



D6.7 Workshop: "Computational Fluid Dynamics-based Process Intensification"

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Document history

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EXECUTIVE SUMMARY

1.1 Description of the deliverable content and purpose

This report describes the activity carried out during the workshop: "*Computational Fluid Dynamics-based Process Intensification*", as well as the organizational procedure. The workshop is part of the Grant Agreement of the IMPROOF project. The workshop was organized by the Laboratory for Chemical Technology of Ghent University. The goal of the workshop was to provide the attendants with a broad overview of the state-of-the-art research related to CFD-assisted process intensification.

1.2 <u>Brief description of the state of the art and the innovation</u> <u>breakthroughs</u>

This part is not relevant for this deliverable, being it focused on the preparation and implementation of the workshop.

1.3 Corrective action

The official title of the workshop was slightly changed with respect to the original one: "3D coupled CFD simulations in cracking furnaces" was changed into "Computational Fluid Dynamics-based Process Intensification". There are two primary reasons for this change. The original topic was deemed to be too niche and there was a concern that the original topic would also overlap too much with the "Furnace Workshop" initially envisioned in Deliverable 6.3. For these reasons, the topic of the workshop was slightly changed to attract a broader audience (not only focussing on the steam cracking process).

One of the originally advertised speakers, namely prof. Hans Kuipers from Eindhoven Technical University, had an accident three days before his expected travel (prof. Kuipers had to go back to the hospital for a check-up on the day of the workshop). The organization of the workshop found a last-minute replacement in prof. Patrice Perreault from the University of Antwerp.



2 PREPARATION OF THE WORKSHOP

2.1 Date and Location

The workshop took place on Monday the 27th of January 2020 in the iGent building of Ghent University, Tech Lane 126 Ghent, across the Laboratory for Chemical Technology. The participants had the opportunity to enrol for the connected workshop *"Novel technologies in steam cracking furnaces"* on the 28th of January 2020.

2.2 <u>Schedule</u>

Table 1 shows the schedule for the 27th of January:

Time	Activity
08:30 - 09:00	Arrival
09:00 - 09:15	Introduction by prof. Van Geem (UGent)
09:15 – 10:15	prof. Thierry Poinsot (CERFACS)
10:15 – 11:15	dr. Victor Francia (Heriot-Watt University)
11:15 – 11:30	Coffee break
11:30 – 12:30	prof. Alberto Cuoci (POLIMI)
12:30 – 13:30	Lunch
13:30 – 14:30	prof. Tony Arts (Von Karman Institute for Fluid Dynamics)
14:30 – 15:30	prof. Kevin Van Geem (Ghent University)
15:30 – 16:00	Coffee break
16:00 - 17:00	prof. Hans Kuipers (Eindhoven Technical University)
	prof. Patrice Perreault (University of Antwerp)

Table 1: Schedule workshop: "CFD-assisted process intensification".

Prof. Hans Kuipers could not make it to the workshop and was replaced by prof. Patrice Perreault from the University of Antwerp.



2.3 Workshop promotion

People were invited to the IMPROOF event through different channels. The Laboratory for Chemical Technology mailing list was used to contact people who had attended previous events organized by the Lab. Each partner ensured that they were properly represented and promotion on the IMPROOF website and on LinkedIn lead to the registration of 50+ participants from various companies and from academia.



Figure 1: Advertising flyer made for the IMPROOF Workshop.



3 WORKSHOP ACTIVITIES

3.1 Speakers

A detailed biography of every individual speaker can be found in Appendix A.

Prof. Poinsot from CERFACS was the first invited speaker. His presentation focused on Large Eddy Simulations (LES) of turbulent reacting flows. The introduction focussed on the implementation of LES in the CERFACS software AVBP. Prof. Poinsot showed work performed both on turbulent premixed flames and related to explosions. At the end, prof. Poinsot gave some insights into ongoing work related to deep learning for turbulence combustion interaction.





Figure 2: prof. Poinsot presenting at the IMPROOF Workshop 27 January 2020.

Dr. Victor Francia, working at the Heriot-Watt University, presented the work he performed in the first years of his academic career related to spray drying and the agglomeration of laundry granular detergents.



Figure 3: dr. Victor Francia presenting at the IMPROOF Workshop 27 January 2020.



