Supercomputing hydrogen combustion and other contemporary problems by open source tools

Computational physics/chemistry perspective

Energy Forum Speaking Event, Thursday, November 23rd 2023
Otaniemi, Espoo

Fig: I. Morev

Associate Prof. Ville Vuorinen
ville.vuorinen@aalto.fi

Aalto-yliopisto
Aalto-universitetet
Aalto University

BUSINESS FINLAND

CSC

Aalto Science-IT project

SUOMEN AKATEMIA

Contents of the talk

1) Prologue

2) Computational fluid dynamics at Aalto in 2023

3) Myths behind hydrogen

4) Aalto participating in international efforts to model hydrogen flames

5) Concluding remarks

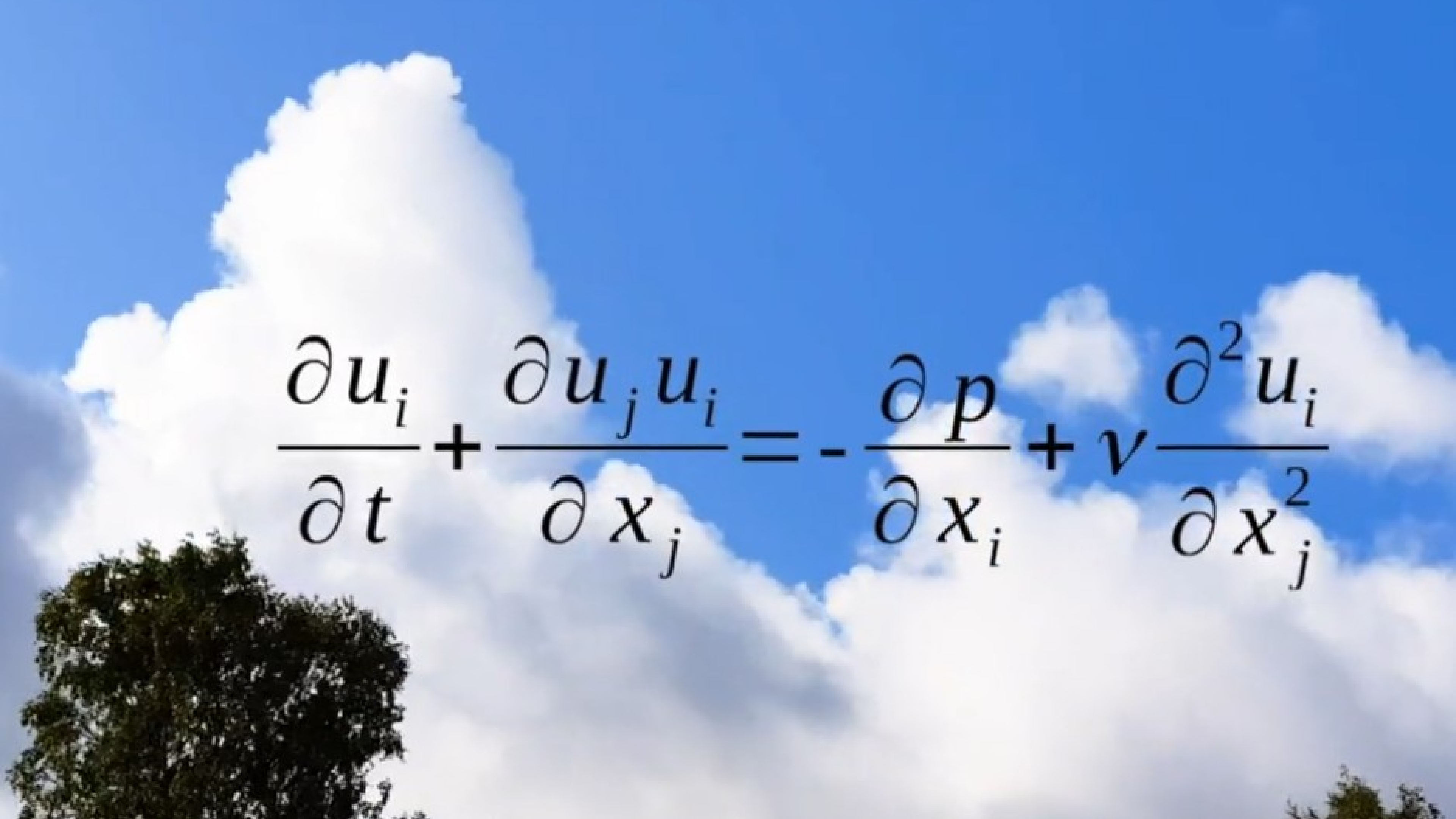
1) Prologue

Artist: Arnold Lakhovsky
https://commons.wikimedia.org/wiki/File:Arnold_Lakhovsky_Conversation.png


Fig: Glen Bowman

https://commons.wikimedia.org/wiki/File:Loule_water_fountain_-_The_Algarve,_Portugal_(13994888880).jpg


Fig: Mike Dorffler



$$\frac{\partial u_i}{\partial t} + \frac{\partial u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2}$$

Millennium Problems

Yang–Mills and Mass Gap

Experiment and computer simulations suggest the existence of a "mass gap" in the solution to the quantum versions of the Yang-Mills equations. But no proof of this property is known.

Riemann Hypothesis

The prime number theorem determines the average distribution of the primes. The Riemann hypothesis tells us about the deviation from the average. Formulated in Riemann's 1859 paper, it asserts that all the 'non-obvious' zeros of the zeta function are complex numbers with real part 1/2.

P vs NP Problem

If it is easy to check that a solution to a problem is correct, is it also easy to solve the problem? This is the essence of the P vs NP question. Typical of the NP problems is that of the Hamiltonian Path Problem: given N cities to visit, how can one do this without visiting a city twice? If you give me a solution, I can easily check that it is correct. But I cannot so easily find a solution.

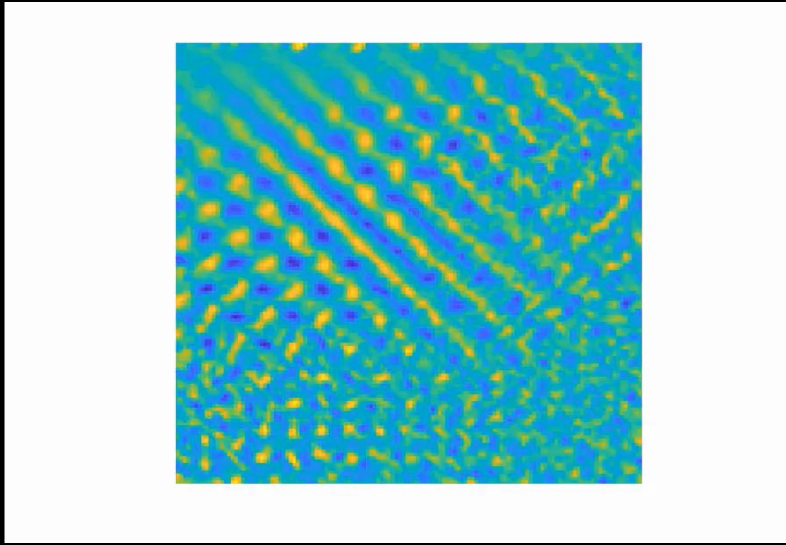
$\$10^6$

Navier–Stokes Equation

This is the equation which governs the flow of fluids such as water and air. However, there is no proof for the most basic questions one can ask: do solutions exist, and are they unique? Why ask for a proof? Because a proof gives not only certitude, but also understanding.

