantique, Nantes)
  Funding: 104 K€, Institut Mines-Télécom
  Dr. Rémi GAUTIER is now a permanent Assistant Professor and a colleague at IMT Lille-Douai, EE-CERI, ECSP, Douai, France

  Two PhD defended (one PhD student supervised at 100% and one PhD student supervised at 30%), and three additional PhD students which are still running:

- **PhD project no.1** (January 2016 – December 2018)
  Student's Name: M. Vignaesh SUBRAMNIAM
  Host Institution: IMT Lille-Douai
  Research Topic: Topology optimization of conjugated heat transfer devices: experimental and numerical investigation
  PhD Defended on: 07 December 2018
  Supervisors: J.L.-HARION, T. DBOUK **(100%)**
  Funding: 50.4 K€ IMT Lille-Douai (ARMINES contract)
  Dr. Vignaesh SUBRAMNIAM is now a permanent R&D Engineer at VALEO®-Thermal Systems Group, working between France and India

- **PhD project no.2** (January 2017 – January 2020)
  Student's Name: M. Hatim BELKHOU
  Host Institution: IMT Lille-Douai
  Research Topic: Heat Transfer Enhancement of Embedded heat exchangers by surface structuring
  PhD to be defended on: December 2019
  Supervisors: D. BOUGEARD (10%), T. DBOUK **(30%)**, S. RUSSEIL (30%), M. MOBTIL (30%)
  Partners: N.-Y. FRANCOIS (VALEO®, Paris)
  Funding: 50.4 K€, VALEO® Group Thermal Systems (thèse cifre – inside a 6 years Industrial chair **NEO (Numerical and Experimental Optimization platform for efficient design of automotive heat exchangers)**)

- **PhD project no.3** (January 2016 – September 2019)
  Student's Name: Mme. Charlène OCTAU
  Host Institutions (external): ALSTOM® and LAMIH, University of Valenciennes
  Research Topic: Particles transport emitted during railway braking systems: an experimental and numerical investigation
  PhD to be defended on: September 2019
  Supervisors: T. DBOUK **(30%)** at IMT Lille-Douai; L. KEIRSBULK et al. (70%) at LAMIH, University of Haut-de-France
  Funding: 250 K€ ALSTOM® (thèse cifre)

- **PhD project no.4** (September 2018 – September 2021)
  Student's Name: M. Hassan KARKABA
  Host Institutions: Lebanese International University (LIU)-Lebanon and IMT Lille-Douai
  Research Topic: Design space exploration to find optimal designs of vortex generators for heat transfer enhancement
  Supervisors: **T. DBOUK (30%)**, S. RUSSEIL (25%), D. BOUGEARD (10%) at IMT Lille-Douai; C. HABCHI (25%) at NDU University Lebanon and T. LEMENAND (10%) at Angers University
  Funding: 50.4 K€, LIU University - Lebanon (50%) and IMT Lille-Douai - France (50%)

- **PhD project no.5** (March 2019 – March 2022)
  Student's Name: M. Masoud MOAZZEN
  Host Institutions: IMT Lille-Douai and IEMN Lille
  Research Topic: Cooling of Electronic Components by using Non-Colloidal Suspensions
  Supervisors: **T. DBOUK (34%)**, D. BOUGEARD (33%) at IMT Lille-Douai; V. THOMY (33%) at IEMN, Institut d'électronique, de microélectronique et de nanotechnologie, Lille
  Funding: 50.4 K€, Haut-de-France Region (50%) and IMT Lille-Douai (50%).

- **Master II-R project no.1** (April 2017 – September 2017)
  Student's Name: M. Trung-Chinh NGUYEN
  Host Institution: IMT Lille-Douai
  Research Topic: Development of spacial filters in CFD for topology optimization technique
  Master: Physique, Mécanique, Sciences de l'Ingénieur, Génie des Systèmes Industriels, Univesity of Rouen
  Supervisor: T. DBOUK **(100%)**
  Funding: 3000 €, An internship funded by IMT Lille-Douai

M. Trung-Chinh NGUYEN is now a research engineer consultant at Aries Consultants Group (Énergie-Air-Aerodynamique), Brussels, Belgium

- **Master II-R project no.2** (July 2018 – November 2018)
  Five months training-ship
  Student's Name: M. Amine KASSOU
  Host Institution: IMT Lille-Douai
  Research Topic: CFD numerical modeling and simulation of indoor polluted air removal by adsorptive walls
  Master2-PEE Procédés, Energie Et Environnement (ENSTA ParisTech)
  Supervisors: T. DBOUK **(50%)**, R. GAUTIER (50%)
  Funding: 2500 € An internship funded by IMT Lille-Douai

- **Master II-R project no.3** (October 2018 – Mars 2019)
  Six months training-ship
  Student's Name: M. Victor VAILLANT
  Host Institution: IMT Lille-Douai
  Research Topic: Pressure Swing Adsorption of Gaseous Mixture: Numerical Simulation and Optimisation Prospects
  Master II-R, Option: Energy Efficiency (IMT Lille-Douai)
  Supervisors: T. DBOUK **(50%)**, R. GAUTIER (50%)
  Funding: An internship funded by IMT Lille-Douai

- **Research Engineering Project** (April 2016 – December 2017)
  Nine months research project
  Researcher's Name : M. Mahdi REZAEI
  Host Institution: IMT Lille-Douai
  Research Topic: CFD 3D modeling and simulation of isothermal turbulent fluid flows in industrial silencers: uncertainty and quantification of pressure drop
  Supervisor: T. DBOUK **(100%)**
  Funding: 60 K€, Boet-Stopson® - Lille
  M. Mahdi REZAEI is now a CFD Researcher at the University of Strasbourg, ICube, CNRS UMR 7357

1.4.3 List of scientific publications

[Note : all my scientific articles are attached in the Appendix]

Published articles in peer-reviewed journals

[1] V. SUBRAMANIAM, **T. DBOUK**, J.-L. Harion, "Topology optimization of conjugate heat transfer systems: A competition between heat transfer enhancement and pressure drop reduction". **International Journal of Heat and Fluid Flow**, 75, 165-184 (**2019**).

DOI: https://doi.org/10.1016/j.ijheatfluidflow.2019.01.002

[2] **T. DBOUK**, "A new technology for CPU chip cooling by concentrated suspension flow of non-colloidal particles". **Applied Thermal Engineering**, 146, 664-673, 5 January (**2019**).

DOI: https://doi.org/10.1016/j.applthermaleng.2018.10.044

[3] **T. DBOUK**, "Heat transfer and shear-induced migration in dense non-Brownian suspension flows: Modelling and simulation". **Journal of Fluid Mechanics**, volume 840, (**2018**).

DOI: https://doi.org/10.1017/jfm.2018.72

[4] V. SUBRAMANIAM, **T. DBOUK**, J.-L. Harion, "Topology optimization of conductive heat transfer devices: An experimental investigation", **Applied Thermal Engineering**, 131, 390-411, (**2018**).

DOI: https://doi.org/10.1016/j.applthermaleng.2017.12.026

[5] R. GAUTIER, **T. DBOUK**, M.A. CAMPESI, L. HAMON, J.-L. Harion and P. PRÉ, "Pressure-swing-adsorption of gaseous mixture in isotropic porous medium : Transient 3D modeling and validation". **Chemical Engineering Journal**, 348, 1049-1062, (**2018**).

DOI: https://doi.org/10.1016/j.cej.2017.05.145

[6] R. GAUTIER, **T. DBOUK**, J.-L. Harion, L. HAMON and P. PRÉ, "Pressure-swing-adsorption of gaseous mixture in isotropic porous medium: Numerical sensitivity analysis in CFD". **Chemical Engineering Research and Design**, 129, 314-326, (**2018**).

DOI: https://doi.org/10.1016/j.cherd.2017.11.007

[7] **T. DBOUK**, "A review about the engineering design of optimal heat transfer systems using topology optimization". **Applied Thermal Engineering**, Vol 112, pp 841–854, (**2017**).

DOI: http://dx.doi.org/10.1016/j.applthermaleng.2016.10.134

[8] **T. DBOUK** "A Suspension Balance Direct-Forcing Immersed Boundary Model for wet granular flows including obstacles". **Journal of Non-Newtonian fluid Mechanics**, 230, 68-79 (**2016**).

DOI: http://dx.doi.org/10.1016/j.jnnfm.2016.01.003

[9] **T. DBOUK**, F. Perales, F. Babik and R. Mozul "A DF-IBM/NSCD coupling framework to simulate immersed particle interactions". **Comput. Methods Appl. Mech. Engrg.**, 309, p. 610–624 (**2016**).

DOI: http://dx.doi.org/10.1016/j.cma.2016.05.041

[10] **T. DBOUK** and J.-L. Harion "Performance of Optimization Algorithms Applied to Large Nonlinear Constrained Problems". **American Journal of Algorithms and Computing**, 2 (1) pp. 32-56 (**2015**).

[11] **T. DBOUK**, P. Montmitonnet, N. Suzuki, Y. Takahama, N. Legrand, T. Ngo and H. Matsumoto "Advanced roll bite models for cold and temper rolling processes". **La Metallurgia Italiana**, 4, (**2015**).

[12] **T. DBOUK**, P. Montmitonnet, N. Legrand "Two-dimentional Roll Bite Model with lubrication for Cold Strip Rolling". **Advanced Materials Research** Vols. 966-967, pp. 48-62 (**2014**).

DOI: 10.4028/www.scientific.net/AMR.966-967.48

[13]**T. DBOUK**, L. Lobry, E. Lemaire, and F. Moukalled, "Shear-induced Particles Migration: Predictions from Experimental Determination of The Particle Stress Tensor". **Journal of Non-Newtonian fluid Mechanics**, 198, pp. 78-95, August (**2013**).

DOI: http://dx.doi.org/10.1016/j.jnnfm.2013.03.006

[14] **T. DBOUK**, L. Lobry, E. Lemaire, "Normal stresses in concentrated non-Brownian suspensions". **Journal of Fluid Mechanics**, Volume 715, pp 239-272, January (**2013**).

DOI: http://dx.doi.org/10.1017/jfm.2012.516

[15] **T. DBOUK**, C. HABCHI, "On the mixing enhancement in concentrated non-colloidal isodense suspensions of rigid particles using helical coiled and chaotic twisted pipes: A numerical investigation". **Chemical Engineering and Processing: Process Intensification**, 141, (**2019**).

[16] **T. DBOUK**, "A computational framework with an Adaptive Mesh Refinement technique for concentrated suspension flows". **Particulate Science and Technology**, 1-10, (**2019**).

Under review **articles in peer-reviewed journals**

[17] S.A. BAHRANI, J.F. MORRIS, **T. DBOUK**, "Destabilization of immersed granular beds by natural convection". **Phys. Rev. Fluids**, under review, submitted April (**2019**).

[18] **T. DBOUK**, S.A. BAHRANI, "Modeling of natural convection in suspension flows: Buoyancy-driven destabilization of immersed granular beds". **Phys. Rev. E**, under review, submitted Mai (**2019**).

[19] C. OCTAU, **T. DBOUK**, M. Watremez, D. Meresse M. Lippert, J. Schiffler, L. Keirsbulck, L. Dubar, "Liquid-solid two-phase jet in a turbulent crossflow: Experiments and simulations". **Chemical Engineering Research and Design**, under review, submitted April (**2019**).

[20] H. BELKHOU, S. RUSSEIL, **T. DBOUK**, M. MOBTIL, D. BOUGEARD, N.-Y. FRANCOIS, "Large Eddy Simulation of boundary layer transition over an isolated ramp-type micro roughness element". **International Journal of Heat and Fluid Flow**, under review, submitted August (**2019**).

[21] M. REZAEI, **T. DBOUK**, F. DELABRE, B. DUMUR, V. FLORQUIN, G. VANDENBOSSCHE, D. BOUGEARD, "Experimental and numerical investigations of turbulent fluid flow in industrial silencers", under review, submitted August (**2019**).

[22] **T. DBOUK**, J. Dirker, V. Fachinotti and L.G. Page. "Necessary factors for robust topology optimization methods: A numerical benchmark applied to generated-heat in surface-to-point removal", under review, submitted August (**2019**).

Published articles in peer-review conference proceedings

[23] H. Belkhou, S. Russeil, **T. DBOUK**, M. Mobtil, D. Bougeard, N. François, “Influence of surface roughness elements on heat transfer in transitional flows: a cfd investigation”. **Proceeding** of the XI International Conference on Computational Heat, Mass and Momentum Transfer, Cracow, Poland, May 21-24 (**2018**).

[24] C. Octau, M. Lippert, **T. DBOUK**, A. Graziani, M. Watremez, L. Keirsbulck and L. Dubar, "Particles transport in railway braking systems: an experimental and numerical investigation". **Proceeding** of the ASME 2017 Fluids Engineering Division Summer Meeting, Waikoloa, Hawaii, USA, 31-July–3-August (**2017**).

[25] R. Gautier, **T. DBOUK**, L. Hamon, P. Pré, D. Bougeard, "Intensification d’un procédé de séparation de gaz par adsorption: étude numérique par simulations CFD 3D et influence de la géométrie du lit adsorbant". **Proceeding** 16ème Congrès de la Société Française de Génie des Procédés, Nancy, du 11 au 13 Juillet (**2017**).

[26] V. Subramaniam, **T. DBOUK**, J.-L. Harion, "Optimisation topologique decomposantsconducteurs de chaleur: étude expérimentale". 25ème Congrès Français de Thermique, Subramaniam-SFT-2017, Marseille, du 30 Mai au 2 Juin (**2017**).

[27] M.-A. Campesi, R. Gautier, **T. DBOUK**, O. Moussa, L. Hamon, F.-X. Blanchet, Y. Gouriou, J.-L. Harion, P. Pré, "Study of a novel heat exchanger asdorber concept for CO2 capture". Physical and Chemical Phenomena in Heat Exchangers and Multifunctional Reactors for Sustainable Technology: Eurotherm Seminar 106, Paris, France, 10-11 Octobre (**2016**).

[28] F. Perales, F. Dubois, Y. Monerie, R. Mozul, F. Babik, **T. DBOUK**, R. Monod, "Xper : une plateforme pour la simulation numérique distribuée d’interactions multiphysiques entre

corps", CSMA2015 proceedings, 12e Colloque National en Calcul des Structures, Presqu'île de Giens, Var, France, 18-22 Mai (**2015**).

[29] **T. DBOUK**, P. Montmitonnet, H. Matsumoto, N. Suzuki, Y. Takahama, N. Legrand, and T. Ngo, "Advanced Roll Bite Models for Cold and Temper Rolling Processes". **Proceeding** of 9th International & 6th European Rolling Conference, Venice, Italy, June (**2013**).

[30] S.A. Bahrani, **T. DBOUK**, J.F. Morris, "Déstabilisation en mode séquentiel d'un lit granulaire immergé par une source thermique". **Proceeding** of XIVe Colloque International Franco-Québécois: Énergies Durables, CIFQ2019, Québéc, Canada, 18 June **2019**.

Pre-prints

[31] **T. DBOUK**, "*AdsorpReactingFoam*®, a computational platform for multi-component adsorption and reactive flows in OpenFOAM®", preprint, July (2019).

[32] **T. DBOUK**, "VOC pollutants reduction in indoor-environment by adsorptive materials and fresh air ventilation: CFD scenarios modeling, simulation and validation in OpenFOAM®", preprint, July (2019).

1.4.4 List of Scientific Communications

Total no. of **oral presentations** = **23**; Total no. of **Posters** = **15**

- 18 June 2019, CIFQ2019 - XIVe Colloque International Franco-Québécois: Énergies Durables. Québéc, Canada. "Déstabilisation en mode séquentiel d'un lit granulaire immergé par une source thermique". (***Oral + Poster***)
- 12 june 2019, 4th French/Belgian OpenFOAM users conference Marseille, France. "Buoyancy-driven instability of immersed granular bed of micro-particles". (***Oral***)
- 11 june 2018, the 25th Anniversary of the European Community on Computational Methods in Applied Sciences (ECCOMAS), the 6th European Conference on Computational Mechanics (Solids, Structures and Coupled Problems) (ECCM 6) and the 7th European Conference on Computational Fluid Dynamics (ECFD 7), Glasgow, UK. "Multiobjective topology optimization applied to conjugate heat transfer problems". (***Oral***)
- 23-24 May 2018, 3rd French OpenFOAM® users conference, Valenciennes, France. "Research and development activities using OpenFOAM at the Energy Engineering Department of IMT Lille Douai". (***Oral***)
- 21-24 May 2018, XI-th International Conference on Computational Heat, Mass and Momentum Transfer (ICCHMT). Cracow, Poland. "Influence of surface roughness elements on heat transfer in transitional flows: a cfd numerical investigation". (***Poster***)
- 16 May 2018, Journée thématique (Thermique dans les écoulements de fluides complexes), Société Français de thermique (SFT), "Heat transfer and shear-induced migration in dense non-Brownian suspension flows: Modelling and Simulation". (***Oral - Invited Speaker***).
- 07 November 2017, Journée Jeunes Chercheurs 2017 (JJC'17) – GEPROC UgéPE, Douai, France. "Infrared Thermal Measurements in Conductive Heat Transfer Tree-Like Structures Obtained by Topology Optimization". (***Poster***)
- 07 November 2017, Journée Jeunes Chercheurs 2017 (JJC'17) – GEPROC UgéPE, Douai, France. "Optimisation de forme d'un adsorbeur échangeur de chaleur" . (***Poster***)
- 07 November 2017, Journée Jeunes Chercheurs 2017 (JJC'17) – GEPROC UgéPE, Douai, France. "Intensification du transfert de chaleur dans les échangeurs embarqués par structurations de surface". (***Poster***)
- 30 May - 02 June 2017, 25ème Congrès Français de Thermique, Marseille, France. "Optimisation topologique des composants conducteurs de chaleur: étude expérimentale". (***Oral + Poster***)
- 03 May 2017, Invited Speaker, Scientific Seminar, Notre Dame University, Zok Mosbeh, Beirut, Lebanon. "Gas separation in packed bed of adsorbing porous medium: Modeling and Simulation". (***Oral***)
- 28 April 2017, IMT National Conference, Colloque « L'énergie en révolution numérique », Paris, France. "Numerical optimization platform developments for designing optimal heat exchangers". (***Poster***)
- 24 April 2017, IMT Research Seminar, University of Lille, Villeneuve d'ascq, France. "Numerical optimization platform developments for designing optimal heat exchangers". (***Poster***)

- 21-22 March 2017, 2ndes journées françaises des utilisateurs de OpenFOAM®, Nevers, France. "TOPOF: Topology Optimization Platform in OpenFOAM®". (***Oral***)
- 30-31 January 2017, 6èmes Journées de l' Association Française de l'Adsorption, Paris, France. "Simulations numériques 3D d'un procédé de séparation de gaz par adsorption (PSA)". (***Oral***)
- 10-11 November 2016, Invited Speaker, Annual Meeting on Rheology, Alicante, Spain. "Dynamic-Scale Modeling of non Brownian suspensions including suspension/structure interactions". (***Oral***)
- 10-11 October 2016, Eurotherm Seminar 106, Paris, France. Physical and Chemical Phenomena in Heat Exchangers and Multifunctional Reactors for Sustainable Technology, "Study of a novel heat exchanger adsorber concept for CO2 capture". (***Oral***)
- 06 October 2016, Journée Jeunes Chercheurs 2016 (JJC'16) – GEPROC UgéPE, Louvain, Belgium. "Topology optimization of conductive heat transfer devices: An experimental investigation". (***Poster***)
- 30 June 2016, Journée des Doctorants 2016 (JDD'16), Douai France. "Topology optimization of conductive heat transfer devices: An experimental investigation". (***Poster***)* (* : Best Poster Award)
- 19-23 June 2016, 5th International Conference on Engineering Optimization, Iguassu Falls, Brazil. "Topology optimization of 2D and 3D heat conduction structures". (***Oral***)
- 31 May - 03 June 2016, Congrès Français de Thermique, Toulouse, France. "Optimisation topologique 3D des systèmes de conduction de la chaleur". (***Poster***)
- 18 May 2016, Journée des utilisateurs OpenFOAM, Rouen, Normandie, France. "Dynamic-Multi-Scale Modeling and Simulation of Immersed Granular Flows over Obstacles". (***Oral***)
- 15-17 July 2015, International conference: 17th British-French-German Conference on Optimization, BFG 2015, Imperial College, London, UK. "An optimization algorithm of high performance for inequality-constrained bounded nonlinear optimization problems". (***Oral***)
- 18-22 May 2015, International conference: 12e Colloque National en Calcul des Structures, CSMA 2015, Presqu'ile de Giens (Var), France. "Xper : une plateforme pour la simulation numérique distribuée d'interactions multiphysiques entre corps". (***Poster***)
- 09-11 July 2014, International conference: Modeling Granular Media Across Scales 2014, Montpellier, France. 'Numerical Modeling of the Dynamics of Immersed Granular Materials'. (***Oral***)
- 22-24 June 2014, The 6th International Conference on Tribology in Manufacturing Processes & Joining by Plastic Deformation, Darmstadt, Germany: 'Advanced Roll Bite Models for Cold and Temper Rolling Processes'. (***Oral***)
- 5-6 Nov 2013, Workshop on Numerical Modelling of Grains/Fluid Flows, ENS, Lyon, France: 'A Suspension Balance Model for the flows of non-Brownian Suspensions of hard spheres'. (***Oral***)
- 10-12 June 2013, The 9th International Rolling Conference and the 6th European Rolling Conference, Venice, Italy: 'Advanced Roll Bite Models for Cold and Temper Rolling Processes'. (***Oral***)

- 05-10 August 2012, The 16th International Congress on Rheology, Lisbon, Portugal: 'Normal Stresses in non-Brownian suspension'. (***Poster***)
- 23 January 2012, Les Rencontres Niçoises de Mécanique des Fluides, Laboratoire Jean-Alexandre Dieudonné, Nice, France: 'Rheology of concentrated suspensions and Shear-induced migration'. (***Oral***)
- 9-13 October 2011, 83rd Annual Meeting of the Society of Rheology, Cleveland, Ohio, USA: 'Normal stresses in concentrated non-colloidal suspensions (Experiments and Simulations)'. (***Poster***)
- 13-16 June 2011, 6th OpenFOAM Workshop, Penn state, USA: 'An Incompressible Multi Phase Solver'. (***Oral***)
- 18-19 Nov 2010, GISEC 2010, Nice, France: 'Normal stress measurements in non-Brownian Suspensions'. (***Oral***)
- 7-9 April 2010, 6th Annual European Rheology Conference (AERC), Göteborg, Sweden: 'Normal stresses in sheared non-Brownian suspensions'. (***Oral***)
- 27 Novembre 2009, le Groupe Français de Rhéologie (GDR MePhy), Paris, France: 'Measurements of Normal Stresses in sheared Stokesian suspensions'. (***Oral***)
- 15-17 April 2009, 5th Annual European Rheology Conference (AERC), Cardiff, United Kingdom: 'Particle migration in suspensions flowing between rotating parallel-plates: The role of the secondary flow'. (***Poster***)

1.4.5 Scientific Missions and Experience

In addition to my contribution in writing the technical annexes, and proposals for the research projects mentioned in section 1.4.2, here below some additional professional experience in developing, writing and depositing (as principal coordinator) of some national and international research projects:

1.4.5.1 additional Experience in Research projects proposals

1- ERC-StG 2016 - European Research Council - project proposal deposit

ERC Panel: PE8 - Products and Processes Engineering.

Project Title: Performance Improvement of Additive-Manufactured Components by Topology Optimization (Acronym: PIACTO).

ERC Keywords: Computational engineering; Energy processes engineering; Simulation engineering and modelling; Scientific computing, Simulation and modelling tools.

Project Duration (months) = 60. **Requested Funding** = 1.497 M€

Final decision: rejected.

2- ERC-StG 2018 - European Research Council - project proposal deposit

ERC Panel: PE3 - Condensed Matter Physics.

Project Title: Topology Optimization Platform for the control of Shear-Induced-Migration phenomenon in suspension flows (Acronym: TOPSIM).

ERC Keywords: Fluid dynamics; Structure and dynamics of disordered systems: soft matter (suspensions); Computational engineering; Application of mathematics in sciences.

Project Duration (months) = 60. **Requested Funding** = 1.499 M€

Final decision: rejected.

3- ANR-JCJC - 2018/2019 - Research project proposal deposit

Project coordinator: T. DBOUK, **Scientific partner**: A. BAHRANI

ERC Panel: PE3 - Condensed Matter Physics.

Project Title: Suspension Structure Interaction in presence of heat transfer (Acronym: ProSSI).

Keywords: suspension structure interaction; non-isothermal non-colloidal suspensions.

Project Duration (months) = 48. **Requested Funding** = 750 K€

External Scientific Collaborators: Prof. Jeffrey F. MORRIS (Levich Institute of Technology, City College University of New York).

Internal Scientific Collaborators: Prof. Jean-Christophe BAUDEZ (IMT Lille Douai).

Final decision: rejected (a new attempt will be done in 2019/2020).

4- Regional PhD thesis funding proposal deposit (2016/2017)

PhD title: Heat transfer intensification in heat exchangers by using non-colloidal suspensions.

Internal Scientific Collaborators: Prof. Daniel BOUGEARD, Dr. Serge RUSSEIL (IMT Lille Douai, Energy Engineering Department).

Final decision: Three years PhD funding was accepted, but the selected foreign student did not get Visa validation for France.

5- Regional PhD thesis funding proposal deposit (2017/2018)

PhD title: cooling of electronic components by using non-colloidal suspension flows.

External Scientific Collaborators: Prof. Vincent THOMY (IEMN, Institut d'électronique, de microélectronique et de nanotechnologie, Lille, France).

Final decision: Three years PhD funding was accepted (50% Region funding, 50% IMT funding). PhD student started on 01 March 2019.

6- Six months funding by China for a foreign PhD researcher (2019/2020)

Research topic: Optimization, modeling and simulation of future generation heat exchangers.

External Scientific Collaborators: Prof. Wang Dingbiao, Zengzhou University, China).

Final decision: Six months funding of $\approx$ 20 K€ was accepted by China. Under the supervision of T. DBOUK, the PhD researcher M. Wang Guanghui will start on 01 October 2019.

1.4.6 Accomplished and on-going research projects, 2014 - Present

Research projects hosted internally at the IMT Lille Douai - ECSP[2], CERI-EE[4]:

A- **Industrial project**: Modeling and simulation of fluid flow in industrial silencers.

Project Period: April 2016 – December 2017

Industrial partner: Boet-Stopson®, SIM-Engineering®, Lille, France.

My role: Principal coordinator of project and co-supervisor.

Affected Researcher: Research Engineer: MSc. M. Mahdi REZAEI.

Scientific Partners: Prof. Daniel BOUGEARD (IMT Lille Douai), MSc. M. Florian DELABRE and Dr. Véronique FLORQUIN (Boet-Stopson®), Dr. Benjamin DUMUR and Dr. Guillaume VANDENBOSSCHE (SIM-Engineering®).

B- **Industrial Chair NEO®**: Two PhD's and one postdoc fundings over 6 years.

Project Period: January 2017 – January 2022

Funding by Industrial partner: VALEO® Thermal Systems Research Group, Paris, France.

My role: Principal coordinator of the Optimization, Modeling and Simulation R&D Tasks, and co-supervisor of students.

PhD no.1: Heat Transfer Enhancement of Embedded heat exchangers by surface structuring (macro-micro-ramp roughness elements): CFD simulations and experimental measurements.

PhD Student (Cifre): M. Hatim BELKHOU; expected PhD defense date: January 2020.

Postdoc: Large-scale inequality optimization algorithms for parallel computing (HPC) applied in CFD simulations. Starting date: January/February 2019.

PhD no.2: Heat transfer intensification in heat exchangers by topology optimization.

Starting date: January 2020.

Scientific Partners: Dr. Serge RUSSEIL, Dr. Mohammed MOBTIL and Prof. Daniel BOUGEARD (IMT Lille Douai), Nicolas-Yoan FRANCOIS (VALEO®).

C- **Industrial Project**: Heat Storage systems - EcoStock-II.

Project Period: January 2018 – July 2019

Industrial partner: EcoTech-CERAM®, Rivesaltes, France.

My role: Principal coordinator of the Optimization, Modeling and Simulation R&D Tasks.

Affected Researchers (collaborator) : Dr. Rémi GAUTIER, IMT Lille Douai, Energy Engineering Department.

Scientific Partners: Dr. Rémi GAUTIER and Prof. Daniel BOUGEARD (IMT Lille Douai), Guilhem DEJEAN (EcoTech-CERAM®), Aubin TOUZO (PROMES, CNRS UPR 8521, Perpignan).

D- **Academic Project**: Optimization, modeling and simulation of future generation heat exchangers.

Project Period: October 2019 – March 2020

My role: Principal coordinator and co-supervisor

PhD Student: M. Wang Guanghui, Zhengzhou University, Zhengzhou, China.

Funding by : National Natural Science Foundation of China.

Scientific Partners: Prof. Wang Dingbiao (Zhengzhou University, Zhengzhou, China).

Research projects hosted at exterior academic and industrial institutions:

E- **Industrial Project**: Particles transport emitted from trains braking systems.

Project Period: January 2017 – January 2022

Funding by Industrial partner: ALSTOM®, France.

My role: Principal coordinator and supervisor of the Modeling and Simulation R&D Tasks.

PhD Student (Cifre): Mme. Charlène OCTAU; expected PhD defense date: September 2019.

Host Institution: LAMIH, CNRS UMR 8201, University of Haut-de-France, Valenciennes, France.

Scientific Partners: Prof. Laurent KEIRSBULCK, Prof. Laurent DUBAR, Dr. Marc WATREMEZ, Dr. Damien MERESSE, Marc LIPPERT and Jesse SCHIFFLER (LAMIH, CNRS UMR 8201, Valenciennes, France).

1.4.7 External Scientific Collaborations and Networks

1.4.7.1 National Universities and Research Institutions

Prof. Elisabeth LEMAIRE, INPHYNI CNRS UMR, **University of Côte d'Azur**, Nice.

Prof. Pierre MOTMITONNET, CEMEF-MinesParisTech, **University of Côte d'Azur**, Sophia Antipolis.

Prof. Pascaline PRÉ, IMT Atlantique, GEPEA CNRS UMR, **University of Nantes**, Nantes.

Prof. Laurent KEIRSBULCK, LAMIH CNRS UMR 8201, **University of Haut-de-France**, Valenciennes.

Dr. Laurent LOBRY, INPHYNI CNRS UMR, **University of Côte d'Azur**, Nice.

Dr. Vincent THOMY, IEMN CNRS UMR, **University of Lille**, Lille.

Dr. Frédéric PERALES, **LPTM, CEA-Cadarache (IRSN)**, St-Paul-Lez-Durance.

Dr. Lomig HAMON, IMT Atlantique, GEPEA CNRS UMR, **University of Nantes**, Nantes.

Dr. Rainier HREIZ, LRGP CNRS UMR, **University of Lorraine**, Nancy.

1.4.7.2 International Universities and Research Institutions

Prof. Jeffrey F. MORRIS, **City College University of New York**, New York, USA.

Prof. Fadl MOKALLED, **American University of Beirut**, Beirut, Lebanon.

Prof. Marwan DARWISH, **American University of Beirut**, Beirut, Lebanon.

Prof. Hiromi MATSUMOTO, **University of Kitakyushu**, Japan.

Dr. Lina BAROUDI, **Manhattan College**, Manhattan, USA.

Dr. Joe ALEXANDERSEN, **Technical University of Denmark** (DTU), Denmark.

Dr. Charbel HABCHI, **Notre-Damme University**, Zouk Mosbeh, Lebanon.

Dr. Jaco DIRKER, **University of Pretoria**, Pretoria, South Africa.

Dr. Victor FACHINOTTI, **Santa Fe University**, Argentina.

Prof. Jean-Marie BUCHELIN, **Von Karman Institute for Fluid Dynamics**, Brussels, Belgium.

Dr. Lilla KOLOSZAR, **Von Karman Institute for Fluid Dynamics**, Brussels, Belgium.

1.4.7.3 Industrial Applied Research Collaborations

M. Nicolas-Yoan FRANCOIS, R&D Project Manager, VALEO® Thermal Systems Research Group, Paris, France.

Dr. Nicolas LEGRAND, R&D Project Manager, ArcelorMittal® Burns Harbor Research, Luxembourg.

Dr. Ludovic Marquant, R&D Project Manager, ARC® International, Arques, France.

1.4.8 Numerical codes developments

Here below an overview list of some of the CFD solvers that I have been personally developing since the last decade:

Several scientific computation codes and tools in CFD (Several millions lines of code):

2010/2011: 3D Solver development for immersed granular flows (suspensions of rigid particles immersed in a fluid).

Solver Name: SbmFoam® (for concentrated suspensions **simple shear flows**)

online link

Integration Library: OpenFOAM® Library (C++) - under the GNU (GPL) General Public Licence.

2011/2012: 3D Solver development for immersed granular flows (suspensions of rigid particles immersed in a fluid).

Solver Name: SbmGeneralFoam® (for concentrated suspensions **general flows**) online link

Integration Library: OpenFOAM® Library (C++) - under the GNU (GPL) General Public Licence.

2012/2013: Advanced 2D Solver development for simulating the rolling loads in a cold strip rolling process (with lubrication).

Solver Name: RollGap®

Integration Library: Fortran90.

2013/2014: 3D solver for fluid/structure interactions (wet granular flows) using the immersed boundary method coupled to a non-smooth contacts dynamics method. **Solver Name**: Xper® online link Integration Library: Xper: IRSN-LMGC90 research laboratories open source C++/Fortran developed library.

2012 - 2015: 3D solver for suspension/structure interactions (suspension flows over obstacles) using the immersed boundary method coupled to a suspension balance model. Solver Name: SbIBMFoam® online link Integration Library: OpenFOAM® Library (C++) - under the GNU (GPL) General Public Licence.

2014/2015: Topology optimization 3D solver for designing optimum heat conduction systems.

Solver Name: TopOptHCFoam®

Optimization Algorithm : MMA, GCMMA (Svanberg, 1987; Svanberg, 2002)

Integration Library: OpenFOAM® Library (C++) - under the GNU (GPL) General Public Licence.

2017/2018: 3D Solver for quasi-compressible immersed granular flows (suspensions of rigid particles immersed in a fluid) including heat transfer, shear-induced migration and buoyancy effects.

Solver Name: SBMHTFoam®

Integration Library: OpenFOAM® Library (C++) - under the GNU (GPL) General Public Licence.

2015 - 2018: 3D Topology Optimization Solver for Multi-Objective Conjugate Heat Transfer Problems (steady laminar flows).

Solver Name: MOadjOptChtFoamMMA®

Optimization Algorithm : MMA, GCMMA (Svanberg, 1987; Svanberg, 2002)

Integration Library: OpenFOAM® Library (C++) - under the GNU (GPL) General Public Licence.

2018 - 2019: 3D CFD Solver for the adsorption/desorption of Multi-component reacting gaseous mixtures in porous media.

Solver Name: AdsorpReactingFoam®

Integration Library: OpenFOAM® Library (C++) - under the GNU (GPL) General Public Licence.

1.4.9 Committee member: organization of scientific events

Organizing of many national and international conferences (+ journées Thématiques):

- Eurotherm Seminar 106, Physical and chemical phenomena in heat exchanger and multifunctional reactor for sustainable technology, 10-11 October 2016, Paris, France.

  https://eurotherm106.sciencesconf.org/

- 9ème Journée des Jeunes Chercheurs, GEPROC et l'UgéPE, 07 November 2017, Douai, France.

  http://conference.mines-douai.fr/JJC-GEPROC-UGEPE-2017

- 3rd French OpenFOAM® users conference (Joint Franco/Belgian OpenFOAM users conference), 23-24 May 2018, Valenciennes, France.

  http://foam-u.fr/3rdfrenchopenfoamconf/

Invitation of several external scientists to conduct internal scientific seminars at our Energy Engineering Department at IMT Lille Douai:

- Dr. Rainier HREIZ, Laboratoire Réactions et Génie des Procédés - UMR 7274, University of Lorraine, Nancy, France.
- Dr. Jaco DIRKER, Department of Mechanical and aeronautical Engineering, University of Pretoria, Pretoria, South-Africa.

1.4.10 Role as a jury member in externally defended PhD's

One participation in a PhD defense as a jury member examinator:

PhD defended by: Dr. Florian DUGAST, on 15 Oct. **2018**.
University of Nantes, LTEN Research Department, CNRS-UMR 6607.
PhD Title: "Développement d'une méthode d'optimisation topologique du composant de transfert par convection".

1.4.11 Scientific Prizes and Awards

- **PhD Grant Award for 3 years**, French Ministry of Higher Education, University of Nice-Sophia Antipolis, September 2008 - September 2011.

- **Best PhD thesis Award**, Best PhD in France in CFD developped with OpenFOAM®. Association Foam-U®, Nevers meeting, Nevers, France, 2017. For more information Click here.

- **Best Paper Award** – Proceeding of 3rd ENFHT-2018 Conference – Budapest - Hungary. Fore more information Click here.

- **Best Poster Award** – JJC-GEPROC-UGEPE 2017 - Douai - France.

1.4.12 Enveloppes soleau - Innovation Potential

For more information about the E-soleau, click here.

Six Enveloppes soleau deposit as the following:

- **T. DBOUK**, Refroidissement des microprocesseurs par un écoulement type suspension des particules solides micrométriques immergées dans un liquide, **INPI enveloppe soleau, no. 581337, 19/01/2017**.
- **T. DBOUK**, Un nouveau liquide de refroidissement dans les échangeurs thermiques : à la base d'une suspension concentrée des particules rigides (micrométriques en taille) immergées dans un liquide Newtonien ou non-Newtonien, et migration de ces particules induite par le cisaillement, **INPI enveloppe soleau, no. 581816, 27/01/2017**.
- **T. DBOUK**, Code de calcul d'optimisation topologique des systèmes de conduction de la chaleur et des systèmes d'écoulement incompressible, **INPI enveloppe soleau, no. 589412, 31/07/2017**.
- **T. DBOUK**, H. BELKHOU, Échangeurs thermiques à plaques brasées et déformées par des géométries de nid d'abeilles, **e-Soleau, DSO2018000806, 22/01/2018**.
- **T. DBOUK**, Échangeurs thermiques éco-intelligents, **e-Soleau, DSO2018001531, 06/02/2018**.
- **K. PRASHANTHA, T. DBOUK, C. DUC**, Sustainable multifunctional wood for advanced applications, **e-Soleau, 30/10/2018**.

1.5 Pedagogic Activities and Responsibilities (September 2014 - Present)

At IMT Lille-Douai, since september 2014, I have approximately about **220 hours per year** as an averaged pedagogic hours (course preparations, course lectures, student reports, supervision of projects, jury member, etc). More details for the pedagogic hours per year are provided in the coming sections (1.5.1.1), (1.5.1.2) and (1.5.1.3).

The total pedagogic hours, between September 2014 and present date, are provided in section (1.5.2).

1.5.1 Constant-rate pedagogic activities (Per Year)

Major : Energy Engineering Students

1.5.1.1 Course Lecturer (20 hours per year)

- **Course Position at IMT Lille-Douai**: Option Master 2 – Postgraduate Students
- **Academic Module in the EE-CERI**[1] : Energy Efficiency.
- **Label of the course** : An Introduction to PINCH Analysis & Process Integration.
- **Keywords**: Thermodynamics cycles and components; Pinch Technology; Heat Integration; Energy versus Exergy;

Course objective: is to introduce to Postgraduate students the Pinch Technology Approach (principles, theory, fundamental concepts and applications). This technique is the most widely used for designing optimized efficient energy systems by saving Energy and both investment and operating costs.

Benefits : The students will be able to :

- Distinguish between exergy, entropy and energy

- Distinguish between efficient and inefficient energy system designs

- Understand the efficient use of energy and the reduction of environmental effects

- Understand the economic potential to improve energy efficiency

- Distinguish between renewable and non-renewable energy resources in an environmental context

- Save Energy and both investment and operating costs by heat recovery in a process design

- Understand the Methodology for minimum energy consumption of processes (PINCH)

- Design thermodynamic efficient processes (precisely : Efficient Heat Exchangers Networks)

- Use Computer Software for doing quick PINCH Analysis end efficient Heat Exchangers Networks

[1] Energie et Environement: Centre Enseignement, Recherche et Innovation

Course materials :

- Lecture slides (pdf)

- Exercises (TD and TP)

- Computer Software Material (& training) ThermOptim®

Pre-requisites (a recall is done in the course) :

- Concepts of Energy, Entropy and Exergy

- Fundamental Thermodynamics Laws

- Cycles of basic energy technologies

- Thermodynamic Machines & Systems

Some of the Course contents :

- Concepts of Energy, Entropy and Exergy : a quick revision

- Thermodynamics Laws : a quick revision

- Calculate thermodynamic feasible Energy cascade and cost targets

- Optimize heat recovery systems

- Size and Integrate a Heat Exchanger into an Existing Exchanger Network

- Identify Cold, Hot, and Utility Streams in a Process

- Extract Data for Process and Utility Streams

- Construct Composite Curves and Grand Composite Curve

- Estimate Minimum Energy Cost Targets

- Estimate Heat Exchanger Network (HEN) Capital Cost Targets

- Estimate Practical Targets for HEN Design

- Design thermodynamic efficient processes (Efficient Heat Exchangers Network)

- Use of a Computer Software for doing PINCH Analysis

1.5.1.2 Research Discovery Projects (2 PDR = 2 x 80 hours = 160 hours per year)

At my research unit at IMT Lille-Douai, i supervised 9 PDR projects (Projets Découverte de la Recherche), 2 PST project (Projets Scientifiques et Techniques) and 1 PO project (Projet Ouvert), which are summarized in the following:

- PDR no.1 : Breakup of viscoelastic filaments
- PDP no.2 : Numerical simulations of fluid flow around an ellipsoidal rotating obstacle
- PDR no.3 : Optimization of nozzles fro fluid injection inside porous media
- PDP no.4 : Mesh generation methodologies for creating representative meshes for porous media
- PDR no.5 : Thermal comfort notion in residential buildings

- PDR no.6 : Structure boundary capturing algorithm in image processing
- PDR no.7 : Potential of open-source softwares in replacing commercial ones : in the simulation of thermodynamics cycles
- PDR no.8 : A numerical study of a new coolant fluid for electronic components based on non-colloidal suspension flows
- PDR no.9 : Micro-pump performance applied to concentrated non-colloidal suspension flows
- PST no. 1 : Modeling of thermal comfort in achitectural and building applications
- PST no. 2 : Modeling of a house of "North of France type", known by "houses 1930" for better thermal insulation enhancement
- PO no. 1 : Solar Decathlon

Note that each PDR project is usually assigned to a group of students made of 3 or 4 students. The PST projects are usually assigned to more than 4 students. Similarly for the open projects (PO).

1.5.1.3 Energy Engineering Students Projects (40 hours per year)

The Energy Engineering Students Projects include several charges like trainingship reports, final year reports, jury member participations, etc.

1.5.2 Total Accomplished Pedagogic hours (2014 - Present)

- Course Lectures (**66 hours**)
- 9 PDR (9 x 80 = **730 hours**)
- 2 PST (Scientific and Technical Projects) (2 x 120 = **240 hours**)
- 1 OP (open project) (**48 hours**)
- 33 Engineering student projects : reports evaluations, corrections and jury member participation (**132 hours**)

1.5.3 Pedagogic projects development responsibility

- New **MOOC** creation in English for 2019/2020 (**20 hours online-Course** : Pinch Analysis and Process Integration)
- New **International Master of Science** program creation (Diplome National de Master, 120 ECTS, 4 semestres) for 2020/2021 (at CERI-EE, IMT Lille Douai, International visibility Working Group)
  Masters title: Intelligent and Sustainable Buildings for future energy, climate change and environmental challenges.

1.6 Author's profiles SWOT analysis

Here below a SWOT analysis (Strengths, Weakness, Opportunities and Threats) for the author's profile:

- **Strengths:**

  Excellent scientific knowledge in physical science combined to computational science at a high level of numerical skills (i.e. programming, debugging, HPC and cloud computing), social, professional and communication competences, experience in national and international projects writing and funding requests, familiar with research in partnership with industrial environments, and an enormous increasing working capacity (i.e. about 10 articles developed in 2018/2019, i.e. published in high impact peer-reviewed journals, and 3 huge CFD solvers)

- **Weakness:**

  A young researcher attached to a small research unit at the IMT Lille-Douai which is not yet very famous as a national/international research institution due to the fusion of Mines-Douai and Télécom Lille on January 2017.

- **Opportunities:**

  An innovative numerical platform creation for topology optimization in CFD. High attractive potential for future collaborations with international researchers and industrial partners.

- **Threats:**

  Saturation capacity might be a threat, but other threats are still yet unknown compared to other junior/senior researchers' profiles.

2 General Introduction

2.1 My three major research and development axes

The major role of Science is to understand and provide logical explanations for observed physical phenomena, through: **R**esearch, **D**evelopment and **I**nnovation (R&D&I).