The last speaker in the morning session was prof. Alberto Cuoci form POLIMI. His talk focussed on chemistry acceleration methods in CFD. He showed examples ranging from combustion to heterogeneous catalysis.





Figure 4: prof. Cuoci presenting at the IMPROOF Workshop 27 January 2020.

Prof. Arts from the von Karman Institute for Fluid Dynamics presented slides comparing aerodynamic and convective heat transfer experiments to computations. He showed work performed on high pressure turbine blades, rotating flows and helically corrugated tubes.





Figure 5: prof. Arts presenting at the IMPROOF Workshop 27 January 2020.

Prof. Van Geem presented the work performed at the Laboratory for Chemical Technology related to steam cracking. The presentation showed the broad research scope of the group. Throughout the years the focus has shifted from experimental work and 1D simulations to 3D CFD.



Figure 6: prof. Kevin Van Geem presenting at the IMPROOF Workshop 27 January 2020.



Prof. Patrice Perreault highlighted his research theme at the University of Antwerp. He also discussed the work he performed during his postdoc stay at the Laboratory for Chemical Technology, where he worked on the scale-up and proof-of-concept study of the so-called gas-solid vortex reactor setup.





Figure 7: prof. Perreault presenting at the IMPROOF Workshop 27 January 2020.



4 ACHIEVEMENTS

Overall, we have received only positive feedback from the participants. During the lunch break a group picture was organized, as shown in Figure 8.



Figure 8: Group picture of the workshop participants

The audience was very heterogeneous with participants both from academia and industry, in total 59 people registered for the event. The final list with signatures can be found in Appendix B.



Figure 9: Distribution of the workshop participants between academia (32) and industry (27) (left) and the distinction between people directly involved in the project (14), people working for one of the IMPROOF partners but not directly on the project (15) and external participants (30) (right).



APPENDIX

A. Speaker biographies

Speaker 1: Thierry Poinsot (CERFACS)

Dr Thierry Poinsot received his PhD thesis in heat transfer from Ecole Centrale Paris in 1983 and his 'These d'Etat' in combustion in 1987 (in those days, the French had a double Phd system...). He is a research director at CNRS, head of the CFD group at CERFACS, senior research fellow at Stanford University, consultant for various companies and member of the French Academy of Sciences since 2019. After his thesis at Ecole Centrale Paris and a two year post-doctoral work at Stanford, he has started combustion activities at CERFACS in 1992 and his group (80 persons in 2020) has produced a significant part of recent research in the field of LES of turbulent combustion in gas turbines. He teaches numerical methods and combustion in many schools and universities (Ecole Centrale Paris, ENSEEIHT, ENSICA, Supaero, UPS, Stanford, Von Karmann Institute, Kanpur, CEFRC Princeton and Beijing). He has authored more than 210 papers in refereed journals and 200 communications. He is the author of the textbook "Theoretical and numerical combustion" with Dr D. Veynante (3000 copies sold) and the editor in chief of «Combustion and Flame ». He has received the first Cray prize in 1993, the BMW prize in 2002, the Grand Prix of French Academy in 2003, the Aeronautics prize of the 3AF (Association d'aeronautique et d'astronautique de France) in 2014, a first ERC advanced grant in 2013 on thermoacoustics and a second one in 2019 on hydrogen combustion for energy storage. In 2017, he has received the Zeldovich Gold medal of the Combustion Institute. He also gave the prestigious Hottel plenary lecture at the last Symposium on Comb. in Seoul (2016).

Speaker 2: Victor Francia (Heriot-Watt University)

Dr Francia is a chemical engineer from the University of Salamanca, Spain. He graduated in 2006 and moved to work in the private sector. Victor has worked in Acciona, managing the operation of desalinisation facilities, as consultant for Exxon Mobil and as engineer in corporate R&D. He spent 4 years at Procter & Gamble working on the design of granulation and spray drying processes, and moved to academia in 2013, first at Imperial College London and later at University College London modelling spray dryers and fluidised beds. Last year, Dr Francia was appointed Assistant Professor in complex multi-phase flows and responsive technology at Heriot-Watt University in Edinburgh, Scotland. His group looks into how we can modulate the formation of dynamic structures in particles flows such as agglomerates, clusters, cakes or fouling layers, to design more robust and efficient manufacturing processes and improve operations in the energy and environmental sectors.