2007-2009: “Re-inventing the wheel”
→ I wanted to program Navier-Stokes solver
→ Fourier pseudo-spectral CFD solver (“turbulent fluid flow”)

Vuorinen et al. (2016) https://www.sciencedirect.com/science/article/pii/S0010465516300388



Sprays

(PhD in 2010: CFD simulation of fuel sprays in 2010)

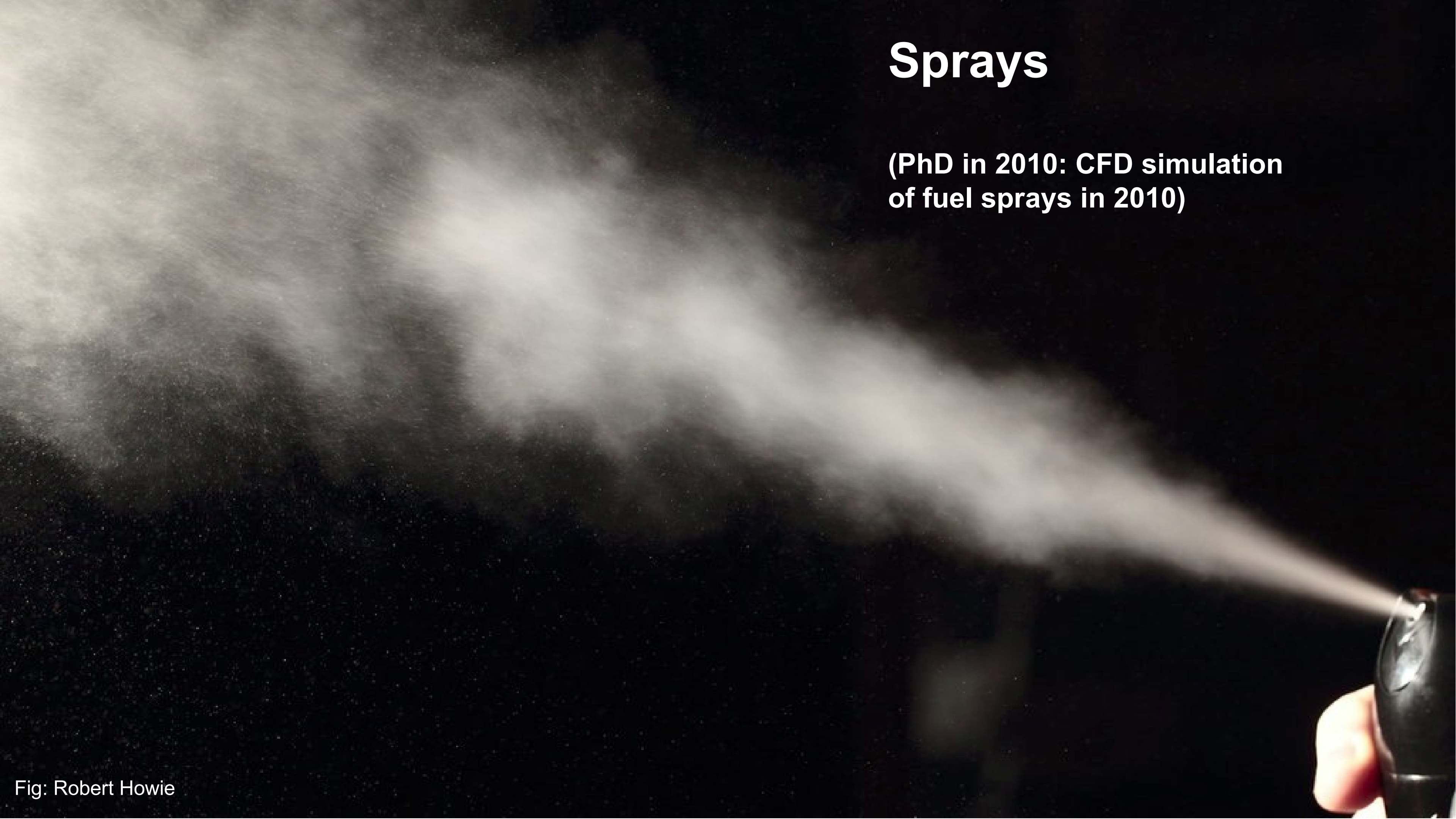


Fig: Robert Howie

Aalto-yliopisto
Aalto-universitetet
Aalto University

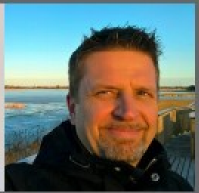
Artist: Arnold Lakhovsky
https://commons.wikimedia.org/wiki/File:Arnold_Lakhovsky_Conversation.png

→ Important ≠ necessary ?

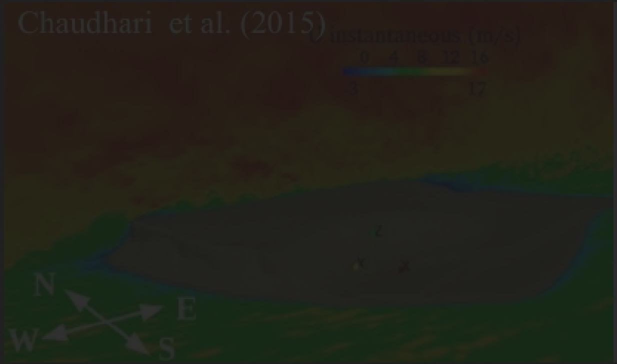
2) Computational fluid dynamics at Aalto in 2023

Computational fluid dynamics team at Aalto University/ENG, Finland

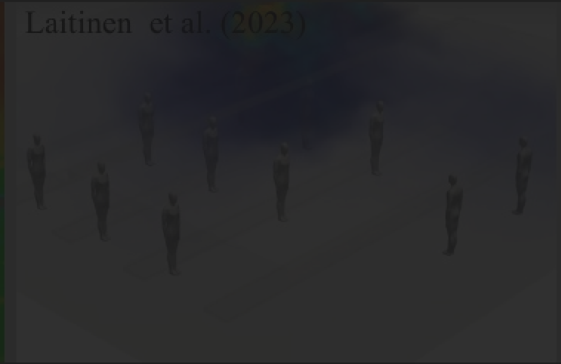
- Prof. V.Vuorinen + Prof. O.Kaario + 20 researchers
- 15 supervised PhD’s, 100+ journal papers
- Hydrogen, e-fuels, reactive multiphase flow, heat transfer, gas-/hydrodynamics
- OpenFOAM, StarCCM+, STAR-CD, LES/DNS/RANS/DES, DLBFoam



Wind power efficiency in landscapes

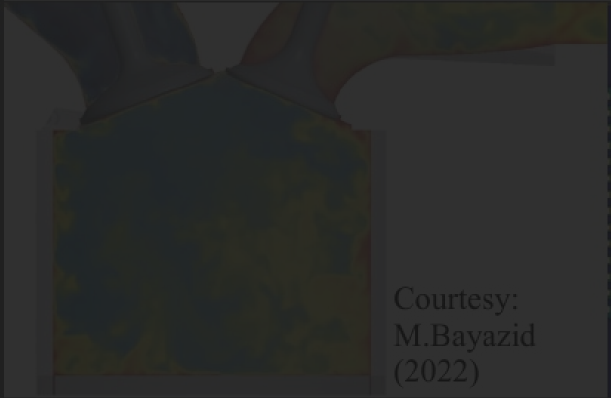


Healthy indoor air/vertical farming



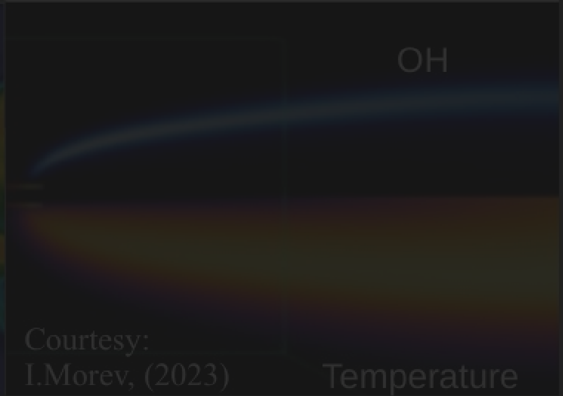
Energy conversion to H2/burners

Energy conversion to H2/engines



Heat transfer and energy

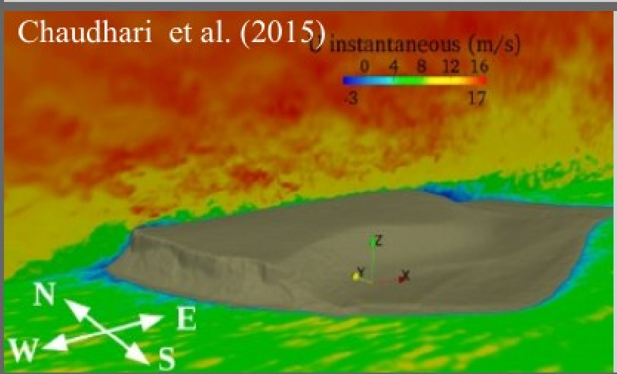
Hydrogen flame physics/chemistry



Computational fluid dynamics team at Aalto University/ENG, Finland

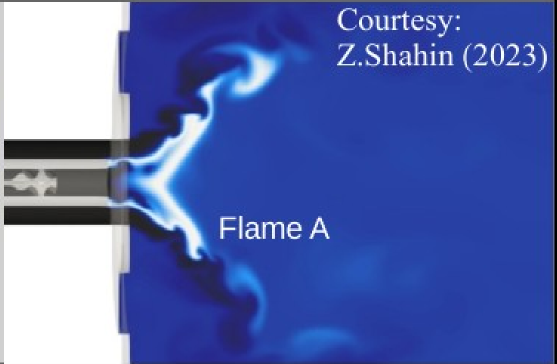
- Prof. V.Vuorinen + Prof. O.Kaario + 20 researchers
- 15 supervised PhD's, 100+ journal papers
- Hydrogen, e-fuels, reactive multiphase flow, heat transfer, gas-/hydrodynamics
- OpenFOAM, StarCCM+, STAR-CD, LES/DNS/RANS/DES, DLBFoam