Research is investigation, solid literature review and **huge gaps identification from the literature**. This leads to new ideas structuring as possible solutions' proposals with the potential for their degree of feasibility.

Development is the management and right placing of overall achieved personal knowledge, competences and experience in specific domains for the seek of founding and/or finding solutions and the corresponding methodologies.

Innovation is to push further both research and development towards more innovative solutions or concepts but which are unique and replies to the human socioeconomic needs and challenges (Diaz and Murnane, 2008). Innovation, solid Networks and animation are all vital key elements that must be taken into account with care if to attract future fundings for the R&D work.

The new challenges today (Environmental Pollution and the increase (-decrease) in Energy demands (-in Energy sources) and their impacts on industry(NAE, 2003) and extremes weather and climate changes) (Diaz and Murnane, 2008), request research and investigation, and efficient fast problems solving techniques. This goes well with new structuring at IMT Lille Douai with the new CERI-EE[1] creation early 2019. Thus any new R&D activity in this context constitute windows fields for innovation. Many projects calls have been rising and supported by most national and international research organizations and institutions concentrated around the topics of: Energy efficient and optimized systems that are Environment-friendly (in a direction towards pollution and toxic gases emissions reduction and elimination, and at a reduced cost (i.e. for mass production feasibility)).

My research and development activities have been concentrated the last 6 years and oriented in that direction, toward numerical modeling, simulation and optimization in CFD (Computational Fluid Dynamics) of thermofluid systems for better performances at lower cost and minimum pollution. These research activities go very well with the R&D targets as defined by the IMT institution in attempts to gain the leadership in 12 domains under 5 transitions as can be seen in figure 2.1. My research axes are concerned with the domain "Optimisation énergétique" (figure 2.1) for environment-friendly, energy efficient, connected and intelligent future systems. My major objectives have been oriented towards solving problems to reply efficiently to the industrial and socioeconomic needs in this context of research and development activities, and to transmit my acquired knowledge and experience to future generations (Dbouk, 2018b).

[1]Centre d'Enseignement, de Recherche et d'Innovation Energie et Environnement

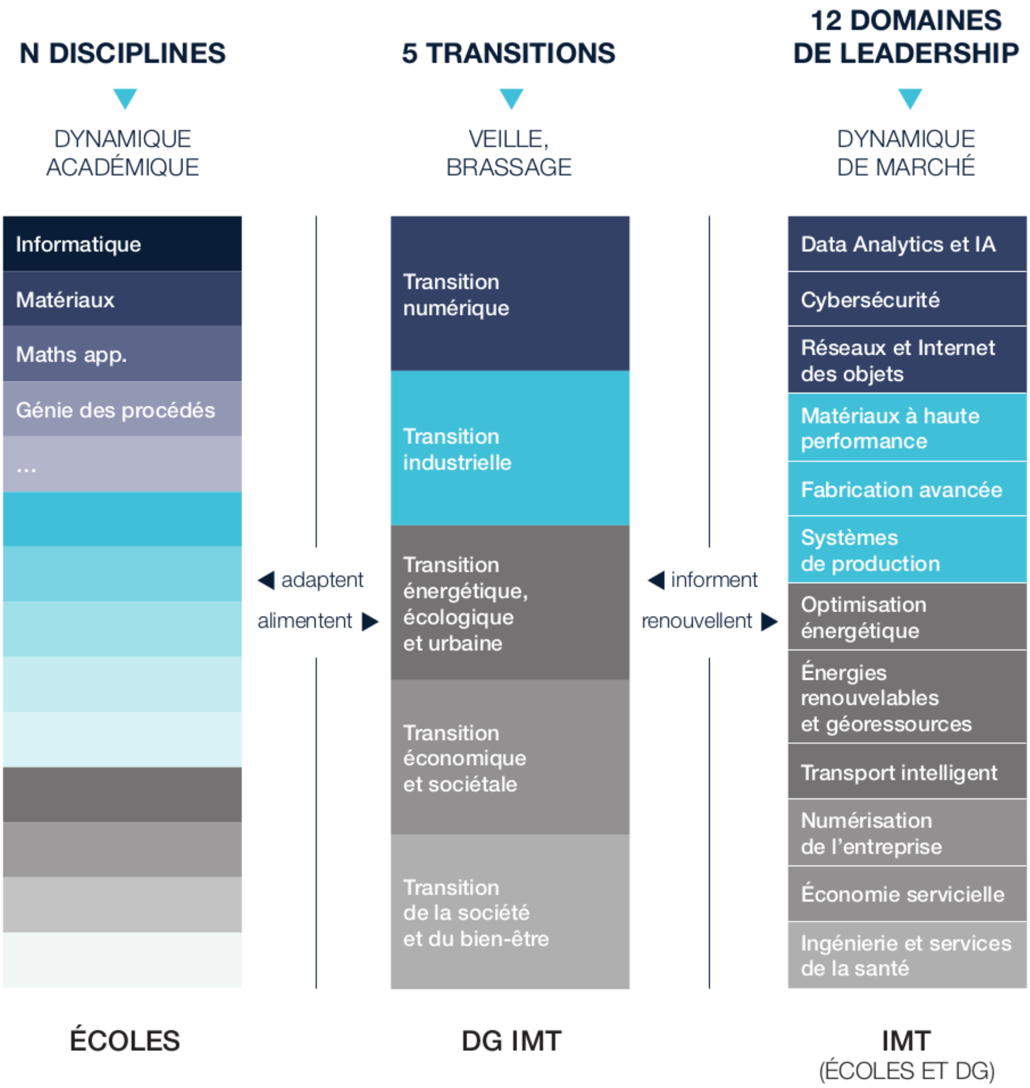


FIGURE 2.1: The twelve research and development leadership domains as defined by the Mines-Telecom Institution (IMT) for the next five years.

Building experimental setups and conducting experimental measurements is essential to better quantify and understand physical phenomena in nature, but they are both time and money consuming. Today thanks to the huge progress in advanced computers and computational power and speed (High Performance, Parallel and Cloud Computing), building numerical models (Algorithms, Artificial Intelligence) is another way that is affordable at lower costs compared to experimental setups and measurements. Of course, experimental measurements will be always required in order to better calibrate, orientate and validate any developed numerical models in the future. In that way, the user gains more confidence in the models to predict and analyze future behaviors of different phenomena with less necessity for numerous experimental setups.

Several numerical methods have been developing to represent the dynamics and behavior of complex thermofluid flows and systems such as: the Finite Difference Method (FDM), the Finite Elements Method (FEM), the Finite Volume Method (FVM), the Lattice Boltzmann Method (LBM), Immersed Boundary Method (IBM), Discrete Elements Method (DEM), etc. My research numerical development activities have been concerned so far with the FVM, IBM and DEM in CFD and their application to optimize, quantify and better understand the dynamics and behavior of complex thermofluid flows and systems at different scales from micro. to macro. (at a Lagrangian flow description, Eulerian description and both coupled Eulerian-Lagrangian), and at different flow regimes: from laminar to turbulent.

In my research and development activities during the last decade i have been working **in parallel** on the following three major R&D&I axes or themes:

Axis no.1 - Complex-fluid flows of non-colloidal suspensions,

Axis no.2 - Topology optimization and design of complex thermofluid flow systems,

Axis no.3 - Multi-component fluid flows in adsorbent porous media

They are summarized briefly in the following:

Axis no.1 - Complex-fluid flows of non-colloidal suspensions:

My first research and development axis focuses on the Rheology of non-colloidal suspensions Stickel and Powell, 2005. Since September 2008, I have been working on this research and development axis to better quantify and understand the Newtonian and non-Newtonian complex behavior of non-colloidal suspension flows that are present in many applications at different scales such as in: chemical engineering, process engineering, civil engineering, geological, biological and mechanical engineering (i.e. detergents, cosmetics, plumes, drilling muds, blood flow, rivers, concrete and cement, oil and fuels transport in pipes, food processing, etc).

The methodology that i have been following is the numerical development (and experimental validation) of different multiscale models (as new CFD codes developments) for quantifying: suspension dynamics, shear-induced migration phenomenon and heat transfer in concentrated non-colloidal suspension flows in different geometries (i.e. via the Finite Volume, Immersed Boundary and Discrete Elements methods, etc).

Understanding the Rheology and the Non-Newtonian complex flow behavior of suspension flows, of particles immersed in liquids, using software engineering tools is essential today for improving and predicting optimal future designs of systems where concentrated suspension flows may be present.

Modeling the dynamics of concentrated rigid particles immersed in a liquid (a "suspension") is a complex task due to the presence of millions of particles, and the manifestation of several phenomena like microstructure orientation changing behavior, shear-induced migration phenomenon as a result of competition between hydrodynamic and friction forces resulting from interactions between the particles and the surrounding fluid, and between the particles themselves (or particle-particle contacts).

Axis no.2 - Topology optimization and design of complex thermofluid flow systems:

My second research and development axis focuses on Topology Optimization Method and Design and its multiphysics applications in multi-scientific disciplines (cross-disciplinary research). One major application that i am enrolled in since September 2014 at the IMT Lille Douai is the optimization of complex thermofluid systems in CFD at different flow regimes and conditions. This is in the objective to propose better energy efficient thermofluid systems and artificially intelligent components (i.e. intelligent heat exchangers, mixers, separators, coolers, heaters, etc).

The topology optimization method Bendsøe and Sigmund, 2004 is an innovative powerful numerical technique that allows one to create and find unpredictable optimal designs for specific predefined objectives and constraints (i.e. equality and inequality constraints). Topology optimization does not require knowing an initial design to be optimized, but it can directly create or find the optimal design (i.e. being the converged solution of the whole optimization problem).

Developing this new advanced research axis at the IMT Lille Douai (at the Energy Engineering Department since September 2014), the methodology i have been following is: the development and validation of macroscopic models and new advanced Algorithms (new CFD codes developments in OpenFOAM®) intended for Topology optimization of thermofluid systems of very large number of degrees of freedom (DOF) (or design variables), and on complex large scale nonuniform unstructured non-stationary meshes or computational grids.

Axis no.3 - Multi-component fluid flows in adsorbent porous media:

My third research and development axis focuses on fluid flows in adsorbent porous media that are present in many applications in nature and industry (i.e. pollutants reduction filters, air purifiers, biogaz seperators, etc). In this third research axis the focus is on surface science with attention to adsorption/desorption phenomena at the gas/solid interface (neglecting chemical reactions between the fluid and solid phases). I have been focusing on this research axis during the last 4 years, and its orientation towards gas separation and gas storage applications or processes through innovative adsorption/desorption modeling and simulation techniques in CFD.

The approach i have been following is the development and validation of macroscopic models (as new CFD codes developments) for better understanding of local adsorption kinematics applied to both: 1- gas separation process in packed beds, and 2- air quality enhancement by removal of pollutants by using adsorptive porous material and air ventilation duct systems.

Today, gas separation and storage process optimization are two important topics for research and investigation. This is due to the fact that energy resources in fuel (petroleum) and oil are decreasing, and the seek of other energy resources like natural or BioGaz (are very important today). This creates a huge opportunity and large potentials for research and developments activities in different applications like in (transport, aerospace, buildings, and industry in general, etc).

Modeling and simulation of adsorption kinematics in adsorptive packed beds in CFD is very important. It permits to:

1. Enhance and optimize the existing industrial systems, applied in gas separation and storage processes, for faster and better adsorption capacity (and thus to increase the natural gas production and storage with an enhanced quality),

2. Investigate new fields/domains of applications like indoor/outdoor air pollution reduction by adsorbent materials.

My scientific competences and maturity degree in each of the three research axes, in addition to the potentials behind for future emerging R&D&I technology and applications are illustrated in figure 2.2. From the Technology Readiness Level scale (TRL) it can be observed that research axis no.1 is more of fundamental research nature than the research axis no.2.

The research axis no.3 is more situated as towards engineering applications and prototypes. Figure 2.3 gives another example of my overall research profile.

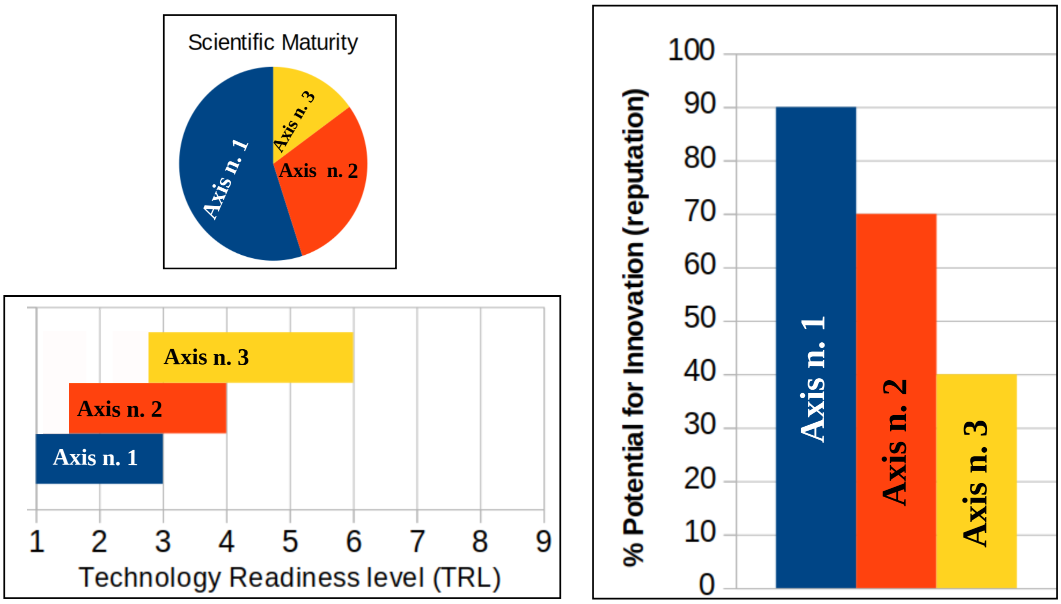


FIGURE 2.2: Author's scientific competences and maturity degree in each of the three research axes.

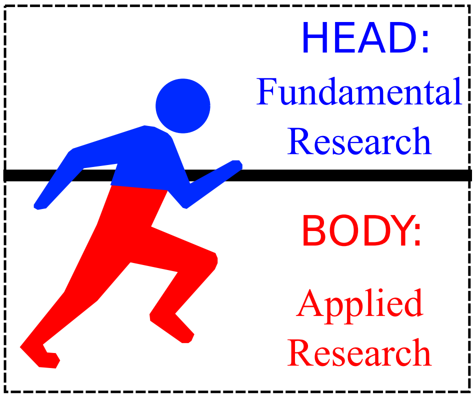


FIGURE 2.3: Author's research profile.

My R&D&I activities are concerned and oriented toward different research topics or keywords as it is illustrated in figure 2.4.

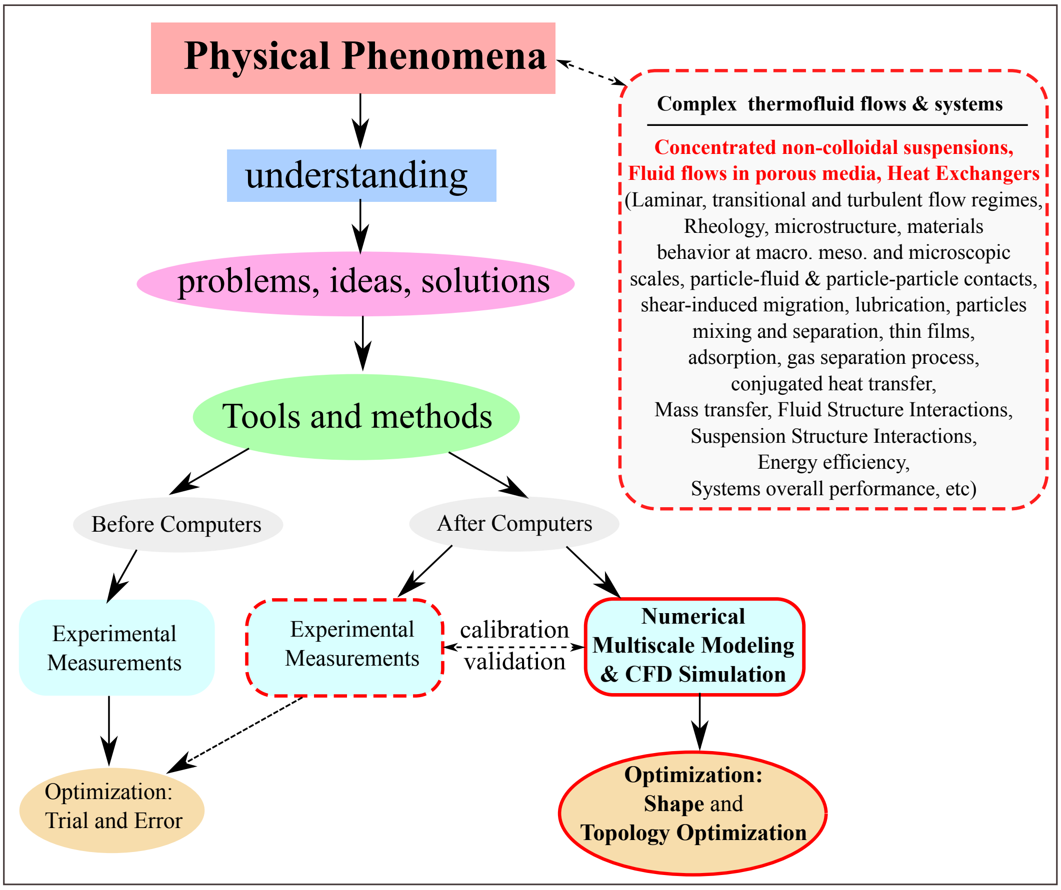


FIGURE 2.4: Overview chart of my scientific research activities domains rounded by red color.

Part II

My Research, Development and Innovation Activities

3 Non-colloidal suspension flows

3.1 Research Axis no.1: Complex-fluid flows of non-colloidal suspensions

Non-colloidal suspensions (see figure 3.1) are complex-fluid flows (particulate material systems) that can be found everywhere and at different scales like in chemical, process, civil, mechanical, geological, biological and industrial engineering applications (e.g. blood, concrete, oil and fuels, cosmetics, detergents, drilling muds, rivers, food processing, etc.). Thus, understanding their flow behavior is essential for predicting different phenomena and optimal future designs where dense suspensions may be present (Guazzelli and Morris, 2011; Guazzelli, 2017).

FIGURE 3.1: An example of complex particulate systems where non-colloidal suspensions are present (**Dbouk2018d**; Dbouk, 2011; Guazzelli, 2017).

3.1.1 Rheology of concentrated suspensions : rigid spheres, isothermal, isodense and Stokes/laminar flows regimes

"Future" might be well imagined (or predicted) if and only if the "past" or history is very well truly known without modification ! Then the "present" constitutes only an interface or a link between "past"-archiving, and the actual building of the "Future". For that reason, here some history about "Rheology" (Doraiswamy, 2002):

"Rheology" (from Greek, *rheo* (flow) and *logia* (study of)) is the Science of matter flow and deformation behavior.

Early beginning: Starting by Archimedes around 250 B.C. scientists started working on Ideal Materials like (Newton, 1687) who worked on Ideal Perfect Rigid Bodies. Then, Ideal Elastic Solids have been tackled throughout the works by Young, 1807, and (Cauchy, 1827) based on efforts by (Boyle, 1660) and (Hooke, 1678). Later by the 1700s, (Pascal, 1663) introduced out the path for both (Bernoulli, 1738) and (Euler, 1755) who studied what is known now by "Inviscid Fluids".

At the early 1800s, Newtonian-Liquids have been born and named thanks to (Navier, 1823; Stokes, 1845) equations which can describe the motion of a fluid in a given geometry such as a (Poiseuille, 1841). At the mid 1800s, Linear Viscoelasticity was introduced and different Models were constituted in order to describe this behavior of liquids, thanks to (Maxwell, 1867), and (Boltzmann, 1878).

After the year 1900: non-Newtonian complex fluids (like dilute suspensions and polymers) have been introduced and studied by (Einstein, 1906) and (Bingham, 1922; Jeffrey, 1922; Herschel, Bulkley, and Z., 1926). During the 3rd decade of the 20th century, the science of Rheology is named officially by E.C. Bingham during the 1920's (Bingham, 1922) and that lead to the foundation of society and Journal of Rheology (Bingham, 1930; Bingham, 1944). So, this is the "Rheology" Science face that we know today, and that has been invading the family of other sciences being the science of deformation and flow of matter (primarily soft matter like liquids, colloids, polymers, foams, gels, granular materials, suspensions, liquid crystals, and a number of biological materials, etc).

After the year 2000: Today, Rheology, this middle-aged science, is continuing to evolve mainly from looking to matter at a "macroscopic scale" to looking and dealing with matter at the "microscopic scale", with huge efforts to better describe the links between both scales (Tanner, 2009). It is no more a single science discipline, but inter-disciplinary sciences that can be combined completely with other sciences like Physics and Chemistry to yield new disciplines like: Rheo-Physics, Rheo-Chemistry and Bio-Rheology, etc.

In my research **axis no. 1** (1.4.6), during the last decade since 2008 i have been conducting R&D&I activities on the Rheology of "non-colloidal concentrated suspension flows" which is placed under the "Condensed and Soft-Matter" ERC (European Research Council) or CNRS (National Center for Scientific Research) panels or sections . First, what kind of suspensions i am talking about ? I am talking about non-colloidal suspensions bi-phase material made of solid particles that are immersed in a Liquid, as shown in table 3.1 and figure 3.2. Thus, depending on the volume fraction of particles $\phi = V_{solid}/V_{total}$ and the flow conditions, different suspension behaviors may occur as it will be shown later (V stands for Volume).

		Dispersed Phase		
		Gas	Liquid	***Solid***
Continuous Phase	Gas		vapors	aero-sol smokes
	Liquid	foams	emulsions	**suspensions**
	Solid	solid foams		alloys, polymers

TABLE 3.1: Classification of Dispersions. (Stickel and Powell, 2005; Dbouk, 2011)

The different forces that might be present in a suspension are illustrated in table 3.2.

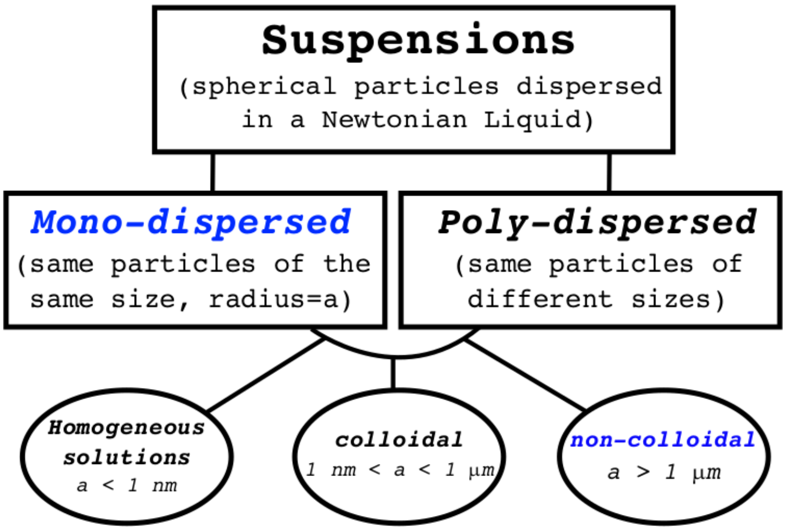


FIGURE 3.2: Classification od Suspensions. (Stickel and Powell, 2005; Dbouk, 2011)

Forces	Mathematical Form	Parameters
Brownian	kT/a	k: Boltzmann's constant $[J{\cdot}K^{-1}]$ T: Absolute Temperature $[K]$
Dispersion or Van der Waals	$\Theta_{effective}/a$	$\Theta_{effective}$: Hamaker constant $[N{\cdot}m]$ $\Theta_{effective} = f\,(\Theta_{particles}\,,\ \Theta_{fluid})$
Electrostatic	$\xi\xi_0\zeta^2$	ξ: dielectric constant of the fluid ξ_0: permittivity of free space $[F\cdot m^{-1}]$ ζ: electrostatic potential of the particles $[V]$
Hydrodynamic or viscous	$\eta a^2\dot{\gamma}$	η: medium viscosity $[Pa\cdot s]$ $\dot{\gamma}$: shear rate $[s^{-1}]$
Gravitational	$a^3\triangle\rho g$	$\triangle\rho$: particle-fluid density difference $[kg\cdot m^{-3}]$ g: gravitational constant $[m\cdot s^{-2}]$
Inertial	$\rho_f a^4\dot{\gamma}^2$	ρ_f: fluid density $[kg\cdot m^{-3}]$

TABLE 3.2: Forces present in a suspension (Dbouk, 2011).

Some order of magnitudes in non-colloidal (or non-Brownian) suspensions being shown in table 3.3. They are usually used when conducting non-dimensional analysis, like the Reynolds number at the particle's scale, the Péclet number and the Schmidt number, given respectively by:

$$Re_p = \frac{\rho_f a^2 \dot{\gamma}}{\eta_f} \tag{3.1}$$

$$Pe = \frac{6\pi\eta_f a^3 \dot{\gamma}}{\kappa T} \tag{3.2}$$

$$Sc = \frac{Pe}{Re} \tag{3.3}$$

where the different variables were defined in table 3.2.

Different Force ratio	Order of magnitude in our work
$\frac{Brownian}{Viscous} \sim \frac{kT}{6\pi\eta a^3\dot{\gamma}}$	$\sim 10^{-09}$
$\frac{Electrical}{Viscous} \sim \frac{\xi\xi_0\zeta^2}{\eta a^2\dot{\gamma}}$	$\sim 10^{-02}$
$\frac{Dispersion}{Viscous} \sim \frac{\Theta_{eff}}{\eta a^3\dot{\gamma}}$	$\sim 10^{-10}$
$\frac{Gravitational}{Viscous} \sim \frac{a\cdot\Delta\rho\cdot g}{\eta\dot{\gamma}}$	$\sim 10^{-03}$
$\frac{Inertial}{Viscous} \sim \frac{\rho_f a^2\dot{\gamma}}{\eta}$	$\sim 10^{-06}$

TABLE 3.3: Orders of magnitude of force ratios in non-colloidal suspensions under non-inertial flow regime. (Dbouk, 2011)

3.1.1.1 Viscometric functions of the suspension

Suspension flows behavior is described by what is known by **material functions** which represent relationships between the applied stress (or forces) and deformation or shear rate. The suspension material functions (called viscometric functions) are the suspension effective dynamic viscosity η_S and the suspension Normal Stress Differences $N_1 = \Sigma_{11} - \Sigma_{22}$ and $N_2 = \Sigma_{22} - \Sigma_{33}$ that can be quantified experimentally through rheometry measurements (i.e. by rheometer instruments). Σ is the suspension stress tensor with its normal stress components $(\Sigma_{11}, \Sigma_{22}, \Sigma_{33})$ where $(1,2,3) \equiv (x,y,z)$ in a 3D Cartesian frame of reference. The stress in the carrier fluid will be denoted by Σ^f, and that of particles by Σ^p. Similarly for other terms where the subscripts f and p wherever appeared in this manuscript, stand for fluid and particles, respectively.

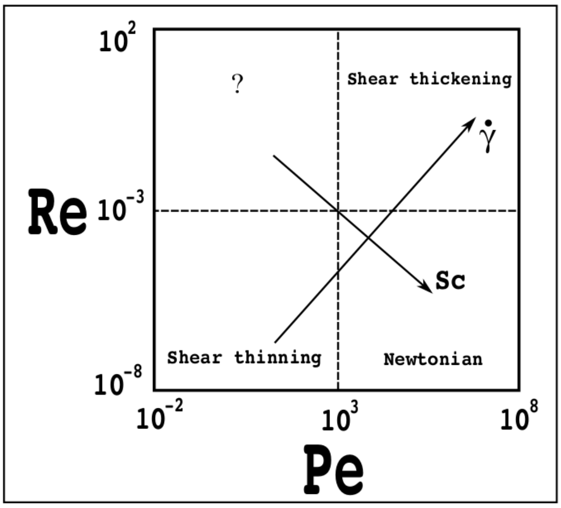


FIGURE 3.3: Phase diagram for suspension rheology, based on a dimensional analysis (Stickel and Powell, 2005).

If a concentrated suspension (monodisperse monodense rigid spheres) is under a flow and isothermal conditions, scientists measured and found that the macroscopic suspension continuum behavior and its effective viscosity η_S may undergo a Newtonian and/or Non-Newtonian behavior (shear-thinning (Vázquez-Quesada, Tanner, and Ellero, 2016), shear-thickening (Denn, Morris, and Bonn, 2018; Morris, 2018), with non-zero N_1 and N_2). This change in suspension's behavior depends on several factors and conditions like the particles bulk volume fraction ϕ, the shear rate $\dot{\gamma}$ and the Schmidt number Sc as illustrated in an example in figure 3.3.

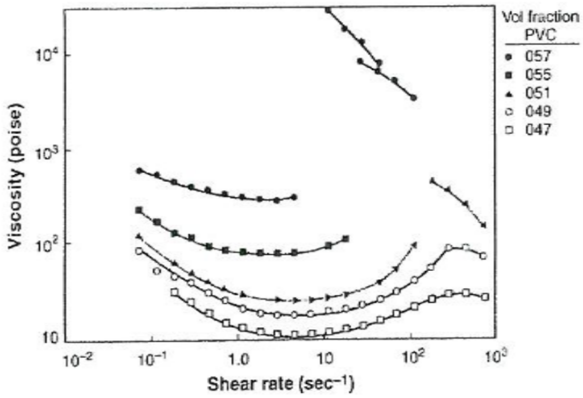


FIGURE 3.4: 1.25 μm PVC particles in dioctyl phthalate (Hoffman, 1972).

Usually, non-colloidal suspensions are considered as viscous materials whose viscosity does not depend on the shear rate (Ovarlez, Bertrand, and Rodts, 2006). But this is only valid for some intermediate shear stress τ_S or shear rate $\dot{\gamma}$ values. This is shown in figure 3.4 where the change in the suspension viscosity behavior depends on the shear rate $\dot{\gamma}$ and volume fraction ϕ (for a suspension of 1.25 μm PVC particles) (Hoffman, 1972).

Since the suspension material functions (η_S, N_1 and N_2) are essential to predict the flow/deformation behavior of these materials, then their measurements are of great importance. If measured accurately and quantified with precision, they can be implemented in CFD codes to create accurate continuum models for concentrated suspension flows.

Several scientists measured the suspension effective viscosity η_S versus ϕ and constituted several laws/fits such as the famous law by (Krieger and Dougherty, 1959) given by:

$$\eta_S = \eta_f (1 - \frac{\phi}{\phi_m})^{-\Xi} \quad ; \quad \Xi = -2.5\phi_m \tag{3.4}$$

where ϕ_m is the maximum packing possible volume fraction of particles that depend on the particles nature (i.e. roughness). For hard spheres it is usually found that $\phi_m \in [0.58, 0.68]$. Many authors constituted different laws of η_S as function of ϕ and ϕ_m (i.e. (Morris and Boulay, 1999) suspension viscosity law).

N_1 and N_2 have been obtained from numerical simulations, or measured by several scientists from the literature who found and all agreed that they are proportional to $\dot{\gamma}$ such that:

$$N_1 = -\alpha_1 \eta_f |\dot{\gamma}|; \quad N_2 = -\alpha_2 \eta_f |\dot{\gamma}| \tag{3.5}$$

where α_1 and α_2 are known by the suspension normal stress coefficients.

Nevertheless the agreements on the proportionality of N_1 and N_2 to $\dot{\gamma}$, the values and signs of N_1 and N_2 were dispersed in the literature, with almost absent knowledge on the particles stress tensor Σ^p quantification. Thus measuring these suspension material functions versus ϕ constituted **a huge gap in the literature** in the Rhology of isodense (or neutrally buoyant) monodisperse rigid spheres suspensions until the works by (Dbouk, 2011; Dbouk, Lobry, and Lemaire, 2013).

In fact several authors from the literature tried to compute the suspension normal stress differences, or to measure them via different techniques. Both situations: different signs, and same signs of N_1 and N_2 were reported (Gadala-Maria and Acrivos, 1980; Yeo and Maxey, 2010; Sierou and Brady, 2002; Deboeuf, Gauthier, Martin, Yurkovetsky, and Morris, 2009; Couturier, Boyer, Pouliquen, and Guazelli, 2011; Zarraga, Hill, and Leighton, 2000; Boyer, Pouliquen, and Guazzelli, 2011) in the literature ! These huge differences in the reported and dispersed results, made it important to continue investigations for better quantification of N_1 and N_2 (i.e. via more advanced measurement technologies) in order to understand the nature behind their unclear behavior.

Thus, the measurements of the suspension normal stress differences in concentrated suspensions was a big challenge for many decades due to the difficulty in achieving accurate measurements, and the limit of the technological level of instruments. Another difficulty lies in the fact that measuring both N_1 and N_2 required at least two different experimental setups (such as rheometer component modules or cells, like parallel-plates, cone-plate and/or concentric cylinders Couette cell, inclined planes, etc).

During my first year PhD (Dbouk, 2011; Dbouk, Lobry, and Lemaire, 2013), for the first time in the litertaure, we developed one innovative single experimental setup (mounted on a parallel-plates rheometer), to measure the suspension α_1 and α_2 coefficients, in addition to the particles normal stress components Σ^p_{11}, Σ^p_{22} and Σ^p_{33} (or their ratios λ_2 and λ_3) given by:

$$\lambda_2 = \frac{\Sigma^p_{22}}{\Sigma^p_{11}} \; ; \; \lambda_3 = \frac{\Sigma^p_{33}}{\Sigma^p_{11}} \tag{3.6}$$

The created innovative rotational parallel-plates rheometer technique (torsional flow), is based on installing pressure transducers in the stationary plate (Dbouk, 2011; Dbouk, Lobry, and Lemaire, 2013). This made it possible to measure the pressure in the liquid P_f as shown in figure 3.5.

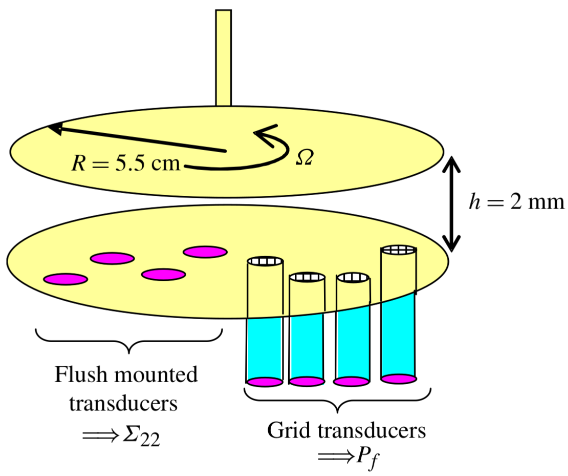


FIGURE 3.5: Innovative parallel-plates rotational rheometer setup mounted by (Dbouk, 2011; Dbouk, Lobry, and Lemaire, 2013).

(Dbouk, Lobry, and Lemaire, 2013) measured the radial profile of the second normal stress, $\Sigma_{22}(r)$ (in the velocity gradient direction) in the parallel-plate configuration. Then α_1 and α_2 were deduced from that profile (see, (Bird, Armstrong, and Hassager, 1977)) using:

$$\Sigma_{22}(r) = -\eta_f \dot{\gamma}_R \left[(\alpha_1 + 2\alpha_2) - (\alpha_1 + \alpha_2) \right] - p_{ref} \; ; \; \dot{\gamma}_R = \Omega R / h \tag{3.7}$$

where p_{ref} is a reference pressure set to zero.

Furthermore, the pore pressure, P^f is measured ($\mathbf{\Sigma} = \mathbf{\Sigma}^f + \mathbf{\Sigma}^p$; $\mathbf{\Sigma}^p = -P^f \boldsymbol{I}$), and allowed (when subtracted from the total normal stress Σ_{22}) to evaluate the particle stress tensor Σ^p_{22} using:

$$\Sigma^p_{22} = \Sigma_{22} - \Sigma^f_{22} = \Sigma_{22} + P^f \tag{3.8}$$

Equation (3.7) made it possible to determine both α_1 and α_2 by measuring the radial profile of Σ_{22} such that the slope gives the combination $-(\alpha_1 + \alpha_2)$ and the origin ordinate gives $(\alpha_1 + \alpha_2)$.

The measurement new methodology developed by (Dbouk, Lobry, and Lemaire, 2013) is summarized in figure 3.6.

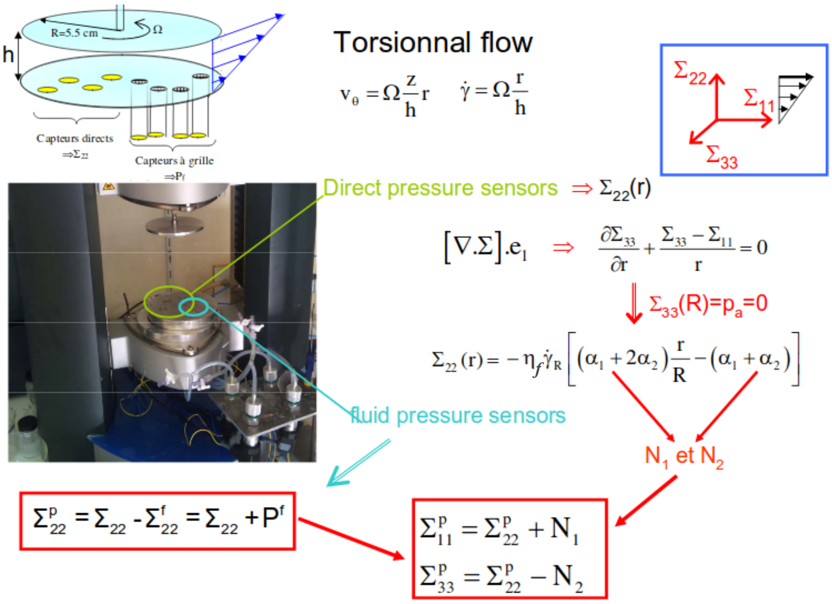


FIGURE 3.6: Measurements methodology of the suspension viscometric functions and particles stress components developed by (Dbouk, 2011; Dbouk, Lobry, and Lemaire, 2013).

An example of these results obtained by (Dbouk, Lobry, and Lemaire, 2013) are shown in figures 3.7 and 3.8, respectively.

All the results by (Dbouk, Lobry, and Lemaire, 2013) were obtained for suspensions of monodisperse polystyrene beads (Dynoseeds TS, Microbeads), 40 and 140 μm in diameter, dispersed in a Newtonian liquid (a mixture of water, UCON oil 75H90000 (Dow) ($\rho_{UCON} = 1090\ kg \cdot m^{-3}$, $\eta_f = 30\ Pa \cdot s$) and zinc bromide). The liquid mixture is then prepared to match the density of the polystyrene particles ($\rho_p \approx 1050\ kg \cdot m^{-3}$).

In (Dbouk, Lobry, and Lemaire, 2013), we measured the particle normal stress components (with their ratios λ_1 and λ_2), and the particles normal visosity (Dbouk, Lobry, and Lemaire, 2013; Morris and Boulay, 1999) as function of ϕ. We found that they are all ϕ-dependent as illustrated in figures 3.9, 3.10 and 3.11. This constituted an interesting new finding in the literature, because previously λ_1 and λ_2 were considered both constant, as for example they were taken by (Morris and Boulay, 1999).

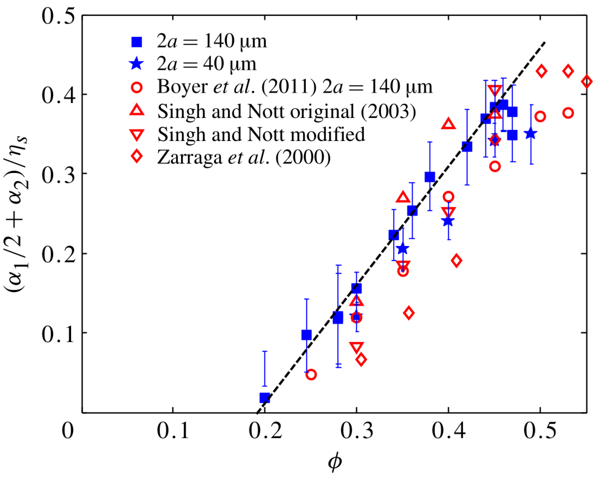


FIGURE 3.7: Linear combination of the normal stress coefficients $(\alpha_1/2 + \alpha_2)/\eta_S$ versus ϕ. Here η_S is normalized by η_f (Dbouk, Lobry, and Lemaire, 2013).

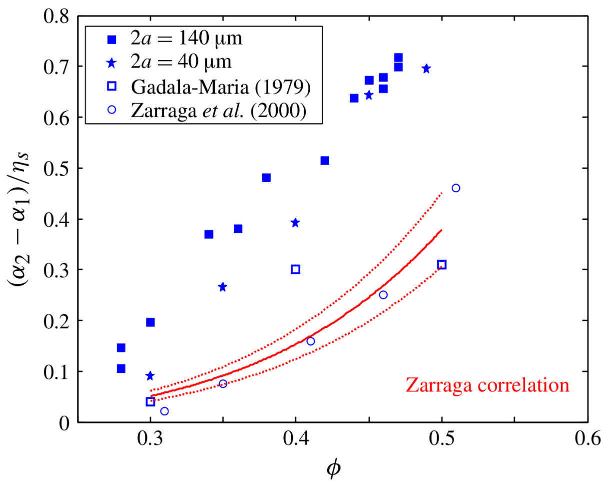


FIGURE 3.8: Linear combination of the normal stress coefficients $(\alpha_2 - \alpha_1)/\eta_S$ versus ϕ. Here η_S is normalized by η_f (Dbouk, Lobry, and Lemaire, 2013).

In contrast to what was expected as usual from the literature, (Dbouk, 2011; Dbouk, Lobry, and Lemaire, 2013) obtained and showed for the first time a negative value for α_1 (a positive first normal stress difference N_1).

This interesting finding by (Dbouk, Lobry, and Lemaire, 2013), pushed further other scientists later to ask more questions and investigate deeper. This was in order to explain this firstly reported what they called like a "contradictory positive sign ?" of N_1 (or $-\alpha_1$) in non-colloidal monodisperse isodense suspensions of spherical beads that are immersed a Newtonian liquid. A very recent seminar by Prof. (Guazelli, 2018) illustrated comparisons between the measurements or data available for α_1 and α_2 as function of ϕ as shown in figure 3.12. This figure 3.12 shows clearly the influence of *bounded versus unbounded* flow on altering the sign of the first normal stress difference coefficient α_1 (Gallier, Lemaire, Lobry, and Peters, 2016) in non-colloidal suspension flows.

Research effort are continuing to more precisely quantify the particles normal stress components in concentrated non-colloidal suspension flows as illustrated in figure 3.13 by d'Ambrosio,

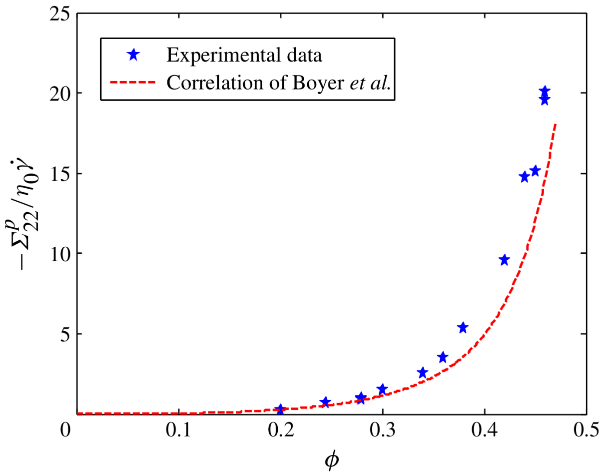


FIGURE 3.9: Σ_{22}^p as function of the particles volume fraction ϕ (Dbouk, Lobry, and Lemaire, 2013).

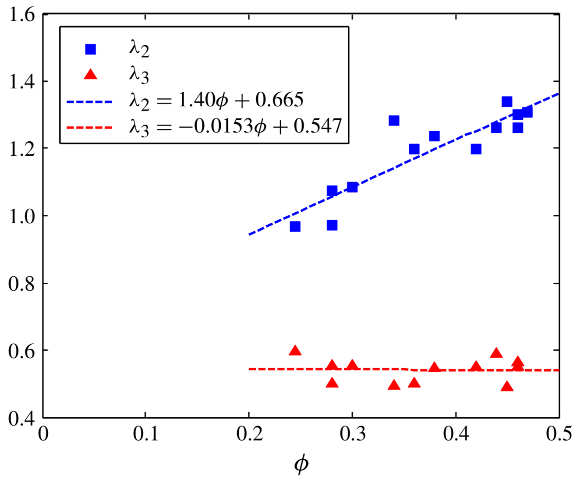


FIGURE 3.10: λ_1 and λ_2 as function of ϕ (Dbouk, Lobry, and Lemaire, 2013).