Speaker 3: Alberto Cuoci (POLIMI)

Alberto Cuoci received his MSc in Chemical Engineering at Politecnico di Milano in 2004. He then carried out a PhD in the same University in collaboration with the University of Utah, on the modeling of NOx and soot emissions from combustion devices. His PhD Thesis was awarded the ENI Award 2009 "Debut in Research Prize". In 2008, Alberto Cuoci was appointed Assistant Professor at the Department of Chemistry, Materials, and Chemical Engineering of Politecnico di Milano and in 2014 he became Associate Professor at the same University. The main scientific interests of Alberto Cuoci are in the field of numerical modeling of reactive flows with detailed kinetics, with special emphasis on: 1) numerical methods for including

complex/large kinetics in CFD codes; 2) formation of pollutants (NO_x and soot) in flames; 3) heterogeneous catalytic processes and reactors.

Speaker 4: Tony Arts (VKI)

EDUCATION

- Docteur en Sciences Appliquées (PhD), Université Catholique de Louvain, Belgium, 1982
- Post-Graduate Diploma Course, von Karman Institute, Belgium, 1979
- Ingénieur Civil Mécanicien, Université Catholique de Louvain (UCL), Belgium, 1978 **CAREER**
- 2008 2012: Special appointment to Graduate Faculty at Purdue University, USA
- 2005 present: Full Professor, von Karman Institute, Belgium
- 2003 present: Head of the Turbomachinery and Propulsion Department, von Karman Institute, Belgium
- 1999 present: Chargé de cours invité (Invited Associate Professor), University of Louvain, Belgium
- 1994 2005: Professor, von Karman Institute
- 1988 1993: Associate Professor, von Karman Institute
- 1982 1987: Assistant Professor, von Karman Institute
- 1980 1981: Military service, research assistant, Royal Military Academy, Belgium

AWARDS and MEMBERSHIPS

- ASME Member since 1996
- Dr. Ernst Zimmerman Memorial Award 1986
- Member at Large, NATO STO/CSO, Applied Vehicle Technology Panel
- International Committee member Japanese Gas Turbine Society
- ASME IGTI Gasturbine conference 2008, Heat transfer Committee "Best Paper award"
- Observer, Board of Directors, CENAERO Belgium
- International Committee member Japanese Gas Turbine Society
- Arthur Charles Main Prize 2011 (Institution of Mechanical Engineers United Kingdom)



Speaker 5: Kevin Van Geem (LCT)

Kevin Van Geem (full professor) is member of the Laboratory for Chemical Technology of Ghent University. Thermochemical reaction engineering in general and in particular the transition from fossil to renewable resources are his main research interests. He is a former Fulbright Research Scholar of MIT and directs the Pilot plant for steam cracking and pyrolysis. He is the author of more than hundred scientific publications and has recently started his own spin-off company.

He is involved in on-line and off-line analysis of complex petrochemical and biochemical samples using comprehensive two-dimensional gas chromatography. Pyrolysis, detailed kinetic modeling, process, scale-up, modeling, and ant-fouling technology belong to his main expertise.

Speaker 6: Hans Kuipers (Eindhoven Technical University)

Hans Kuipers graduated in 1985 at the department of Chemical Engineering of the University of Twente. In December of the same year he started with his Ph.D. study at the Reaction Engineering group of University of Twente on detailed micro balance modeling of gas-fluidized beds. In June 1990 he received his Ph.D. degree in Chemical Engineering and was appointed as assistant professor in the Reaction Engineering group headed by Prof. W.P.M. van Swaaij. In 1994 he was appointed as associate professor in the same group. In 1999 he became fulltime professor in Fundamentals of Chemical Reaction Engineering at the University of Twente. From 2006 until 2010 he was Scientific Director of the Institute of Mechanics Processes and Control (IMPACT) at the University of Twente. Since August 2010 he is a fulltime professor at Eindhoven University of Technology and heads the group Multiphase Reactors. He teaches amongst others introductory and advanced courses on transport phenomena and multiphase reactors. His research interests are in the area of multiphase chemical reactors. He participates in the Gravitation Program Multi-scale Catalytic Energy Conversion (MCEC) and acts as program director Process Technology and member of the Executive Board (EB) of the Advanced Research Center (ARC) Chemical Building Blocks Consortium (CBBC). Since 2019 he is Honorary Professor of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences.

B. List of participants

(see following pages)