Wind power efficiency in landscapes

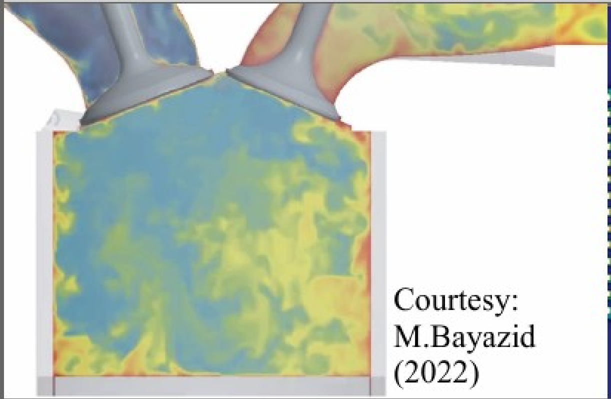


Healthy indoor air/vertical farming

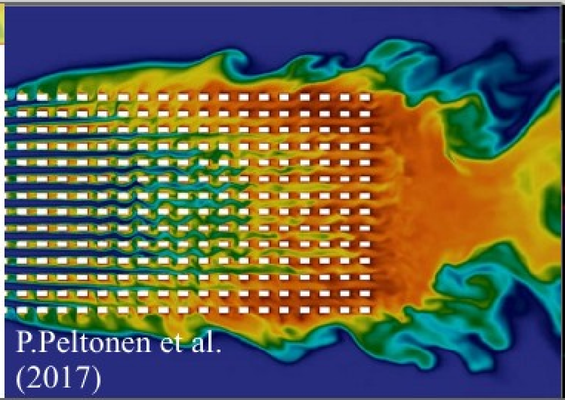
Energy conversion to H2/burners



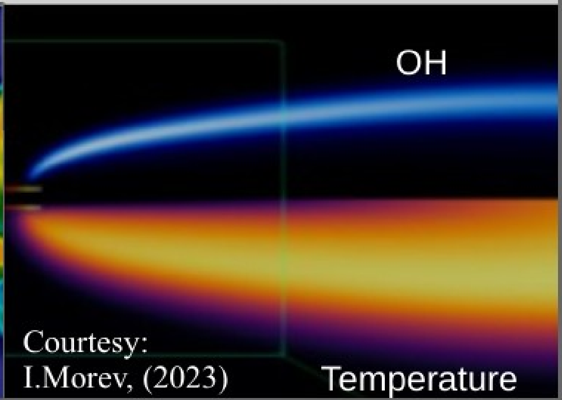
Energy conversion to H2/engines



Heat transfer and energy



Hydrogen flame physics/chemistry



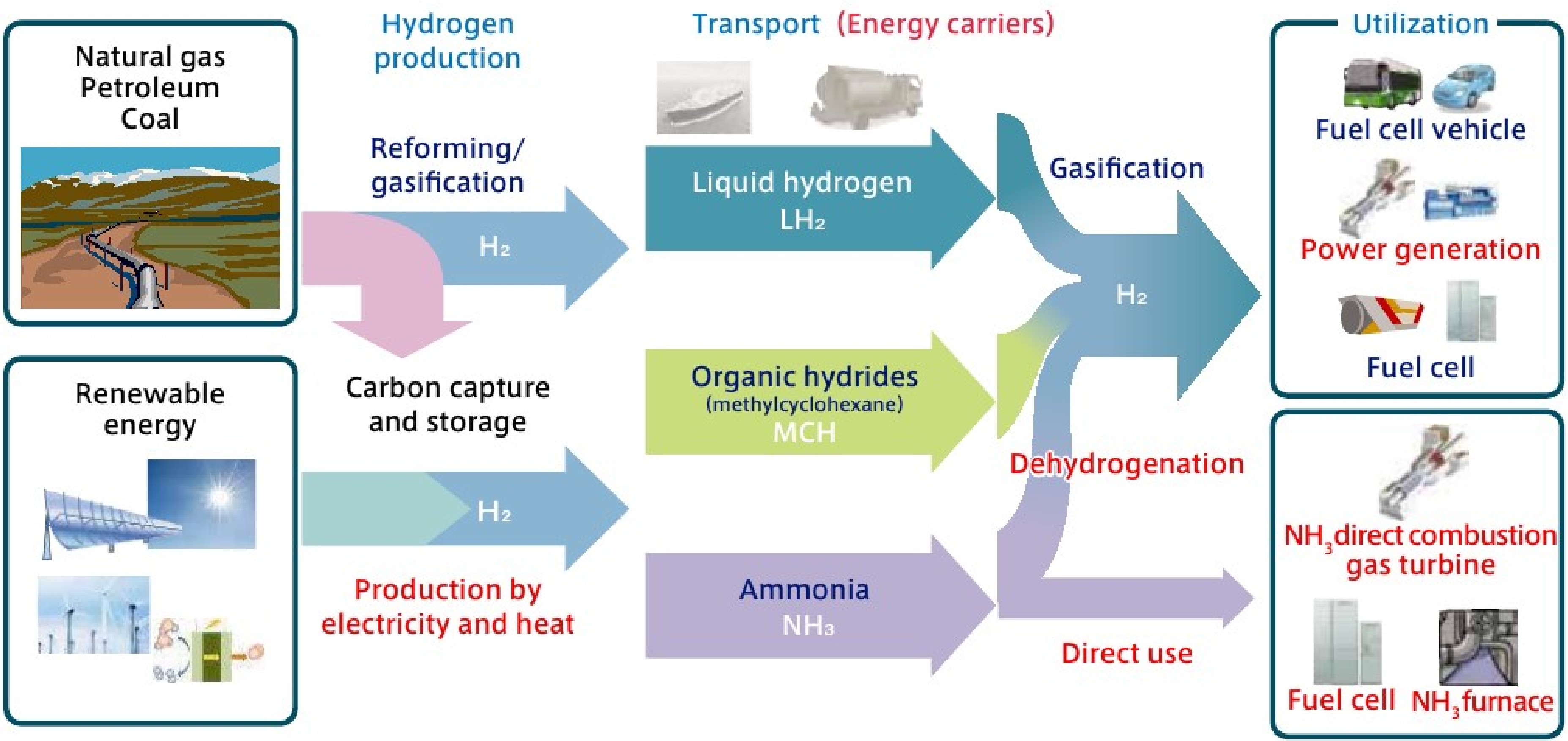
Supercomputer Mahti, BullSequana XH2000 from Atos. Image: CSC 2020.

3) Myths behind hydrogen

Myth 1: Hydrogen is fossil free

Fossil vs green hydrogen. Most hydrogen nowadays from fossil sources.

Japan Science and Technology Agency, available at http://www.jst.go.jp/sip/pdf/SIP_energycarriers2016_en.pdf



Myth 2: Hydrogen is the primary future fuel

Other synthetic fuels needed to solve the hydrogen storage problem

→ **E.g. easy to liquify:** ammonia (NH_3), methane (CH_4), propane (C_3H_8) or methanol (CH_3OH)

Table 1
Thermal properties and fundamental combustion characteristics of ammonia and hydrocarbon fuels. Data of boiling point and condensation point are from NIST database [8].

Fuel	NH_3	H_2	CH_4	C_3H_8
Boiling temperatureat 1 atm (°C)	−33.4	−253	−161	−42.1
Condensation pressure at 25 °C (atm)	9.90	N/A	N/A	9.40
Lower heating value, LHV (MJ/kg)	18.6	120	50.0	46.4
Flammability limit (Equivalence ratio)	0.63~1.40	0.10~7.1	0.50~1.7	0.51~2.5
Adiabatic flame temperature (°C)	1800	2110	1950	2000
Maximum laminar burning velocity (m/s)	0.07	2.91	0.37	0.43
Minimum auto ignition temperature (°C)	650	520	630	450

H. Kobayashi et al. / Proceedings of the Combustion Institute 37 (2019) 109–133

Myth 3: Hydrogen is simple: $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$

"Hydrogen + Oxygen → Water"

Hydrogen combustion is complex and also produces nitric oxide emissions

E.g. Westbrook et al. (2004)
→ 19 chemical reactions
→ 11 molecule species

O'Connaire, M., H. J. Curran, J. M. Simmie, W. J. Pitz, and C. K. Westbrook,
" ,"
Int. J. Chem. Kinet., 36:603-622, 2004 (UCRL-JC-152569).