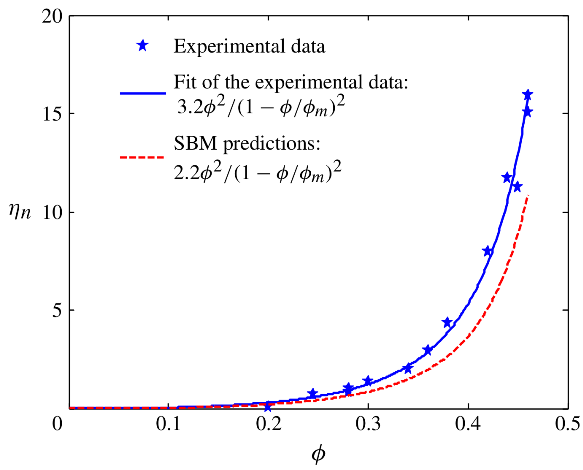


FIGURE 3.11: Particles stress normal viscosity as function of ϕ (Dbouk, Lobry, and Lemaire, 2013).

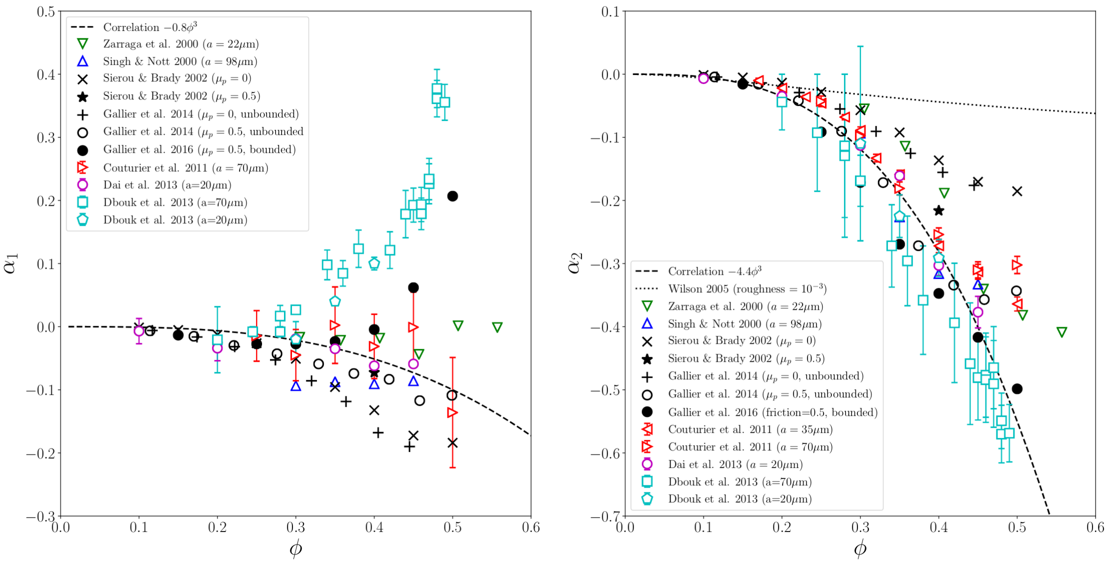


FIGURE 3.12: α_1 and α_2 as function of ϕ (Guazzelli, 2018). Note that here $N_{1,2}$ were defined as $(N_{1,2} = \alpha_{1,2}\, \eta_f\, |\dot{\gamma}|)$.

Blanc, and Lemaire, 2019. The latter authors showed that the third component Σ^p_{33} fits better the old correlation by Zarraga, Hill, and Leighton, 2000 compared to a recent one proposed by Boyer, Guazzelli, and Pouliquen, 2011.

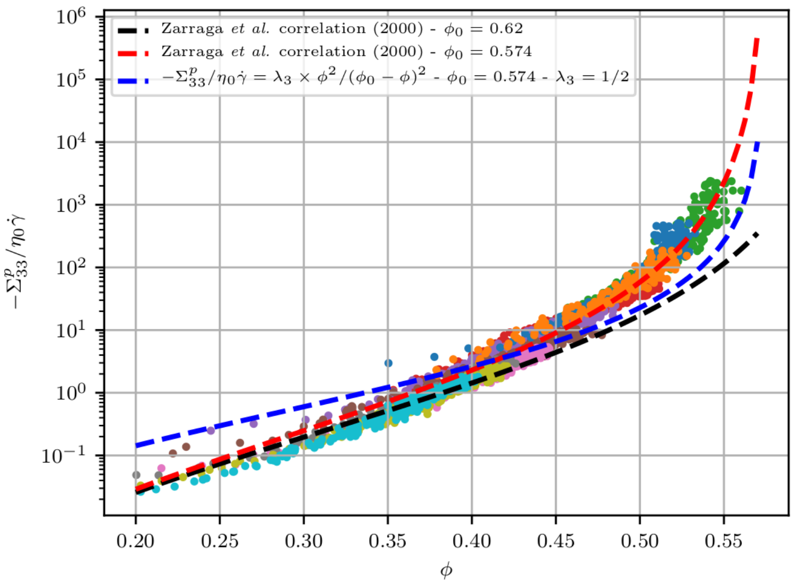


FIGURE 3.13: Third particle normal stress normalized by the product of the fluid viscosity and the local shear rate versus the local particle volume fraction. The agreement with the correlation proposed by Zarraga, Hill, and Leighton, 2000 where $\phi_0 = 0.574$ is very good (red line). In contrast, it is not possible to represent the experimental results by the correlation obtained by Boyer, Guazzelli, and Pouliquen, 2011 for Σ^p_{22} together with $\lambda_3 = 1/2$ (blue line). Adopted from (d'Ambrosio, Blanc, and Lemaire, 2019).

So far, this was a part of my R&D productions that i accomplished during my PhD period at the l'INPHYNI (Institut de Physique de Nice, University of Nice Sophia Antipolis a member of the University of Côte d'Azur). My PhD period experience (and multi national and international conferences) allowed me to gain and develop national and international research networks, respect and reputation in the Rheology scientific community:

- **National scientific collaborations and discussions with:**

  R&D units in France like the Mobile Particulate Systems Research Group at the IUT of the University of Marseille (Prof. E. GUAZELLI, Prof. O. POULIQUEN and Prof. B. METZGER, etc - a GDR (Groupe de Recherche) on Suspensions Rheology)

- **International scientific collaborations and discussions with:**

  - The Computational Fluids Dynamics Research Group, at the American University of Beirut (AUB) in Lebanon, Headed by Prof. MOUKALLED and Prof. M. DARWISH (in the context of a **CEDRE research collaboration program**, **Partnership: Hubert Curien (PHC), French-Lebanese**).

  - The Complex Fluids Research Group at the Levich Institute of Technology, City College University of New York, Headed by Prof. Jeffrey F. MORRIS.

3.1.1.2 Lubrication and frictional forces

Lubrication and frictional forces (solid-solid contacts) are very important when considering solid and liquid mixtures. In concentrated suspensions of non-colloidal particles, studies from the literature (Blanc, Peters, and Lemaire, 2011; Blanc, Lemaire, Meunier, and Peters, 2013; Gallier, Lemaire, Lobry, and Peters, 2016) have shown that the particles roughness may alter the suspension microstructure as function of the concentration and the local shear rate. The numerical modeling challenges can be described as a question : how to build reliable and robust **micro**scopic scale models that may project correctly the physics up to the **macro**scopic scale ?

In order to deepen my knowledge and answer this question later, i conducted a first postdoc research and development activity at the CEMEF (Center of Material Forming), Surfaces & Tribology Research Group, Headed by Prof. Pierre MOTMITONNET at Mines-ParisTech, Sophia Antipolis, France.

This R&D project was in the context of an industrial project funded by Arcelor-Mittal® R&D team (Dr. Nicolas LEGRAND), and in collaboration with Japanese researchers from Nippon-Steel® and Prof. Hiromi MATSUMOTO from the University of Kitakyushu, Japan.

The main mission in this Postdoc research activity was to develop (for online rolling process) a fast model for **friction control by lubrication in thin films** by **developing an asperity deformation model at the microscopic scale** (asperity scale). The lubrication theory and models that i developed (Dbouk, Montmitonnet, and Legrand, 2014; Dbouk, Montmitonnet, Suzuki, Takahama, Legrand, Ngo, and Matsumoto, 2014) have been applied to the lubrication (thin film of order $\sim O(1)\ mm$) of online strip rolling process (Montmitonnet, 2006). The mixed lubrication theory was applied representing contact mechanics between rough bodies with thin film fluid flow (lubricant). The lubricant flow is described by a generalized Reynolds' equation (that is enhanced by flow factors) (see Patir and Cheng, 1979). In metal forming, it has been recognized that roughness crushing is dependent on the plastic state of the underlying bulk metal, namely *macroplasticity* that helps *asperity flattening* (Montmitonnet, 2006; Dbouk, Montmitonnet, and Legrand, 2014; Dbouk, Montmitonnet, Suzuki, Takahama, Legrand, Ngo, and Matsumoto, 2014).

The metal solid strip is deformed in a roll-bite (a rolling zone of order $\sim O(1)\ mm$) between two rotating cylinders (called rolls) as shown in figure 3.14. The roll-bite zone is an elastic/plastic zone where elastoplastic deformation occurs. The originality in this model compared with other models from literature is that it takes into account the roll deformation with respect to the deformation of the strip at the roll-strip interface. The objective in such rolling process is to predict friction, in order to better control (in online mode) and reduce the solid-solid contacts severity. This is also to control and improve the final product surface quality (the metals strip tribology) (Montmitonnet, 2006).

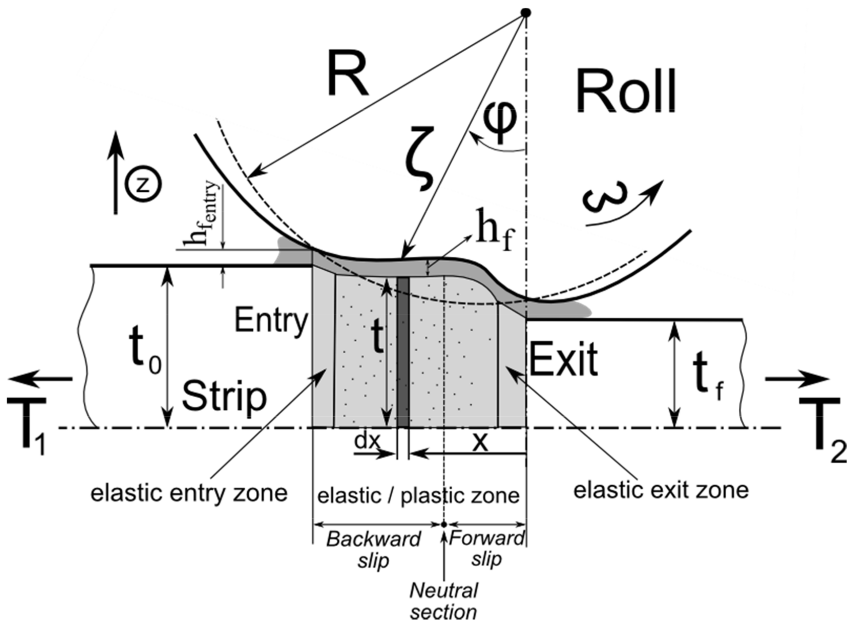


FIGURE 3.14: Cold metal strip rolling with thin lubrication of thickness h_f (Dbouk, Montmitonnet, and Legrand, 2014; Dbouk, Montmitonnet, Suzuki, Takahama, Legrand, Ngo, and Matsumoto, 2014). T_1 and T_2 represents the tension forces at the inlet and exit of the roll-bite, respectively.

Figure 3.16 shows the dimensionless effective friction coefficient at the roll-bite as function of the non-dimensional lubrication film thickness H as obtained by the lubrication microscopic asperity-deformation model by (Dbouk, Montmitonnet, and Legrand, 2014; Dbouk, Montmitonnet, Suzuki, Takahama, Legrand, Ngo, and Matsumoto, 2014). The developed asperity model (figure 3.15) was validated to the experimental measurements by (Tabary, Sutcliffe, Porral, and Deneuville, 1996).

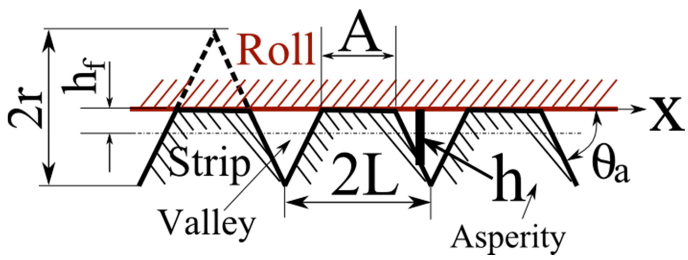


FIGURE 3.15: Asperity model for lubrication in thin films (see (Dbouk, Montmitonnet, and Legrand, 2014; Dbouk, Montmitonnet, Suzuki, Takahama, Legrand, Ngo, and Matsumoto, 2014)).

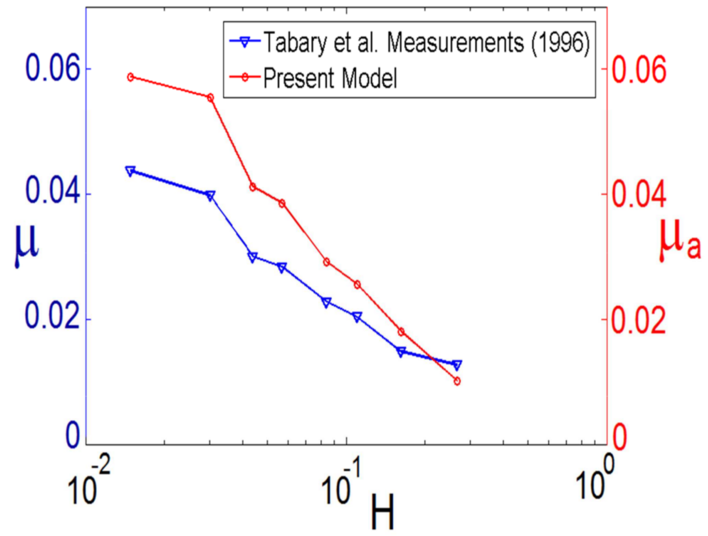


FIGURE 3.16: The dimensionless effective friction coefficient at the roll-bite as function of the non-dimensional lubrication film thickness H (see (Dbouk, Montmitonnet, and Legrand, 2014; Dbouk, Montmitonnet, Suzuki, Takahama, Legrand, Ngo, and Matsumoto, 2014)).

A future challenge will be how to extend this asperity modeling approach to even lower scale to be applied as lubrication films and particles roughness models in non-colloidal suspension flows.

Thus from all above, the first **huge gap in the literature** (3.1.1.1) was filled by quantifying the suspension viscometric functions, explanation of N_1 altering sign, importance of friction and lubrication forces at the microscopic scale, and the measurements of the particles normal stress components in concentrated non-colloidal suspension flows.

After all above, I was interested during my PhD (the last two years of PhD) in developing a macroscopic (Eulerian mixture) CFD model (fed by the measured viscometric functions) for particles transport in suspension flows (Dbouk, Lobry, Lemaire, and Moukalled, 2013) via the Finite Volume Method (Ferziger and Peric, 2002; Versteeg and Malalasekera, 2007; Moukalled, Mangani, and Darwish, 2015). The main mission or (benefit will be) is to predict the phenomenon of shear-induced migration in complex geometries where isodense (or neutrally buoyant) and polydense non-colloidal suspension flows may be present as it will be shown in the next paragraphs.

3.1.1.3 Shear-Induced Migration

What is shear-induced migration (SIM) ? When a non-colloidal suspension of neutrally buoyant particles is under a flow, the SIM phenomenon may occur as a self-diffusion phenomenon depending on the inertial forces, viscous forces, flow type, flow development entry length (thus the geometry type), in addition to the suspension properties (viscosity, particles roughness, particles polydispersity and the contact interactions frequency, etc).

The SIM phenomenon can be explained as a transition state towards an equilibrium. Many researchers have been trying to accurately quantify and predict the SIM in different suspension flow geometries. For example, experiments in a Couette cell showed that the SIM occurs from the inner to the outer cylinder, while in the parallel-plate geometry, no SIM was observed (Chapman, 1990; Chow, Sinton, IWAMIYA, and Stephens, 1994; Merhi, Lemaire, Bossis, and Moukalled, 2005; Bricker and Butler, 2006; Kim, Lee, and Kim, 2008).

In pressure-driven flows in channels, the SIM occurs from the wall to the centerline from a homogeneous ϕ of particles at inlet toward a non-homogeneous one like in the example of figure 3.17 (Phillips, Armstrong, Brown, Graham, and Abbott, 1992; Lyon and Leal, 1998; Miller and Morris, 2006; Semwogerere, Morris, and Weeks, 2007). Several authors have investigated the SIM in many different geometries like (Gadala-Maria and Acrivos, 1980; Leighton and Acrivos, 1987a; Leighton and Acrivos, 1987b; Lhuillier, 2009; Dbouk, 2011).

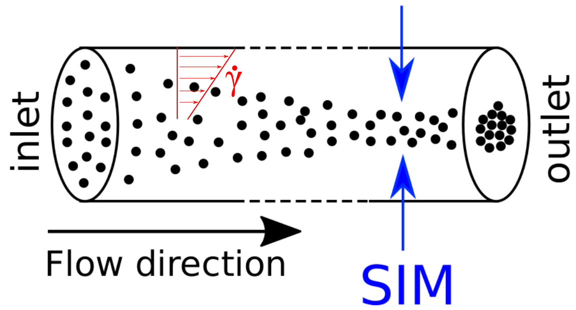


FIGURE 3.17: Shear-induced migration phenomenon in a pipe/channel flow.

3.1.1.4 CFD Modeling approaches of solid/liquid multiphase flows

Modeling multiphase flows (laminar and/or turbulent) in Computational Fluid Dynamics (CFD) is a complex task due to the locally varying time and length scales in the flow. The modeling task becomes even more complex in the case of large number of particles (e.g. concentrated suspensions), and it is still a topic for going research and investigation. The complexity in the modeling lies in the fact that multi-way coupling techniques must be employed to take into account particle-particle collision/interactions that take place.

Figure 3.18 lists the different modeling approaches that can be applied in computational Fluid Dynamics showing the increase of accuracy on the trade of an increase in the computational cost.

The advantage of the Euler-Euler Approach lies in the small computational cost compared to the Euler-Lagrange approach. Its disadvantage lies in the validity-limit of the applied correlations or constitutive models.

Modeling and simulation of the SIM in CFD:

For multiple years, many efforts were made to model and predict accurately the phenomenon of SIM through Eulerian modeling mixture approach. Nevertheless the efforts by (Phillips, Armstrong, Brown, Graham, and Abbott, 1992) based on diffusive-flux models, **a huge gap in the literature** was still present because no totally physical models existed yet! For example, the diffusive flux model principle by (Phillips, Armstrong, Brown, Graham, and Abbott, 1992) includes numerical parameters that must be fitted for each specific case of the suspension and flow conditions. Generally speaking, two schools in fact exist in modeling of suspension dynamics that can predict shear-induced migration: the French school and the American school. Both are complementary to each other. The first school tends more towards granular rheology to describe the suspension (Boyer, Pouliquen, and Guazzelli,

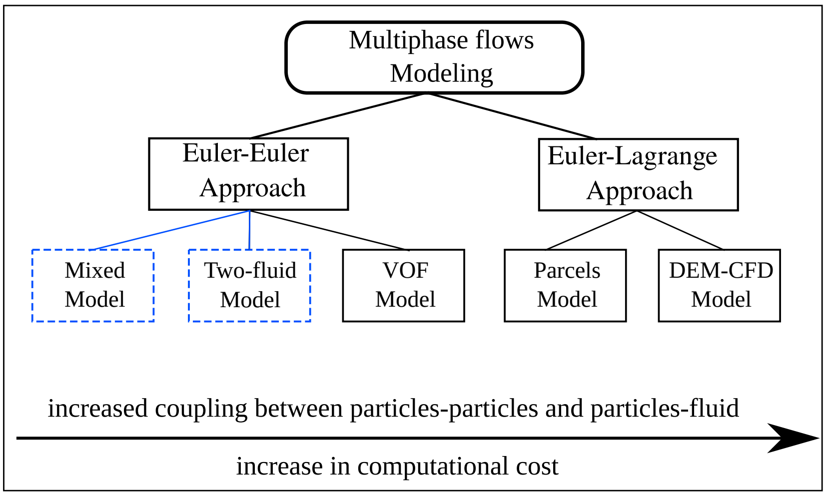


FIGURE 3.18: Multiphase flows modeling approaches. DEM: Descrete Elements Method; VOF: Volume of Fluid. A focus in this manuscript is given to the Euler-Euler approach (the Mixed Model, precisely the SBM).

2011), while the latter adopts more the liquid/solid mixture or simply the whole suspension rheology principle (Morris and Brady, 1998; Nott and Brady, 1994; Nott, Guazzelli, and Pouliquen, 2011). Several examples in the literature showed how to well move and interact between suspension rheology and granular rheology (Boyer, Guazzelli, and Pouliquen, 2011).

(Dbouk, Lobry, Lemaire, and Moukalled, 2013) followed the second school to model the shear-induced migration in both neutrally buoyant, and polydense non-Brownian suspension flows. (Dbouk, Lobry, Lemaire, and Moukalled, 2013) applied the Suspension Balance Model (SBM) of (Morris and Boulay, 1999; Morris and Brady, 1998; Nott and Brady, 1994; Nott, Guazzelli, and Pouliquen, 2011) modified for the measured viscometric functions in (Dbouk, Lobry, and Lemaire, 2013) and implemented in the open source CFD library (OpenFOAM, 2019). OpenFOAM is a huge C++ platform based essentially on the Finite Volume Method (FVM) (Ferziger and Peric, 2002; Versteeg and Malalasekera, 2007; Moukalled, Mangani, and Darwish, 2015) and C++ programming language (Stroustrup, 2013).

The SBM model is an Euler-Euler mixture model that is based on: a migration flux $\mathbf{J}$ that is proportional to the divergence of the particles stress tensor $\mathbf{\Sigma}^p$, such that:

$$\mathbf{J} = \frac{2a^2}{9\eta_f} f(\phi)[\nabla \cdot \mathbf{\Sigma}^p] \tag{3.9}$$

where $f(\phi)$ is a sedimentation hindrance function that represents the mobility of the particles phase (see (Dbouk, Lobry, Lemaire, and Moukalled, 2013)).

In the SBM model by (Dbouk, Lobry, Lemaire, and Moukalled, 2013), the equation of $\mathbf{J}$ (3.9) is developed and implemented in (OpenFOAM, 2019) as a source term in a particles transport or **advection equation** coupled to the continuity and momentum continuum bulk equations to predict SIM through the variable ϕ (local volume fraction of particles), such that:

$$\frac{\partial \phi}{\partial t} + \mathbf{U} \cdot \nabla \phi = -\nabla \cdot \mathbf{J} \tag{3.10}$$

where $\mathbf{U}$ is the suspension averaged velocity vector such that ($\mathbf{J} = \phi(\mathbf{U}^p - \mathbf{U})$) and $\mathbf{U}^p$ the particles averaged velocity vector (see (Nott and Brady, 1994; Morris and Boulay, 1999)).

An example of the SIM prediction, of an isodense monodisperse suspension flow in rectangular cross-section channel, is illustrated in figure 3.19. The numerical results are compared to experimental data by (Lyon and Leal, 1998). Another example for SIM phenomenon prediction by (Dbouk, Lobry, Lemaire, and Moukalled, 2013), but in a concentric cylinders Couette cell, is illustrated in figure 3.20.

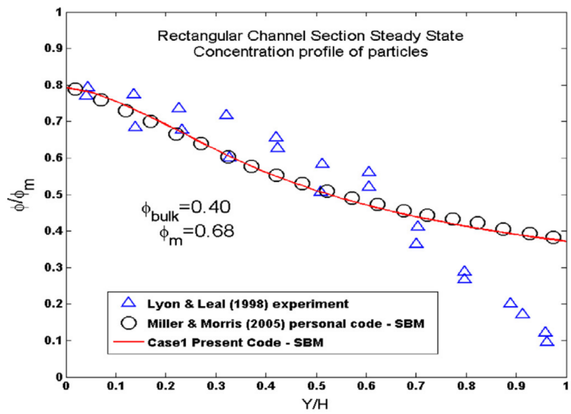


FIGURE 3.19: Shear-induced migration prediction in a channel flow of rectangular cross-section (Dbouk, Lobry, Lemaire, and Moukalled, 2013). Neutrally buoyant monodisperse non-colloidal suspension of spherical beads in Newtonian liquid.

The SBM solver (a first version) that i developed and implemented in (OpenFOAM, 2019) as a new CFD solver(Dbouk, Lobry, Lemaire, and Moukalled, 2013), was intended for **simple shear flows** of **neutrally buoyant** monodisperse suspensions (where orientation of $\mathbf{\Sigma}^p$ components is obligatory). Due to that restriction, i extended then the solver into a new second version in order to account for **general 2D flows of suspensions** and **buoyancy effects** (particles-liquid density difference). This interesting contribution by (Dbouk, Lobry, Lemaire, and Moukalled, 2013) made the orientation of the particles stress tensor components, (Σ^p_{11}, Σ^p_{22}, Σ^p_{22}) in the directions of (velocity, velocity-gradient and vorticity, respectively), to be no more an obligatory. The principle idea behind the general 2D flow modeling of a suspension is that it can be expressed as a local flow that vary as: simple shear, extensional and/or pure rotational, as illustrated in figure 3.21. For that objective, the particles stress tensor is transformed into another general one that is rotated based on the local eigen values/vectors of local strain rate tensor $\mathbf{E} = 0.5(\nabla\mathbf{U} + \nabla\mathbf{U})^T$.

The CFD solver developed by (Dbouk, Lobry, Lemaire, and Moukalled, 2013) was validated and applied to the experimental measurements case by (Rao, Mondy, Sun, and Altobelli, 2002) for viscous resuspension of polydense suspension in horizontal concentric cylinders Couette cell as shown in figures 3.22 (CAD geometry in CFD) and 3.23 (transient CFD results for resuspension and mixing).

My numerical programming and developments in the early versions of the (OpenFOAM, 2019) CFD platform in C++ (Stroustrup, 2013) were later rewarded after six years by the Foam-U French Association prize : "Best PhD thesis in France in CFD, developed within (OpenFOAM, 2019)".

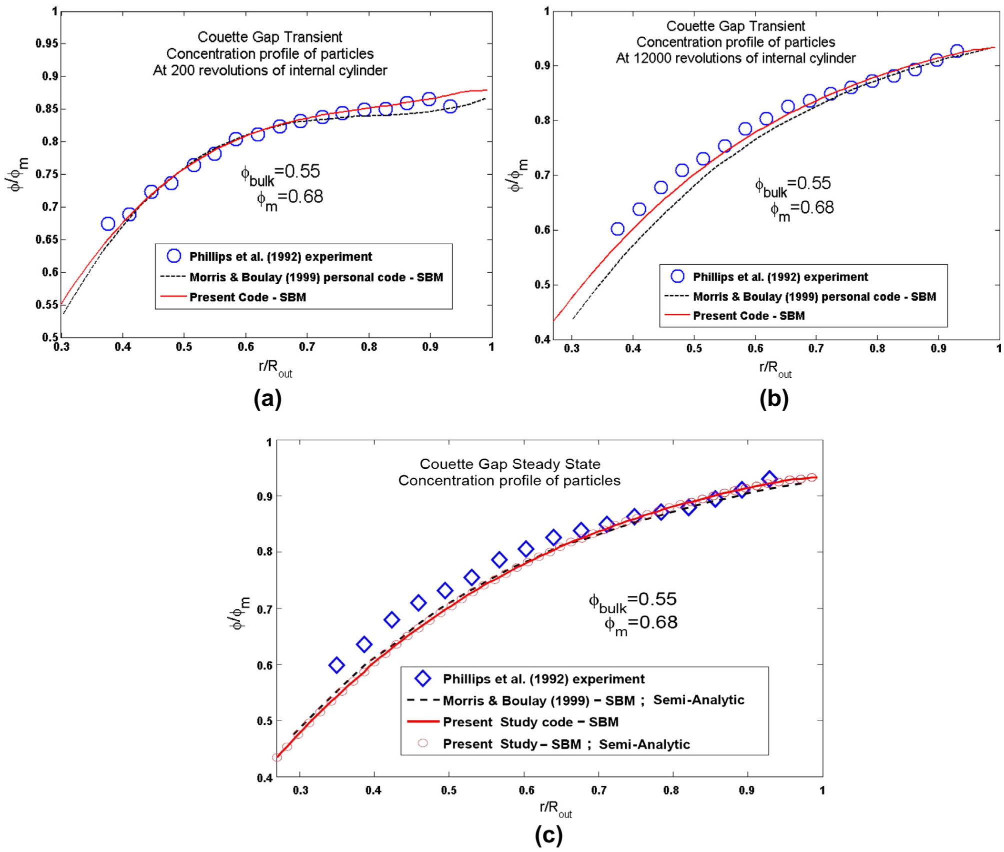


FIGURE 3.20: Shear-induced migration prediction in a concentric cylinders Couette cell rotational flow (Dbouk, Lobry, Lemaire, and Moukalled, 2013; Phillips, Armstrong, Brown, Graham, and Abbott, 1992; Morris and Boulay, 1999). Neutrally buoyant monodisperse non-colloidal suspension of spherical beads in Newtonian liquid. Stationary mesh or grid.

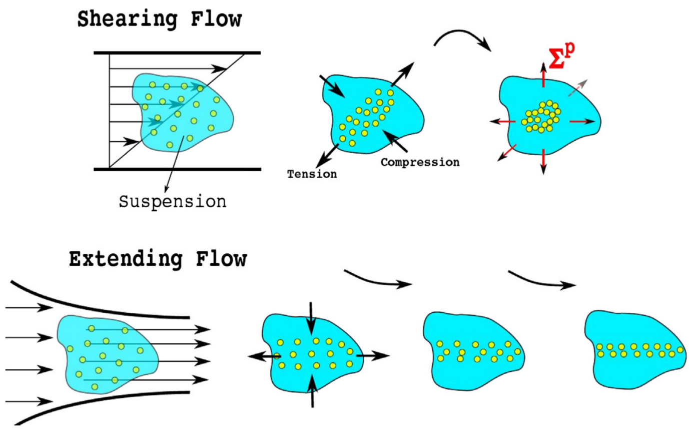


FIGURE 3.21: General 2D suspension flow is expressed as: simple shear, extension and rotation (Dbouk, 2011; Dbouk, Lobry, Lemaire, and Moukalled, 2013).

3.1.1.5 Suspension Structure Interaction: a step towards dynamic multiscale modeling

We have seen in the previous section the dynamics of suspensions as continuum media that has been well quantified experimentally in the literature for isothermal suspensions of

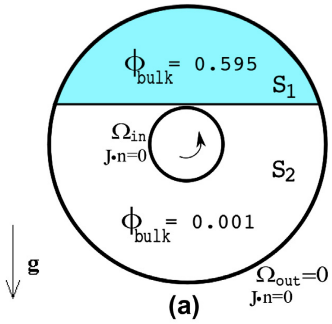


FIGURE 3.22: Geometry and boundary conditions (Dbouk, 2011; Dbouk, Lobry, Lemaire, and Moukalled, 2013; Rao, Mondy, Sun, and Altobelli, 2002).

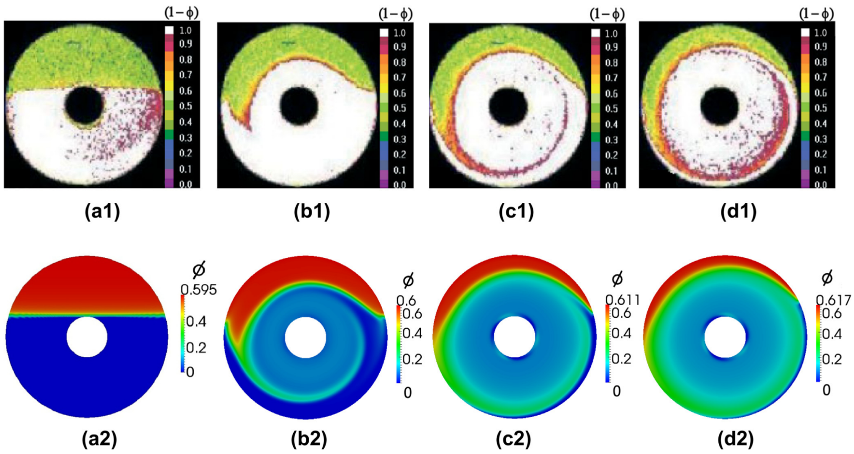


FIGURE 3.23: Resuspension evolution after several turns of the inner cylinder (Dbouk, 2011; Dbouk, Lobry, Lemaire, and Moukalled, 2013; Rao, Mondy, Sun, and Altobelli, 2002). [(a1), (a2)] 0 turn; [(b1), (b2)] 45 turns; [(c1), (c2)] 135 turns and [(d1), (d2)] 225 turns. $\rho_p^i/\rho_f^i = 0.94$, $a = 397\ \mu m$, $\eta_f = 0.588\ Pa \cdot s$.

monodisperse spherical beads. Moreover, a macroscopic model based on the SBM model has been developed for SIM and particles transport prediction in general 2D suspensions flows. The advantages of the macroscopic scale modeling approach in CFD, on Eulerian stationary grids or meshes, is that it permits computations of a large number of particles ($\approx O(10^6)$) transport in the carrier liquid at a very low computational cost. The number of particles n can be estimated using ($n = \frac{3\phi}{4\pi a^3} V$) where V represents the total mixture volume being in consideration.

Nevertheless the huge advantages behind the continuum modeling at a macroscopic scale, the numerical modeling of a suspension at a microscopic scale (Euler-Lagrange) is still necessary and constitutes **a huge gap in the literature**. It is important because, it can provide a deeper vision and thus more understanding of the physics at the particles' scale (particle-particle contact), which can be then extended to the macroscopic scale where the macro models prediction accuracy can be then enhanced. In (Dbouk, Perales, Babik, and Mozul, 2016), we investigated Fluid Structure Interaction (FSI) and conducted R&D on the numerical modeling and simulation at the particles' scale by implementing a direct-forced Immersed Boundary Method (IBM) (Peskin, 1972; Peskin, 1977) in ("PELICANS software platform") in order to account for the FSI forces between the solid particles and the surrounding fluid.

To solve the particle-particle contacts or interactions at the particles' scale, in (Dbouk, Perales, Babik, and Mozul, 2016) we applied the non-smooth contacts dynamics method (NSCDM) that was developed by (Jean, 1999). We then coupled the ("PELICANS software platform") framework to a Contact-Mechanics framework named LMGC90 (F Dubois, 2006) such that the resulting CFD-NSCDM package was named **Xper** (Dbouk, Perales, Babik, and Mozul, 2016; Perales, Dubois, Monerie, Mozul, Babik, Dbouk, and Monod, 2015).

The coupling algorithm based on the IBM that i developed and the resulting software (named "Xper" (Perales, Dubois, Monerie, Mozul, Babik, Dbouk, and Monod, 2015; Dbouk, Perales, Babik, and Mozul, 2016)), were a success story after several scientific discussions and collaborations with many scientists in several national institutions, like:

- **1** - the Scientific Computation Research Group Headed by Prof. F. DUBOIS (LMGC, Laboratory of Mechanics and Civil Engineering, University of Montpelier).
- **2** - the Laboratoire de physique et de thermomécanique des matériaux (LPTM) at the IRSN, the Institute of Radio-protection and Nuclear Safety, Cadarache, France.

  The collaborations between the above research units (**1** and **2**) and others, were in the context of a huge research group named **Mist** (Laboratoire de Micromécanique et Intégrité des Structures).

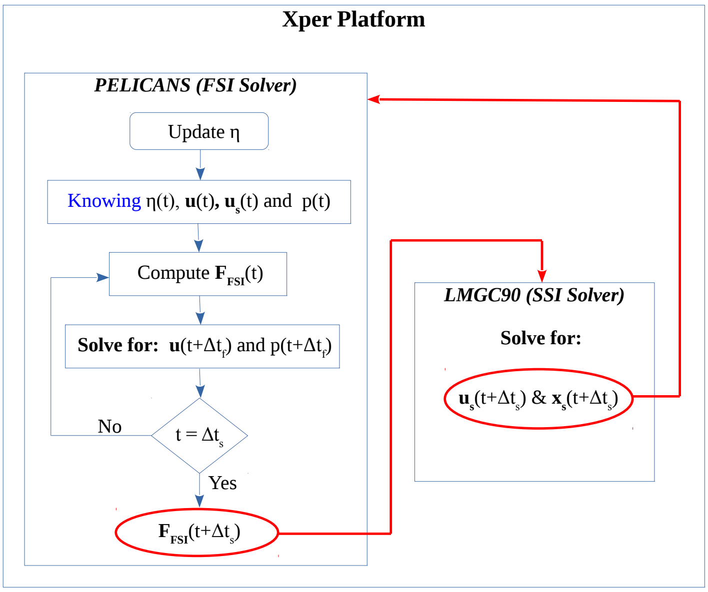


FIGURE 3.24: Xper: PELICAN-LMGC90 coupling algorithm ("PELICANS software platform"; F Dubois, 2006; Dbouk, Perales, Babik, and Mozul, 2016; Perales, Dubois, Monerie, Mozul, Babik, Dbouk, and Monod, 2015). η is the numerical parameter that defines a fluid/solid element cell on the computational grid. F_{FSI} is the fluid/structure interaction force and $\mathbf{u}_s$ the immersed solid body velocity at its mass center, and $\mathbf{u}$ the fluid velocity.

Validation results for **Xper** are obtained for a 3D settling sphere problem such that the velocity values are found to be in good agreement with data from the literature (Cate, Nieuwstad, Derksen, and Akker, 2002; Wachs, 2010) as shown in figure 3.25.

Additionally, in (Dbouk, Perales, Babik, and Mozul, 2016), we investigated the influence of imposing a numerical fluid cells film, around two identical settling cylindrical particles in a stationary fluid, on the particle-particle contacts and dynamics behavior. This is an important point, because usually many authors in literature have the habit to impose this

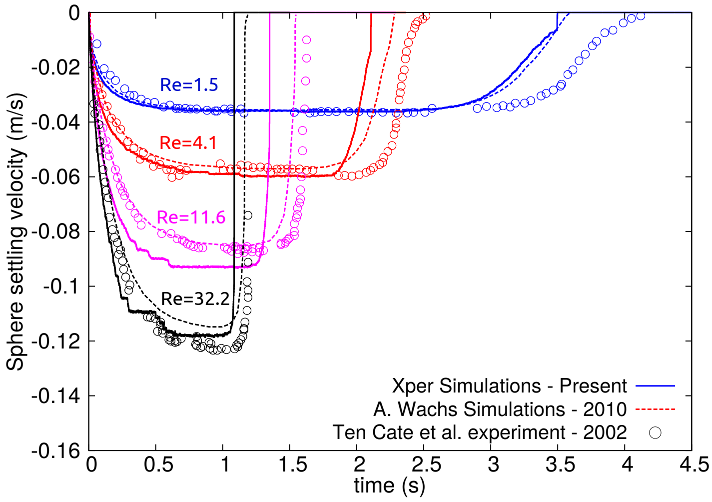
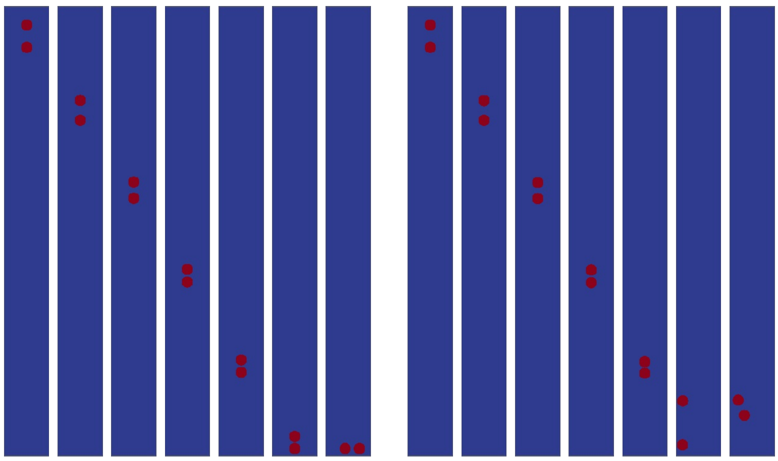


FIGURE 3.25: Settling velocity of a sphere in viscous fluid (Cate, Nieuwstad, Derksen, and Akker, 2002; Wachs, 2010; Dbouk, Perales, Babik, and Mozul, 2016)

numerically to reduce numerical instabilities by adding a virtual-lubrication-like thin film protection layer. Interestingly in (Dbouk, Perales, Babik, and Mozul, 2016) i showed that, imposing this numerical fluid ring (of thickness of the order of a one mesh space) around the particle to neglect friction alters the particles trajectories as illustrated in figures 3.26 and 3.27.

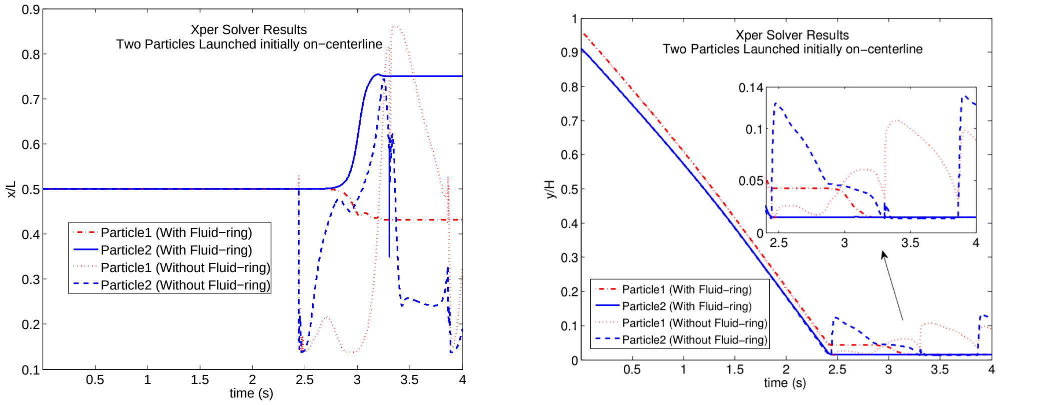


(a) With fluid ring (b) Without fluid ring

FIGURE 3.26: Settling of two cylinders (Dbouk, Perales, Babik, and Mozul, 2016)

This is an interesting new finding in the literature concluding that: imposing even a small fluid ring, the resulting dynamics is different from the real dynamics. Thus, this point must be taken with care, because it contributes to the final macroscopic behavior when many particles enter in contact, such as in non-colloidal suspensions flows.

The DF-IBM developed for pure-fluids in (Dbouk, Perales, Babik, and Mozul, 2016) is then extended in (Dbouk, 2016) to account for immersed rigid bodies in concentrated suspension flow. (Dbouk, 2016) introduced to the scientific community, for the first time, **a dynamic multiscale modeling approach, on Eulerian stationary grids**, with a new terminology named "**Suspension Structure Interaction (SSI)**" as illustrated in figure 3.28.



(a) Normalized x-positions versus time (b) Normalized y-positions versus time

FIGURE 3.27: Settling of two cylinders: trajectories of particles shown in figure 3.26 (Dbouk, Perales, Babik, and Mozul, 2016)

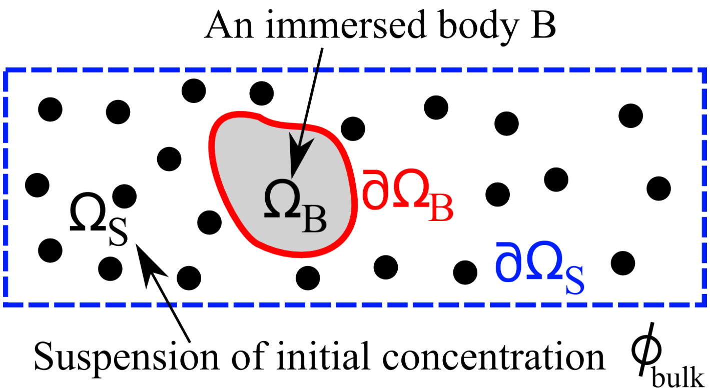


FIGURE 3.28: Suspension Structure Interaction (SSI) between a concentrated suspension and a rigid immersed body (Dbouk, 2016)

The SSI solver developed by (Dbouk, 2016) and implemented in the (OpenFOAM, 2019) C++(Stroustrup, 2013) CFD platform is then applied to investigate for the first time the influence of a concentrated neutrally buoyant suspension flow of monodisperse beads, on the drag and lift coefficients of a stationary immersed cylinder in a Poiseuille flow. Figure 3.29 shows an example for the numerical results obtained by (Dbouk, 2016).

Moreover, in (Dbouk, 2016), the SSI solver was interestingly applied to investigate a new phenomenon from the literature observed experimentally by (Haddadi, Shojaei-Zadeh, Connington, and Morris, 2014) in a suspension flow over an immersed stationary cylinder inside a microchannel (neutrally buoyant particles). As shown in figure 3.30, (Haddadi, Shojaei-Zadeh, Connington, and Morris, 2014) observed that the wake region behind the cylinder witnesses a pure-fluid wake (with recirculation and particles trap-release) that can extend depending on the flow inertia or the Reynolds number.

The SSI continuum solver in (Dbouk, 2016), captured well the pure-fluid wake extension phenomenon that was observed experimentally by (Haddadi, Shojaei-Zadeh, Connington, and Morris, 2014) as it is illustrated in figure 3.31.

This SSI solver will be applied in further research activities such as investigating other applications and possible phenomena that may appear when studying non-colloidal suspensions flows with suspension structure interactions (both numerical and experimental

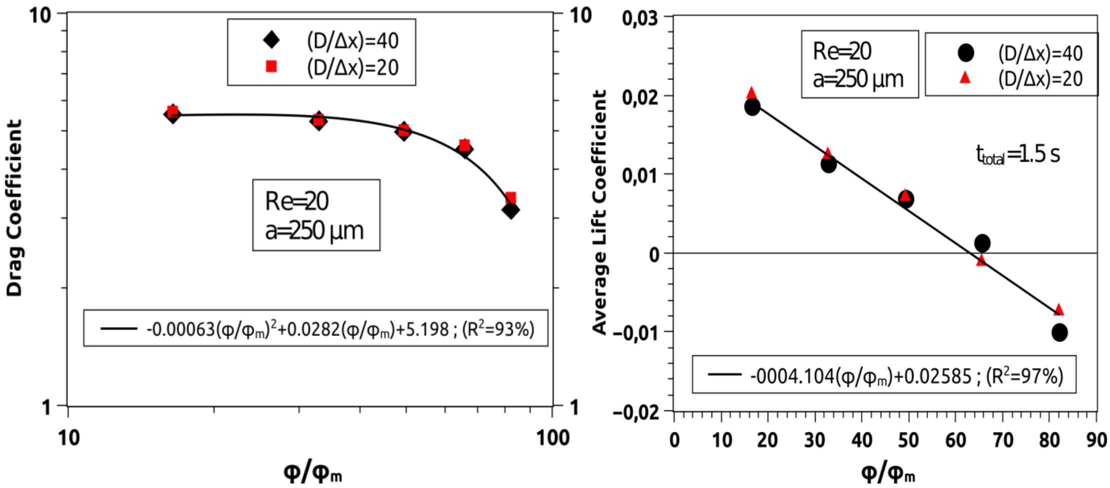


FIGURE 3.29: Drag and average lift coefficients acting on a stationary cylinder immersed in a concentrated suspension flow in a channel (see (Dbouk, 2016))

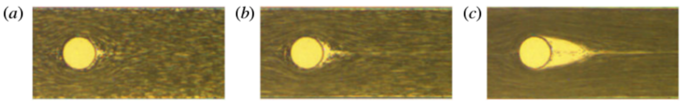


FIGURE 3.30: The experimental observation of the flow of a $\phi_{bulk} = 0.084$ suspension of neutrally buoyant particles over a cylindrical obstacle confined in a microchannel at (a) Re = 60, (b) Re = 120 and (c) Re = 300. It should be noted that because of the geometry of the channel, which is similar to a Hele-Shaw cell, the onset of vortex shedding is larger than that in uniform flow over a circular cylinder, i.e. $Re_{cr} \approx 55$ (Bearman and Zdravkovich, 1978; Zovatto and Pedrizzetti, 2001). Figure from (Haddadi, Shojaei-Zadeh, Connington, and Morris, 2014).

investigations).

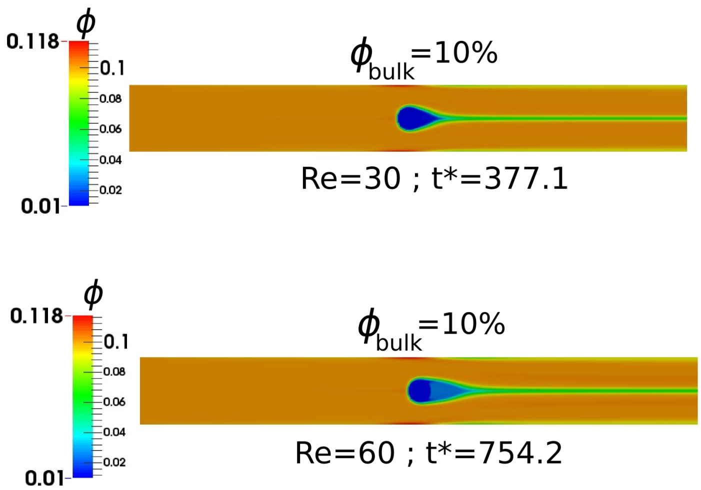


FIGURE 3.31: Numerical results for the flow of a suspension of neutrally buoyant particles over a cylindrical obstacle confined in a microchannel (see (Dbouk, 2016))

3.1.2 Rheology of concentrated suspensions : Introducing non-isothermal situations

So far, we have seen in the above sections that literature is rich with numerous research and development activities conducted on the Rheology of **isothermal** non-colloidal suspensions, both experimentally and numerically. However, by the early of 2018, (Dbouk, 2018a) payed attention surprisingly that the scientific community has not been giving yet enough attention to heat transfer in non-colloidal suspension flows of monodisperse particles immersed in a Newtonian liquid. This was identified as **a huge gap in the literature** that should be filled as soon as possible. The only experimental works on this topic identified from the literature are those by (Metzger, Rahli, and Yin, 2013), and numerically by (Wu, Zhou, Aubry, Antaki, and Massoudi, 2017).

Nevertheless the important numerical efforts by (Wu, Zhou, Aubry, Antaki, and Massoudi, 2017), their modelling was neither 100% correct nor complete. (Wu, Zhou, Aubry, Antaki, and Massoudi, 2017) did not consider the influence of the shear rate $\dot{\gamma}$, volume fraction ϕ and Péclet number ($Pe_{d_p} = \dot{\gamma} d_p^2 / \alpha_f$) on the suspension effective thermal properties as observed experimentally by (Metzger, Rahli, and Yin, 2013).

In (Dbouk, 2018a), I was the first to propose a more complete modeling in CFD (thanks to old measurements on porous materials by Eucken, 1932; Russell, 1935; Ribaud, 1937; Sugawara and Yoshizawa, 1961; Sugawara and Yoshizawa, 1962). My CFD model was validated, after comparing my numerical results to those obtained experimentally by (Metzger, Rahli, and Yin, 2013) as illustrated in figure 3.32.

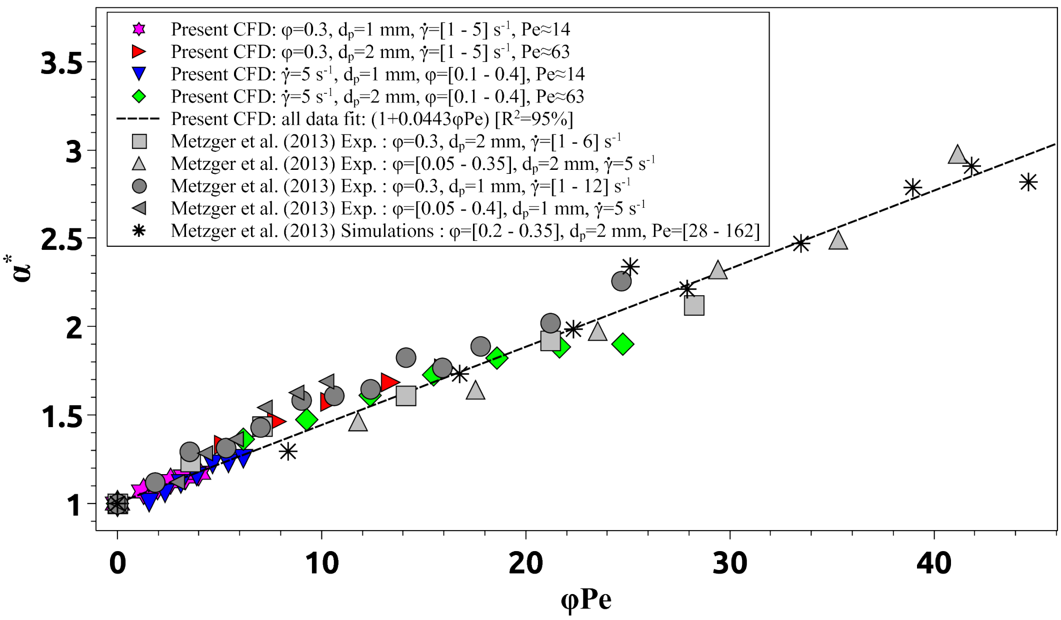


FIGURE 3.32: Numerical results for the dimensionless suspension effective thermal diffusivity as function of ϕPe (Dbouk, 2018a; Metzger, Rahli, and Yin, 2013). $\alpha^* = \alpha_{susp.}(\dot{\gamma}) / \alpha_{susp.}(\dot{\gamma} = 0)$

The new CFD solver, developed in (Dbouk, 2018a), is then applied to investigate heat transfer enhancement in channels by means of a suspension flow inside a square cross-section conduit of aspect ratio $L/D_h = 800$. Interesting numerical CFD results were obtained as it can be seen from figures 3.33 and 3.34 showing that non-colloidal suspensions may contribute well to heat transfer enhancement depending on the particles/fluid thermophysical and concentration properties, and the geometry or flow regime conditions. An advantage

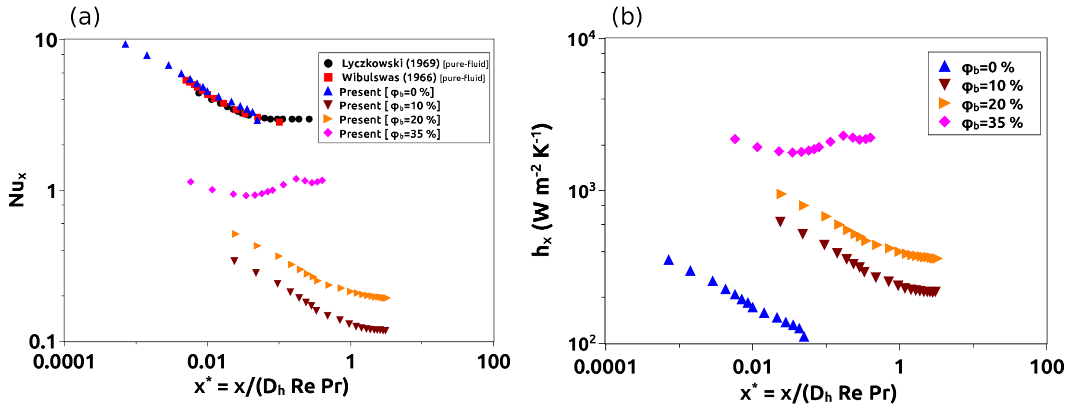


FIGURE 3.33: Suspension flow in a square cross-section channel of aspect ratio $L/D_h = 800$. Local thermal properties at the steady-sate for different initial ϕ_{bulk} values: (a) Local Nusselt number; (b) Local heat transfer coefficient. The initially applied simulation data are: $k_p/k_f = 5$; $n = 1$; $C_1 = 2.3$; $C_2 = 50\ K$; $T_c = 180\ K$; $d_p = 100\ \mu m$; $\eta_{f_i} = 8 \cdot 10^{-7}\ m^2 \cdot s^{-1}$; $T_{f_i} = 293\ K$; $\beta_0 = 3 \cdot 10^{-4}\ K^{-1}$; $\rho_f = \rho_p = 1180\ Kg \cdot m^{-3}$; $C_{p_f} = C_{p_p} \approx 1\ KJ \cdot Kg^{-1} \cdot K^{-1}$. From (Dbouk, 2018a)

of using non-colloidal suspensions as cooling or heating fluids is that they are not harmful to human respiratory system compared to their nano-fluids counterpart.

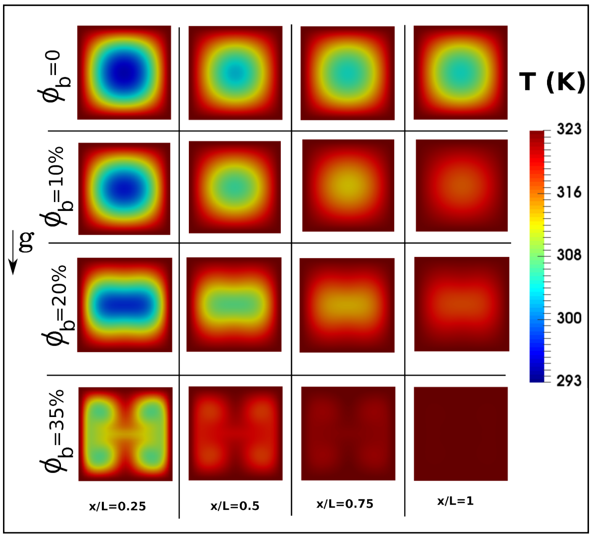


FIGURE 3.34: Snapshots of the local temperature at four different cross-section locations along the flow direction at the steady-sate for different initial ϕ_b values.
The initially applied simulation data are: $k_p/k_f = 5$; $n = 1$; $C_1 = 2.3$; $C_2 = 50\ K$; $T_c = 180\ K$; $d_p = 100\ \mu m$; $\eta_{f_i} = 8 \cdot 10^{-7}\ m^2 \cdot s^{-1}$; $T_{f_i} = 293\ K$; $\beta_0 = 3 \cdot 10^{-4}\ K^{-1}$; $\rho_f = \rho_p = 1180\ Kg \cdot m^{-3}$; $C_{p_f} = C_{p_p} \approx 1\ KJ \cdot Kg^{-1} \cdot K^{-1}$. From (Dbouk, 2018a).

This non-isothermal innovative CFD solver by (Dbouk, 2018a) has huge potentials for future R&D&I activities, for example for investigating other applications like new cooling or thermal insulation techniques by using non-colloidal suspension flows like in the very recent work in (Dbouk, 2019b) that will be described later.

The developments by (Dbouk, 2019b) constituted a key success element to found a new axis on **microfluidics** and to collaborate with the BioMEMS Research Group represented by Prof. Vincent THOMY (who is co-directing a common PhD project that started on March 2019 by the PhD student M. Masoud MOAZZEN on the cooling of electronic components by using non-colloidal suspension flows). The BioMEMS group develops advanced technological solutions dedicated to biosensors, **microfluidics** for handling and studying bio-species and solutions to control surface wettability.

3.1.3 Rheology of non-colloidal suspensions: a continuing large field for research and development

The variety of types of non-colloidal suspensions (like Newtonian vs non-Newtonian liquid carrier (i.e. Yield-stress fluids), particles shape (spheres, fibers,..), particles polydispersity, flow type, etc) constitute a large scientific discipline for future research, development, and innovation where new studies can take place and emerge everyday. For example, moving from shearing flows to extensional or oscillatory flows, moving from spheres to fibers, moving from monodisperse to polydisperese systems, very recent research activities have been emerging in order to explore and deepen our understanding of the Rheology of non-Brownian suspensions at different scales (A Franceschini, 2014; Snook, Davidson, Butler, Pouliquen, and Guazzelli, 2014; Ovarlez, Mahaut, Deboeuf, Lenoir, Hormozi, and Chateau, 2015; Gamonpilas, Morris, and Denn, 2016; Bounoua, Lemaire, Férec, Ausias, and Kuzhir, 2016; Tapia, Shaikh, Butler, Pouliquen, and Guazzelli, 2017; Seto, Giusteri, and Martiniello, 2017; Tanner, 2018; Butler and Snook, 2018).

In my opinion, the Rheology of non-colloidal suspensions is still a huge discipline in Rheology science for R&D&I with many research gaps to be filled during the next decade. This constitutes a huge potential for further R&D&I activities that if conducted at the IMT Lille Douai, would contribute well and enhance the overall scientific network and reputation of our department or research unit. This creates huge potential for future fundings attractions like additional industrial partners and the recruitment of junior researchers (post-docs, PhD's, Master's, research engineers, etc).

Finally, i am still continuing several R&D activities and developments, on this **research Axis 1** that have huge potentials for future innovations and scientific collaborations with national/international research units. The potentials behind this research Axis 1 are presented and discussed in chapter 4.

4 Shape and Topology Optimization

4.1 Research Axis no.2: Topology optimization and design of complex thermofluid flow systems

Today, heat exchangers or thermofluid flows and heat transfer systems can be found everywhere such as in industrial or domestic heat exchangers (in home, vehicle radiators, etc), electronic devices, aerospace and automotive industries, chemical engineering process, submarines, rockets, satellites, process and food engineering, etc.

So, Design and optimization of thermofluid engineering devices to obtain better designs that are more compact with less mass, less frictional losses and increased overall thermal efficiency has been always a vital topic for R&D&I (Gero, 1985; Bertsekas, 1999). Design optimization has been very well developing the last decade thanks to the progress in computational power and technology (i.e. High Performance Computing (HPC), Cloud Computing, Computing via Graphical Processing Units (GPU), Artificial Intelligence(AI), etc) in order to improve the existing designs or create directly optimal intelligent ones (Bendsøe and Sigmund, 2004; Shah and Sekulić, 2007) and thus overcome the socioeconomic challenges (Diaz and Murnane, 2008) efficiently. This is also important if we would like to follow correctly the next decade energy strategies as defined by the European Union (i.e. less waste materials, energy efficient systems, less pollutant emissions, etc). One excellent solution that may contribute well to the accomplishment of these EU objectives is Shape and Topology Optimization (TO) which fit well in the R&D&I activities at the CERI-EE[2] at the IMT Lille Douai.

An example of shape versus topology optimization applied to solid mechanics (a struss structure) is shown in figure 4.1. Another example but applied to CPU cooling heat sink design is illustrated in figure 4.2. Topology optimization has been very well developed for solid mechanics applications, but not yet well developed for thermofluid applications (see Dbouk, 2017a).

Topology optimization is very expensive computationally compared to shape and size optimization due to a larger number of degrees of freedom (design variables). However, an optimal design obtained through a shape optimization process may serve as an important starting point for a topology optimization design process.

4.1.1 Shape Optimization Design

4.1.1.1 Vortex generators

The objective in this research activity is to find different optimal designs of vortex generators (VG) through shape optimization techniques in CFD. The goal is to enhance mixing

[2] Centre d'Enseignement, de Recherche et d'Innovation Energie et Environnement

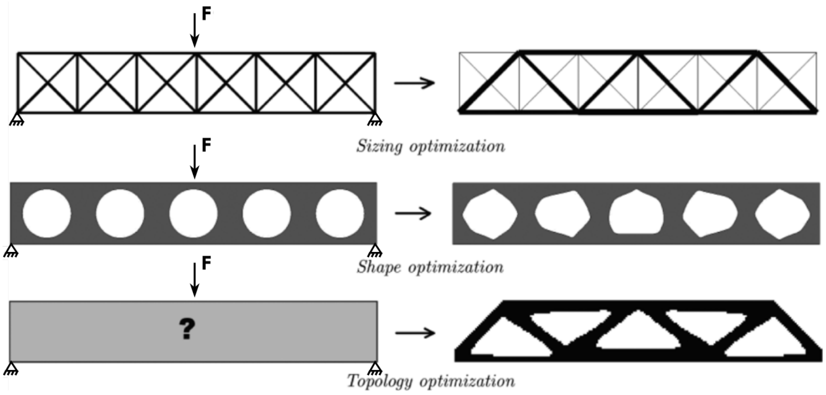


FIGURE 4.1: Size, shape and topology optimization. The initial problems are shown at the left side and the optimal solutions are shown at the right side. Adapted from Bendsøe and Sigmund, 2004.

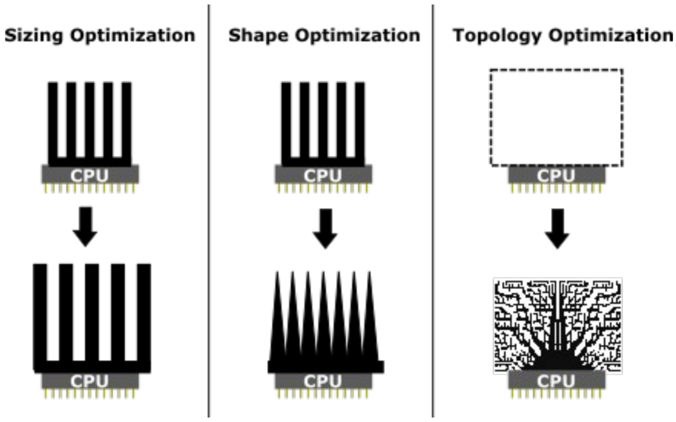


FIGURE 4.2: Optimization of a CPU heat sink.

and heat transfer in channel flows at an acceptable cost of pressure drop by finding optimal VG designs that adapt to flow regime (e.g. laminar, turbulent, forced, free and mixed convection, etc).

Optimization techniques in CFD based on Surrogated-based-Models (or surface response methods), Machine Learning (ML) or Artificial Intelligence (AI) methods (L. Hertel, 2018; Red-Cedar-Technology, 2016) have been investigated in this purpose. A research project in this context is the PhD of M. Hassan KARAKABA, **co-supervised by the author (at 30%)** with Dr. Serge RUSSEIL (25%), Dr. Charbel HABCHI (25%) from NDU University in Lebanon, Prof. Daniel BUGEARD (10%), and Prof. Thierry LEMENAND (10%) from Angers University.

The objective in the PhD project of M. Hassan KARAKABA is to find different optimal designs of vortex generators as shown in figure 4.3 (for heat transfer intensification) where each design can perform in an optimal way depending on the type of the flow regime (H. Karkaba, Dbouk, Habchi, Russeil, Lemenand, and Bougeard, 2019).

This PhD project is funded as 50% from IMT Lille Douai and 50% from LIU University of Lebanon. M. Hassan KARAKABA is now at the end of his first year PhD. The main idea behind vortex generators to enhance heat transfer is that by perturbing the flow dynamics to create local transitional phenomena. The latter enhance the fluid flow vortices creation that induce heat transfer intensification enhancement (compared to similar flow but in empty channels).

Of course the challenge is to enhance heat transfer but at an acceptable cost in pressure drop augmentation (e.g. a Thermal Enhancement Factor (TEF) $\zeta > 1$). The TEF ζ is defined as :

$$\zeta = (Nu/Nu_0)(f/f_0)^{-1/3} \tag{4.1}$$

The subscript *0* stands for the empty channel geometry, and the local Nusselt number Nu_x is defined as:

$$Nu_x = \frac{h_x \times D_h}{k} \tag{4.2}$$

The global Nusselt number $Nu(=\bar{Nu_x})$ (used in eqn. 4.1) is obtained after integrating Nu_x along the flow direction and at different sections between inlet and outlet.

D_h is the hydraulic diameter of the channel, h the heat transfer coefficient integrated from local h_x along the flow direction (mass flow averaged), and k the thermal conductivity.

The local heat transfer coefficient h_x inside the channel is defined as the following:

$$h_x = \frac{q''_x}{T_w - T_x} \tag{4.3}$$

where q''_x is the computed boundary heat flux, T_x the computed temperature at each section position and T_W the imposed wall temperature.

The local friction coefficient f_x is defined as the following:

$$f_x = \frac{P_x - P_{in}}{\rho u^2} \frac{H}{L} \tag{4.4}$$

The effective friction factor f is computed by integrating f_x at different sections along the flow direction between inlet and outlet.

In the PhD of H. KARKABA, two optimization methods have been investigated: a sweep method (with no optimization algorithm), and a SHERPA®(L. Hertel, 2018; Red-Cedar-Technology, 2016) artificial intelligence optimization search algorithm. The obtained Pareto-frontier results are illustrated in figures 4.4 and 4.5 for a forced convection and laminar flow regime (at Re = 1020). The optimal design (OD) obtained is shown in table 4.1 with comparisons to previous designs from the literature T. and Li, 2018; Tian, He, Lei, and Tao, 2009 comparing Diagonal Vortex Generator (DVG), Rectangular Vortex Generator (RVG), Delta Winglet Pair (DWP) and Rectangular Winglet Pair (RWP).

In the SHERPA® artifical intelligence method, a wide range of the design parameters is investigated by taking a smaller parameter intervals for the predefined parameters. Each vortex generator design CFD case was run on 64 processors in parallel, and required approximately $t = 6$ min. as a computational time to reach the steady state. As for the computational time, the SHERPA® method obtained the optimal design after computing a total of 1516 design cases. Using SHERPA® method, the overall computational time of the Pareto frontier designs was reduced by a factor of **6.18** (compared to the Pareto frontier obtained by the *sweep* method and that required much more number of design cases).

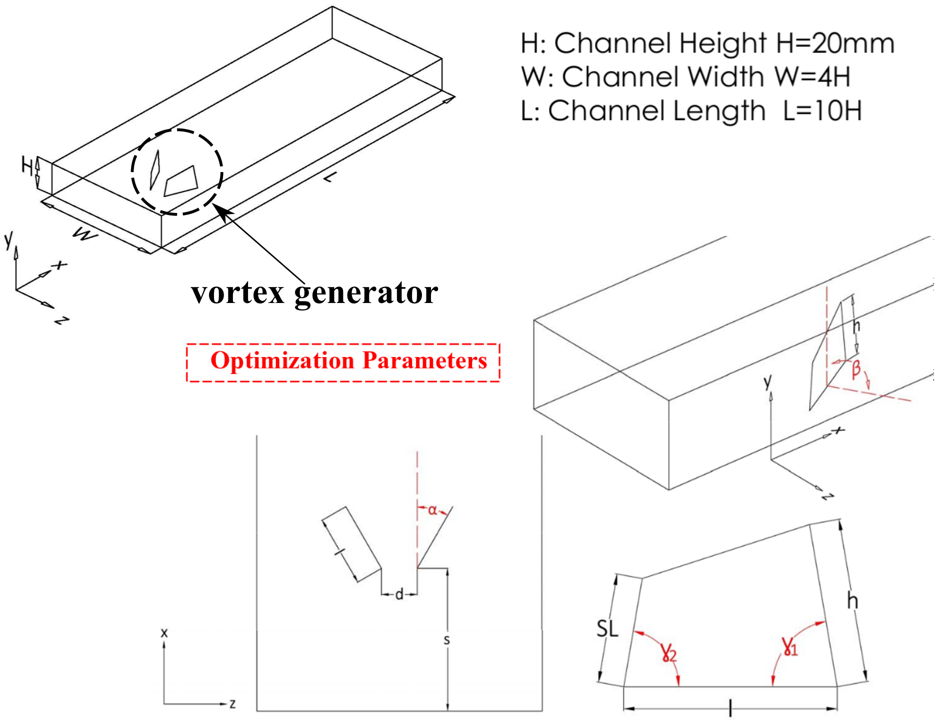


FIGURE 4.3: Shape optimization in CFD of a vortex generator showing the design variables in red color. From H. KARKABA PhD 2018/2021 (H. Karkaba, Dbouk, Habchi, Russeil, Lemenand, and Bougeard, 2019). Flow direction is along the x-axis.

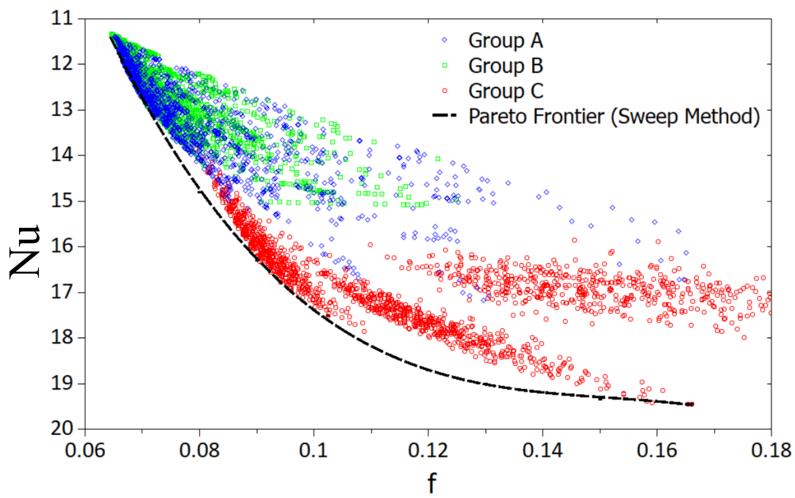


FIGURE 4.4: Pareto-frontier of the shape optimization of vortex generator (H. Karkaba, Dbouk, Habchi, Russeil, Lemenand, and Bougeard, 2019) showing the effective Nusselt number versus the effective friction factor for the different designs. Results from the PhD of H. KARKABA using multigroup sweep method without an optimization algorithm.

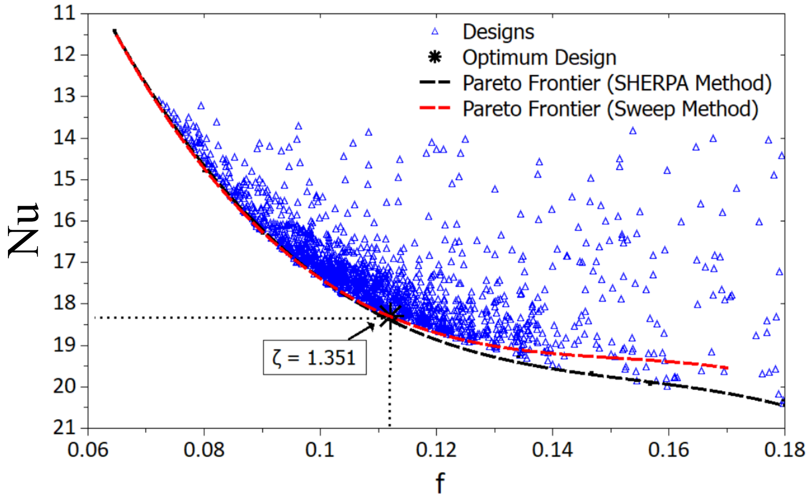


FIGURE 4.5: Pareto-frontier of the shape optimization of vortex generator (H. Karkaba, Dbouk, Habchi, Russeil, Lemenand, and Bougeard, 2019) showing the effective Nusselt number versus the effective friction factor for the different designs. Results from the PhD of H. KARKABA using the artificial intelligence (IA) optimization search algorithm SHERPA® (L. Hertel, 2018; Red-Cedar-Technology, 2016).

Optimum Present Design (H. KARKABA et al. 2019)								
α	β	γ_1	γ_2	h	SL	l	d	s
°	°	°	°	mm	mm	mm	mm	mm
45	55	110	125	19	19	20	10	40

Comparison to previous Designs from the literature					
Author	Khan et al. 2018		Tian et al. 2009		Present Design
Case	DVG	RVG	DWP	RWP	OD
$\frac{Nu}{Nu_0}$	1.151	1.309	1.200	1.370	1.628
$\frac{f}{f_0}$	1.155	1.384	1.161	1.448	1.747
ζ	1.097	1.119	1.142	1.211	1.351

TABLE 4.1: Design parameters of the optimal design (OD) vortex generator obtained by (H. Karkaba, Dbouk, Habchi, Russeil, Lemenand, and Bougeard, 2019) compared to the designs obtained by (T. and Li, 2018) and (Tian, He, Lei, and Tao, 2009). Results from the PhD of H. KARKABA using the artificial intelligence (IA) optimization search algorithm SHERPA® (L. Hertel, 2018; Red-Cedar-Technology, 2016).

4.1.1.2 Vortex generators: from micro to macro, a deep understanding of the induced transition to turbulence

The objective in this research activity is to analyze (from a microscopic to a macroscopic scale), both numerically and experimentally, heat transfer enhancement in channels using vortex generators. The purpose is to own a deep understanding of the induced transition to turbulence phenomena while employing VG inside empty channels. This will help us to propose optimal heat exchangers (HE) configurations to be applied in the automotive industry for a wide range of HE functionality conditions interval (e.g. different temperature difference, Reynolds numbers, indutrial constraints, etc).

The PhD of M. Hatim BELKHOU (at 30%) started on January 2017 lies in this context (A confidential PhD project where the defense is expected on January 2020). This PhD project is funded by VALEO® Thermal Systems Research Group in the context of a 6-years industrial "chair NEO®" between our research unit and VALEO®. This project (**co-supervised by the author at 30%**) is in internal scientific collaboration and partnership with the colleagues: Prof. Daniel BOUGEARD (*PhD director*), Dr. Serge RUSSEIL and Dr. Mohammed MOBTIL at IMT Lille Douai, and in external collaboration with M. Nicolas-Yoan FRANCOIS at VALEO® Thermal Systems Research Group, Paris (La Verrière).

Several work packages (WP) have been defined and investigated in the PhD of M. Hatim BELKHOU as the following:

- Conduct CFD shape optimization on heat exchangers (HE) for better thermal performance enhancement and pressure drop reduction (via RANS turbulence modeling approaches) (Dbouk, 2018c; Dbouk, 2018d).
- Conduct Large Eddy Simulations (LES) for turbulence (Lesieur, Métais, and Comte, 2005; Hinze, 1975) to quantify transitional flow induced by micro-ramp-roughness elements, to be applied in specific HE designs for the automotive industry. The main goal here is to validate a numerical methodology based on LES technique, by comparing numerical CFD results to experimental data obtained recently by tomographic PIV (Ye, Schrijer, and Scarano, 2016b; Ye, Schrijer, and Scarano, 2016a).
- Conduct new experimental measurements to validate the numerical models applied above but extended for turbulent flows with heat transfer (via inverse method measurements techniques).
- Finally, propose innovative solutions coupling macro and micro ramp structures fro better heat transfer and pressure drop reduction.

According to the above mentioned work packages, LES simulations were conducted by (Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2018; Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2019) in order to induce transitional flow to turbulence by micro-ramp-surface roughness rigid elements as shown in figure 4.6.

Preliminary results are obtained in (Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2019; Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2018) through Large-Eddy-Simulations (Lesieur, Métais, and Comte, 2005; Hinze, 1975) using a CFD commercial software. We found numerically that the backflow region behind the micro-ramp ($x/h \leq 4$) is dominated by the trailing edge pair of vortices, with a quasi-steady behavior without any significant fluctuations. However, Kelvin-Helmholtz instabilities appear downstream (x/h=5), and lead to vortex structures formation and fluctuations in the upper shear layer. These fluctuations were in agreement with the presence of a momentum deficit (or inflection point) illustrated in figure 4.7.

Moreover, as show in figure 4.8, a hairpin vortex system is formed behind the micro-ramp. These structures are composed of a head portion and a leg portion. Moving downstream, the swirling hairpin vortices are stretched, distorted and then break down such that their geometrical shape moves from hairpin to ring. These vortex structures observed numerically in (Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2018) are in good agreement with the experimental PIV (Particles Image Velocimetry) observations published by (Ye, Schrijer, and Scarano, 2016b; Ye, Schrijer, and Scarano, 2016a).

The contours visualization of the non-dimensional mean velocity superimposed with projected streamlines at three streamwise positions y-z(x/h=5, 15, 25) are shown in figure 4.9. Our present LES simulations were compared to recent experimental data obtained by (Ye,

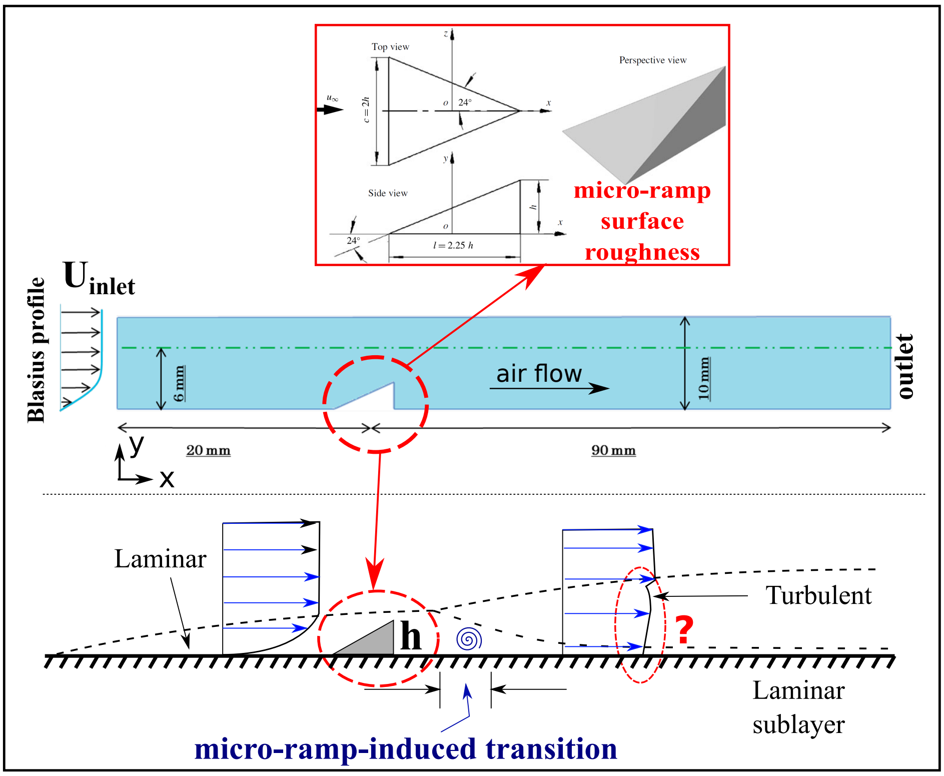


FIGURE 4.6: Micro-ramp-induced transition to turbulent flow. From (Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2019; Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2018).

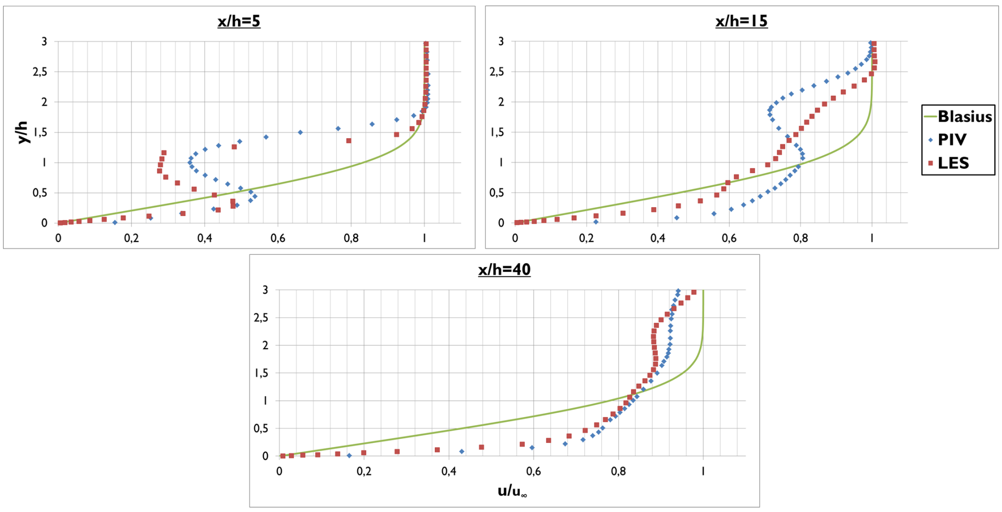


FIGURE 4.7: Profiles of mean streamwise velocity component in the center plane at three positions: $x/h = 5$; 15; 40. From (Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2019).

Schrijer, and Scarano, 2016b; Ye, Schrijer, and Scarano, 2016a). The corresponding cross-sectional contours of streamwise velocity fluctuations are illustrated in figure 4.10.

After the PhD of M. Hatim BELKHOU, another PhD is expected to take place early 2020 on the topic of topology optimization, that will be introduced later as a more advanced optimization technique, for designing innovative HE designs to be applied in the automotive industry (it will be a second PhD to be funded by the industrial partner Valeo® in the

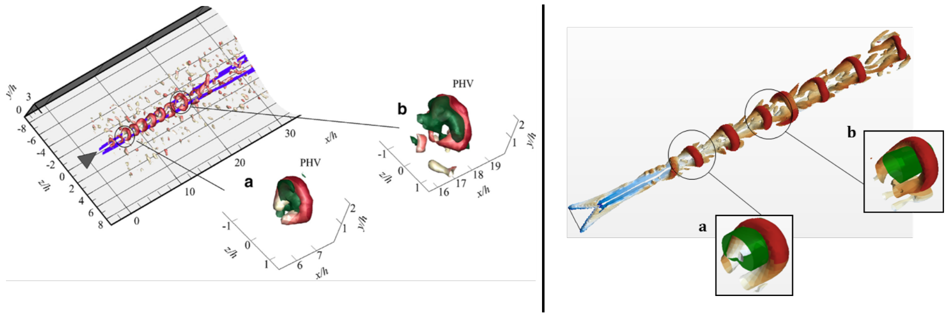


FIGURE 4.8: Instantaneous flow organization color coded by u/u_∞; (a,b) perspective views at precise streamwise locations. (left) experiment by Ye, Schrijer, and Scarano, 2016b; (right) present LES results. From (Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2018).

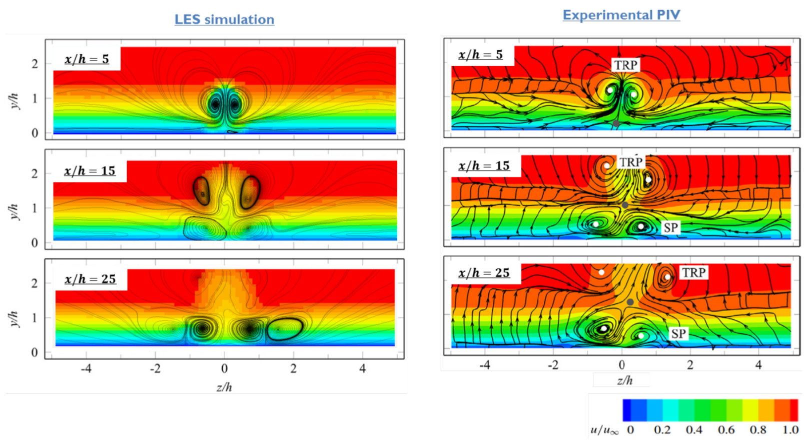


FIGURE 4.9: Color contours visualization of the non-dimensional mean velocity superimposed with projected streamlines at three streamwise positions y-z : x/h=5, 15, 25. (TRP) trailing-edge pair, (SP) secondary pair. Adopted from (Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2019).

context of our industrial chair NEO®).

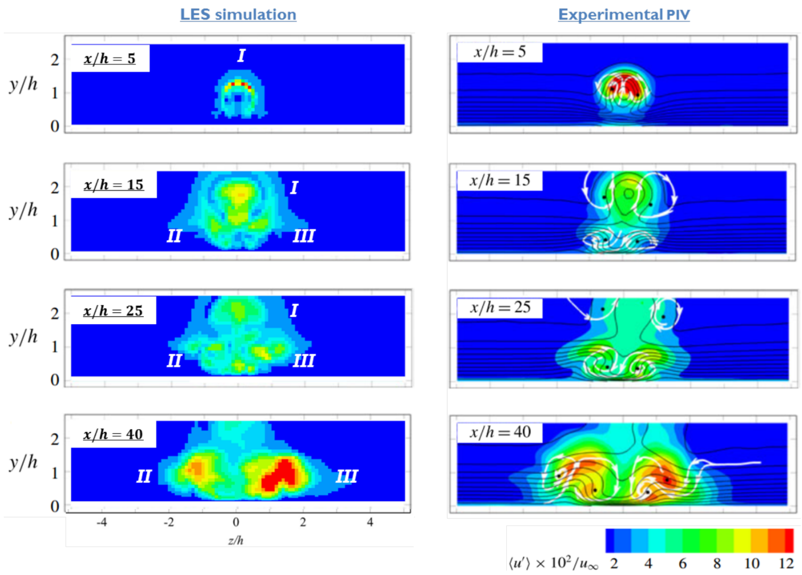


FIGURE 4.10: Cross-sectional contours of streamwise velocity fluctuations. Adopted from (Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2019).

4.1.2 Topology Optimization: Definition, Challenges and Techniques

Topology Optimization (TO) is a recent and emerging methodology (or science or technology) that is not very well developed yet in the optimization of conjugate heat transfer systems or devices as shown in figure 4.11 from a recent literature review article by (Dbouk, 2017a). This makes it a huge field or discipline for investigations, developments and thus with huge potentials for innovations, especially today thanks to the 3D-printing techniques that can fabricate any complex design (Zegard and Paulino, 2016).

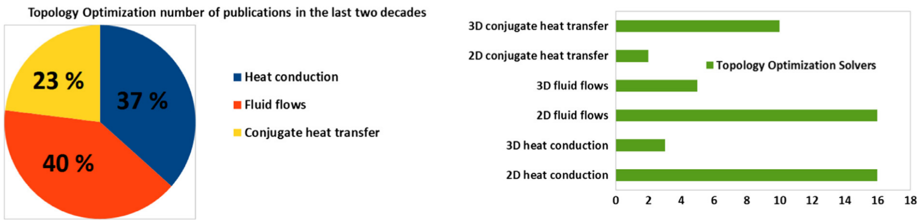


FIGURE 4.11: Number of publications for topology optimization heat transfer systems (Dbouk, 2017a).