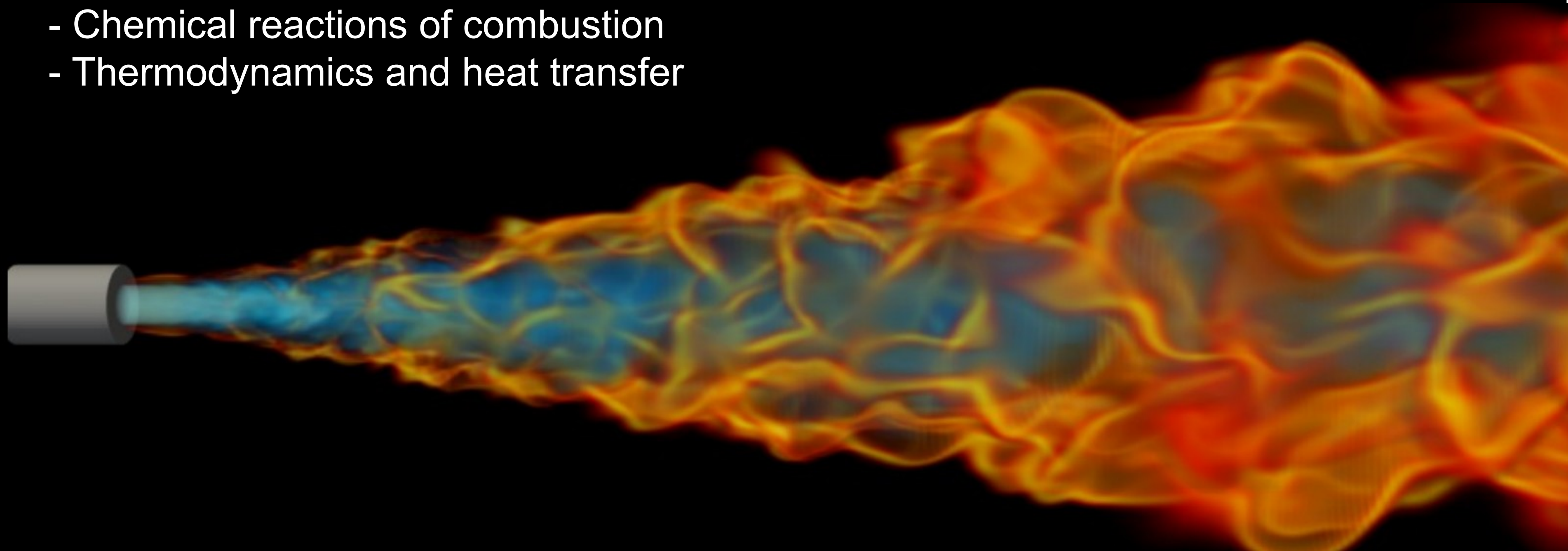
Aalto-yliopisto
Aalto-universitetet
Aalto University

	Reaction	A	n	E_a	Ref.
	H_2/O_2 Chain Reactions				
1	$\dot{H} + O_2 = \dot{O} + \dot{O}H$	1.91×10^{14}	0.00	16.44	[39]
2	$\dot{O} + H_2 = \dot{H} + \dot{O}H$	5.08×10^{4}	2.67	6.292	[40]
3	$\dot{O}H + H_2 = \dot{H} + H_2O$	2.16×10^{8}	1.51	3.43	[41]
4	$\dot{O} + H_2O = \dot{O}H + \dot{O}H$	2.97×10^{6}	2.02	13.4	[42]
	H_2/O_2 Dissociation/Recombination Reactions				
5[a]	$H_2 + M = \dot{H} + \dot{H} + M$	4.57×10^{19}	−1.40	105.1	[43]
6[b]	$\dot{O} + \dot{O} + M = O_2 + M$	6.17×10^{15}	−0.50	0.00	[43]
7[c]	$\dot{O} + \dot{H} + M = \dot{O}H + M$	4.72×10^{18}	−1.00	0.00	[43]
8[d,e]	$\dot{H} + \dot{O}H + M = H_2O + M$	4.50×10^{22}	−2.00	0.00	[43] ×2.0
	Formation and consumption of $H\dot{O}_2$				
9[f,g]	$\dot{H} + O_2 + M = H\dot{O}_2 + M$	3.48×10^{16}	−0.41	−1.12	[44]
	$\dot{H} + O_2 = H\dot{O}_2$	1.48×10^{12}	0.60	0.00	[45]
10	$H\dot{O}_2 + \dot{H} = H_2 + O_2$	1.66×10^{13}	0.00	0.82	[6]
11	$H\dot{O}_2 + \dot{H} = \dot{O}H + \dot{O}H$	7.08×10^{13}	0.00	0.30	[6]
12	$H\dot{O}_2 + \dot{O} = \dot{O}H + O_2$	3.25×10^{13}	0.00	0.00	[46]
13	$H\dot{O}_2 + \dot{O}H = H_2O + O_2$	2.89×10^{13}	0.00	−0.50	[46]
	Formation and Consumption of H_2O_2				
14[h]	$H\dot{O}_2 + H\dot{O}_2 = H_2O_2 + O_2$	4.2×10^{14}	0.00	11.98	[47]
	$H\dot{O}_2 + H\dot{O}_2 = H_2O_2 + O_2$	1.3×10^{11}	0.00	−1.629	[47]
15[i,f]	$H_2O_2 + M = \dot{O}H + \dot{O}H + M$	1.27×10^{17}	0.00	45.5	[48]
	$H_2O_2 = \dot{O}H + \dot{O}H$	2.95×10^{14}	0.00	48.4	[49]
16	$H_2O_2 + \dot{H} = H_2O + \dot{O}H$	2.41×10^{13}	0.00	3.97	[43]
17	$H_2O_2 + \dot{H} = H_2 + H\dot{O}_2$	6.03×10^{13}	0.00	7.95	[43]×1.25
18	$H_2O_2 + \dot{O} = \dot{O}H + H\dot{O}_2$	9.55×10^{06}	2.00	3.97	[43]
19[h]	$H_2O_2 + \dot{O}H = H_2O + H\dot{O}_2$	1.0×10^{12}	0.00	0.00	[50]
	$H_2O_2 + \dot{O}H = H_2O + H\dot{O}_2$	5.8×10^{14}	0.00	9.56	[50]

Myth 4: Hydrogen combustion is purely chemistry

Hydrogen flames are 3D and they involve complex physics and chemistry

- Fluid dynamics (gas velocity/temperature/density variation)
- Chemical reactions of combustion
- Thermodynamics and heat transfer

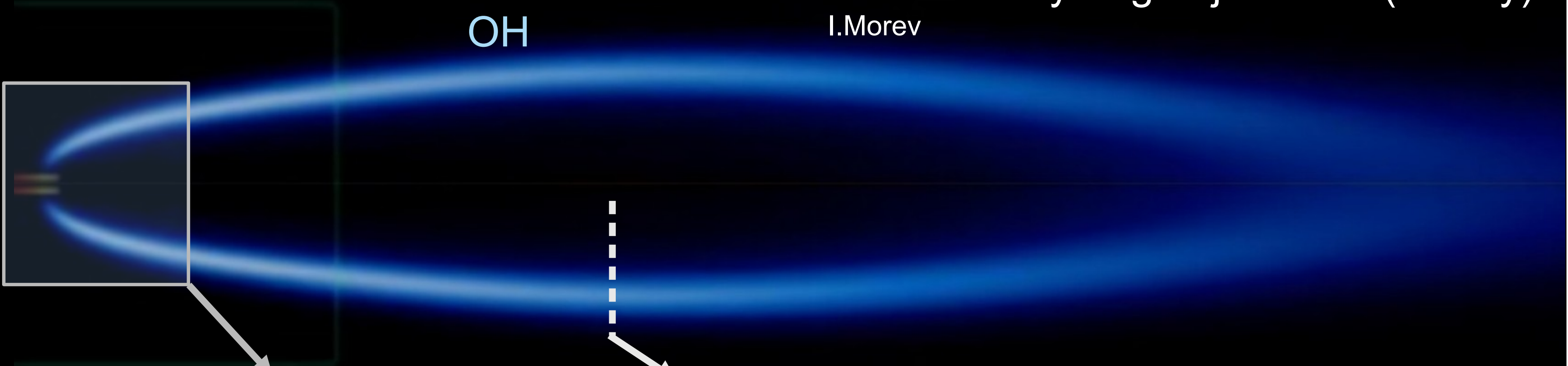


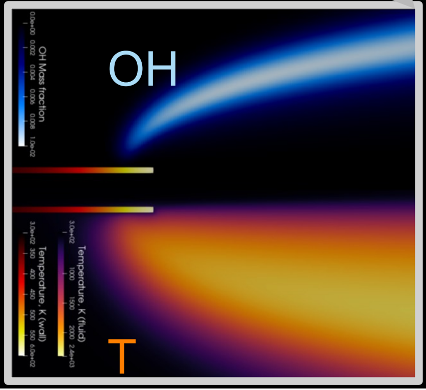
Simulated hydrogen jet flame (turbulent)
I.Morev