TO optimization is about creating a design in an optimal manner by filling some initial volume with material points to constitute and build this optimal design (of course for predefined objective functions and problem constraints) (Bendsøe and Sigmund, 2004). Mathematically speaking, a TO problem can be written as the following:

$$\left\{ \begin{array}{c} min.\ f_0(\mathbf{x}) \quad such\ that: \\ G_i(\mathbf{x}) = 0, \quad \forall i = 1,2,...,m \\ R_k(\mathbf{x}) \leq 0, \quad \forall k = 1,2,...,e \\ \mathbf{x} \in \mathbf{X} \end{array} \right\} \tag{4.5}$$

where $\mathbf{x} = (x_1, x_2, ..., x_n)^T \in \mathbf{R}^n$ are called the design variables of n degrees of freedom (DOE).

$\mathbf{X} = \mathbf{x} \in \mathbf{R}^n | x_j^{min} \leq x_j \leq x_j^{max},\ j = 1, ..., n\ (x_j^{min} \leq x_j^{max})$. The design variable vector $\mathbf{x}$ is thus bounded numerically such that its final value represents only one value, either x^{min} or x^{max}. This can be seen as design variables interchanging between continuous and discrete variables nature. Going from continuous to discrete design variables is usually achieved via interpolation or penalization techniques like the Solid Isotropic Material with Penalization (SIMP) technique (Bendsøe and Sigmund, 2004), Level-Set Methods (Allaire, Jouve, and Toader, 2004; Dugast, Favennec, Josset, Fan, and Luo, 2018), coupled methods (Xia, Shi, and Xia, 2018), etc. f_0, G_i, R_k are real-valued twice continuously differentiable functions.

$G_1, G_2, ..., G_e$ represents the state equations or "equality constraints" for the physical problem to be solved. In case of a pure steady heat conduction example, $[G]$ is then the steady heat conduction equation. In case of TO problem applied to fluid flows with no heat transfer, then $[G]$ should represent the mass and momentum conservation system equations, etc. Moreover, $[R]$ represents "inequality constraints" that can be defined in different manners depending on user objectives. For example, for imposing a certain maximum volume fraction of a material in the domain, $[G]$ will be then just a maximum volume input percentage to be satisfied under an inequality constraint.

4.1.2.1 Optimization problems solving : Iterative Methods

In optimization, there are three basic iterative approaches to find a local or global minimum of an objective function (Bertsekas, 1999): **A: the line-search strategy approaches**, **B: the trust region approaches** and **C: Coupled approaches**.

A, **B** and **C** methods can be applied directly to *unconstrained* optimization problems. However, they can be applied to *constrained* optimization problems but after doing specific treatments and obeying necessary conditions (i.e. Lagrangian multipliers, Augmented Lagrangian multipliers, KKT (Karush-Kuhn-Tucker) conditions for equality and/or inequality constraints, etc.).

A- Line search strategy approaches (Classical or old Methods):

Named Line-search approaches which first choose a step direction and then a step size. Such methods obtain a search direction in each iteration, and search along this direction to obtain a better point. The search direction is a descent direction, normally computed by solving a subproblem that approximates the original optimization problem near the current iterate. Therefore, unless a stationary point is reached, there always exist better points along the search direction.

- **Gradient-based methods:** All methods that require the gradient (and/or higher order gradients) or their approximations. Some examples are: Secant Method (which is a Quasi-Newton method); Steepest Descent or Gradient Descent method; Newton's method; Quasi-Newton's methods. When a Gradient-based method is applied, usually a local optimum will be found.
- **Gradient-free methods:** All methods that neither require the gradient nor its approximation (i.e. Evolutionary Algorithms (EA) like Genetic Algorithms (GA), etc.). An example is the **Bi-Section** method (two starting points are needed).

B- Trust Region strategy approaches (More Recent Methods):

Named Trust region approaches which first choose a step size (the size of the trust region) and then a step direction (see Wenyu and Ya-Xiang, 2006; Bertsekas, 1999; Harth, Sun, and Schafer, 2007). Trust region algorithms (TRA) are a class of relatively new algorithms. The trust region approach is strongly associated with approximation (a solution of the approximate model can be taken as the next iterate point). In fact, most line search algorithms also solve approximate models to obtain search directions. However, in a TRA, the approximate model is only "**trusted**" **in a region near the current iterate**. Because of the boundedness of the trust region, TRA's **can use non-convex approximate models**. This is one of the advantages of TRA's compared to line search algorithms. Trust region algorithms are reliable and robust, they can be applied to ill-conditioned problems, and they have very strong convergence properties. For comparisons between Line-search and trust-region methods, see Harth, Sun, and Schafer, 2007.

C- Coupled Methods: Like Genetic Algorithms (GA) coupled to line-search-trusted-region

methods (for more details see(Xiaowei, 2007; JingHui, Rui, Donglian, Hongfang, and Shuhua, 2011)).

4.1.2.2 Topology optimization problems solving : Specific algorithms

The topology optimization problem in (4.5) is usually a large-scale, highly non-linear, non-convex, numerically-unstable optimization problem with equality and inequality constraints that requires specific treatments like: optimality necessary conditions to be satisfied (like the KKT conditions), advanced numerical techniques (like duality and convex analysis, line search techniques, Lagrange Multipliers, adjoint methods, etc) and advanced gradient-based optimization algorithms (like MMA, GCMMA, SNOPT, etc) (Svanberg, 1987; Svanberg, 2002; Gill, Murray, and Saunders, 2005; Bertsekas, 1999) to be solved efficiently and to achieve convergence. For example, in a topology optimization problem (4.5), numerical instabilities (Sigmund and Petersson, 1998) may arise such as:

- Checkerboards problems formation of regions of alternating solid and void elements that are ordered in a checkerboard-like fashion,
- Mesh-dependence problems (qualitatively different solutions for different mesh-sizes or discretizations),
- Local minima (i.e. obtaining different solutions to the same discretized problem when choosing different algorithmic parameters),
- Etc...(Sigmund and Petersson, 1998)

4.1.3 A review of Topology Optimization Method applied to Heat transfer and fluid flows

In (Dbouk, 2017a), I conducted a detailed review about TO solvers and algorithms applied to heat transfer systems (see table 4.2). I found that there is still **a huge gap in the literature**, where TO must be developed to the optimization of thermofluid flows and heat transfer systems.

For that reason, since September 2014 (Dbouk, 2017a) I have been developing a recent research axis on Topology Optimization applied to three-dimensional conjugate heat transfer systems and devices. For those developments, I had the chance to supervise (at 100%) the PhD of M. V. SUBRAMANIAM between Jan. 2016 and Dec. 2018 at our research unit. The developments of this R&D&I axis at the IMT Lille Douai goes towards the objectives of developing an advanced numerical platform for TO. This new numerical platform is based on the (OpenFOAM, 2019) open source (opensource.com, 2018) CFD library. I have been coupling it to advanced optimization algorithms like the Method of Moving Asymptotes (MMA) by (Svanberg, 1987) and the Globally Convergent Method of Moving Asymptotes (GCMMA) by (Svanberg, 2002), and other open source interior-point optimization algorithms (like the Coin-or project).

4.1.4 Internally developed CFD solver for topology optimization of heat conduction problems : An Experimental validation

In (Dbouk and Harion, 2015), I implemented in OpenFOAM, 2019 and investigated the MMA algorithm performance and proposed a new strategy with new set of parameters that performed well when solving a complex topology optimization problem (problem 1) from the literature (Svanberg, 2002; Gomes-Ruggiero, Sachine, and Santos, 2010; Gomes-Ruggiero, Sachine, and Santos, 2011) as illustrated in figure 4.12. The MMA algorithm is based on a primal-dual interior point method.

Study	Mesh	Flow State	Discretization	Adjoint	Optimizer	Reference
1	3D Structured Uniform	Transitional Steady Incomp.	FEM	Discrete	MMA/ SLP	Lee [17]
2	2D Structured Uniform	Laminar Steady Incomp.	FVM	Discrete	MMA	Marck et al. [60, 61] Marck [16]
3	3D Structured Uniform	Laminar Steady Incomp.	FEM	Continuous	MMA	Dede [18]
4	3D Structured Uniform	Laminar Steady Incomp.	FEM	Discrete	MMA in parallel	Alexandersen et al. [4, 5]
5	3D Structured Uniform	Turbulent Steady Incomp.	FVM	Continuous	ALM* Steepest-Descent	Kontoleontos et al. [101]
6	3D Structured Uniform	Laminar Steady Incompr.	FVM	Continuous	MMA	Oevelens & Baelmans [103]
7	3D Structured Uniform	Laminar Steady Incompr.	FEM	Discrete	n/a	Koga et al. [36]
8	3D Structured Uniform	Laminar Steady Incompr.	FEM	Continuous	n/a	Yaji et al. [104]
9	2D Structured Uniform	Laminar Steady Incompr.	FEM	Discrete	MMA	Yoon [87]
10	3D Structured Uniform	Laminar Steady Incompr.	FEM	n/a	MMA	Yoon [88]
10	3D UnStructured Uniform	Laminar Transient Incomp.	XFEM†	Discrete	GCMMA	Coffin & Maute [43]
11	3D UnStructured Uniform	Laminar Steady Incomp.	XFEM†	Discrete	GCMMA	Coffin & Maute [105]
12	3D UnStructured Uniform	Laminar Steady Incomp.	FEM	n/a	n/a Gradient-Based	Zhou et al. [106]

*ALM: Augmented Lagrange Multipliers; † XFEM: Extended Finite Elements Method.

TABLE 4.2: Some topology optimization solvers developed for conjugate heat transfer applications. All the references can be found in (Dbouk, 2017a) from which this table was taken from.

After a deep analysis of the MMA algorithm and other existing topology optimization algorithms in the literature (Svanberg, 1987; Gomes-Ruggiero, Sachine, and Santos, 2011; Gill, Murray, and Saunders, 2005; Bertsekas, 1999), I coupled the MMA to (OpenFOAM, 2019) and solved for TO applied to a heat conduction of bi-material volume-to-point (VP) problem (Subramaniam, Dbouk, and Harion, 2018a) using gradient-based technique based on the continuous adjoint method (Giles and Pierce, 2000; Othmer, 2008a). The VP heat conduction topology optimization problem is known in the literature (Gersborg-Hansen, Bendsøe, and Sigmund, 2006) as the filling of a domain in an optimal way by a first material that has different thermal diffusivity from that of another second material. Applying a heat generation source and a heat sink at one edge of the boundary domain, the objective function is to minimize the averaged temperature in the whole domain (thus to find the optimal structure of the bi-material distribution) (see figure 4.13). The equality constraint is the state equation defined by the heat conduction and the inequality constraint is the volume constraint imposed on the highly conductive material.

In order to achieve fast computations at a lower computational cost or number of iterations, a sensitivity analysis is conducted and developed in the (OpenFOAM, 2019) platform based

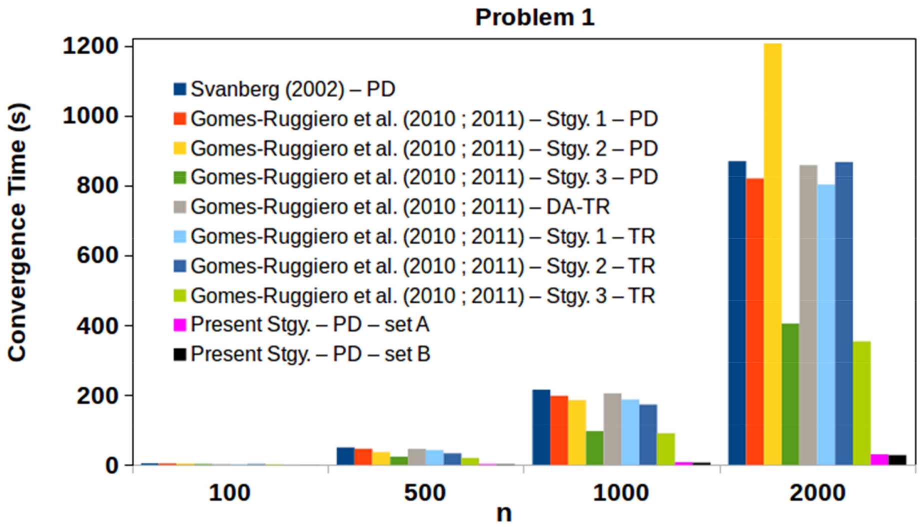


FIGURE 4.12: Performance of the MMA algorithm (Dbouk and Harion, 2015; Svanberg, 1987; Svanberg, 2002; Gomes-Ruggiero, Sachine, and Santos, 2010; Gomes-Ruggiero, Sachine, and Santos, 2011).

on the Continuous Adjoint Method (Othmer, 2008b; Hinterberger and Olesen, 2011). This is in order to compute efficiently (using the same (OpenFOAM, 2019) CFD solvers) the gradient of the objective function with respect to the design variables (here have the role to be either material 1, or material 2 (black, or white, respectively)). The whole procedure of the algorithm developed in (OpenFOAM, 2019) applied to steady heat conduction topology optimization is illustrated in the flow chart of figure 4.13.

The optimal designs obtained by (Subramaniam, Dbouk, and Harion, 2018a) had the form of tree-like structures as shown in figure 4.13 which is know from the literature. However, thermal experimental validations of such structures have never been conducted before ! This was identified as **a huge gap in the literature** to be filled. For that reason, (Subramaniam, Dbouk, and Harion, 2018a) developed an experimental infra-red thermography setup for that purpose as illustrated in figure 4.14.

The fabrication of two optimal tree-like structures obtained by the numerical TO solver was a serious challenge. After huge efforts in selecting the appropriate materials, the tree-like structures have been fabricated by using aluminum (cut by water jet technique) and polymer resin materials. The final structures are then created as shown in figure 4.15 (after being inserted in a fitting mold where the liquid polymer solidified inside an oven at around 80 °C).

Since heat transfer in VP problems is manifested by an important conduction mode, then the interface between the two materials (aluminum/polymer) was verified to ensure an excellent interface adhesion quality (observed under a microscope) as shown in figure 4.16. The water jet cutting technique overcomed the laser jet cutting one in terms of better quality at the interface (figure 4.16).

Interestingly, in (Subramaniam, Dbouk, and Harion, 2018a) we showed a good agreement between the experimental measurements and the numerical results with very close values of the objective function (average temperature at steady state), as illustrated for two tree-like optimal designs in figures 4.17 and 4.18, respectively.

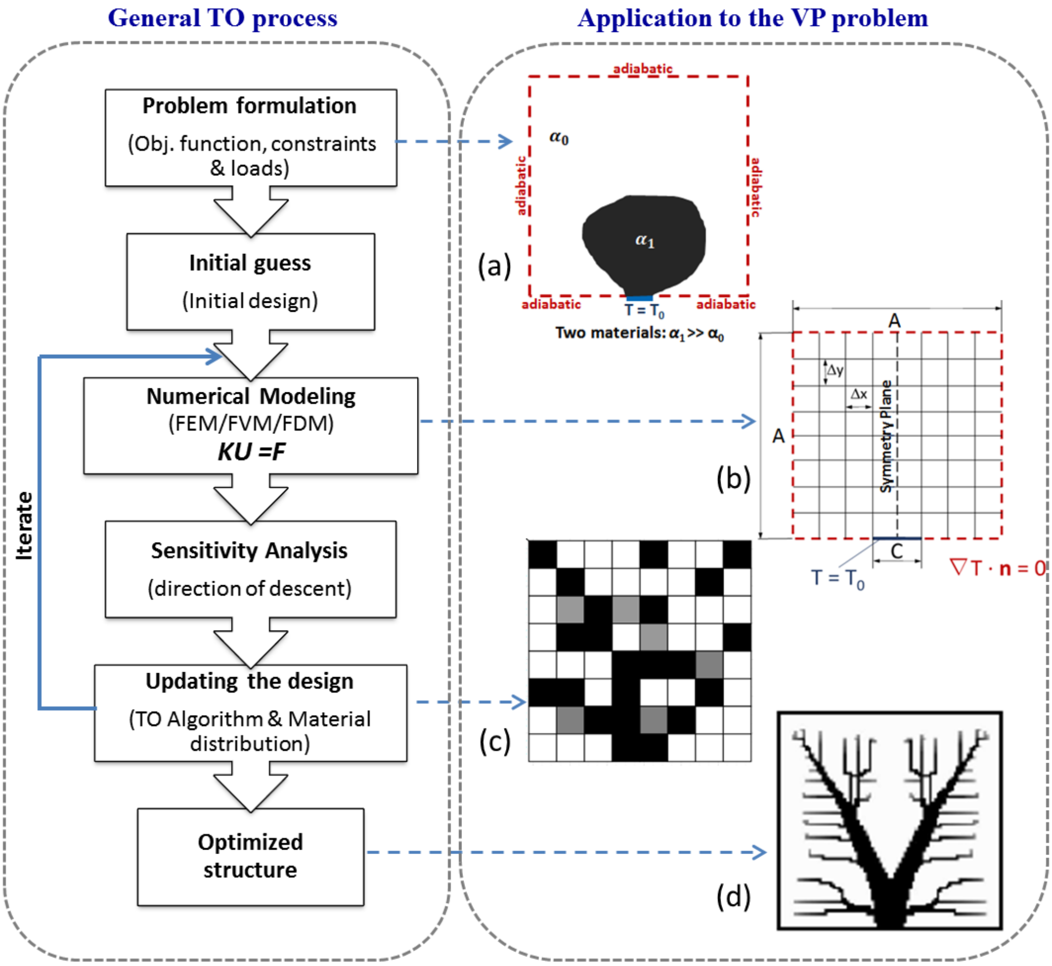


FIGURE 4.13: Topology optimization algorithm applied to steady heat conduction problem in 2D (Subramaniam, Dbouk, and Harion, 2018a).

During the PhD period of V. SUBRAMANIAM at our research unit at the IMT Lille Douai, I initiated international collaborations and network development. I conducted several scientific discussions and invited Prof. J. DIRKER who is a teammate of Prof. J. MEYER who is the Clean Energy Research group Head of Department and Division Head at the University of Pretoria in South Africa. Moreover a collaborative work (Dbouk, Dirker, Fachinotti, and Page, 2019) is still going on with Prof. V. FACHINOTTI at the Computational Methods Center Research Group at Santa Fe University, Santa Fe, Argentine. I also invited Dr. R. HREIZ, from the Optimization and Simulation Research Group at the Process Engineering and Reaction Laboratory (LRGP), CNRS (UMR 7274), University of Lorraine, France.

With Professors DIRKER, and FACHINOTTI (mentioned above), I initiated some collaborative work in order to investigate the influence of:

- the adjoint method (Continuous Adjoint(CA) or Discrete Adjoint(DA)) for objective function gradient computation (Giles and Pierce, 2000),
- the numerical discretization method (Ferziger and Peric, 2002) (i.e. FVM (Finite Volumes Method), FEM (Finite Elements Method), FDM (Finite Differences Method)),
- the grid or mesh cells type (i.e. structured, unstructured, uniform, nonuniform, cells shape, etc),

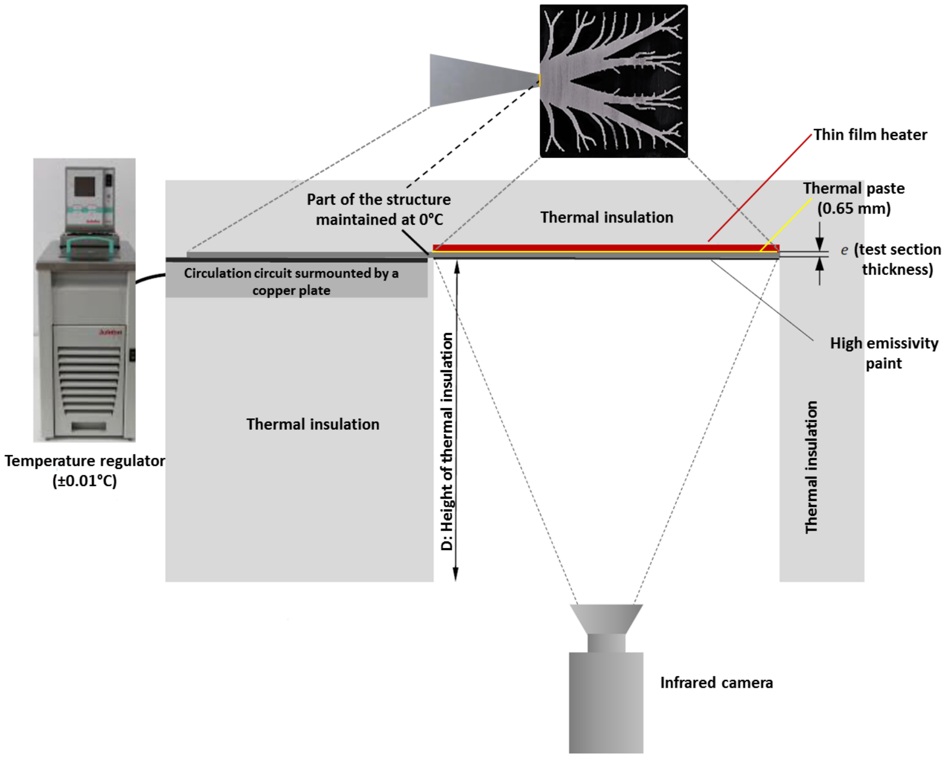


FIGURE 4.14: The topology optimization experimental infra-red thermography setup developed by (Subramaniam, Dbouk, and Harion, 2018a).

- the interpolation techniques for material distribution (Bendsøe and Kikuchi, 1988; Bendsøe, 1989; Bendsoe and Sigmund, 2013; Stolpe and Svanberg, 2001), the spatial filters type (Guest, Prevost, and Belytschko, 2004; Sigmund, 2007),
- etc

on the optimality of the topology optimization solutions (& the robustness of TO solvers) obtained with the MMA (Svanberg, 1987) and/or interior-point (IP) methods. This is illustrated in figures 4.19 and 4.20, and it is still a large filed for further research and investigations.

Very recently the team by Prof. Ole SIGMUND, at the Department of Mechanical Engineering and Solid Mechanics (Technical University of Denmark), showed that the optimal structure for these kind of heat conduction or volume-to-point problems is a hair-pins-like structure (Yan, Wang, and Sigmund, 2018).

In this research axis no.2, I also initiated very recently for a future collaboration (as Masters-II research project, as common internship) with Dr. Lilla KOLOSCZAR, and Prof. Jean-Marie BUCHLIN from the Environmental and Applied Fluid Dynamics Research Group at Von-Karman Institute for Fluid Dynamics in Belgium. This an advantage with huge potentials for future collaborations especially that our two departments in Douai (North of France) and Belgium are very close geographically to each other.

Furthermore, in another contribution through a 6-months Masters2 internship project, i supervised (at 100%) the research works by T.-C. NGUYEN. During his 6-months internship a new OpenFOAM, 2019 library has been developed and implemented for several spatial filters (Sigmund, 2007) intended for topology optimization solvers. Such filters are essential in topology optimization in order to have a minimum length control of the final designs and thus better final description of the optimal structures. In (Nguyen and Dbouk, 2017),

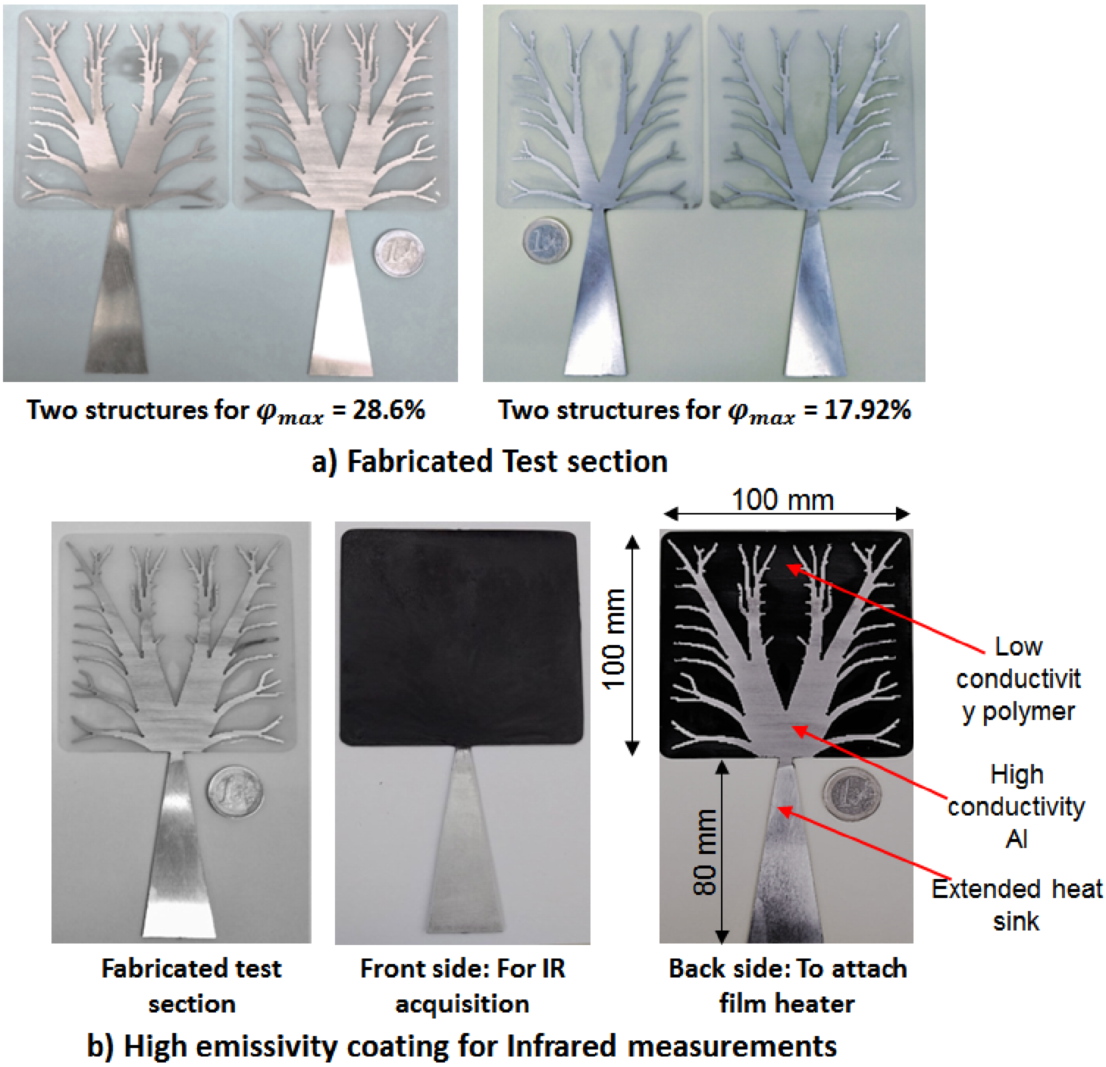


FIGURE 4.15: Fabricated topology optimization tree-like bi-material structures. From (Subramaniam, Dbouk, and Harion, 2018a).

we investigated the influence of different spatial filters on the computational speed, on the final tree-like structures design, and overall algorithm performance. The tree-like structures were obtained for a 2D heat conduction topology optimization problem (or VP problem). The strategy that we followed in the OpenFOAM, 2019 library, on generalized collocated mesh types, is illustrated in figure 4.21.

The computational time affected by the application of the different spatial filters (Nguyen and Dbouk, 2017) are illustrated in figure 4.22 for 10^4 design variable or degrees of freedom (DOF). It can bee seen clearly that the filter's choice and its implementation or coding inside OpenFOAM, 2019 affects well the computational time. An example piece-of-code is illustrated in figure 4.23 for the HeavySide-Erode filter type (Sigmund, 2007).

The influence of filters' type (Nguyen and Dbouk, 2017) on the final optimal structures is shown in figures 4.24 and 4.25.

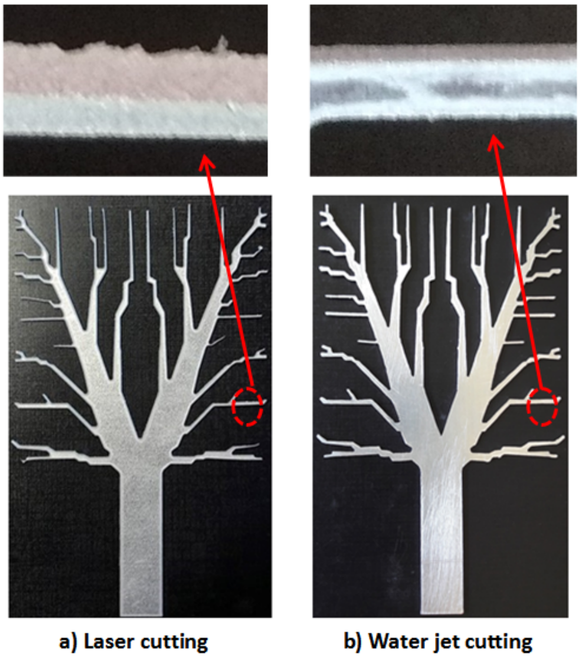


FIGURE 4.16: Interface quality after using two cutting techniques (Subramaniam, Dbouk, and Harion, 2018a).

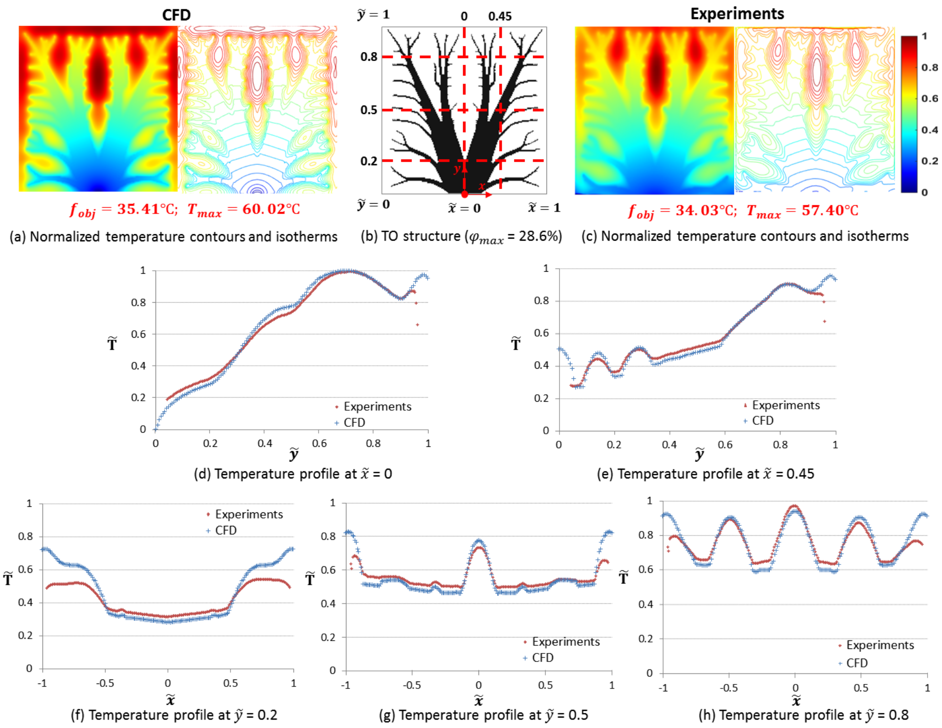


FIGURE 4.17: Thermal measurements on optimal structure of 28.6% volume constraint applied on the aluminum material (in black). From (Subramaniam, Dbouk, and Harion, 2018a).

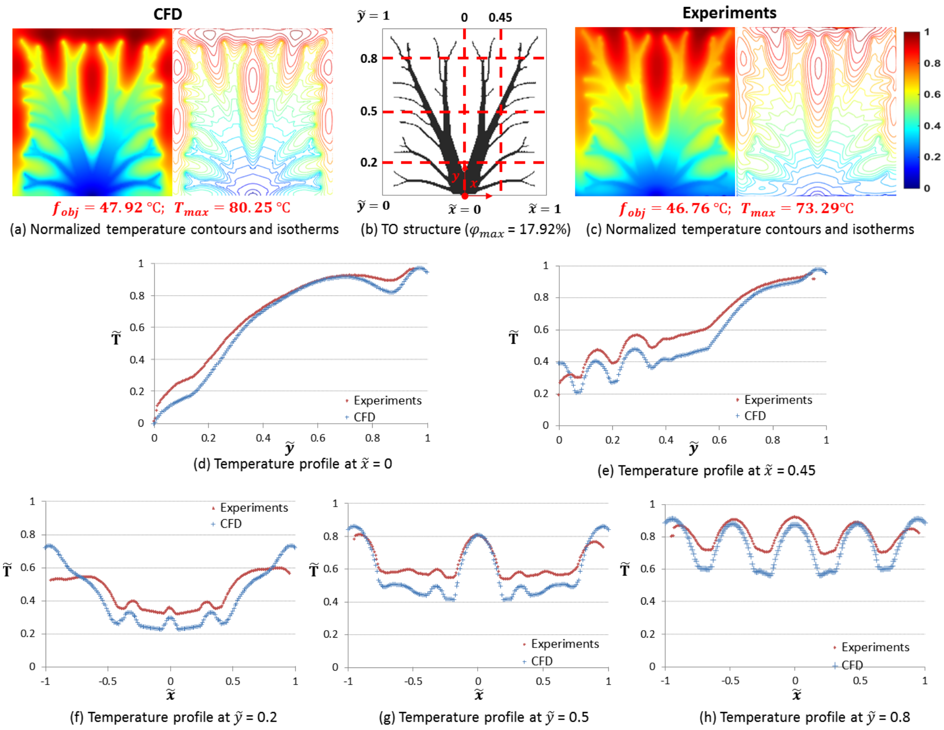


FIGURE 4.18: Thermal measurements on optimal structure of 17.92% volume constraint applied on the aluminum material (in black). From (Subramaniam, Dbouk, and Harion, 2018a).

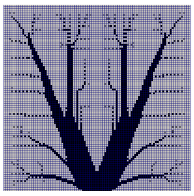
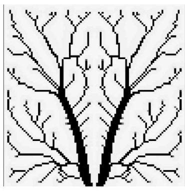
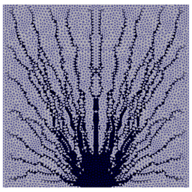
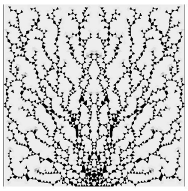
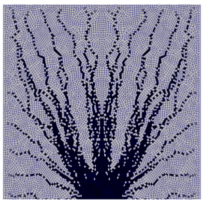
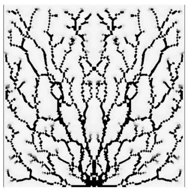
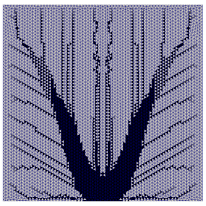
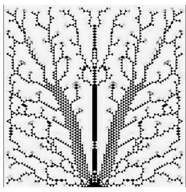
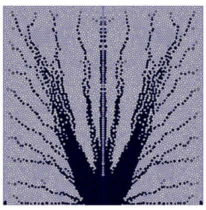
Mesh type	FVM-MMA-CA	FEM-IPOPT-CA
Structured Square cells	 0.96089	 0.753452
Unstructured Triangular cells	 0.96975	 0.638434
Unstructured Quadrangular cells	 0.97665	 0.735470
Structured Triangular cells	 0.96343	 0.730092
Unstructured Polyhedral cells	 0.97120	

FIGURE 4.19: Steady temperature distribution of the optimal structures, with normalized value of the thermal coefficient (lower: is better). Influence of mesh cells type on optimal tree-like structures obtained with topology optimization applied to heat evacuation volume-to-point problem (average temperature minimization). From (Dbouk, Dirker, Fachinotti, and Page, 2019).

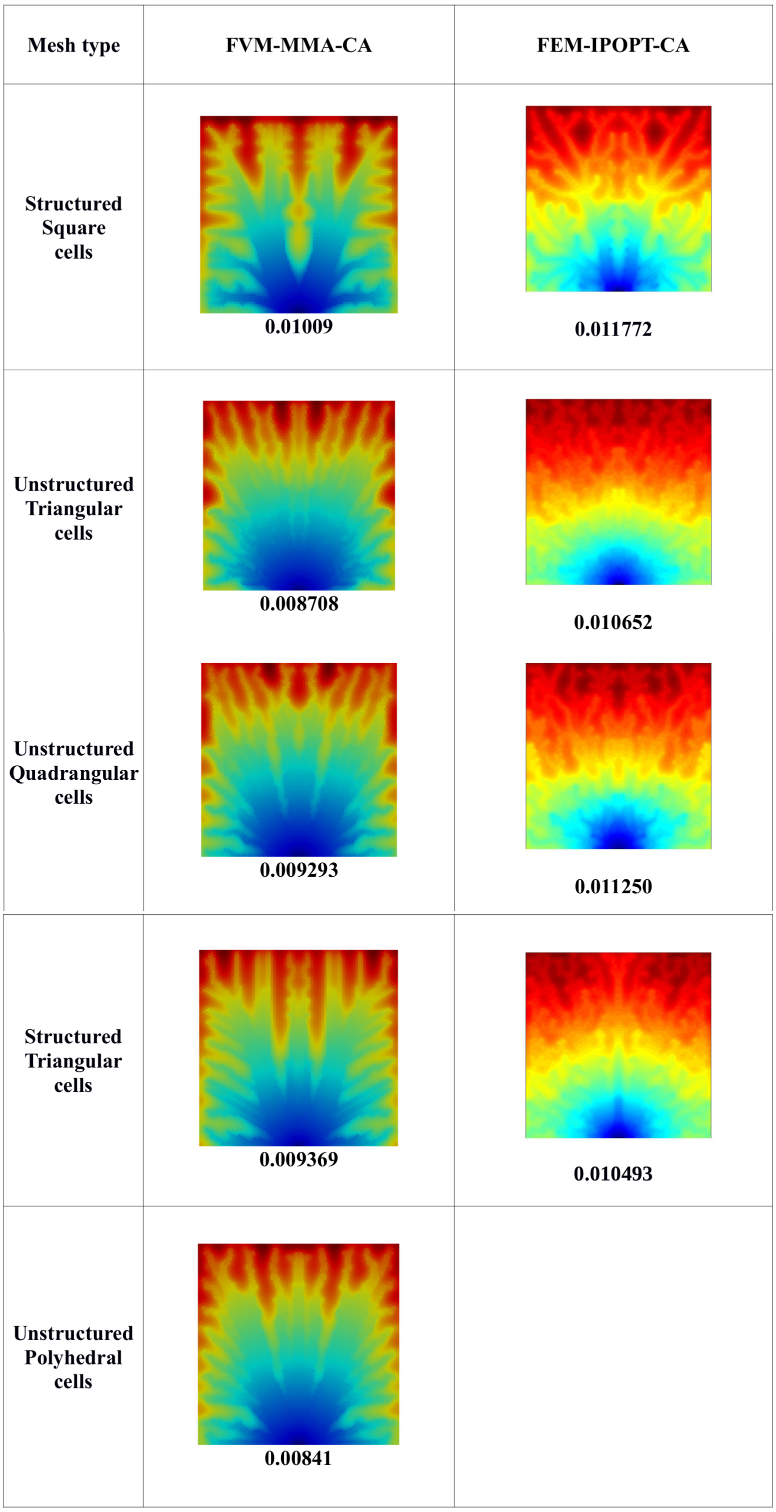
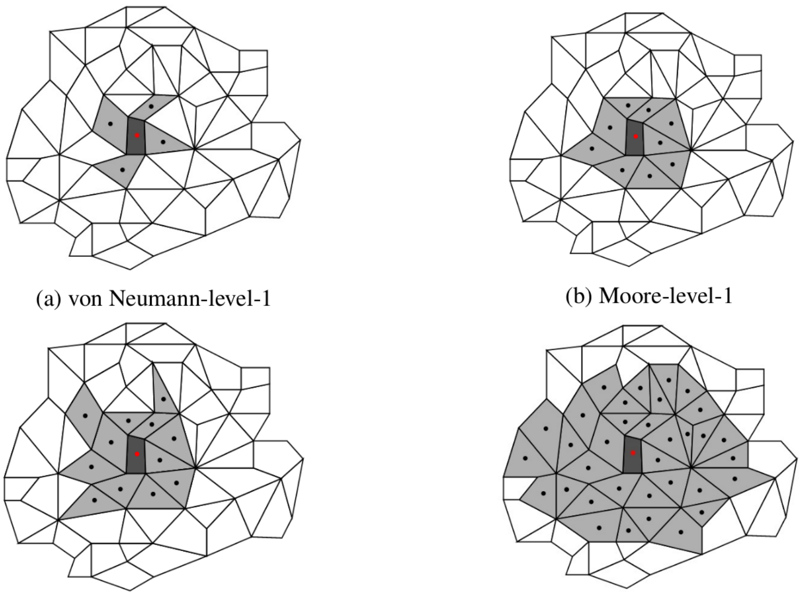


FIGURE 4.20: Steady temperature profiles for optimal structures with value of intermediate-material error degree (high error: lower values). Influence of mesh cells type on optimal tree-like structures obtained with topology optimization applied to heat evacuation volume-to-point problem (average temperature minimization). From (Dbouk, Dirker, Fachinotti, and Page, 2019).



(a) von Neumann-level-1 (b) Moore-level-1

(c) von Neumann-level-2 (d) Moore-level-2

FIGURE 4.21: General spatial filtering technique applied numerically on collocated grids as Neighborhood and Levels (Nguyen and Dbouk, 2017).

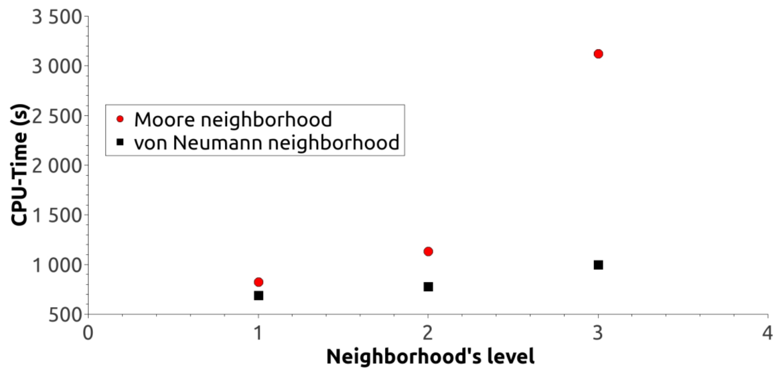


FIGURE 4.22: CPU-Time increases with the neighborhood's level for a basic density filter (Svanberg and Svärd, 2013) using the algorithm MMA (Svanberg, 1987; Nguyen and Dbouk, 2017). $DOF = 10^4$.

```
#include "FilterHeavySideErode.H"
// FilterHeavySide_Erode
Foam::volScalarField FilterHeavySideErode::HeavySideErode_Filtering
(Foam::volScalarField etaa, double RMIN, double beta1) {
Foam::volVectorField C = etaa.mesh().C(); // OpenFOAM Mesh cells-coordinates
Field

double SS=0.; double SS2=0.;
double H=0.;
// based on one levels in OpenFOAM (cellPoints and pointCells)
forAll(etaa.mesh().C(),i)
{
        const unallocLabelList& neigh = etaa.mesh().cellPoints()[i]; // ne:
neigbor
        forAll(neigh, neighI)
        {

                const unallocLabelList& neigh_of_adj = etaa.mesh().pointCells()
[neigh[neighI]];
                forAll(neigh_of_adj, neigh_of_adjI)
                {
```

FIGURE 4.23: A C++ piece-of-code example in OpenFOAM, 2019 for the Erode type filter (Nguyen and Dbouk, 2017; Sigmund, 2007).

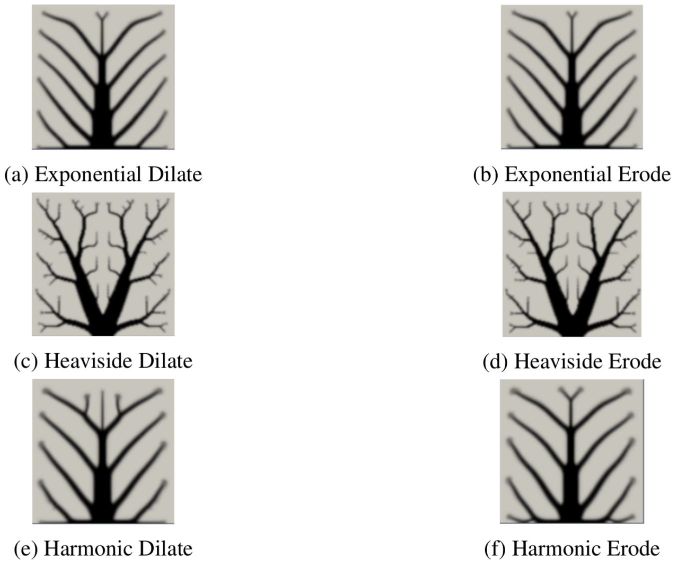


FIGURE 4.24: Optimal structures with using an innovative "TopoStep" algorithm (Nguyen and Dbouk, 2017). $DOF = 10^4$.

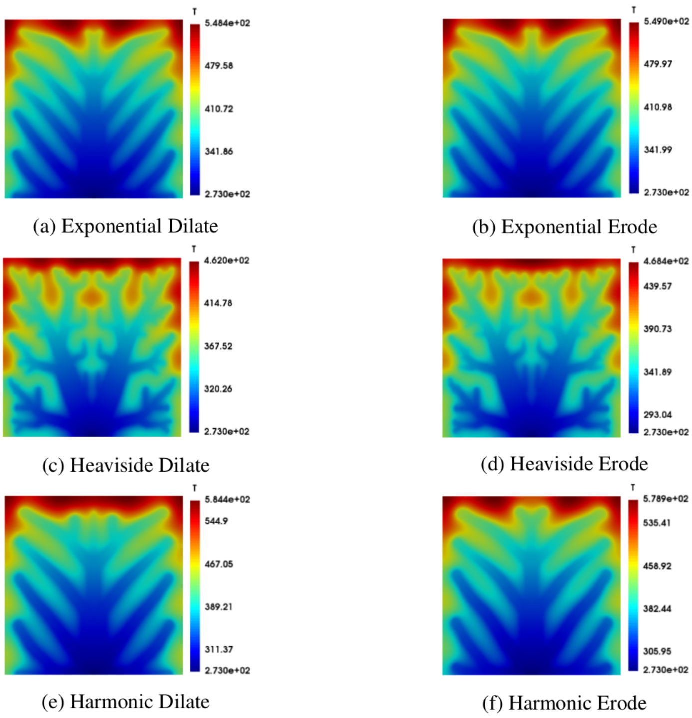


FIGURE 4.25: Temperature profiles of figure 4.24 (Nguyen and Dbouk, 2017). $DOF = 10^4$.

4.1.5 Internally developed CFD platform for topology optimization of conjugate heat transfer systems

After the experimental validation of the heat conduction topology optimization CFD solver, I continued developing and creating, at the research unit at IMT Lille Douai, a new topology optimization platform in CFD (OpenFOAM, 2019) to account for topology optimization of conjugate heat transfer systems (under forced convection steady laminar flow regimes).

Some topology optimization solvers have been developing in the literature (Dbouk, 2017a) for conjugate heat transfer systems, but they are still of very few number and limited for simple cases (single objective, 2D, small number of design variables, uniform structured meshes, etc). This was identified as **a huge gap in literature**. For that reason, to fill this huge gap, during the PhD of V. SUBRAMANIAM (**supervised by the author at 100%**) we developed several numerical work packages (WP) such as: a multi-objective function derivation for reducing pressure drop and maximizing the thermal power in a conjugate heat transfer fluid flow problem (Subramaniam, Dbouk, and Harion, 2018b) as shown in figure 4.26. The newly developed topology optimization platform may handle 2D and 3D configurations on all types of grid or mesh cells, and it allows applying wide variety of different numerical schemes and spatial filters (Sigmund and Petersson, 1998; Guest, Prevost, and Belytschko, 2004; Sigmund, 2007).

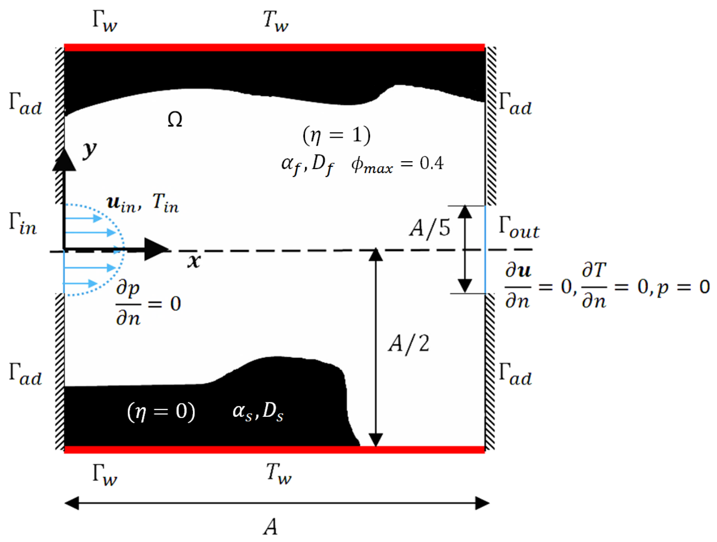


FIGURE 4.26: Two-dimensional topology optimization domain of fluid flow with conjugate heat transfer (with boundary conditions shown). Selected from (Subramaniam, Dbouk, and Harion, 2018b).

The objective function is:

$$F = \omega_1 J_f + \omega_2 J_{th} \tag{4.6}$$

where:

$$J_f(\boldsymbol{u}, p) = -\int_{\Gamma} \left(p + \frac{1}{2}|\boldsymbol{u}|^2\right) \boldsymbol{u} \cdot \boldsymbol{n} \, d\Gamma \tag{4.7}$$

and

$$J_{th}(\boldsymbol{u}, T) = \int_{\Gamma} (\rho C_p T) \boldsymbol{u} \cdot \boldsymbol{n} \, d\Gamma \tag{4.8}$$

$\boldsymbol{u}$ is the fluid velocity vector field, p the pressure field, ρ the density, C_p the heat capacity and $\boldsymbol{n}$ the unit normal vector to the boundary. ω is a pondering or weighting variable ($\omega \in [0, 1]$) that places like a priority degree between the two objective functions defined in (4.7) and (4.8) depending on the users' choice, type and/or cost of application.

The topology optimization problem is solved in (OpenFOAM, 2019) for low Reynolds numbers $Re \in [3, 100]$ and moderate temperature differences $\Delta T = T_w - T_{in} \in [10 - 80]$. Its mathematical description is given as the following:

Minimize:

$$F(\boldsymbol{u}, p, T, \eta) \tag{4.9a}$$

subject to:

$$\nabla \cdot \boldsymbol{u} = 0 \tag{4.9b}$$

$$(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \nabla \cdot (\nu \nabla \boldsymbol{u}) - \alpha(\eta)\boldsymbol{u} \tag{4.9c}$$

$$(\boldsymbol{u} \cdot \nabla)T = \nabla \cdot (D(\eta)\nabla T) \tag{4.9d}$$

$$\frac{1}{V} \sum_{j=1}^{nCells} \eta_j \leq \phi_{max} \tag{4.9e}$$

where η is the design variables field (solid or fluid, see figure 4.26), D the effective thermal diffusivity, ν the fluid kinematic viscosity, T the temperature field, ϕ_{max} the maximum allowed volume fraction or porosity and α stands for the Brinkman forcing or penalization term (Khadra, Angot, Parneix, and J-P, 2000; Dbouk, Perales, Babik, and Mozul, 2016).

Material distribution technique: The final solution of the topology optimization problem knows only discrete variable values, which is not the case with the continuous modeling formulation. To solve this issue, the density based TO approach by (Bendsøe and Sigmund, 2004; Bendsoe and Sigmund, 2013), can overcome this issue by introducing a continuous design field, $\eta(\boldsymbol{x})$ that is modified iteratively via a material interpolation technique. This is applied by (Subramaniam, Dbouk, and Harion, 2018b) such that the friction coefficient (α) and the effective thermal diffusivity (D) change with η by applying a Rational Approximation of Material Properties (RAMP-type interpolation functions) (see Stolpe and Svanberg, 2001) as the following:

$$\alpha(\eta) = \alpha_s + (\alpha_f - \alpha_s)\eta \frac{1+k}{\eta + k} \tag{4.10a}$$

$$D(\eta) = D_s + (D_f - D_s)\eta \frac{1+k}{\eta + k} \tag{4.10b}$$

knowing:

$$(\alpha(\eta), D(\eta)) = \begin{cases} (\alpha_s, D_s), & \text{if } \eta = 0 \text{ (solid material)} \\ (\alpha_f, D_f), & \text{if } \eta = 1 \text{ (fluid material)} \end{cases} \tag{4.11}$$

So, for all $0 \leq \eta \leq 1$, $k > 0$ is a parameter that governs the shape of the functions $\alpha(\eta)$ and $D(\eta)$ (for example α is interpolated between the two extrema of $\alpha_f \approx 0$ and $\alpha_s \approx \infty$). In the fluid domain, the Brinkman penalization term $\alpha \boldsymbol{u}$ approaches zero to recover the classical Navier-Stokes equation in 4.9. However in the solid domain, α has a very large value in order to force the local velocity to approach zero ($\alpha_f \approx 0$ and $\alpha_s \approx 10^5$ were considered in Subramaniam, Dbouk, and Harion, 2018b).

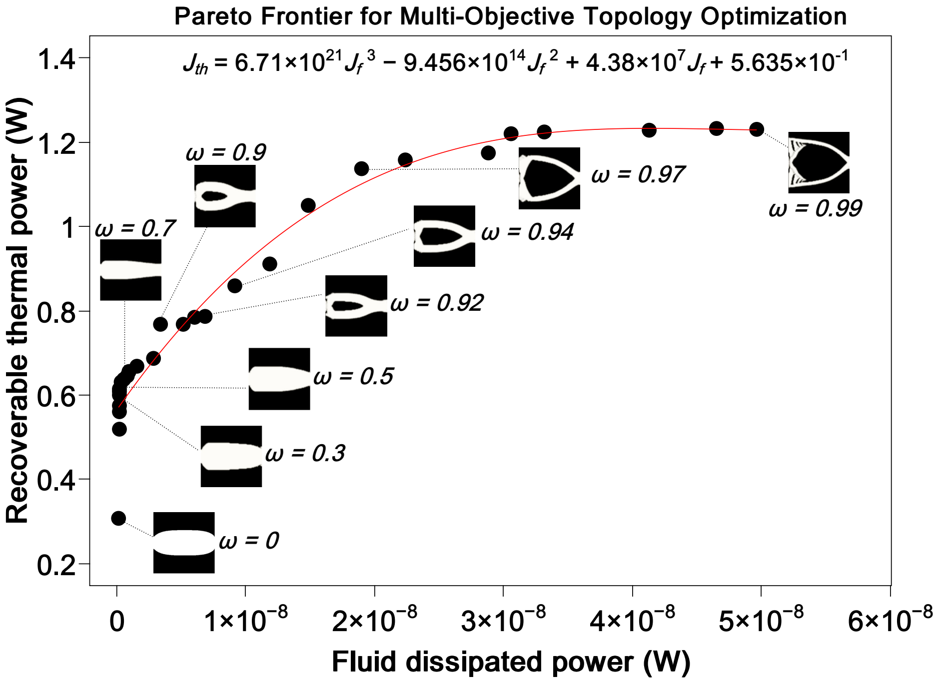


FIGURE 4.27: Topology optimization problem of conjugate heat transfer system (steady state - Pareto front: bi-objective function). Selected from (Subramaniam, Dbouk, and Harion, 2018b).

The optimal thermofluid designs obtained after solving the topology optimization problem in (4.9) are shown in figures 4.27 and 4.28. They represent the multi-objective Pareto-Frontier (or Pareto-Set) of the steady state designs with their local dimensionless temperature and velocity values defined as the following:

$$\tilde{T} = \frac{T - T_{in}}{T_w - T_{in}} \tag{4.12}$$

$$\tilde{u} = \frac{|\boldsymbol{u}|}{|\boldsymbol{u}_{in}|_{max}} \tag{4.13}$$

where T_{in} is the fluid temperature at the inlet boundary and T_w is the temperature at the top and bottom walls boundaries Γ_w (see figure 4.26). $|\boldsymbol{u}_{in}|_{max}$ is the maximum fluid velocity at inlet and $|\boldsymbol{u}|$ is the velocity magnitude.

In the PhD works by V. SUBRAMANIAM, we investigated the influence of different conditions on altering the final optimal designs such as the Reynolds number, temperature boundary value, and the influence of the thermal diffusivity ratio $(\frac{D_s}{D_f})$ as shown in figure 4.29 (Subramaniam, Dbouk, and Harion, 2018b). From figure 4.29 it can be observed clearly that when the diffusivity of the solid material is imposed initially lower than that of the fluid, the optimization algorithm places fluid branches or cells, more near to the boundary upper and lower walls, so that to enhance heat transfer (and thus the thermal power maximization objective at $\omega = 0.9$).

4.1.6 Topology optimization of thermofluid components: a continuing field for research, development and innovation

My R&D&I activities are continuing on the **research Axis 2** for both topology and shape design optimization, that have huge potentials for future innovations, funding attractions (from public, private, region, national, international R&D associations) and thus future job opportunity creation for junior researchers.

This research axis no.2 constitute an important perspective for expanding and founding new further industrial and scientific national/international collaboration networks.

This will importantly contribute to the research unit scientific reputation, and to the next HCERES research committee evaluations of our research unit.

Some additional potentials and new ideas for future developments and strategies behind this research Axis no.2 will be presented and discussed in chapter 6.

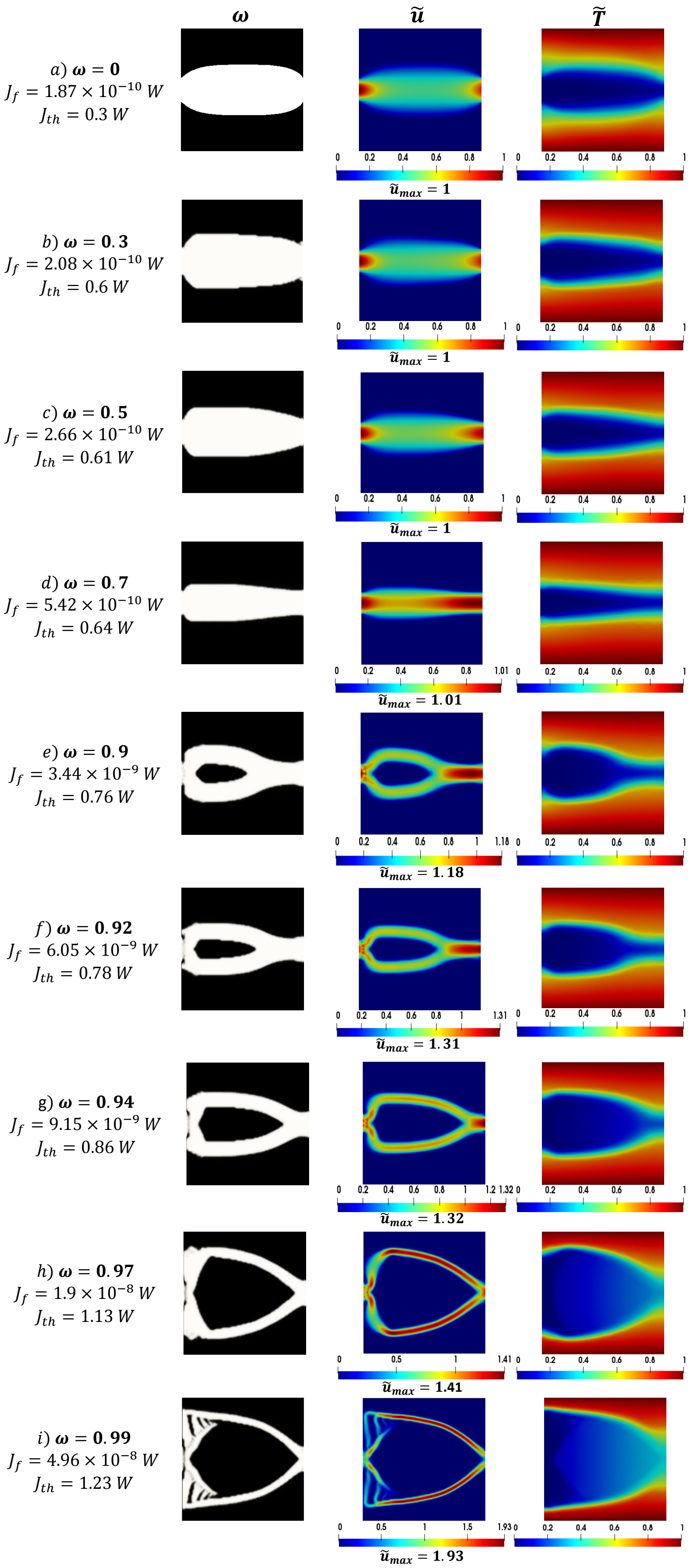


FIGURE 4.28: Topology optimization designs performance (Pareto front of figure 4.27). Selected from (Subramaniam, Dbouk, and Harion, 2018b).

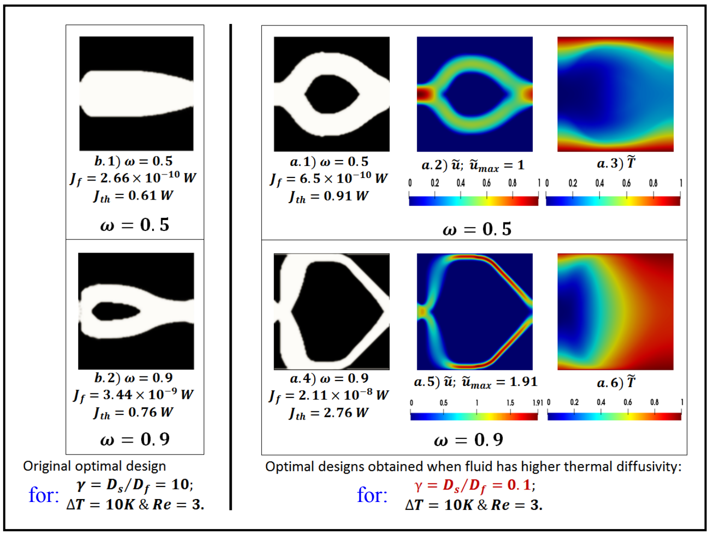


FIGURE 4.29: Topology optimization designs: Influence of the thermal diffusivity ratio ($\frac{D_s}{D_f}$). Selected from (Subramaniam, Dbouk, and Harion, 2018b).

5 Fluid flows in complex porous media

5.1 Research Axis no.3: Multi-component fluid flows in adsorbent porous media

The demand in energy is keep rising every day where the consumption of fossil fuels (as energy usual sources) has lead to huge amounts of greenhouse gases emissions. CO_2 in coal is an attractive carbon sequestration technology with huge potentials. It enhances CH_4 as methane natural gas production from coal-beds, and it has a potential to result or be a carbon neutral or a carbon sink (Harris and Zoback, 2008).

After a literature study (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018), we found that the most modeling and simulation techniques that exist in the literature are based on one- or two- dimensional simplified models with a huge need for developing 3D CFD models for gas separation by pressure and/or temperature swing adsorption (PSA, TSA) in adsorbent packed beds of porous material. Another gap identified is that the existing gas separation systems should be optimized for enhancing the adsorption capacity, and thus the quantity of gas being separated per unit time (of course with control on the local temperature in beds and the temperature front optimal local distribution). All these were identified as **a huge gap in the literature** that should be filled rapidly.

For that reason, this research axis no. 3 has been emerging three years ago at our research unit, and it is thus less scientifically mature compared to axes no.1 and no.2 with huge potentials for further investigations and developments. This R&D axis no.3 is focused on developing 3D CFD robust models (to be experimentally validated) for multi-component gaseous flow in adsorbent porous media including heat transfer and optimization in CFD.

The applications in this research axis are mainly oriented towards:

- **A** - Gas separation processes (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018; Gautier, Dbouk, Harion, Hamon, and Pré, 2018) (i.e. for CO_2 gas emissions reduction and storage, methane CH_4 gas production and storage, and recovery of oil and natural gas, etc),
- **B** - Pollutants transport in air prediction and thus control,
- **C** - Pollutants reduction in indoor and outdoor environments such as in industrial indoor zones, airplanes cabins, vehicles and buildings by using both: adsorbent porous walls/materials and air ventilation systems (Kassou, Gautier, and Dbouk, 2018),
- **D** - Natural and/or BioGaz production and storage (energy storage applications).

In the first application **A** mentioned above (Gas separation processes and storage), i had the opportunity to supervise (at 100%) and guide a first R&D activity of a one-year postdoc (April 2015 - April 2016). This project was funded by IMT where the Postdoc researcher was

Dr. R. GAUTIER (today recruited as a permanent researcher at our research unit in Douai). This Postdoc project has been developing in an external collaboration with Prof. Pascaline PRÉ and Dr. Lomig HAMON, from the Energy and Environmental Systems research Group at the IMT Atlantique. A 3D CFD macroscopic model (validated experimentally) has been developed for simulating pressure swing adsorption (PSA) process in a packed bed of isotropic porous media (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018; Gautier, Dbouk, Harion, Hamon, and Pré, 2018). The porous material is based on carbon molecular sieves (for CO_2 adsorption or separation from a bi-component CO_2/CH_4 gaseous mixture).

In this 3D CFD modeling (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018; Gautier, Dbouk, Harion, Hamon, and Pré, 2018), only the adsorption kinematics with exo(-endo)thermic heat release(-absorb) have been considered such that chemical reactions are neglected. Another drawback is that this 3D model is limited to bi-component or binary adsorption in packed beds in a commercial CFD code.

Due to the above limiting reasons, further R&D efforts have been conducted very recently to extend the modeling into multi-components adsorption and chemical reactions. A computational platform has been developed in that purpose to account for multi-component adsorption and reactive flows in OpenFOAM® (Dbouk, 2019c; Dbouk, 2019d).

5.1.1 CFD modeling and simulation of gas separation by pressure swing adsorption in packed beds

Separation processes (physical and chemical) are very important in chemical engineering, chemical manufacturing, petroleum processing, and other engineering and industrial processes. Due to the new industries that are emerging every day such as in intelligent materials, biotechnology, oil and natural gas production and storage, gas separation process is a continuing important R&D topic in chemical and process engineering (Wankat, 1994) and design optimization.

Most separation processes are governed by Heat and Mass transfer where one or more components migrate from one phase to the interface between the two phases in contact (Welty, Wicks, Rorrer, and Wilson, 2007). In a**d**sorption processes, the components remain at the interface, however in gas a**b**sorption and liquid-liquid extraction processes, the components penetrate the interface, and then moves into the second phase bulk (Welty, Wicks, Rorrer, and Wilson, 2007). In multi-components or gaseous mixtures, mass transfer is governed by a macroscopic transport mode that is "molecular diffusion" (**convection independent**), such that the transport phenomena can be deduced from the *kinetic theory of gases* (Welty, Wicks, Rorrer, and Wilson, 2007).

Adsorption can be of two type Physisorption (physical) or Chemisorption (chemical). But i will focus only on physical adsorption where chemical reactions are not considered. In adsorbent porous materials (porous so that to have a high internal surface area for solute adsorption), **molecular diffusion** takes place **inside** the porous material **pores** or solids. The adsorptive molecules attaches onto the surface (adsorbent) and become (adsorbate or admolecules), and desorption is when adsorbate detaches from the adsorbent (spontaneously or induced) as shown in figure 5.2. The **amount of the substance adsorbed** at equilibrium **depends** mainly **on**: **the temperature**, **the gas vapour pressure**, and **the specific surface area of the solid** (adsorbent).

According to (Do, 1998), three are 3 different kinds of pores as the following:

- Micropores such that $D_{pores} \leq 2\ nm$,

- Mesopores such that $2 \leq D_{pores} \leq 50\ nm$,
- Macropores such that $D_{pores} \geq 50\ nm$.

Almost all adsorption isotherms (Physisorption) can be classified according to the International Union of Pure and Applied Chemistry (**IUPAC**) as it is shown in figure 5.1.

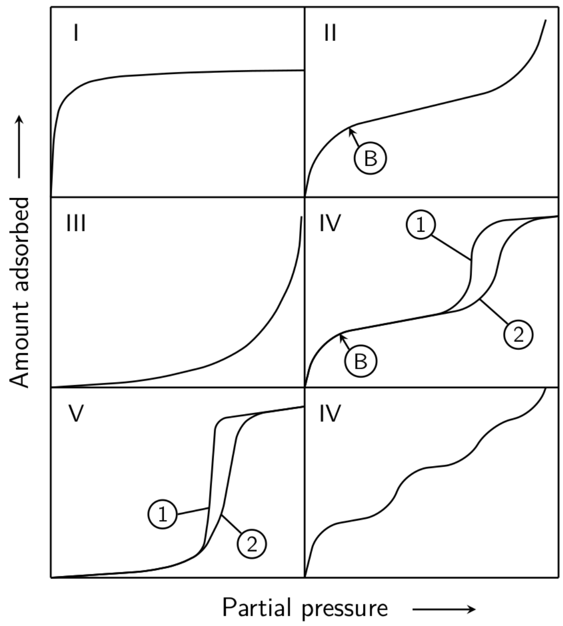


FIGURE 5.1: The six types of physisorption according to the IUPAC (International Union of Pure and Applied Chemistry), 1: adsorption, 2: desorption, B: beginning of multimolecular layers adsorption. Adapted from (Sing, 1985).

In fact, at low pressure values, all types are known as referred to by *Henry's Law*. The other types can be described as the following:

- Type I: reversible, adsorption limit, referred to as *Langmuir isotherm*.
- Type II: reversible, multilayer adsorption on a non-porous or macroporous adsorbent. Point B indicates beginning of multimolecular layers adsorption.
- Type III: curve convex to the partial pressure curve (rare and uncommon).
- Type IV: adsorption with hysteresis, i.e. for capillary condensation in mesopores. Again, point B indicates beginning of multimolecular layers adsorption (with an adsorption limit).
- Type V: similar to type III (with an adsorption limit and hysteresis) (rare and uncommon).
- Type VI: stepwise multimolecular layers adsorption takes place at this type, on a uniform non-porous surface. Monomolecular layer capacity: height of each step.

Additionally, in an adsorption process, when a component or solute attaches onto the solid surface that is attractive to this solute, this defines what is known by "material selectivity for a component" (as shown in figure 5.3).

Figure 5.4 shows the different types of porous diffusion where D_{Ae} represents the effective diffusivity of species A in a binary mixture of A and B (Welty, Wicks, Rorrer, and Wilson, 2007), and D_{KA} the Knudsen diffusivity for diffusing species A (*kinetic theory of gases*). It

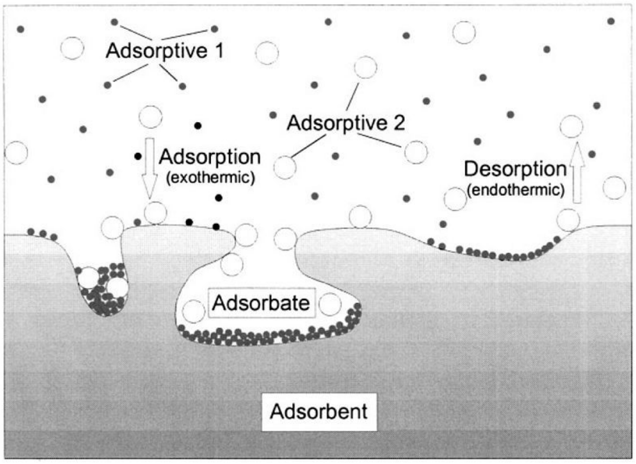


FIGURE 5.2: Physical adsorption and desorption mechanisms. Adopted from (Keller, 2005).

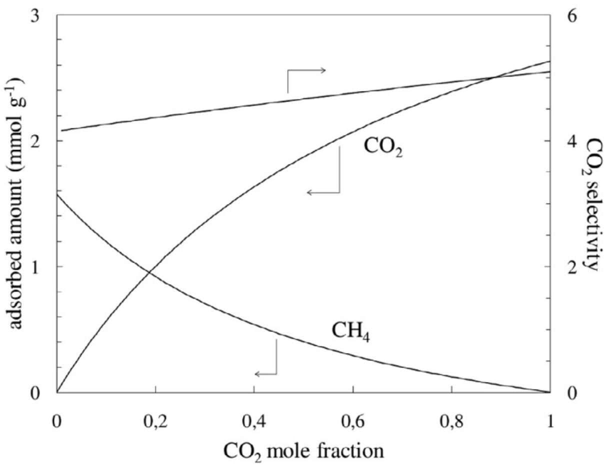


FIGURE 5.3: Derived IAST (Ideal Adsorbed Solution Theory (LeVan and Vermeulen, 1981; Myers and Prausnitz, 1965)) equilibrium data of a binary CO_2/CH_4 mixture: adsorbed quantities and CO_2 selectivity versus CO_2 initial molar fraction. Adopted from (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018).

is important to note that the Knudsen diffusion is usually significant only at low pressure values and small pore diameters. Nevertheless, in some instance both Knudsen diffusion and molecular diffusion (D_{AB}) can be important.

Figure 5.5 shows an example of the adsorbent packed bed with the 3D CFD CAD model and boundary conditions for CO_2 adsorption from bi-component CO_2/CH_4 gaseous mixture. The adsorption process in this packed bed is a pressure-swing-adsorption (PSA) multistage or cyclic process where each cycle is made of 4-steps sequence as shown in figure 5.6.

Figures 5.7 shows the transient 3D CFD results of the temperature filed, adsorption quantity and adsorption rate in the adsorbent packed bed column. Figure 5.7 illustrates the numerical predictions of the local temperature profiles which are in good agreement with the ones measured experimentally.

The linear driving force (LDF) model (considers diffusion inside spherical particles, (Glueckauf and Coates, 1947; Glueckauf, 1955)) was used and implemented in the CFD package

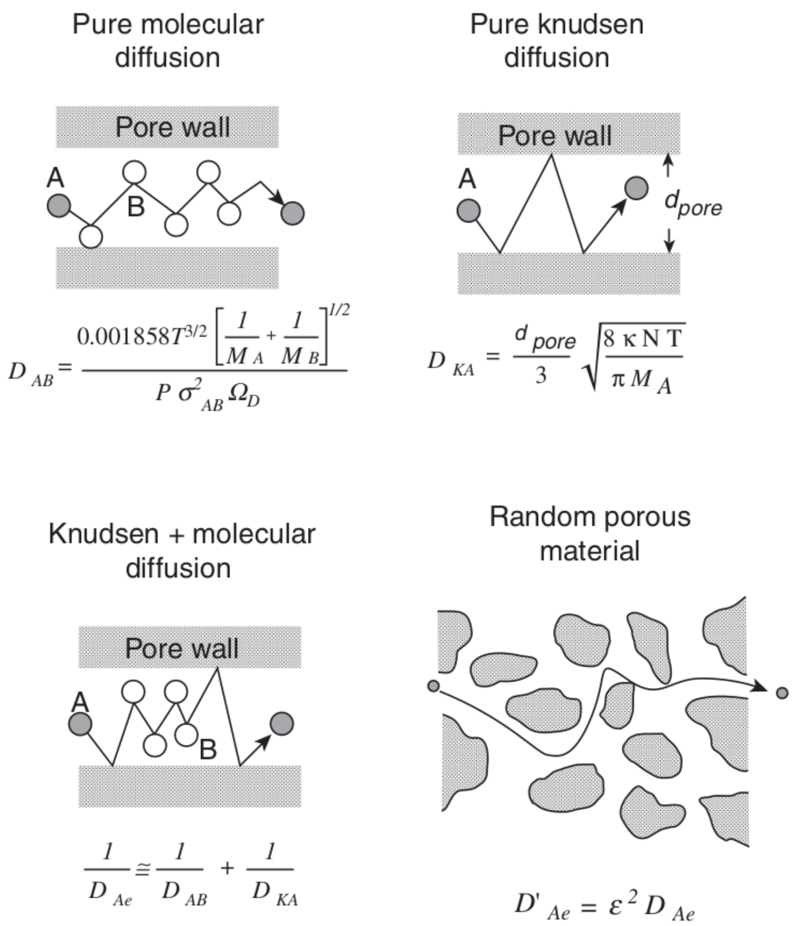


FIGURE 5.4: Types of porous diffusion. Shaded areas represent nonporous solids. Adopted from (Welty, Wicks, Rorrer, and Wilson, 2007).

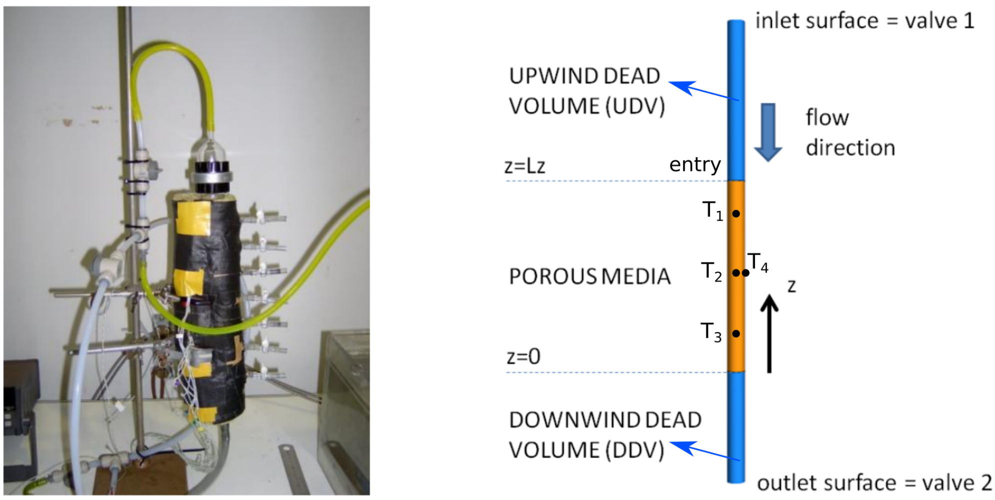


FIGURE 5.5: CO_2 adsorption or CH_4 separation and production from a bi-component CO_2/CH_4 gaseous mixture. Adsorbing packed bed experiment (left), and 3D CFD CAD model and boundary conditions (right). From (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018).

SIEMENS® StarCCM+® to compute the adsorption rate in the packed bed as the following:

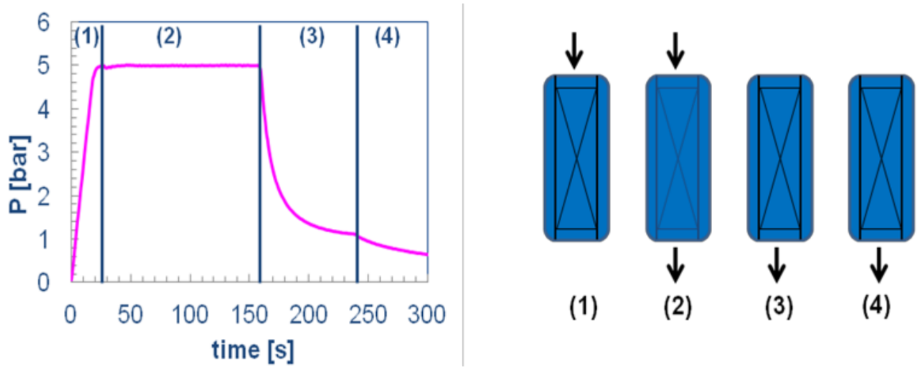


FIGURE 5.6: Pressure Swing Adsorption Process. (1) Pressurization or Feed in, (2) CO_2 adsorption or CH_4 production, (3) CO_2 desorption or evacuation or blow-down and (4) Vacuum regeneration. From (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018).

$$\frac{d}{dt}(q) = k_{p,i} \left({q^*}_{m,i} - q_i \right) \tag{5.1}$$

where q_i is the adsorbed quantity or concentration ($mol \cdot kg^{-1}$), ${q^*}_{m,i}$ is the equilibrium adsorbed quantity of the adsorbed phase for component i for binary mixture, and $k_{p,i}$ is the mass transfer coefficient (s^{-1}) for the i^{th} component.

For the adsorption isotherm equilibrium models, the Ideal Adsorbed Solution Theory (IAST) model by (LeVan and Vermeulen, 1981) was implemented in the CFD model by (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018; Gautier, Dbouk, Harion, Hamon, and Pré, 2018) and compared to other two simpler models (Langmuir, and extended-Langmuir) as shown in figure 5.9. The adsorption isotherm correlates, at a constant temperature, between the adsorbed amount of gas and the equilibrium gas pressure.

In (Gautier, Dbouk, Harion, Hamon, and Pré, 2018) several sensitivity analysis have been conducted using the 3D CFD model developed in (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018). This is in order to investigate the sensitivity of the CFD model to different physical and numerical parameters like: the effective thermal conductivity value of the adsorbent packed bed (KS) as shown in figure 5.10, the mass transfer coefficient (see figure 5.11), the heat transfer coefficient at the packed bed wall, etc.

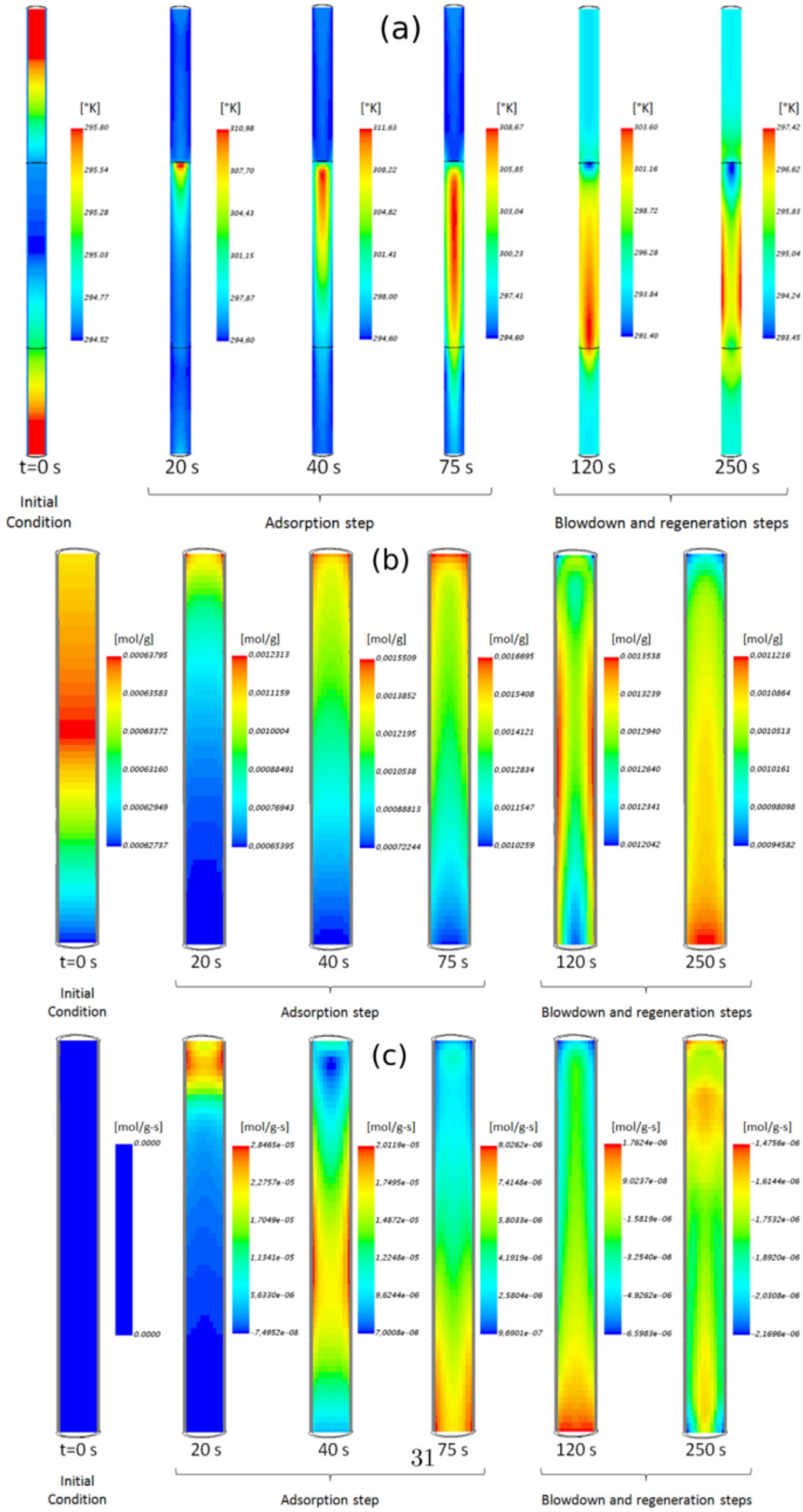


FIGURE 5.7: 3D CFD simulation results at different time steps of the PSA cycle. Streamwise direction is downward. (a) Temperature fields. (b) Adsorbed quantity. (c) Adsorption rate. From (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018).

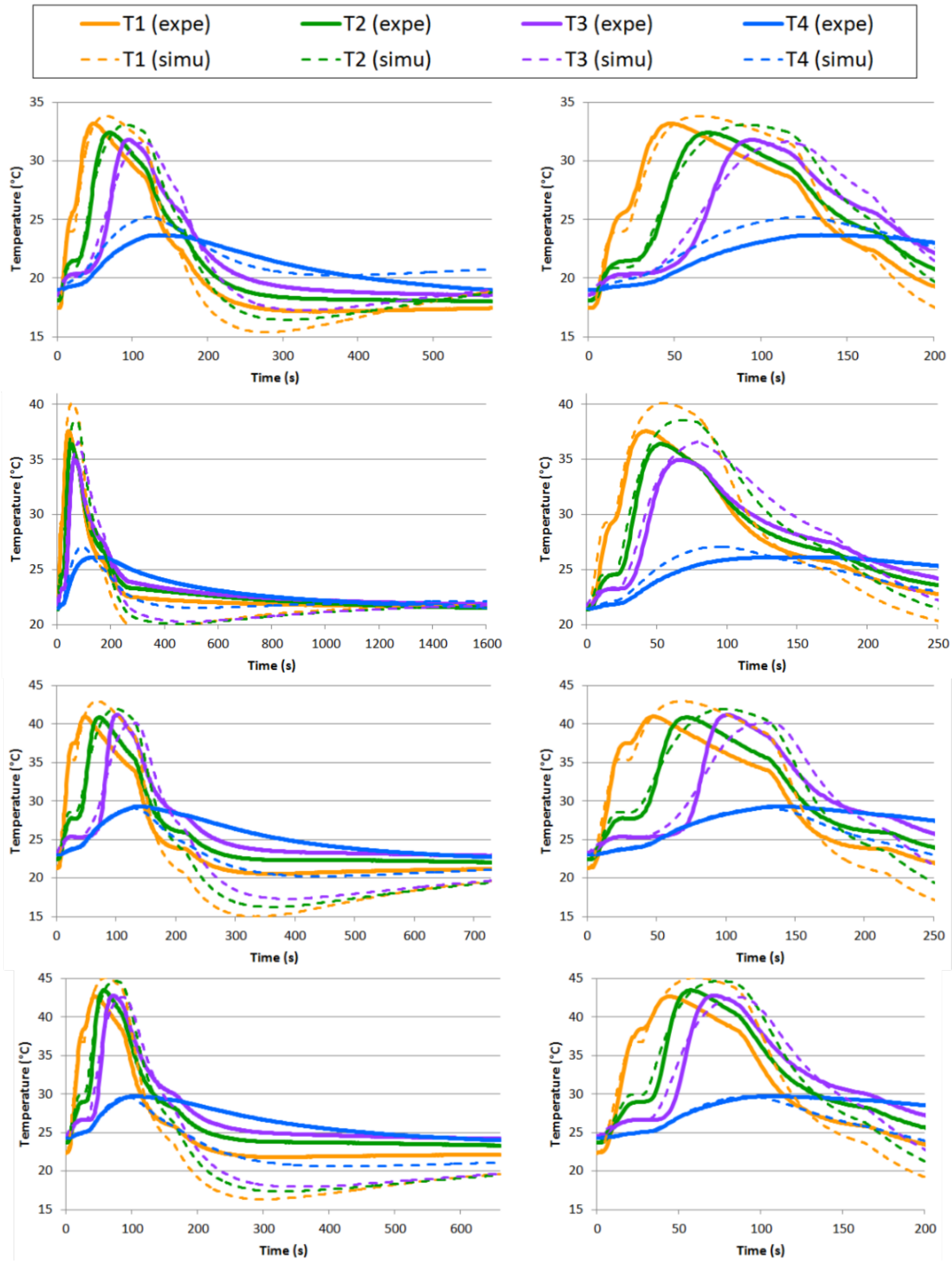


FIGURE 5.8: Time evolution of temperature for packed bed thermocouples T1, T2, T3 and T4 (see fig. 5.6) at steady-state cycle for different four operating conditions. (Left): entire cycle; (Right): zoom in over pressurization, adsorption and blowdown steps. Adopted from (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018).

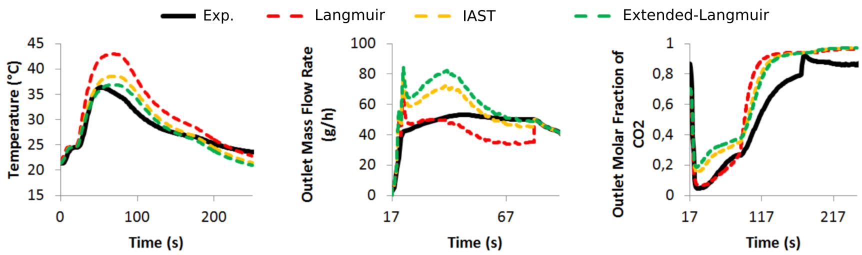


FIGURE 5.9: Comparisons of isotherm models using Langmuir isotherm with or without mixture assumption. (left) Temperature for thermocouple T2; (middle) outlet mass flow rate; (right) outlet molar fraction of CO_2. Adopted from (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018).