3D flame structure essential (e.g. flame stability)

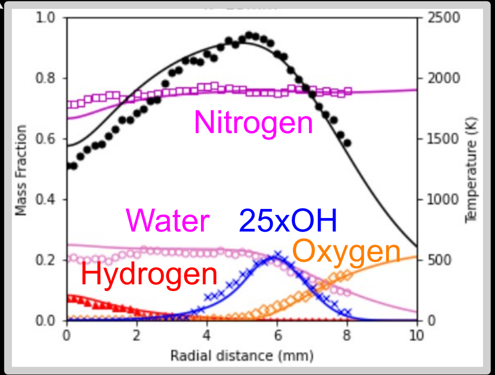
Simulated hydrogen jet flame (steady)

I.Morev





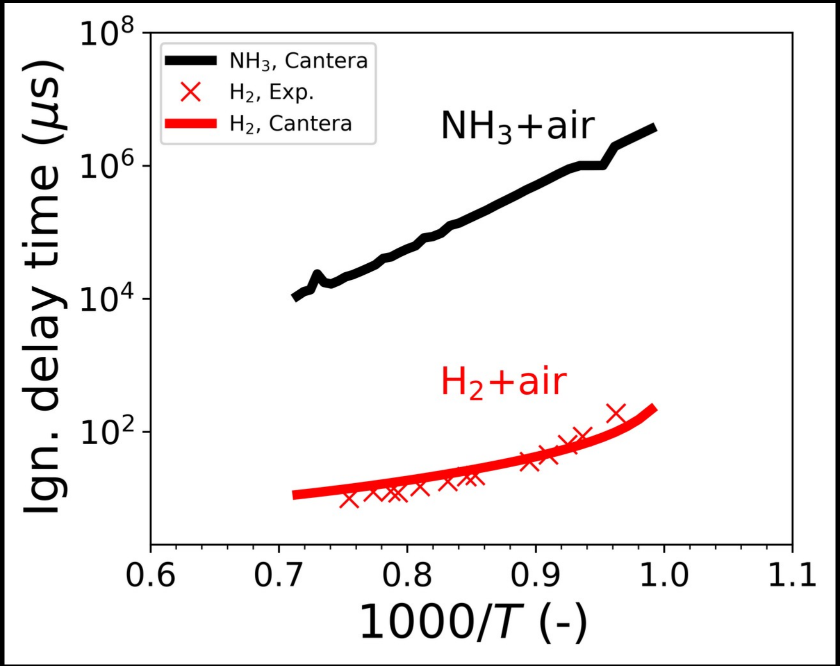
Zoom to injector

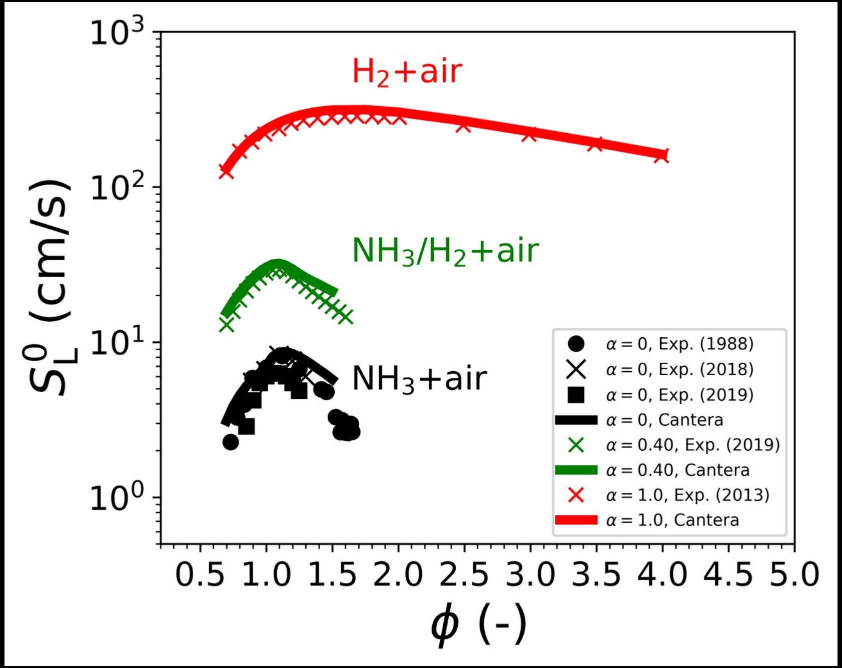


Experiment vs simulation

Myth 5: Hydrogen + green fuels: “just use them”

Different fuels – including green fuels – may have very different burning characteristics (ignition time and flame speed) affecting combustion dynamics strongly. Hydrogen is a very different fuel than what we are used to. Retrofitting, optimization, combustion research needed!





Aalto-yliopisto
Aalto-universitetet
Aalto University

Courtesy: P.Tamadonfar

Myth 6: Green fuels → no emissions

Green fuels: not automatically clean! E.g. hydrogen gives NOx emissions. Ammonia N_2O emissions.

Comment | Published: 05 October 2022

Using ammonia as a shipping fuel could disturb the nitrogen cycle

Paul Wolfram, Page Kyle, Xin Zhang, Savvas Gkantonas & Steven Smith

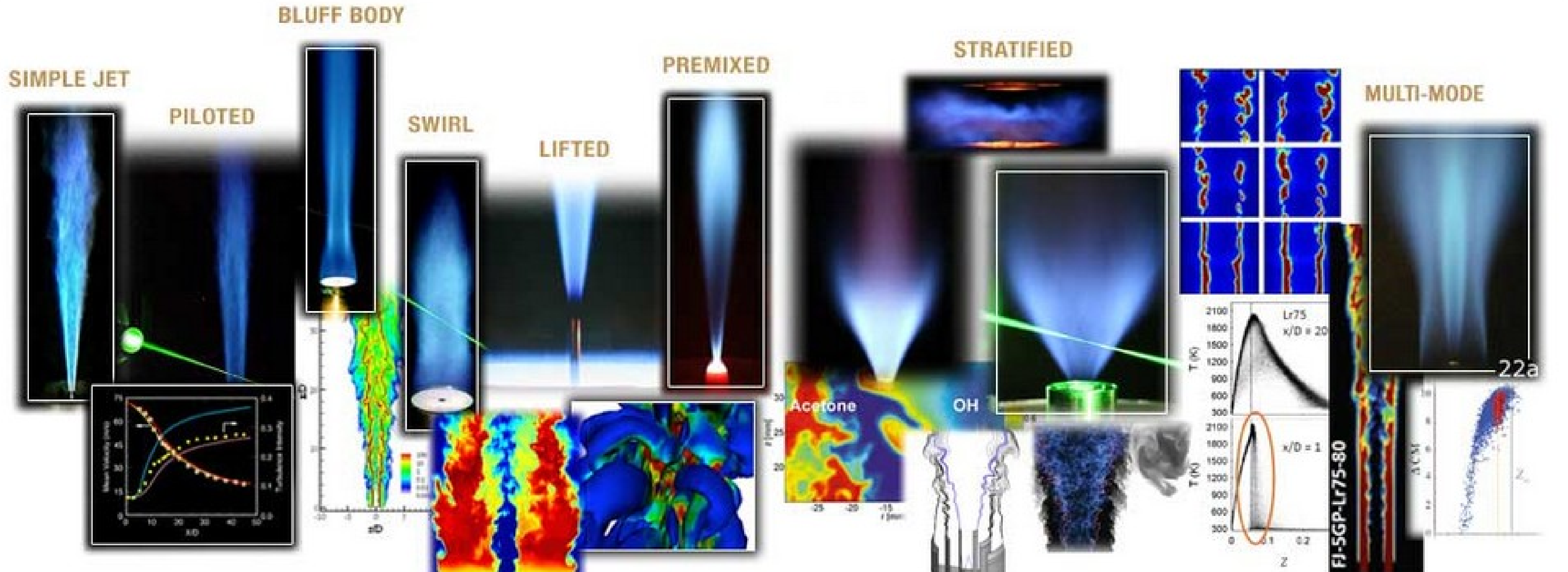
Nature Energy **7**, 1112–1114 (2022) | Cite this article

[just 0.4% of ammonia converting into N_2O (GWP_{N2O}=273) may negate climate benefits of green ammonia ...]

4) Participation of Aalto University in international efforts to understand hydrogen flames via the HENNES Business Finland project

TNF Workshop

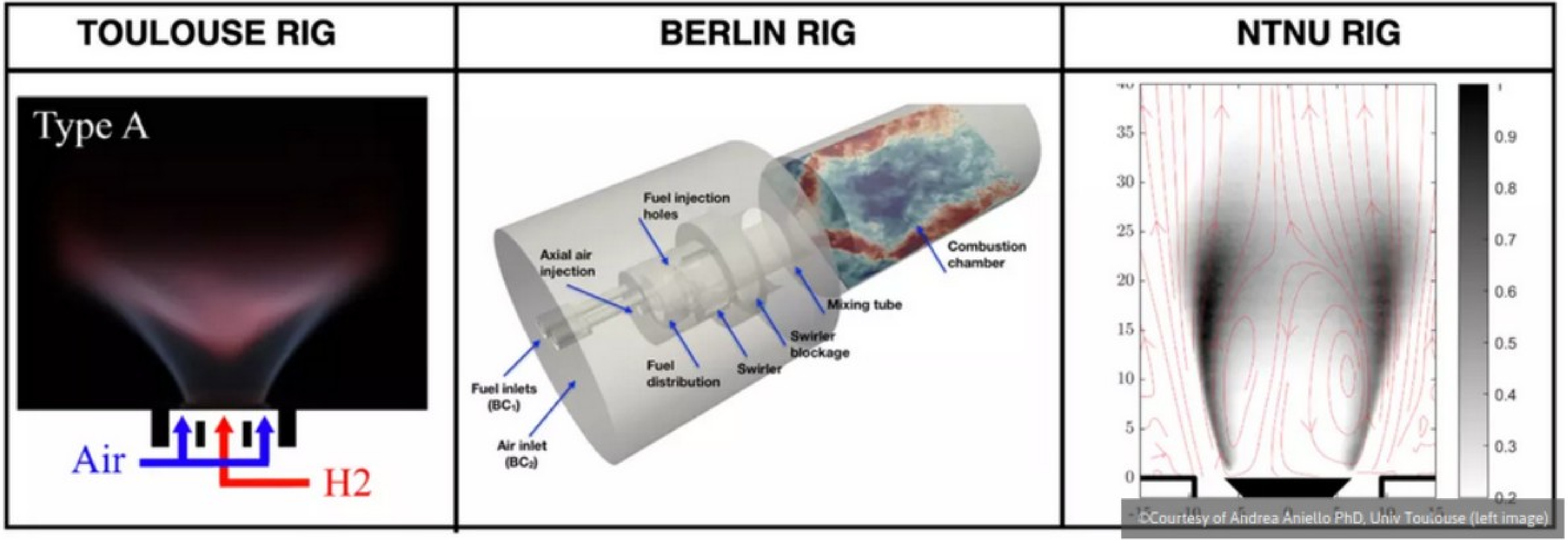
International Workshop on Measurement and Computation of Turbulent Flames



May 2023: International initiative to compare different CFD codes against High quality experimental data on three hydrogen flame rigs

Clean Aviation working group on CFD codes for hydrogen-air combustion

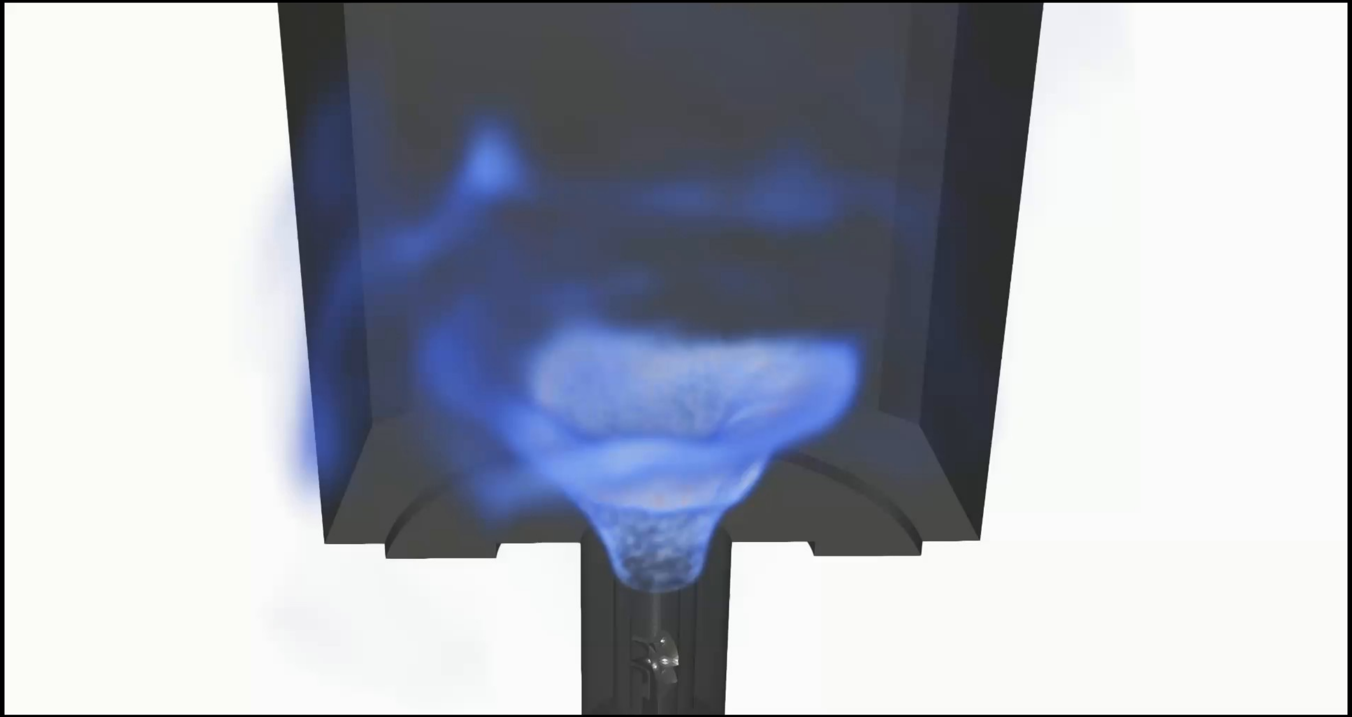
Experimental, high-precision data will be made available from **three experiments**: the **HYLON rig** in Toulouse, the **TU Berlin rig** in Berlin and the **NTNU rig** in Trondheim. Only pure hydrogen-air flames will be considered in the frame of this workshop.



©Courtesy of Andrea Aniello PhD, Univ Toulouse (left image)

Large-eddy simulation of HYLON Flame A setup (TOULOUSE rig): non-premixed hydrogen combustion

Courtesy: Z.Shahin (M.Sc. thesis 2023)



Large-eddy simulation of HYLON Flame A setup (TOULOUSE rig): non-premixed hydrogen combustion → predictive methods

Courtesy: Z.Shahin (M.Sc. thesis 2023)

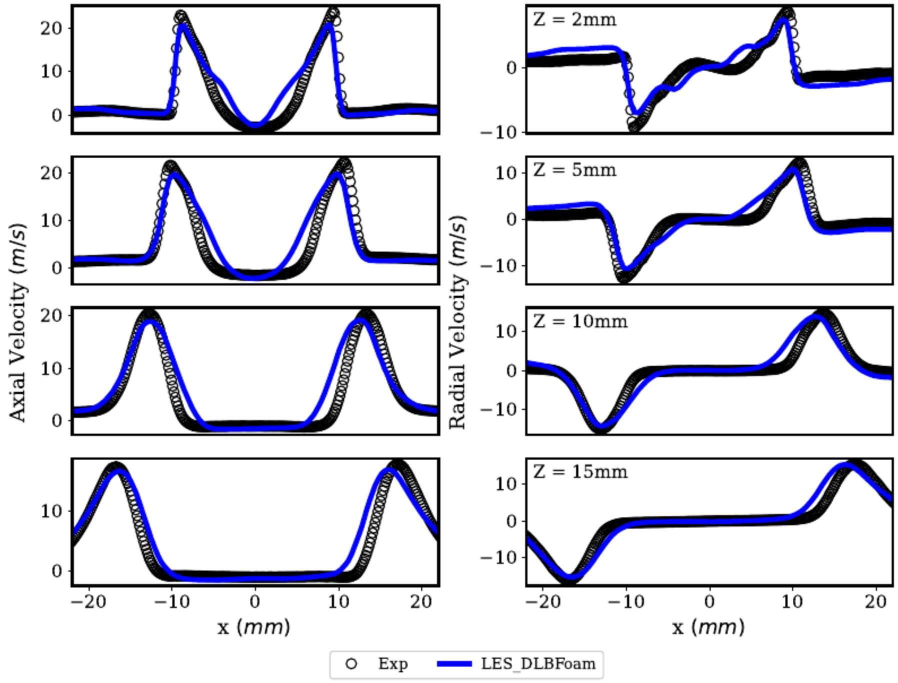


Figure 28: Comparison between reacting flow PIV data (depicted by symbols) at z = 2, 5, 10, and 15 mm on the axial plane versus LES results for the mean axial U_z a) and radial b) velocity U_r.