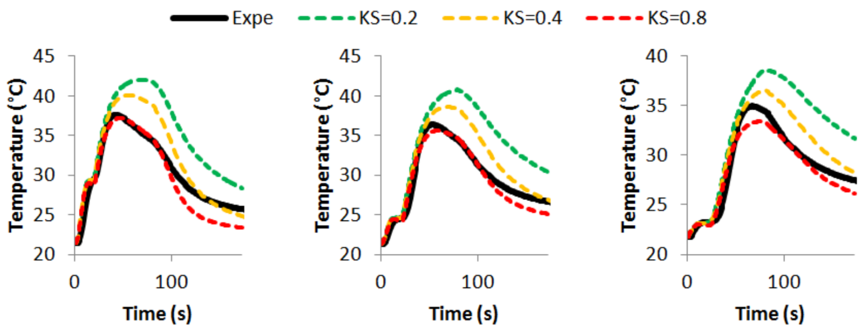


FIGURE 5.10: Influence of adsorbent thermal conductivity KS on the local temperature profiles inside the bed. (left): At position T1; (middle): at position T2; (right): at position T3 (See figure 5.5). From (Gautier, Dbouk, Harion, Hamon, and Pré, 2018).

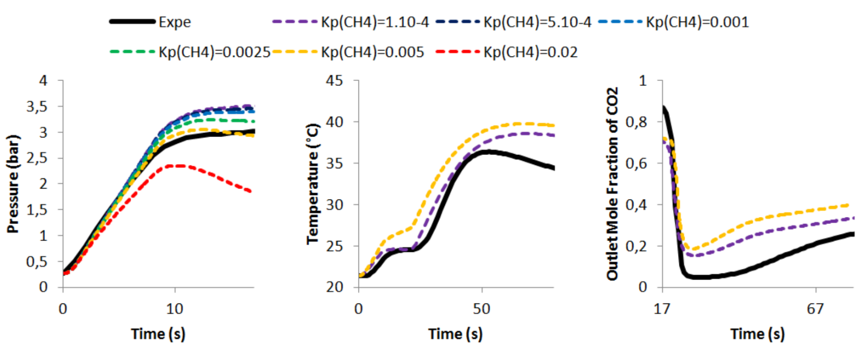


FIGURE 5.11: Influence of the mass transfer coefficient $k_{p_{CH_4}}$ in (s^{-1}) on: the pressurization step (left); the temperature profile at T2 (center) and the outlet molar fraction of CO_2 (right). From (Gautier, Dbouk, Harion, Hamon, and Pré, 2018).

5.1.2 Pollutants transport in air and their reduction in indoor environments by adsorbent materials and air ventilation

The second and third applications **C, D** (in section 5.1), on pollutants transport prediction and reduction, is a very recent and rising application at our research unit. It is very important and goes well with the new structuring R&D strategies defined by the IMT Lille Douai research direction (CERI-EE[3]).

Since July 2018, I have been developing another new R&D activity on this research axis no.3. We had 5-months Masters' internship project (funded by IMT Lille Douai), where I supervised (at 50%) the works of M. Amine KASSOU. The objective is to apply the 3D CFD adsorption models, developed previously in (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018; Gautier, Dbouk, Harion, Hamon, and Pré, 2018), but to investigate the potentials behind the CFD models to predict well pollutant transport in air, and pollutants reduction (i.e. by applying adsorbent walls in indoor environment).

In (Kassou, Gautier, and Dbouk, 2018) masters internship, preliminary CFD results were obtained for reducing toluene pollutant in air by applying (indoor) an adsorbent wall, in the presence of air ventilation. Several investigations have been conducted such as the influence of the flow rate and the adsorbent wall capacity on the characteristic time of pollutant reduction (i.e. below the international indoor threshold) as shown in figures 5.12 and 5.13.

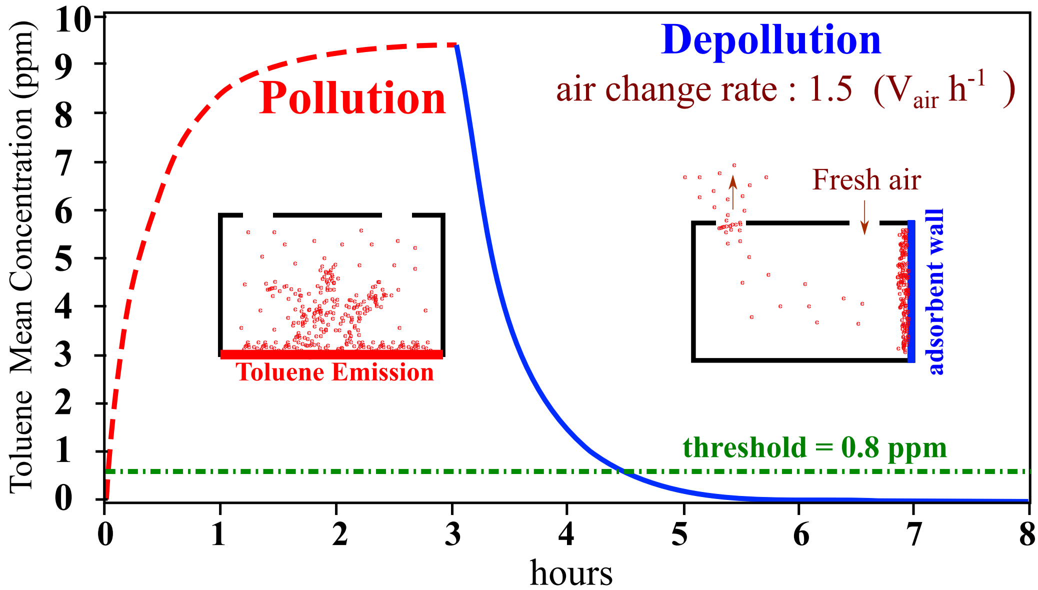


FIGURE 5.12: 3D CFD simulation results for pollution emission of toluene from the ground (left), and its reduction by applying adsorbent wall combined with air ventilation (right). From (Kassou, Gautier, and Dbouk, 2018).

The works by (Kassou, Gautier, and Dbouk, 2018) were limited to binary adsorption in commercial CFD code. For that reason, very recently a new computational platform has been developed in order to account for multi-component adsorption and reactive flows in OpenFOAM® applied to pollutants reduction in indoor environment (Dbouk, 2019d).

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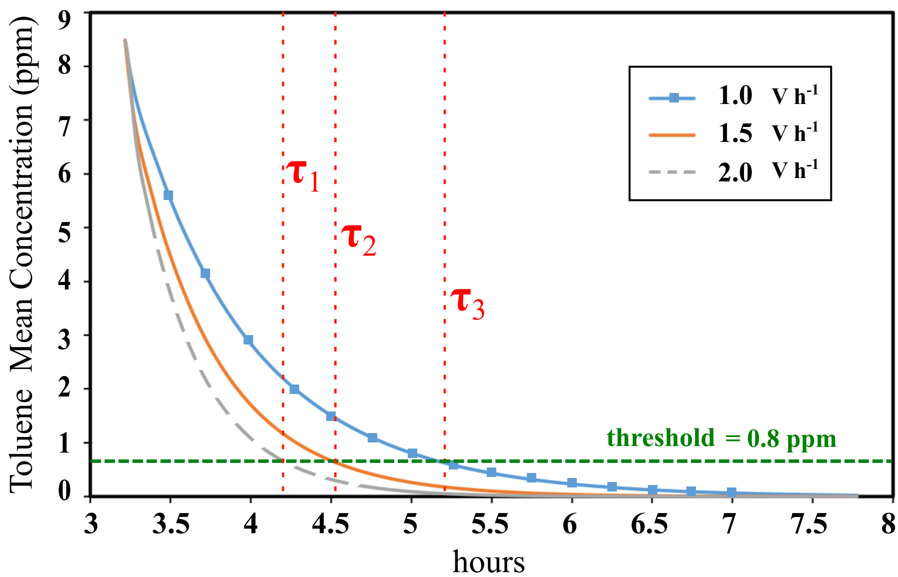

FIGURE 5.13: Influence of air change rate ventilation (in $V_{airroom} \cdot h^{-1}$) on the characteristic time (in τ $(hours)$) of toluene pollution reduction. Adapted from (Kassou, Gautier, and Dbouk, 2018).

5.1.3 Gas production and energy storage applications

Concerning the fourth application **D** (in section 5.1) in my research axis no.3, it is also a recent research activity that i have been contributing to its development 18 months ago. It is in the context of an industrial project named "EcoStock-II©" funded by the industrial partner EcoTech-CERAM®. I have been working on this **confidential project** at our research unit where the main objective is to develop a macroscopic numerical model in CFD to predict (and optimize) the energy-charge-discharge time and thermal behavior (with pressure drop) in plug-and-play container-unit (the "EcoStock-II©") (for example see figure 5.14). The developed CFD model is validated experimentally through measurements by the industrial partner. Optimization in CFD (see figure 5.15) has been conducted in attempts to find innovative novel designs (e.g. material storage thermophysical properties, immersed particles diameter, etc) as new waste heat energy storage systems.

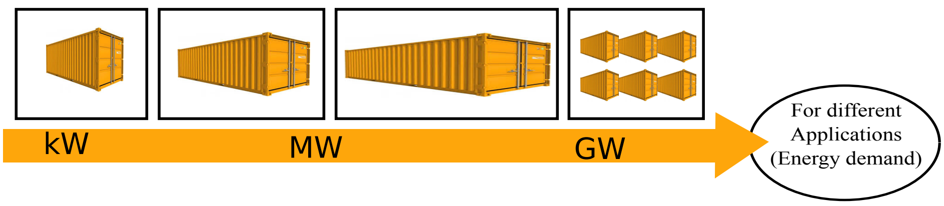

FIGURE 5.14: An example of plug-and-play energy storage system.

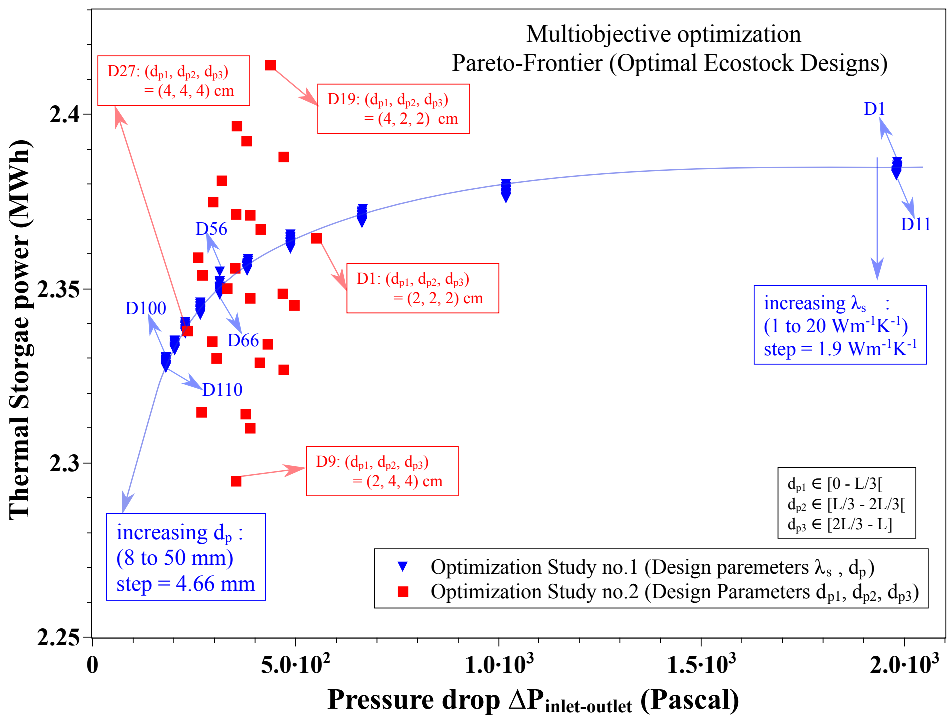

FIGURE 5.15: An example of plug-and-play energy storage system optimization.

5.2 Conclusion of Part II

As a conclusion of Part II, we have seen three different R&D&I axes that the author is involved in their developments, with several scientific contributions, students supervision (Postdoc, PhD, Masters students) and huge potentials for further developments and scientific collaborations (see figure 2.2). Moreover, it can be observed that there is a good synergy between these three axes and the author's scientific profile which is oriented towards: numerical coding and developments, scientific computing, optimization techniques, which all converge to the "Topology Optimization and MultiPhysics Multiscale Modeling & Simulation of Complex Thermofluid flows and Systems" which is the title of this manuscript. In fact the axis no.2 which is focused on Topology Optimization constitutes a joint core that can feed (and get feeded from) both axis no.1 and axis no.3, and even other possible future axes or scientific themes as illustrated in figure 5.16. Of course with the attention not to disperse a lot towards new research axes.

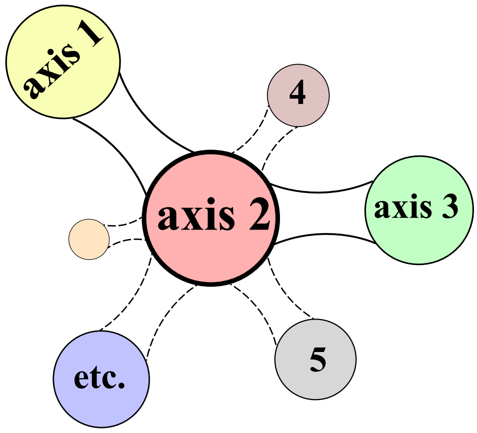

FIGURE 5.16: Evolutionary Research: core axis no.2 (Topology optimization) and its interconnecting links with the other research axes.

Part III

Future R&D Strategies

6 Perspectives for further R&D&I

In this chapter 6, i will introduce some of my research and development project-plans, new ideas and perspectives for the next decade, and their position in the new CERI-EE[1] and in the new research strategies defined recently by the IMT Lille Douai.

6.1 Research strategy and targets for the year 2030

The recent strategy presented by IMT Lille Douai's new director of research, through a program entitled "Lille Douai 2030" will change clearly the scientific identity of the institution. IMT Lille Douai was born in January 2017 after merging Mines-Douai and Telecom-Lille. Some vital points as a summary of this new research and development strategy are :

6.1.1 Research units and governance plan

Research at the IMT Lille Douai will be grouped into main research, innovation and teaching centers (named CERI[2]), coordinated by the Research and Innovation Department and linked to the IMT's main areas of expertise: *digital and communication systems in industry*, *energy and environment*, and *materials and processes*. The new governance will include the setting up of an internal scientific council, representative of the CERI[2], whose mission will be to guide the research strategy inside each CERI[2].

6.1.2 IMT : leadership in strong themes

The "IMT Lille Douai 2030" research strategy plans intend to structure the institution research strengths around a few strong scientific themes, in order to gain a national (and international) leadership that meets the strategic plan of the IMT (as for example in the fields of Digital Manufacturing).

With the aim to improve the visibility and image of IMT Lille Douai, the Research and Innovation Department wants to put in place tools which enable scientists to target Horizon 2020 ERC Grants and 2030 Appeals and young-researchers projects at the ANR (French National Research Agency). For this purpose, competitive calls for projects will be organized internally to identify research subjects and scientists, potential winners at the ERC and Young Researchers of the ANR in the coming few years.

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6.1.3 Partnerships and the influence of IMT Lille Douai

The "IMT Lille Douai 2030" strategy is so ambitious such that the college wants to strengthen its partnership research, by sustaining its industrial partnerships through industrial chairs and joint laboratories.

To broaden its scientific offer, IMT Lille Douai wants, on one hand, to be part of a unifying regional dynamic research, and on the other hand an innovation player seeking to join other regional research teams (CNRS, universities, research institutes, etc.).

More generally, the main goal is to no longer to have an "isolated" research teams by 2030 but to promote exchanges of IMT researchers, with French academic partners, international, and industrial researchers. IMT will be setting up a new welcome program to encourage well for visiting researchers worldwide.

My future R&D activities are presented below, contributing well to the CERI-EE[3] R&D activities and reputation. Moreover, they contribute also to the overall scientific community (i.e. future scientific collaborations opportunities, research projects and funding plans, industrial sectors targeting, etc). My research and development activities converge to (and fit inside) the research strategies and targets for the year 2030, as they were defined by the IMT[4].

6.2 Perspectives and potentials: research axis no.1

After my R&D activities presented in chapter 3 section 3.1 on non-colloidal suspension flows, very recently, I identified another **huge gap in the literature** related to non-colloidal suspension flows where the dynamics is induced by thermal heating (i.e. thermally natural or thermally free-convective suspension flows). This new research activity is of huge potential at the CERI-EE[3] for treating several interesting research topics of many potential for further applications and industrial aspects (plumes, volcanic eruptions, crystallization problems, oil and gas production, slurry flows, etc).

6.2.1 Non-isothermal non-colloidal suspension flows (free laminar convection)

Immersed granular beds (IGB) are weak solids that can be remobilized, and thus may be seen as concentrated suspension. The dynamics of settled particle beds arises in geophysical situations, as sediments and wet soils, as well as in water treatment and process engineering applications. Various phenomena are observed when liquid flows through these beds: these include plumes, chimney formation and local bed fluidization during the passage of water through a sandy environment (Zoueshtiagh and Merlen, 2007); advection of particles by the rise of bubbles and the formation of craters (G. Varas and Géminard, 2009; C. Picard and Joubaud, 2016); and destabilization of an immersed granular bed (IGB) by buoyancy (C. Morize and Sauret, 2017; E. Herbert, 2018). While this is a long-standing problem, new tools are being applied in this field of study. For example, M. Houssais and Morris, 2019 recently experimentally investigated in a microscale model of a sediment bed the slow dynamics and eventual rapid destabilization induced by an imposed Darcy flow. This use of lab-on-chip technology allows understanding of the particle rearrangement and the bed compaction and

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dilation mechanisms in different flow regimes. Natural convection in miscible two viscous fluids had been studied in the literature by (Bars and Davaille, 2002; Bars and Davaille, 2004). They quantified the interface deformation as a result of chemical diffusion through a critical effective buoyancy number. However, Rayleigh-Bénard convection in particle-laden liquids was rarely studied in the literature. It goes back to the early works by T. Girasole and Roze, 1995 who studied the influence of polystyrene particles (solid volume fraction between 1% and 10% and diameters from 0.1 to 100 μm) on the first Rayleigh-Bénard bifurcation. They observed a growth of the thermal relaxation time and decrease of the buoyancy time due to an increase of the convective threshold with the volume fraction.

The phenomenon of destabilization has been considered previously for pure fluids in a number of scenarios, but in the case of a settled bed of solid particles, a range of different phenomena and mechanisms are observed, including particle transport and sedimentation, multiphase Rayleigh-Bénard-like convection and particle resuspension (C. Morize and Sauret, 2017). Similar multiphase phenomena can be found in nature as plume eruptions or black smokes (V. S. Solomatov and Stevenson, 1993; Martin and Nokes, 1988; Martin and Nokes, 1989), as well as in process and chemical engineering, in underground stratified oil and gas layers, and micro-bubbles in biogas production (G. Lavorel and Bars, 2009; F.E. Loranca-Ramos and Pacheco-Vázquez, 2015).

Improved knowledge on natural convection and the associated IGB dynamics will thus affect an important number of R&D topics.

From a physics point of view, in analogy with a pure-fluid, thermal convection in a concentrated suspension medium (i.e. IGB of initial height h^0) can be seen as heat transport by mass transport phenomenon. It can be explained as a competition between a driving force (gravitational acceleration) and resistance forces (thermal and viscous suspension diffusion).

The driving force inside the IGB witnesses a characteristic response time τ_g as the following:

$$\tau_g = \sqrt{\frac{h^0}{g\,{\beta^0}_s\,\Delta T}} \tag{6.1}$$

The thermal diffusion that tends to reduce the temperature gradients inside the fluid has a characteristic time given by:

$$\tau_\alpha = \frac{{h^0}^2}{{\alpha^0}_s} \tag{6.2}$$

The characteristic time corresponding to the resistance viscous diffusion is:

$$\tau_\nu = \frac{{h^0}^2}{{\nu^0}_s} \tag{6.3}$$

${\alpha^0}_s$, ${\beta^0}_s$ and ${\nu^0}_s$ represent the suspension initial properties at $\phi^0 = 0.66$, and $\Delta T = T_h - T_c$.

Based on the above three characteristic times, a dimensionless *suspension Rayleigh number* Ra_s can be defined as the following:

$$Ra_s = \frac{\tau_\nu \times \tau_\alpha}{{\tau_g}^2} \tag{6.4}$$

In this study, the bed destabilization behavior is quantified by its sequential mode period τ_n, partial ($t_{d,\text{onset}}$) and total ($t_{d,\text{total}}$) characteristic times as a function of h^0 and Ra_s.

In this context, in a very recent work in (Dbouk and Bahrani, 2019; Bahrani, Morris, and Dbouk, 2019), a new solver in OpenFOAM, 2019 (intended only for forced-convective non-colloidal suspension flows) has been developed to take into account **thermally free-convective** *non-colloidal suspension flows*, and **resuspension and mixing induced by thermal heating** (see figure 6.1). It has been developed (Dbouk and Bahrani, 2019; Bahrani, Morris, and Dbouk, 2019) with experimental validations to investigate the resuspension, of an immersed compact suspension bed, induced by thermal heating. The objective was to understand the Rayleigh-Bénard-like instabilities in such kind of complex non-isothermal concentrated suspensions. Some examples of the preliminary results are illustrated in figure 6.2 showing the destabilization modes phenomenon.

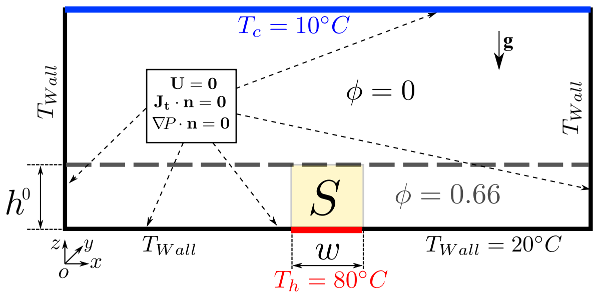

FIGURE 6.1: The geometry and boundary conditions applied in the numerical CFD simulations. $T_{wall} = 20°C$, S, and $\mathbf{J_t}$ is the total flux detailed in Dbouk, 2018a. Adopted from (Dbouk and Bahrani, 2019; Bahrani, Morris, and Dbouk, 2019).

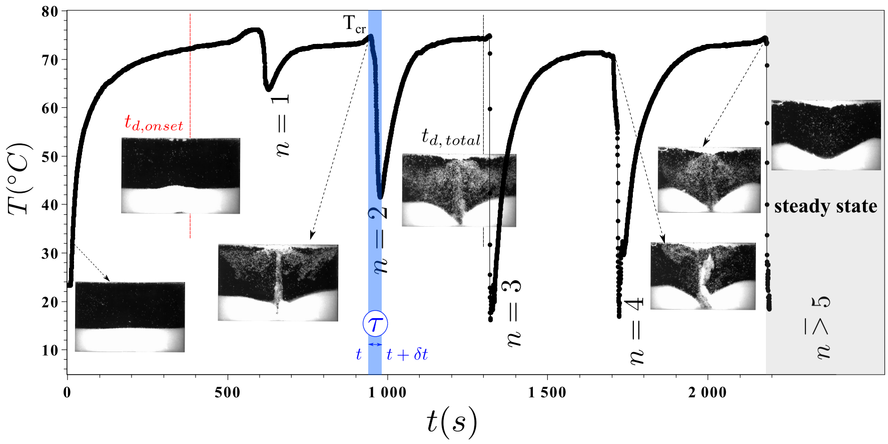

FIGURE 6.2: Measured local temperature T for $h^0/H = 0.38$ illustrating multiple destabilization modes. Each mode includes a characteristic period τ. Critical temperature T_{cr} measured at different τ, illustrating the corresponding images for the local destabilization of the immersed granular bed, and the steady state denoting no further change in the bed/liquid interface. The *onset* or *partial* destabilization time $t_{d,\text{onset}}$ represents the characteristic time at which the IGB destabilization onset occurs. The *total* destabilization time $t_{d,\text{total}}$ describes the time where a first complete particles removal occurs in the zone where heating is applied at the bottom ($b \times w$). Adopted from (Dbouk and Bahrani, 2019; Bahrani, Morris, and Dbouk, 2019).

To better quantify the instability induced in IGB by thermal heating, two modified critical numbers Rayleigh Ra^*_{cr} and Buoyancy B^*_{cr}, based on the IGB destabilization onset ($t = t^*$)

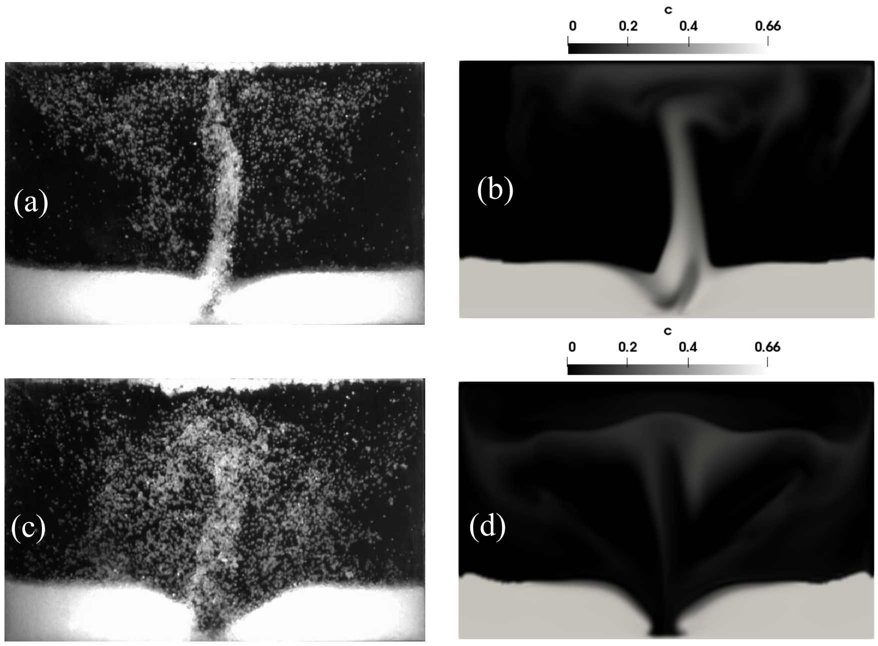

FIGURE 6.3: Frontal views at plane $y = 0$ and as captured by the camera for the particles ejection and local bed surface deformation with time for immersed granular bed initially at $h^i = 15\ mm$. (a) Experiment image captured at $t = 400$ seconds, (b) Numerical CFD results at $t = 400$ seconds. (c) Experimental image captured at $t = 700$ seconds, (d) Numerical CFD results at $t = 700$ seconds. White: rigid particles, black: liquid. Adopted from (Dbouk and Bahrani, 2019).

and its local volume fraction ($\hat{\phi}$), have been defined respectively as:

$$Ra^*_{cr}(\hat{\phi},\ t = t^*) = \frac{g\hat{\beta}_s \Delta T_{cr} H^3}{\hat{\nu}_s \hat{\alpha}_s}, \quad t^* = t_{d,\text{onset}} \tag{6.5}$$

$$B^*_{cr}(\hat{\phi},\ t = t^*) = \frac{\Delta\rho^0}{\hat{\rho}_s \hat{\beta}_s \Delta T_{cr}}, \quad t^* = t_{d,\text{onset}} \tag{6.6}$$

where the local volume fraction $\hat{\phi}$ is computed as:

$$\hat{\phi} = \frac{1}{S} \iint_{S=h^0 \times w} \phi(x,z)\, dx\, dz \tag{6.7}$$

$\hat{\rho}_s$, $\hat{\beta}_s$, $\hat{\nu}_s$ and $\hat{\alpha}_s$ are the thermophysical properties of the IGB (or suspension) that depend on $\hat{\phi}$ in the local zone $[S = h^0 \times w]$ (see figure 6.1).

$$\hat{\zeta}_s = \frac{1}{S} \iint_{S=h^0 \times w} \zeta_s(x,z)\, dx\, dz \tag{6.8}$$

where ζ_s is a mathematical operator that is applied to ρ, ν, β and α such that:

$$\zeta_s = \zeta_p \phi + (1 - \phi)\zeta_l \tag{6.9}$$

with $\beta_p = 8 \cdot 10^{-4}$ K^{-1} and $\alpha_p = 10^{-7}$ m$^2\cdot$ s^{-1}. α_l and β_l are, respectively, water thermal diffusivity and thermal expansion coefficients that depend on the temperature; we neglect the influence of the salt on these properties.

Figure 6.4 shows the numerical CFD predictions obtained for the critical Buoyancy number, compared to the recent experiments by (E. Herbert, 2018; C. Morize and Sauret, 2017; Bahrani, Morris, and Dbouk, 2019).

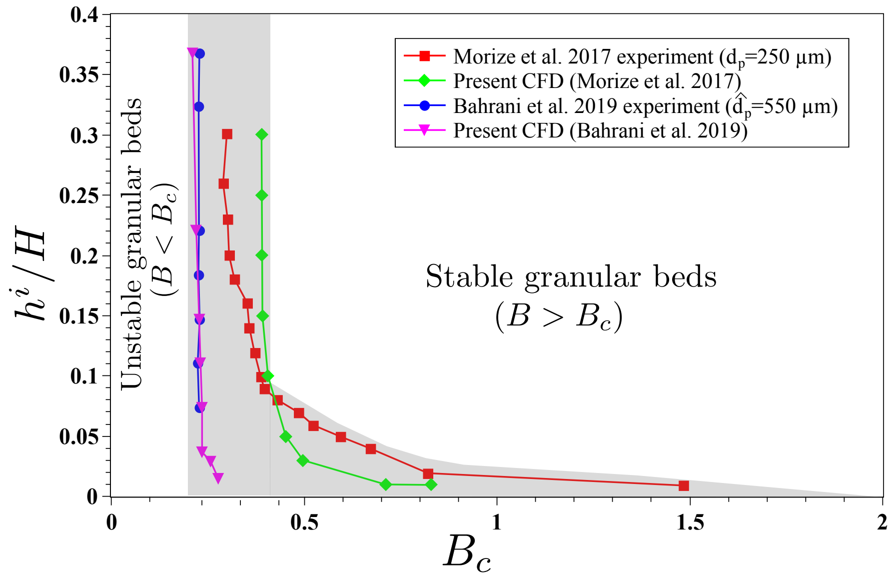

FIGURE 6.4: Critical Buoyancy number as function of initial h^0/H ($h^0 = h^i$). Right side arrow: stable immersed granular beds for $(B > B_c)$. Left side arrow: Unstable immersed granular beds for $(B < B_c)$. Adopted from (Dbouk and Bahrani, 2019).

A thermal phase stability diagram (TPSD), with the novel feature that it is based on the modified critical Rayleigh number (Ra^*_{cr}) as a function of h^i/H for immersed granular beds of polydispersed particles, is illustrated in figure 6.5 (black circles and black dashed line). The critical Rayleigh number for the pure fluid case is shown by the black crosses, corresponding to the case of $h^i = 0$. This TPSD defines two regimes: "stable" (blue region in figure 6.5) and "unstable" (red region in figure 6.5) depending on Ra^*_{cr} versus h^i/H. For $Ra < Ra^*_{cr}$ the IGB is stable meaning that there is zero deformation of the initial bed surface in the presence of the applied thermal heating source. However, for $Ra > Ra^*_{cr}$ the IGB becomes unstable such that the bed surface starts to deform and destabilization onset occurs, upon reaching a critical threshold temperature $T_{cr}(\phi',\ t = t^*)$.

This new recent innovative research activity, on free convection in non-colloidal suspension flows, adds an important value to our research unit, and opens a window for future topics for R&D&I where suspensions (as intelligent materials) may invade other interdisciplinary scientific domains like, medical science (blood flows), biomechanics, electronics, telecommunication, geology, chemistry, etc.

This recent R&D activity have been mounted with a new external collaboration with Prof. Jeffrey. F. Morris at the Complex Fluids Research Group at the Levich Institute of Technology, City College University of New York. Another internal collaboration have been started on this topic with Dr. Amir BAHRANI from IMT Lille Douai.

GDR objective: An objective is to create soon (around 2019/2020) a new GDR (Groupe de Recherche) in order to animate, and better develop this new research activity in France

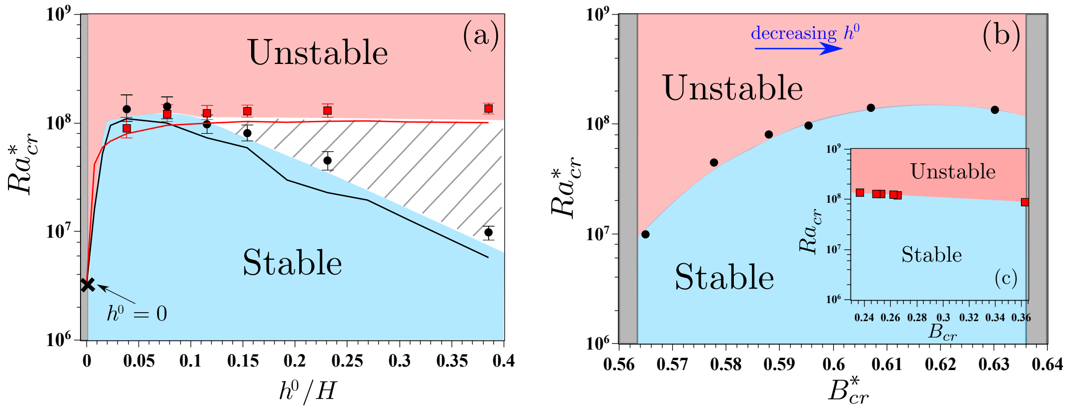

FIGURE 6.5: Thermal phase stability diagram (TPSD), (a) for the modified Ra^*_{cr} as a function of initial bed's height h^0/H, (b) for Ra^*_{cr} as a function of the modified B^*_{cr}, (c) for the classical Ra_{cr} versus the classical B_{cr}. Classical Ra_{cr}: experimental measurements (red squares) versus numerical simulations (red solid line). Modified Ra^*_{cr} : experimental measurements (black circles) versus numerical simulations (black solid line). The Rayleigh number value for a pure fluid (black **x** point). Adopted from (Bahrani, Morris, and Dbouk, 2019).

concentrated around heat transfer in non-colloidal suspensions. This will gather several junior and senior researchers, which can attract also several regional and external industrial partners in the future (further research network development).

6.2.2 Cooling of electronic components (forced laminar convection)

End 2016 early 2017, we have recently created and launched the idea for a new window for R&D&I in the topic of **cooling of electronic components** (i.e. see Enveloppes Souleau (Dbouk, 2017b; Dbouk, 2017c), and Dbouk, 2019b).

In very recent R&D&I efforts in Dbouk, 2019b, a novel heat sink design was proposed for CPU cooling applications, based on non-colloidal suspension flows. The attraction behind non-colloidal suspensions applied as new coolant, lies in the fact that: non-colloidal suspensions (made of micro-particles) are usually human health and environmentally friendly compared to nano-fluids counterparts (threshold PM10, PM2.5, see RespireAsso, 2018). An example of this new heat sink design (& working and boundary conditions, and installation circuit) are illustrated in figures 6.6, 6.7 and 6.8 (Dbouk, 2019b).

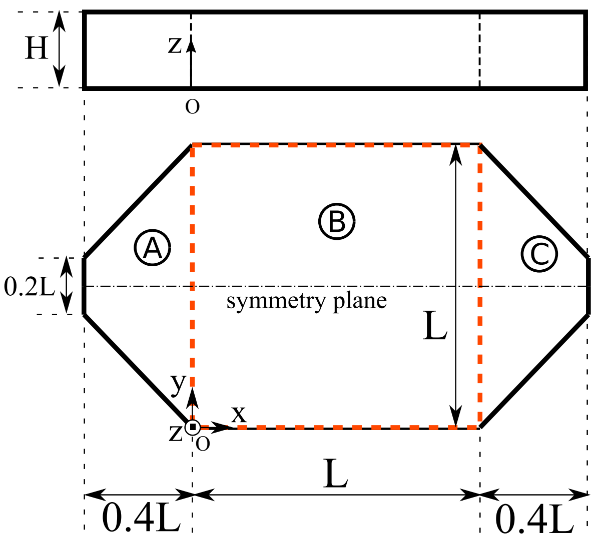

FIGURE 6.6: A schematic representation of the 3D geometry of the CPU cooling device. (A): Diverging nozzle zone; (B): CPU zone with heat generation; (C): Converging nozzle zone. $H = 0.2L$; $L = 0.05\ m$. From (Dbouk, 2019b).

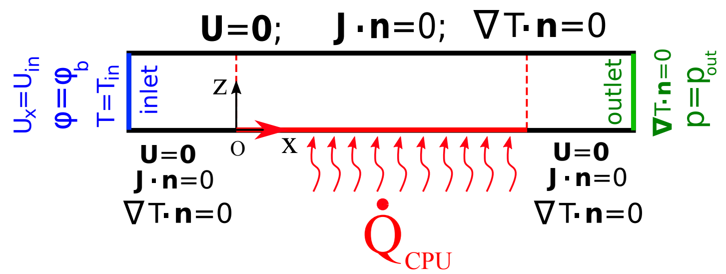

FIGURE 6.7: The boundary conditions (BC) applied in the present CFD simulations with $T_{in} = 293\ K$ and $\dot{Q}_{CPU} = 3800\ W\ m^{-2}$. From (Dbouk, 2019b).

Figures 6.10 and 6.11 show as an example that upon increasing the CPU power from 9.5 W to 47.5 W, the suspension at $k_p = 100k_f$ is still very well performing in terms of cooling where the mean CPU temperature holds $T_{mean} = 296.06\ K$ (a $T_{max} = 298.23\ K$). However at such high CPU power of 47.5 W, the suspension at $k_p = k_f$ is less performing in terms of maximum point temperature that reaches 365.33 K, but still accepted ($T_{mean} = 326.19\ K$) by being below the maximum usually allowed temperature for CPU units.

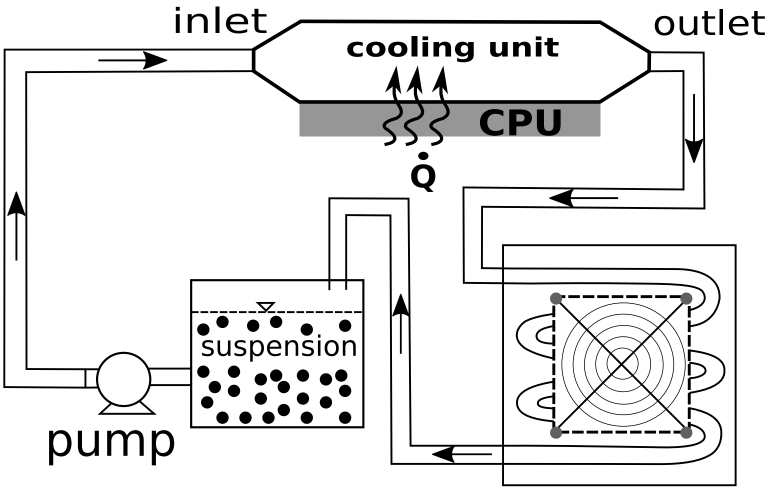

FIGURE 6.8: A schematic representation of the CPU cooling device installation in a circuit of circulating suspension flow within different components. From (Dbouk, 2019b).

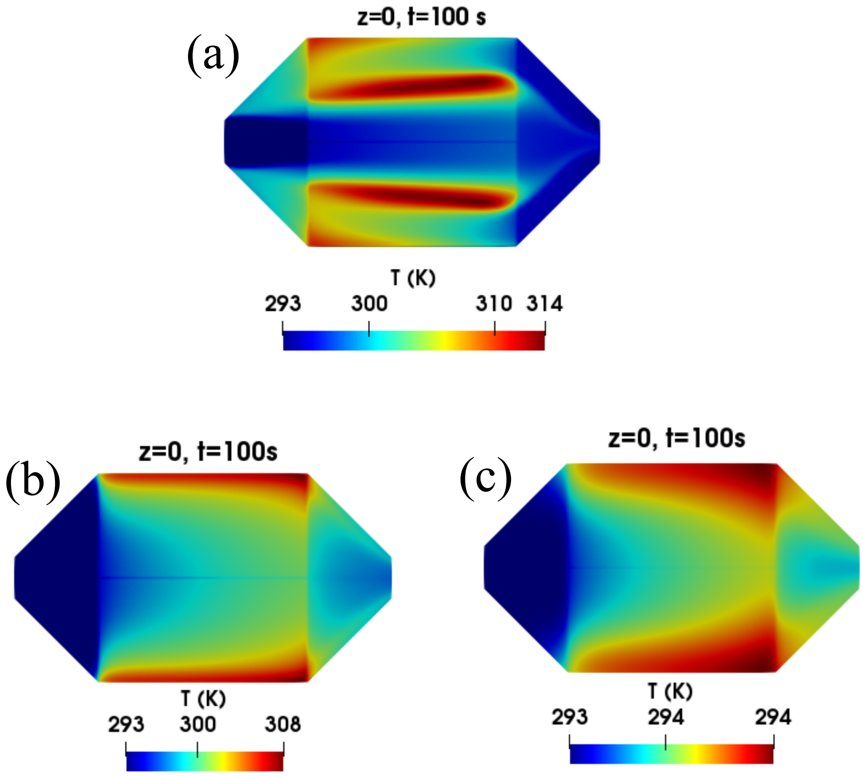

FIGURE 6.9: Temperature profiles at the steady state (t=100 s). (a) Pure water fluid; (b) Suspension no.1 of table 6.1; (c) Suspension no.2 of table 6.1. From (Dbouk, 2019b).

On March 2019, a new PhD thesis was launched at our department, to deepen our understanding in this new emerging field of non-colloidal suspension being as new coolants (numerical and experimental investigations). It is external collaboration with Prof. Vincent THOMY at the BioMEMS Research Group at IEMN (Institut d'Électronique, de Microélectronique et de Nanotechnologie, Lille, France). Prof. THOMY has a wide experience in the

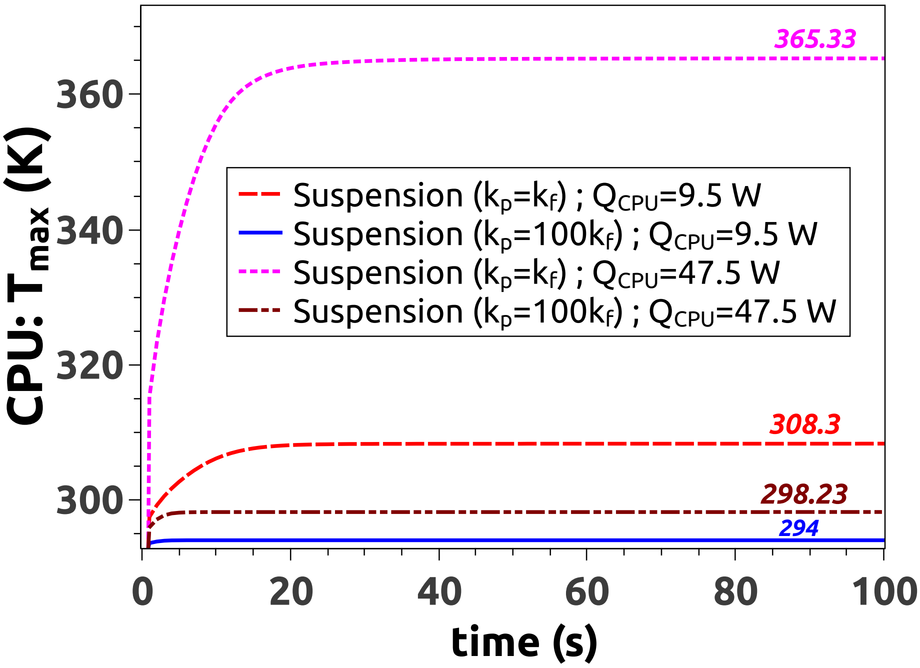

FIGURE 6.10: Influence of imposed heat flux on the CPU maximum temperature using the different cooling-fluids applied in table 6.1. From (Dbouk, 2019b).