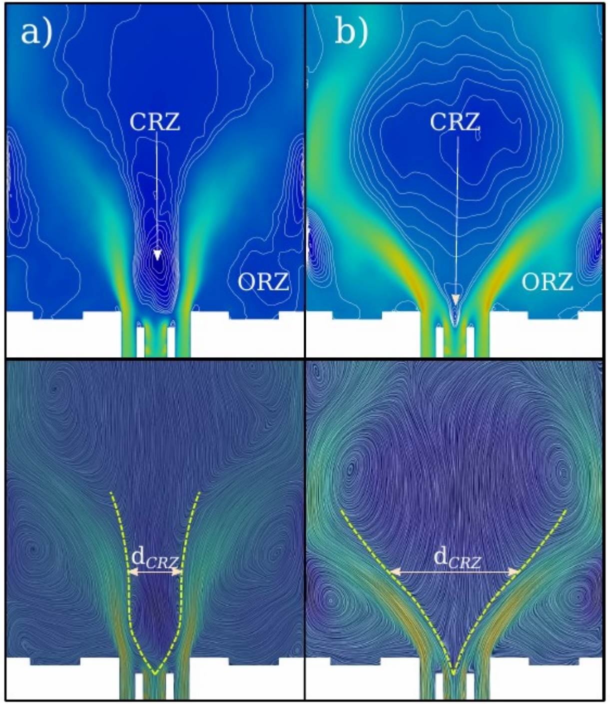


Figure 33: Comparison of the velocity fields in cold a) and reactive b) conditions in the axial plane with white isolines for negative U_z in the upper panel part and the streamlines of the axial velocity in the lower panel part.

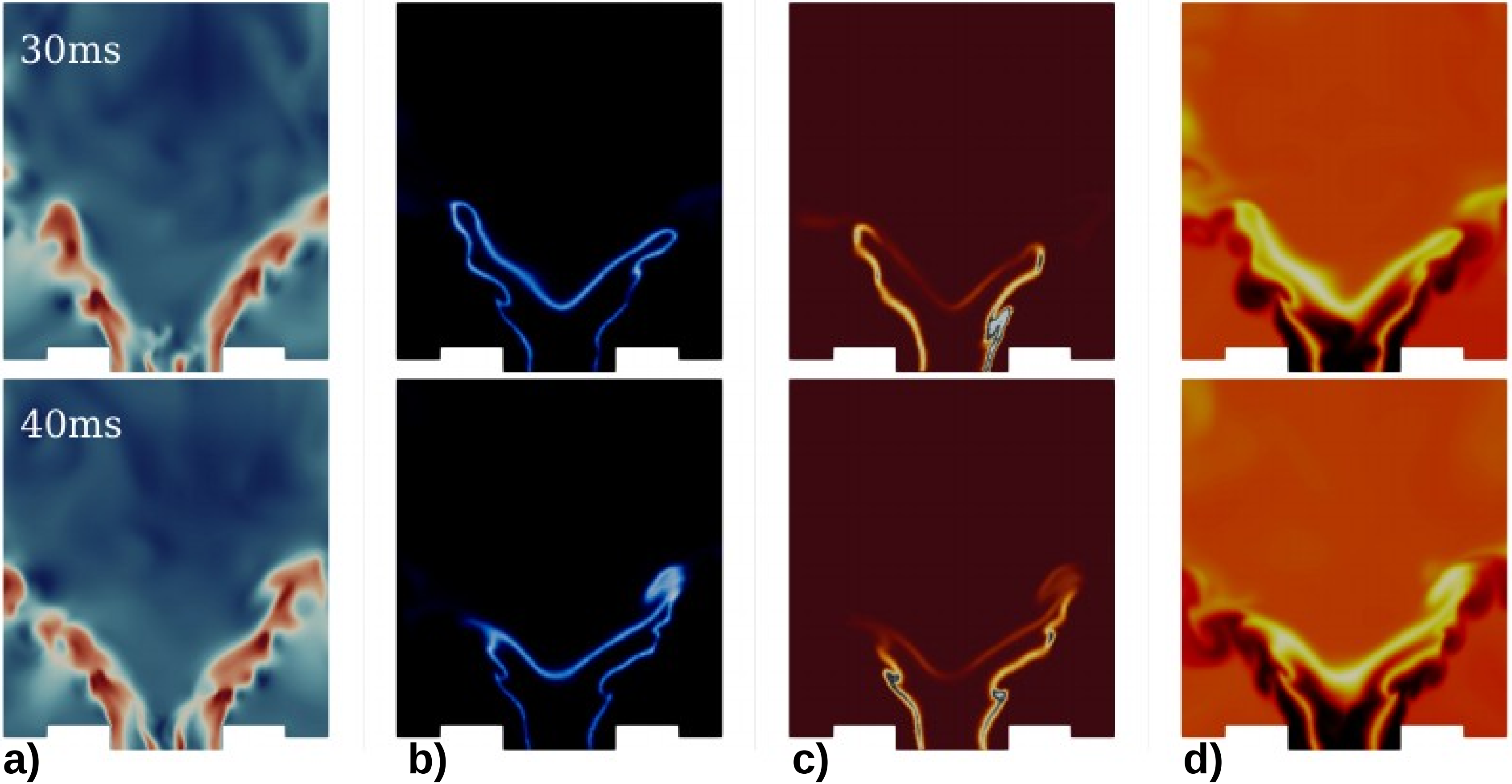


Figure 40: Instantaneous axial cut planes displaying the axial velocity a), OH mass fraction b), heat release rate HRR_{norm}c), and temperatures d) at four distinct time snapshots

Courtesy: Z.Shahin (M.Sc. thesis 2023)

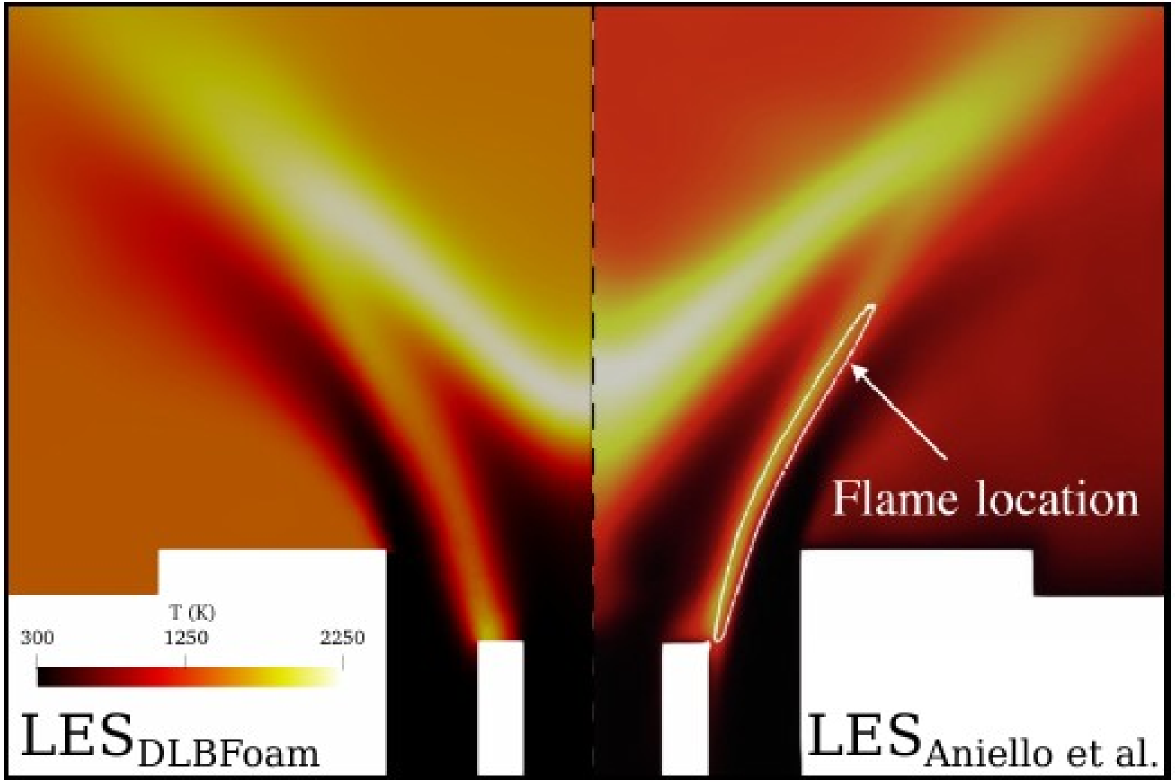
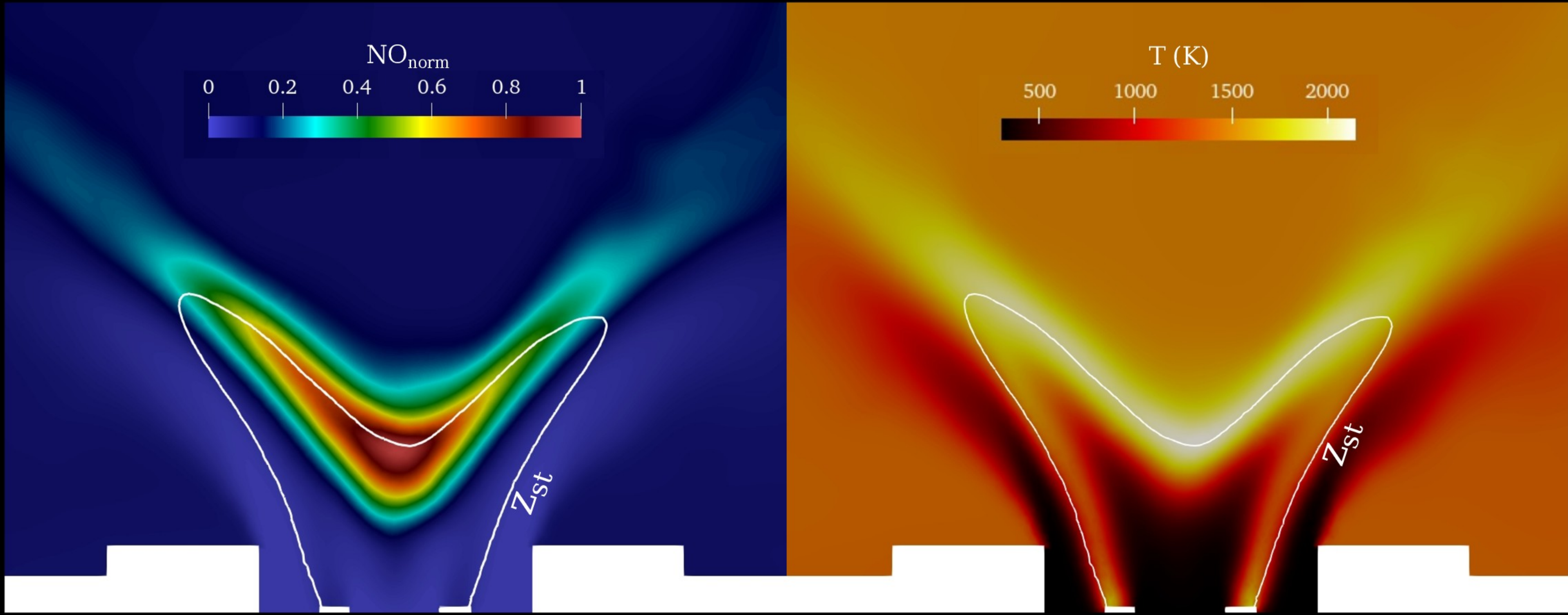


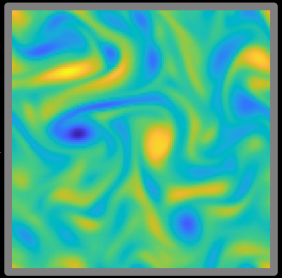
Figure 36: Contour map of the the temperature observed from the current work a) and the LES values from [14]b) for the anchored flame A.

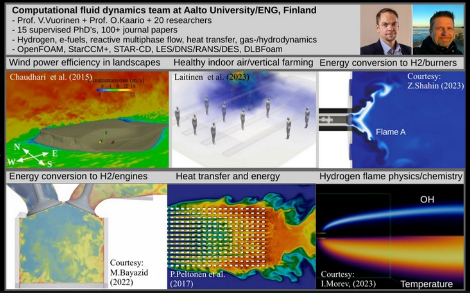
Courtesy: Z.Shahin (M.Sc. thesis 2023)



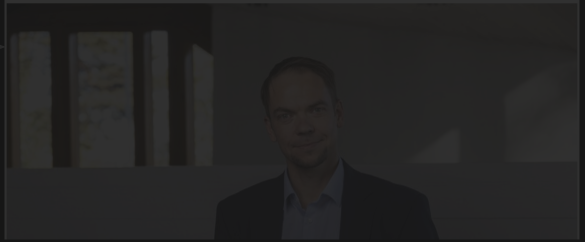
5) Concluding remarks

My career 1/2: Energy story and towards hydrogen





H2 flame A (Z.Shahin)


The Academy of Finland awards Ville Vuorinen for his research on the spread of the COVID-19 disease

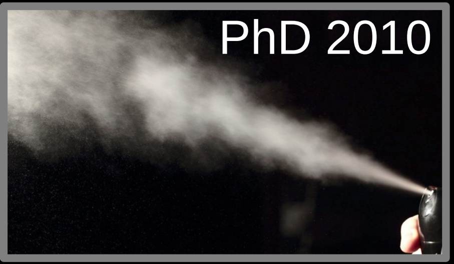
Published: 26.5.2023

Ville Vuorinen, who studies the physics of air and fluid flows, is awarded for his exceptional scientific courage and creativity, as well as for his work to promote the social impact of science.

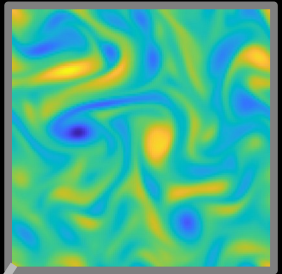
My career 2/2: From basic research to societal relevance – airborne transmission COVID-19

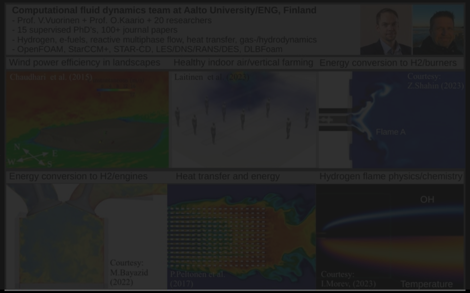
Aalto-yliopisto
Aalto-universitetet
Aalto University

My career 1/2: Energy story and towards hydrogen



+





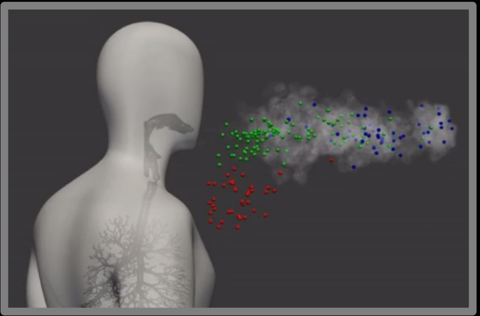
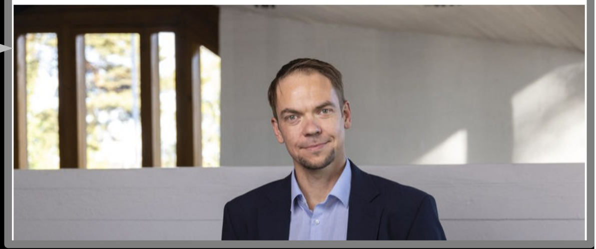


Fig. M.Korhonen

Sim. M.Auvinen&A.Hellsten



The Academy of Finland awards Ville Vuorinen for his research on the spread of the COVID-19 disease

Published: 26.5.2023

Ville Vuorinen, who studies the physics of air and fluid flows, is awarded for his exceptional scientific courage and creativity, as well as for his work to promote the social impact of science.

My career 2/2: From basic research to SCICOM and societal relevance – airborne transmission of COVID-19

Aalto-yliopisto
Aalto-universitetet
Aalto University

Vuorinen et al. (2020) https://www.sciencedirect.com/science/article/pii/S0925753520302630

Summing up what matters

1) *"God is in the details"*

2) Power of team collaboration and multidisciplinary work

3) Investments in research + education (PhD & MSc degrees)

4) Wave the flag

5) *"Simulation has become the third scientific pillar alongside theory and experiments"* (Prof. C.Hasse/Nov. 6th 2023)

Aalto University

Aalto-yliopisto
Aalto-universitetet
Aalto University