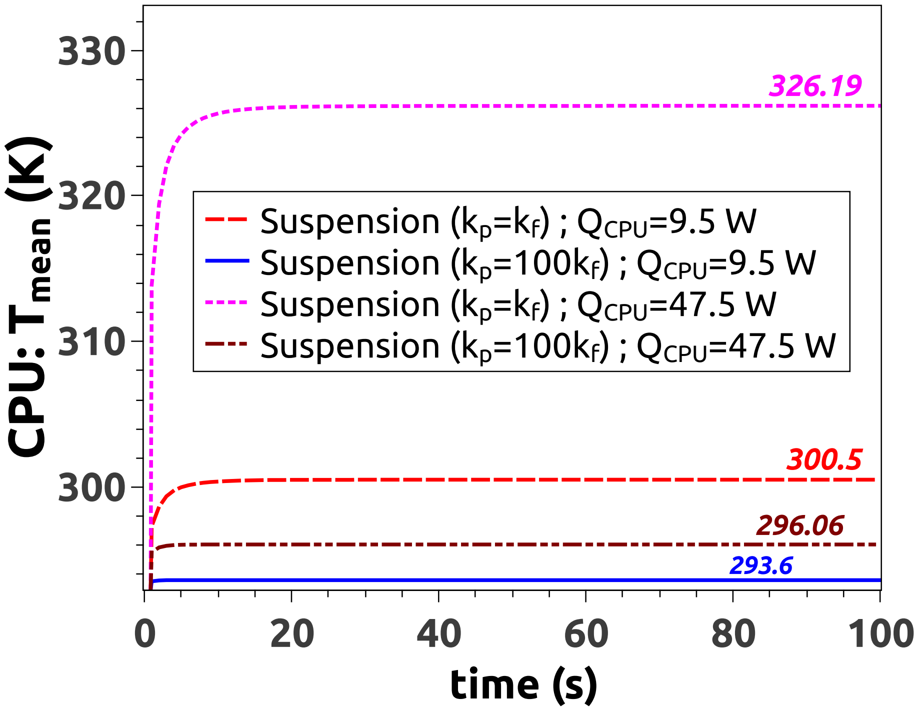

FIGURE 6.11: Influence of imposed heat flux on the CPU mean temperature versus time using the different cooling-fluids applied in table 6.1. From (Dbouk, 2019b).

field of microelectronics and microfluidic research applied to different applications (like in physical and life sciences).

Pure fluid: **Water**	Suspension **no.1**	Suspension **no.2**
$\phi_b = 0$	$\phi_b = 0.35; d_p = 50\ \mu m$	$\phi_b = 0.35; d_p = 50\ \mu m$
$k_f = 0.6\ W\ m^{-1}\ K^{-1}$	$k_p = k_f$	$k_p = 100\ k_f$
$\rho_f = 10^3\ Kg\ m^{-3}$	$\rho_p = \rho_f$	$\rho_p = \rho_f$
$c_{p_f} = 900\ J\ kg^{-1}\ K^{-1}$	$c_{p_p} = 4180\ J\ kg^{-1}\ K^{-1}$	$c_{p_p} = 4180\ J\ kg^{-1}\ K^{-1}$
$Re = 2 \cdot 10^3$ ($U_{in} = 0.16\ m\ s^{-1}$)	$Re_S = 294$ ($U_{in} = 0.1\ m\ s^{-1}$)	$Re_S = 294$ ($U_{in} = 0.1\ m\ s^{-1}$)

TABLE 6.1: Operating conditions using three different CPU cooling-fluids. From (Dbouk, 2019b).

6.2.3 Research toward turbulence modeling in non-colloidal suspensions

In the PhD project of Mme. C. OCTAU (hosted externally at LAMIH laboratory, University of Valenciennes) that i have been supervising (at 30%) since 3 years (defense expected in September 2019), I have been working on turbulence modeling in non-colloidal suspensions (to consider particles-induced turbulence with particle-particle and particles-fluid interactions, knwon as 4-way coupling).

The project of the PhD program of Mme C. OCTAU is funded by the industrial partner ALSTOM® (thèse CIFRE) and it is in collaboration between my research unit and the LAMIH, UMR CNRS 8201 (Laboratoire d'Automatique, de Mécanique et d'Informatique Industrielles et Humaines).

The main objective in the PhD of C. OCTAU is to develop and validate numerical models in CFD (Euler-Euler and/or Euler-Lagrange), for predicting particles transport emitted after rail-way braking of a train (i.e. high speed trains (TGV[4])). Due to the complexity of the problem, a first approach was followed, where we studied suspension jet in cross-flow of water, both experimentally and numerically.

In the PhD project of Mme. C. OCTAU, (macroscopic modeling in CFD, including RANS turbulence models, particles/fluid drag coefficients, lift, etc) (Gidaspow, 1986; Bouillard, Lyczkowski, and Gidaspow, 1989; Schiller and Naumann, 1933), primarily results were obtained in (Octau, Dbouk, Watremez, Meresse, Lippert, Schiffler, Keirsbulck, and Dubar, 2019).

Compared to single-liquid and liquid-liquid jets in crossflow (JICF), liquid-solid two-phase JICF is rarely studied in the literature. Modeling *multiphase turbulent* flows is a complex task due to the locally varying *time* and *length* scales in the flow. The modeling task becomes even more complex in the case of large number of particles (which is the present case of this contribution), and it is still a topic for research and investigation. The complexity in the modeling lies in the fact that 4-way coupling technique must be employed so that the modeling to be complete, for different ratios of the particle response time τ_p to the Kolmogorov time scale τ_K, as illustrated in figure 6.12 by (Elghobashi, 1994) for different regimes. The one-way coupling regime means that particles have negligible effect on turbulence. In other words, it means that particle dispersion depends on the state of turbulence of the continuous phase, due to very low particles concentration (the particles to turbulence momentum transfer posses insignificant effect on the flow). The two-ways coupling regime means that momentum transfer from the particles is large enough to modify the local turbulence structures (e.g. an increase in the turbulence energy dissipation rate, or enhanced production of turbulence energy depending on the particles diameter). The four-way coupling regime dense suspensions) means that in addition to the two-way coupling between the particles and turbulence, particle-particle collision/interactions takes place.

Modeling of turbulent multiphase flows in CFD might be achieved, at an accepted accuracy level versus acceptable computational cost, depending on the modeling approach that is adopted.

A new experimental setup has been developed to investigate a vertical jet of liquid-solid mixture in water turbulent crossflow. A 6% volume fraction of rigid micro particles in water is injected vertically in a horizontal pure-water turbulent flow. The jet trajectory, penetration and the particles concentration were recorded via a high resolution camera with

[4] Train à Grande Vitesse

particles tracking technique. Three-dimensional CFD simulations have been conducted using two different Eulerian models: a Two-Fluid model in the commercial CFD code Star-CCM+® , and a new CFD solver developed in the opensource code OpenFOAM® based on a Mixture model to predict the hydrodynamics, jet trajectory and the particles transport. A modified-$k-\varepsilon$ model (to account for particle induced turbulence, and turbulent dispersion), and a modified-buoyant-$k-\varepsilon$ model have been employed in the commercial and open-source codes, respectively. The developed new solver Mixture Model in the open-source CFD package captured better the Liquid-solid jet's bend compared to the Two-Fluid Model in the commercial CFD code. It constitutes a better compromise due to its good accuracy associated with a computational cost that is reduced by a factor of 7.

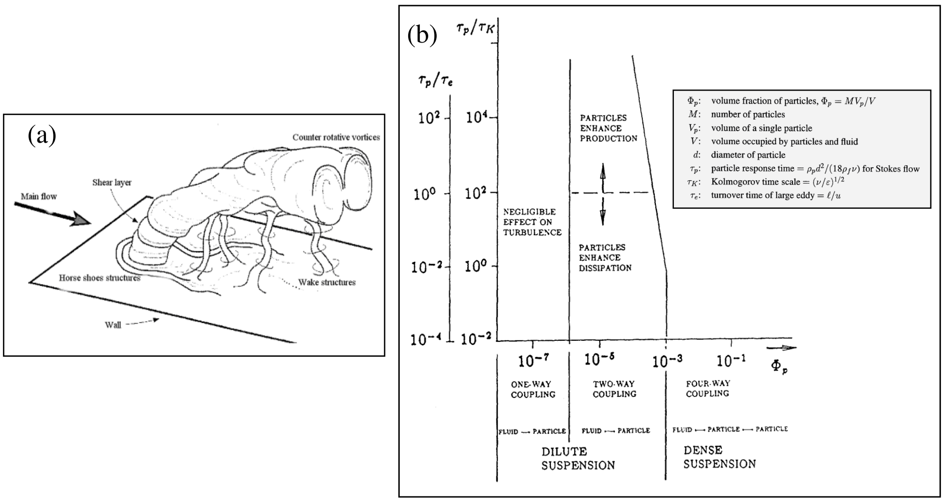

FIGURE 6.12: (a) The vortical structures of a jet in a crossflow, adopted from (Fric and Roshko, 1994). (b) Map of regimes of interaction between particles-in-fluid and turbulence, reproduced from (Elghobashi, 1994).

Figure 6.13 shows the experimental setup developed during the PhD period of Mme C. OCTAU (2016-present).

Figure 6.14 shows the geometry of the 3D channel and the applied boundary conditions in OpenFOAM® and Star-CCM+®.

The concentration profiles for the liquid-solid jet's bend are shown in figure 6.15. It can be clearly observed that the numerical results are very close to the experimental data at the different times 400, 800 and 2500 ms. The new solver developed in OpenFOAM® as a new mixture model predicted better the jet's bend or jet's trajectory at all time steps compared to the experimental data as shown in figure 6.15-(j,k,l).

For local analysis, three points of the experimental concentration field located at the jet's bend were considered: A ($x/h = 0, y/h = 0.1$), B ($x/h = 0.05, y/h = 0.25$) and C ($x/h = 0.1$, $y/h = 0.3$) as shown in figure 6.15. These three points correspond to local line probes positions that have been considered at each point (A, B, and C) rather than only local single points. This is in order to do an averaging of the concentration values in the direction perpendicular to the plane of visualization by the camera.

The obtained normalized local concentration values located at these points A, B and C are plotted as function of time as shown in figure 6.16. The new solver in OpenFOAM® based on a modified Mixture Model is found to predict better the averaged concentration values at different local positions (points A, B and C) compared to experimental data.

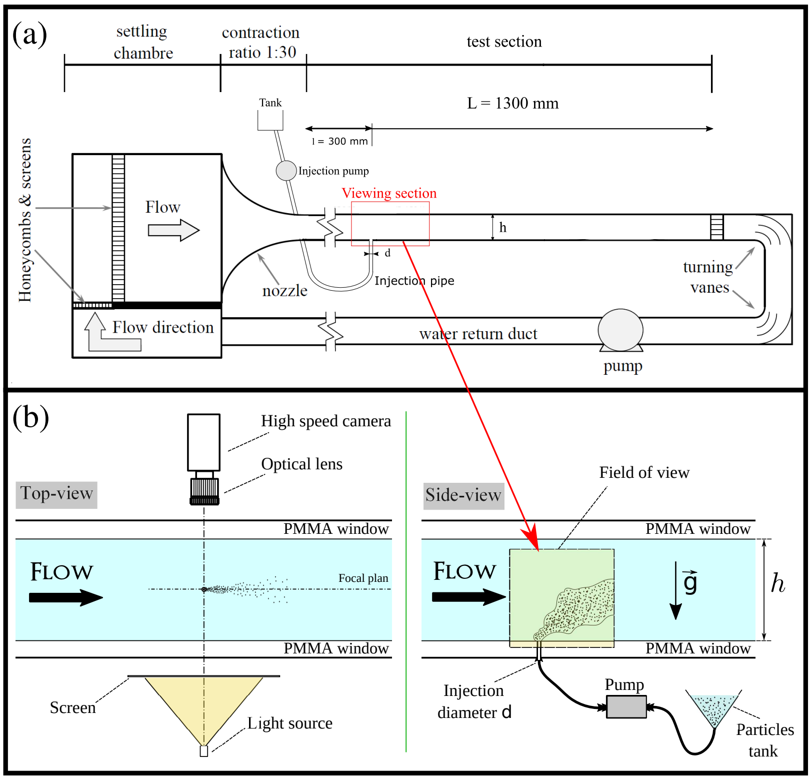

FIGURE 6.13: (a) Hydrodynamic channel description and apparatus. (b) Sketch of the shadowgraphy technique applied to the field of view. Adopted from (Octau, Dbouk, Watremez, Meresse, Lippert, Schiffler, Keirsbulck, and Dubar, 2019).

Using the new solver Mixture model developed in opensource CFD code OpenFOAM® (for simulating a total physical time of 4 seconds), the solution required 22.08 hours as computational time, solved in OpenFOAM® in parallel on a cluster of 32 intel processors (each 2.3 GHz).

Using the Two-Fluid model in the commercial CFD code Star-CCM+® required more additional computational time of about 142.4 hours, solved in parallel on the same cluster of same number of processors.

The new developed CFD solver via a mixture model approach in OpenFOAM® required a computational time that is reduced by a factor of 7, compared to the commercial Two-fluid model in Star-CCM+® . Further investigations are still going on in attempts to improve the overall accuracy of the models.

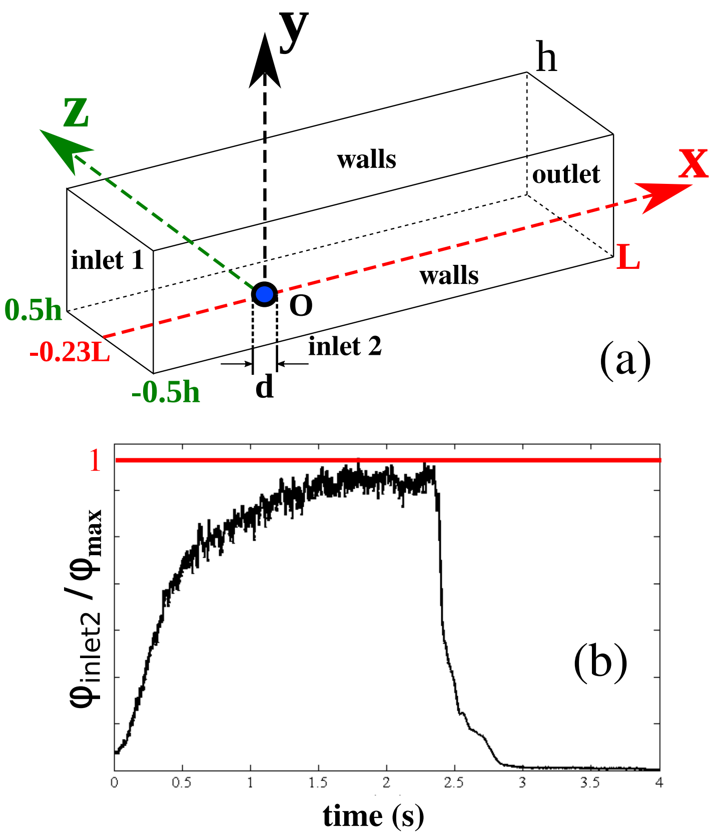

FIGURE 6.14: (a) The geometry of the 3D channel and the applied boundary conditions. (b) Volume fraction $\phi^*(t)$ boundary condition imposed at the vertical injection inlet 2 ($\phi_{max} = 6\%$). Adopted from (Octau, Dbouk, Watremez, Meresse, Lippert, Schiffler, Keirsbulck, and Dubar, 2019).

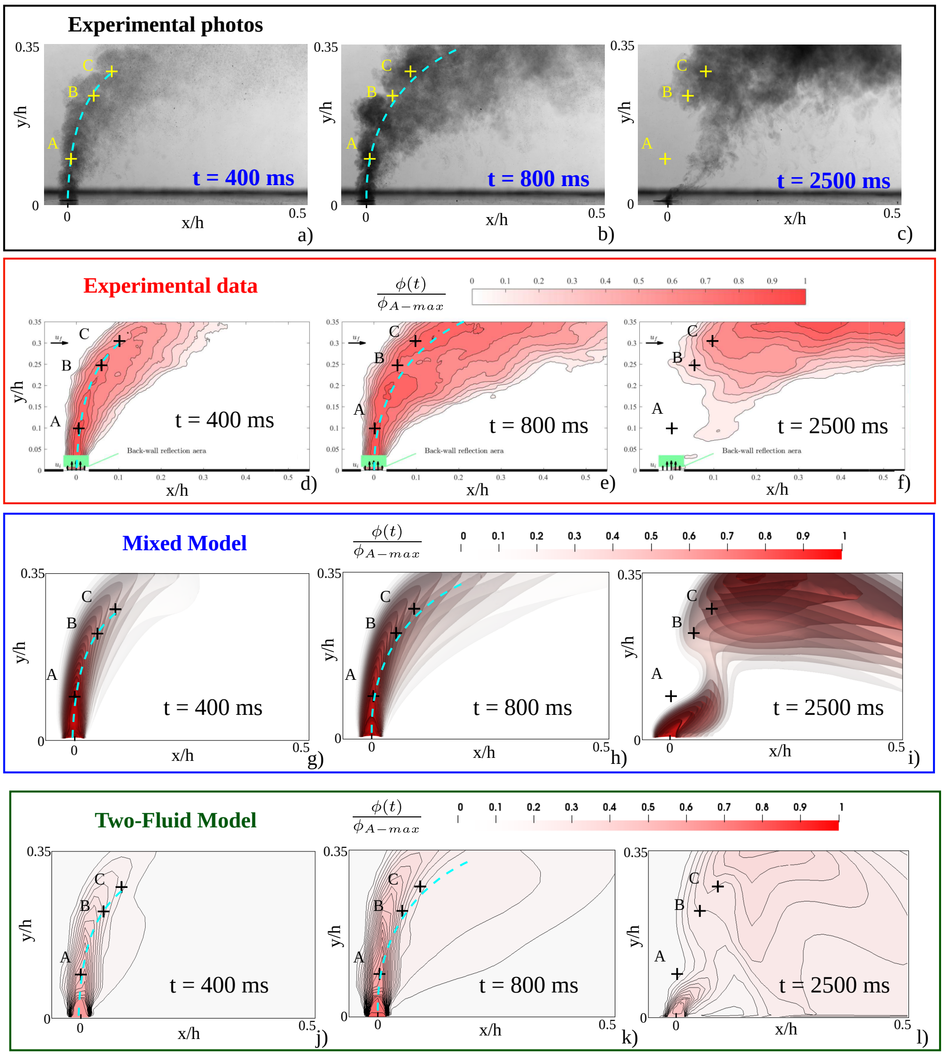

FIGURE 6.15: Experimental and numerical normalized concentration fields at t=400, 800 and 2500 ms. a-f) experimental results; g-i) numerical results at $z = 0$ applying the Mixture model new solver in OpenFOAM®; j-l) numerical results at $z = 0$ applying the Two-Fluid model in Star-CCM+. Adopted from (Octau, Dbouk, Watremez, Meresse, Lippert, Schiffler, Keirsbulck, and Dubar, 2019).

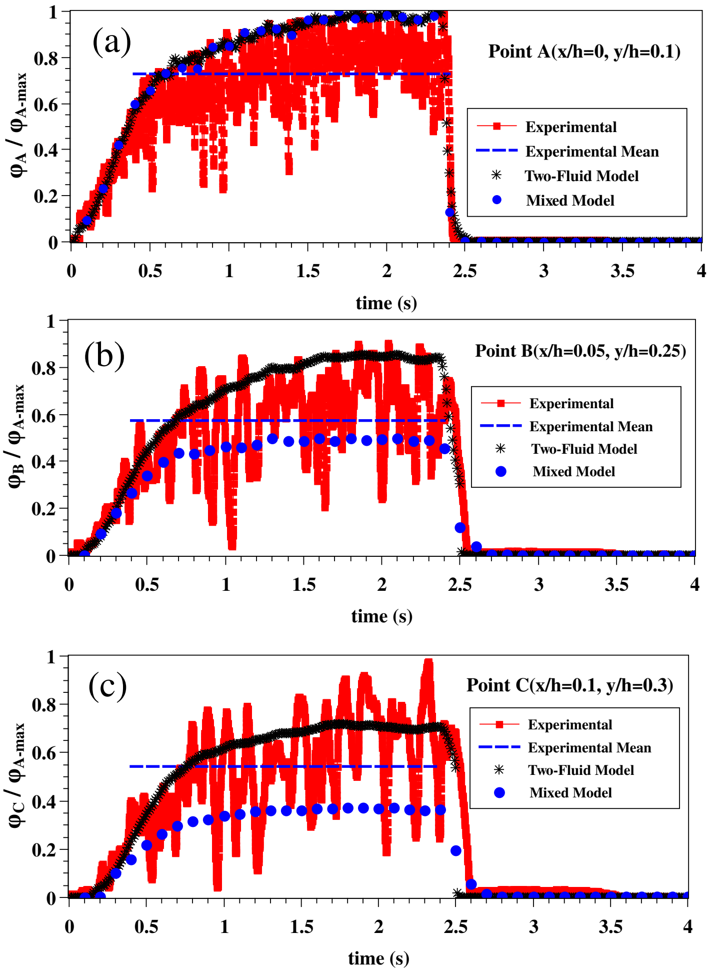

FIGURE 6.16: The normalized particle's concentration value at the point A($x/h = 0$, $y/h = 0.1$), B($x/h = 0.05$, $y/h = 0.25$) and C($x/h = 0.1$, $y/h = 0.3$) as function of time using the Mixture model in OpenFOAM®, and the two-Fluid model in Star-CCM+®. ϕ_{A-max} corresponds to the maximum value obtained at the point A between t=0 and t=4 s. Adopted from (Octau, Dbouk, Watremez, Meresse, Lippert, Schiffler, Keirsbulck, and Dubar, 2019).

6.2.4 Mixing enhancement (solid-particles-liquid multiphase flows)

Recently, in Dbouk and Habchi, 2019, I started applying for the first time in our research unit, non-colloidal suspension in chaotic advection flows in multifunctional heat exchangers (Habchi, Ouarets, Lemenand, Della Valle, Bellettre, and Peerhossaini, 2009; Habchi, Lemenand, Della Valle, and Peerhossaini, 2009). The major objective is to study numerically in CFD the potential of chaotic and helical pipes in mixing of non-colloidal *isodense* suspensions of rigid microparticles as illustrated in figure 6.17. The idea is to place static mixers to solve the problem of shear-induced migration in concentrated non-colloidal isodense suspension flows.

This new research activity at our research unit, I launched recently in collaboration with Dr. Charbel HABCHI from the Notre-Dame University, in Lebanon. It is also good to mention that i previously conducted research and development activity on similar research topic in the past (during my early Master-II-research studies at the research unit: LTEN, UMR CNRS 6607, at the University of Nantes), where i worked on the numerical modeling and simulation of liquid-liquid dispersion in a chaotic advective flows.

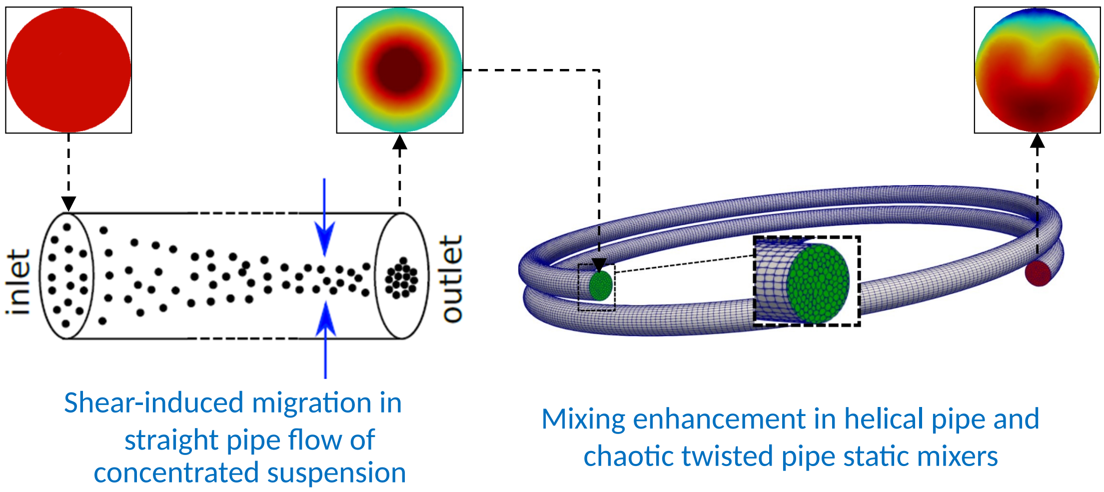

FIGURE 6.17: Shear-induced migration and mixing enhancement in helical pipe and chaotic twisted pipe static mixers. Solid particles are in black; Newtonian liquid is in white. A graphical abstract adopted from (Dbouk and Habchi, 2019).

In this research study, to quantify the mixing process, we adopted the mixing index MI based on the coefficient of variation (CoV) of the particles concentration as follows:

$$MI = 1 - \frac{CoV_{outlet}}{CoV_{inlet}} \tag{6.10}$$

where the coefficient of variation CoV is obtained as follows:

$$CoV = \frac{\sigma_\phi}{\hat{\phi}_b} \tag{6.11}$$

σ_ϕ is the standard deviation of the volume fraction at outlet with respect to the mean value $\hat{\phi}_b$. The mixing index is represented in % and it is directly related to the degree of homogeneity of the particles which is quantified by the CoV. Good mixing is reflected by high values of MI, and vice-versa.

Some examples of the numerical CFD results obtained on mixing in isodense suspensions, via an advanced new solver that was developed internally in OpenFOAM, 2019, are illustrated in figures 6.18 and 6.19 (i.e. mixing index MI).

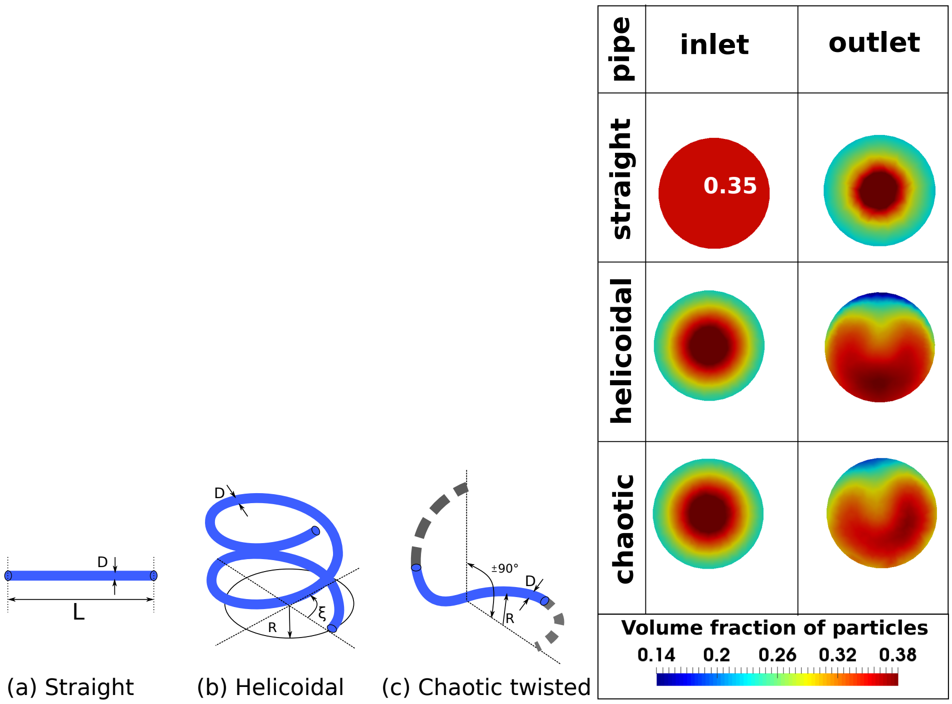

FIGURE 6.18: Non-colloidal *isodense* suspension: mixing in multi-functional heat exchangers; (right-hand-side) at exit of the 7^{th} elbow; $D_p = 400\ \mu m$; $Re = 100$; inlet volume fraction = 0.35 (steady state). From (Dbouk and Habchi, 2019).

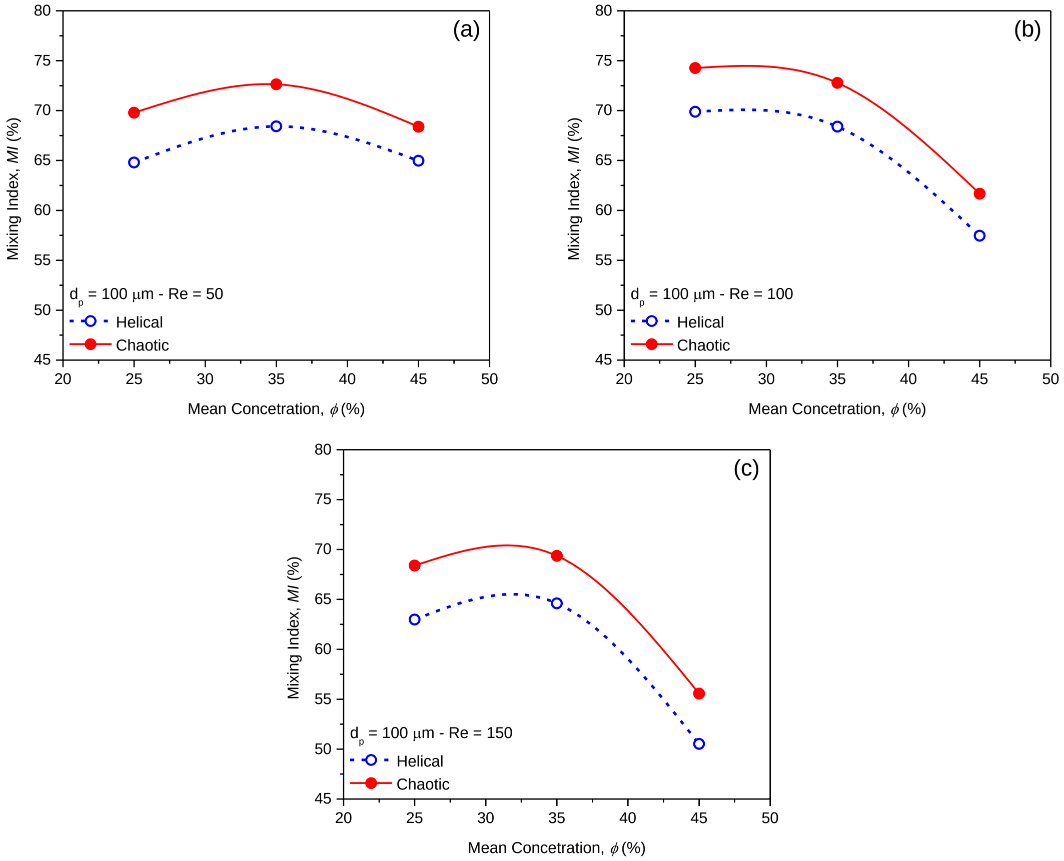

FIGURE 6.19: Non-colloidal *isodense* suspension: mixing index as function of the volume fraction ϕ and the Reynolds number (steady state). From (Dbouk and Habchi, 2019).

6.2.5 Adaptive Mesh Refinement Techniques

In a recent effort, I have been also working on the topic of adaptive mesh refinement (AMR) techniques on hexahedral mesh (in both 2D and 3D) and their applications in the CFD solvers that i have developed previously for non-colloidal suspension flows (with and without heat transfer). The importance behind AMR techniques is the allowance for computational time reduction versus an increase in accuracy, especially at the suspension/liquid interface regions in the computational domain.

The new developed algorithm intended for the recent developed AMR technique is illustrated in figure 6.20.

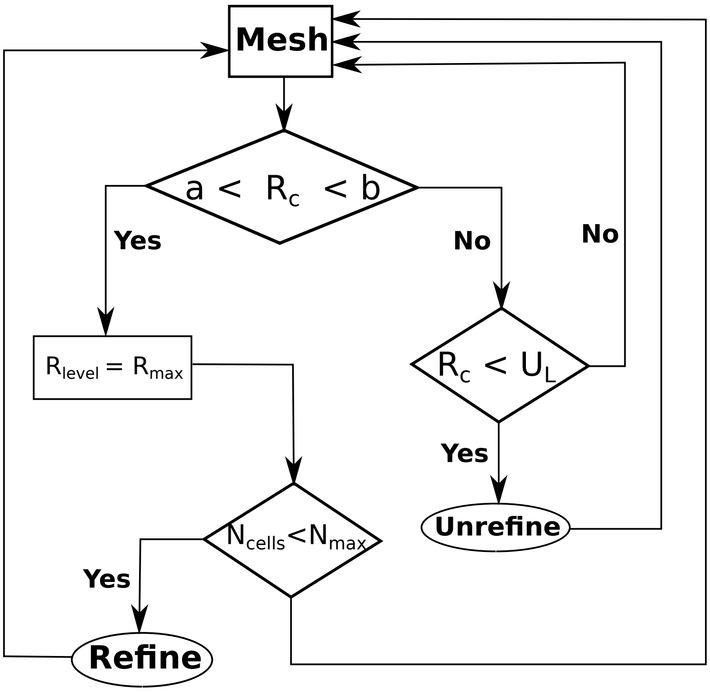

FIGURE 6.20: The flow chart of the Adaptive Mesh Refinement algorithm. Adopted from (Dbouk, 2019a).

If we look again to the mixing and resuspension case of figure 3.23, presented in Chapter 3, it solved again but applying now an advanced 2D AMR technique as illustrated in figures 6.21 and 6.22.

A similar example but applied to shear-induced migration in a channel flow is illustrated in figure 6.23.

Finally, i can state that my research axis no.1 is still full of huge potentials for further developments and new applications to be developed at IMT Lille Douai, such as in automotive industry (electric vehicles, battery cooling, etc), medical science field applications (blood flow Rheology), geological and civil engineering applications (cement flow, volcanic eruptions, undersea level plumes, petroleum extraction, etc) and chemical and process engineering, etc.

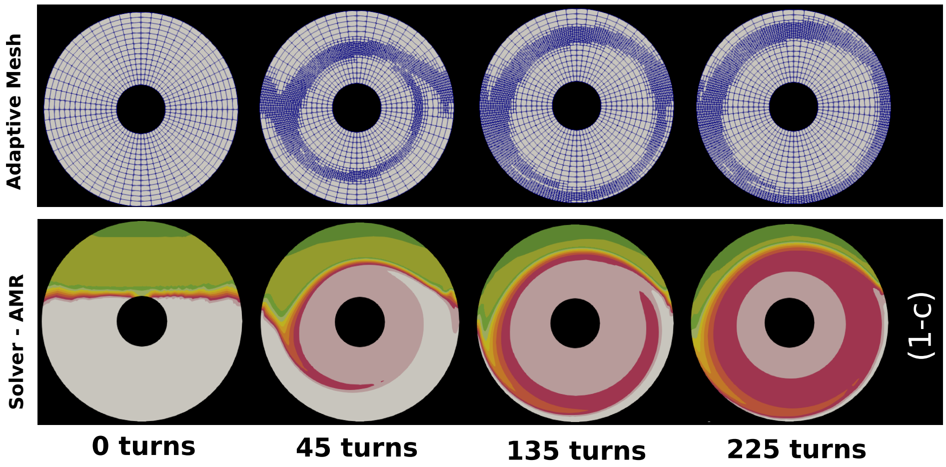

FIGURE 6.21: The particle concentration maps as (1-c) values versus **2D** adaptive mesh refinement; From left, to right at: 0, 45, 135, and 225 turns of the inner cylinder, respectively. ***Suspension Properties***: $a = 397\ \mu m$, $\rho_0 = 1.253\ g/cm^3$, $\rho_p = 1.18\ g/cm^3$, $\mu_0 = 0.588\ Pa \cdot s$. Adopted from (Dbouk, 2019a).

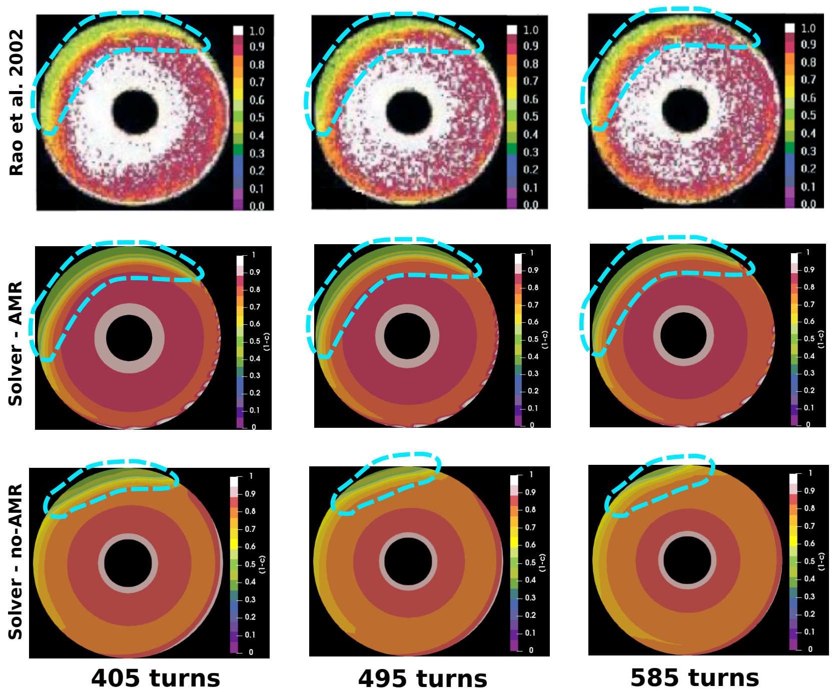

FIGURE 6.22: The particle concentration maps as (1-c) values obtained: experimentally by (Rao, Mondy, Sun, and Altobelli, 2002) (upper row); numerical solver with **AMR** technique (middle row); numerical solver without **AMR** technique (lower row).From left, to right at: 405, 495 and 585 turns of the inner cylinder, respectively. ***Suspension Properties***: $a = 397\ \mu m$, $\rho_0 = 1.253\ g/cm^3$, $\rho_p = 1.18\ g/cm^3$, $\mu_0 = 0.588\ Pa \cdot s$. Adopted from (Dbouk, 2019a).

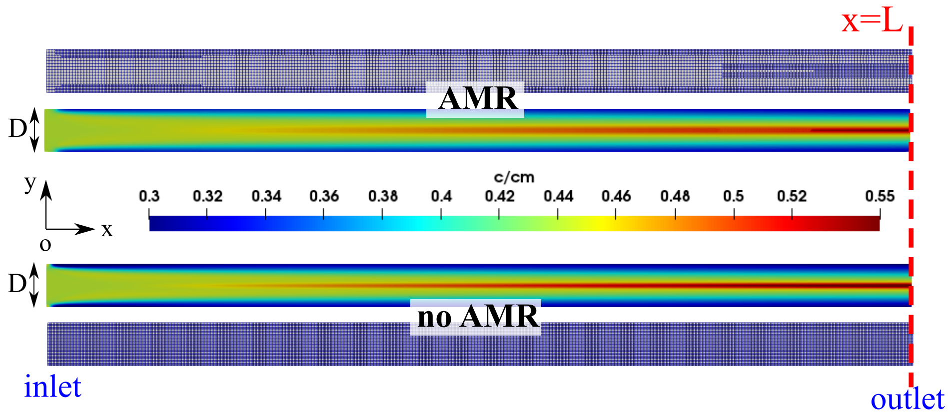

FIGURE 6.23: Dimensionless particles concentration inside the channel at the steady state. The AMR technique reduces the computational cost importantly by a factor of 4 (for an initial uniform mesh of base $D/30$ cells) while retaining a very good accuracy of results for the shear-induced migration prediction. Adopted from (Dbouk, 2019a).

6.3 Perspectives and potentials: research axis no.2

6.3.1 Topology Optimization Design

Some perspectives for the topology optimization R&D&I axis, are the extension of the actual topology optimization solvers, that I have been developing, into:

- Large-scale 3D problems with optimization algorithms that can perform efficiently in parallel runs over multiple CPU and GPU units. For example, very recently, a one-year extendable Postdoc recruitment position is opened, November 2018, (click here to see this postdoc tasks description) to contribute to the development of this R&D task at our research unit, funded by the industrial partner VALEO® Thermal Systems Research Group (in the context of the industrial chair "NEO").
- MultiPhysics applications (such as turbulent flows with heat transfer), fluid structure interaction, thermo-mechanical stresses, adsorbent porous media, energy storage, gas separation, etc).

6.4 Perspectives and potentials: research axis no.3

Some of my future objectives for axis no.3 (on Multi-component fluid flows in adsorbent porous media) are as the following:

- First objective is to pursuit our collaboration with the team at IMT Atlantique in order to extend our previous research activity in (Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018; Gautier, Dbouk, Harion, Hamon, and Pré, 2018) towards new innovative design of multi-functional adsorbent-heat-exchangers (AHE) (i.e. see figure 6.24).
- Second objective is to validate experimentally the recent works by (Kassou, Gautier, and Dbouk, 2018) on air pollution reduction and pollutant transport prediction in indoor environment (bi-component adsorption). This mission can be done in internal collaboration with researchers from the Atmospheric and Environmental Research Department at IMT Lille Douai, and it fits well in the new strategies defined for the new CERI-EE[3].
- Third objective is to initiate future international collaborations with other researchers who are working on similar topics in CFD applied to pollution prediction and reduction by adsorbent materials in various applications (vehicles, industry zones, airplane cabins, residential buildings).
- Fourth objective is to validate the recent CFD solvers for multi-component adsorption developed in (Dbouk, 2019c; Dbouk, 2019d).
- Final objective is to apply the topology optimization solvers that I have been developing to the optimization and design of thermofluid systems where adsorption (& desorption) phenomena may be present. This will be in attempts to approach and initiate a collaboration with the researchers: (Amigo, Prado, Paiva, Hewson, and Silva, 2018) (at Imperial College, London) who are working recently on a similar R&D topic.

[3] Centre d'Enseignement, de Recherche et d'Innovation Energie et Environnement

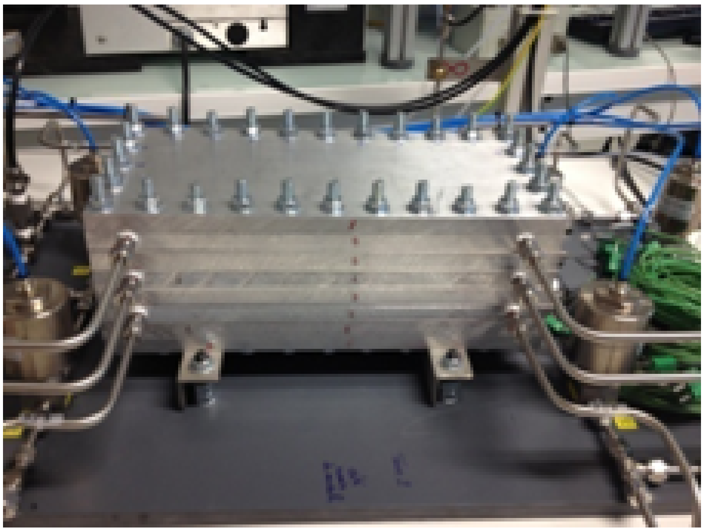

FIGURE 6.24: An example of an innovative multi-functional adsorbent-heat-exchanger prototype. A collaboration project with Prof. PRÉ, at IMT Atlantique, University of Nantes.

6.5 Conclusion

As a final conclusion, since September 2014 which is the date of my arrival to IMT Lille Douai:

- I have been both teaching and directing research through intense supervision of several Postdoc, PhD and Masters research students inside and outside the hosting research unit, and their good insertion into a prospective successful future R&D&I career (Dr. R. GAUTIER, Dr. V. SUBRAMANIAM, M. H. BELKHOU, Mme. C. OCTAU, M. H. KARKABA, M. M. MOAZZEN, M. T.C. NGUYEN, M. A. KASSOU and M. V. VALLANT)
- I have brought and introduced new research axes into my hosting research unit ECSP (CERI-EE): (Dbouk, 2018a; Dbouk, 2019b),
- I have been adding value by contributing to the hosting research unit overall scientific reputation, development, research direction and orientation, research supervision/co-supervision and scientific collaborations (**Dbouk2019preprintbb**; Dbouk and Harion, 2015; Dbouk, Perales, Babik, and Mozul, 2016; Dbouk, 2016; Dbouk, 2017a; Nguyen and Dbouk, 2017; Subramaniam, Dbouk, and Harion, 2018a; Gautier, Dbouk, Campesi, Hamon, Harion, and Pré, 2018; Gautier, Dbouk, Harion, Hamon, and Pré, 2018; Dbouk, 2018a; Dbouk, Dirker, Fachinotti, and Page, 2019; Dbouk and Habchi, 2019; Dbouk, 2019a; Dbouk, 2019c; Dbouk, 2019d; Dbouk and Bahrani, 2019; Kassou, Gautier, and Dbouk, 2018; Vaillant, Gautier, and Dbouk, 2019; Octau, Dbouk, Watremez, Meresse, Lippert, Schiffler, Keirsbulck, and Dubar, 2019; Belkhou, Russeil, Dbouk, Mobtil, Bougeard, and François, 2019; H. Karkaba, Dbouk, Habchi, Russeil, Lemenand, and Bougeard, 2019),
- I have been also generating new ideas (Dbouk, 2017b; Dbouk, 2017c; Dbouk, 2018c; Dbouk, 2018d), as innovative research topics for future research projects developments and new applications, national and international scientific collaborations and networking with both academia and industry (Dbouk, 2019b),

- I have been also mounting a new Masters program on intelligent buildings, and a new course for postgraduate students (Dbouk, 2018b) on pinch analysis and process integration methods, for a better and efficient use of energy resources (such as the optimization of energy consumption in different applications, and in the context of a future environment-friendly socioeconomic world).
- The last 5 years, I contributed importantly to the preparations of last wave of French HCERES research committee evaluations (with good synergy between my different R&D activities and those present at the hosting research unit).

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