Producing and using clean hydrogen: three related fluid mechanical problems

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Collaborators on the hydrogen topics.

Gretar Tryggvason, Ragha Ragavendran, Wei Qin, Seyed Mohammadamin Taleghani, Arnaud Malan, Yusufali Omar, Jean Robin, Wiilemijn Van Rooejen

Current Students and postdocs

Cesar Pairetti, Basil Ahmed Kottilingal, Jacob Maarek, Yash Kulkarni, Xiangbin Chen, Damien Thomas, Jieyun Pan, Tian Long,Tianyang Han,

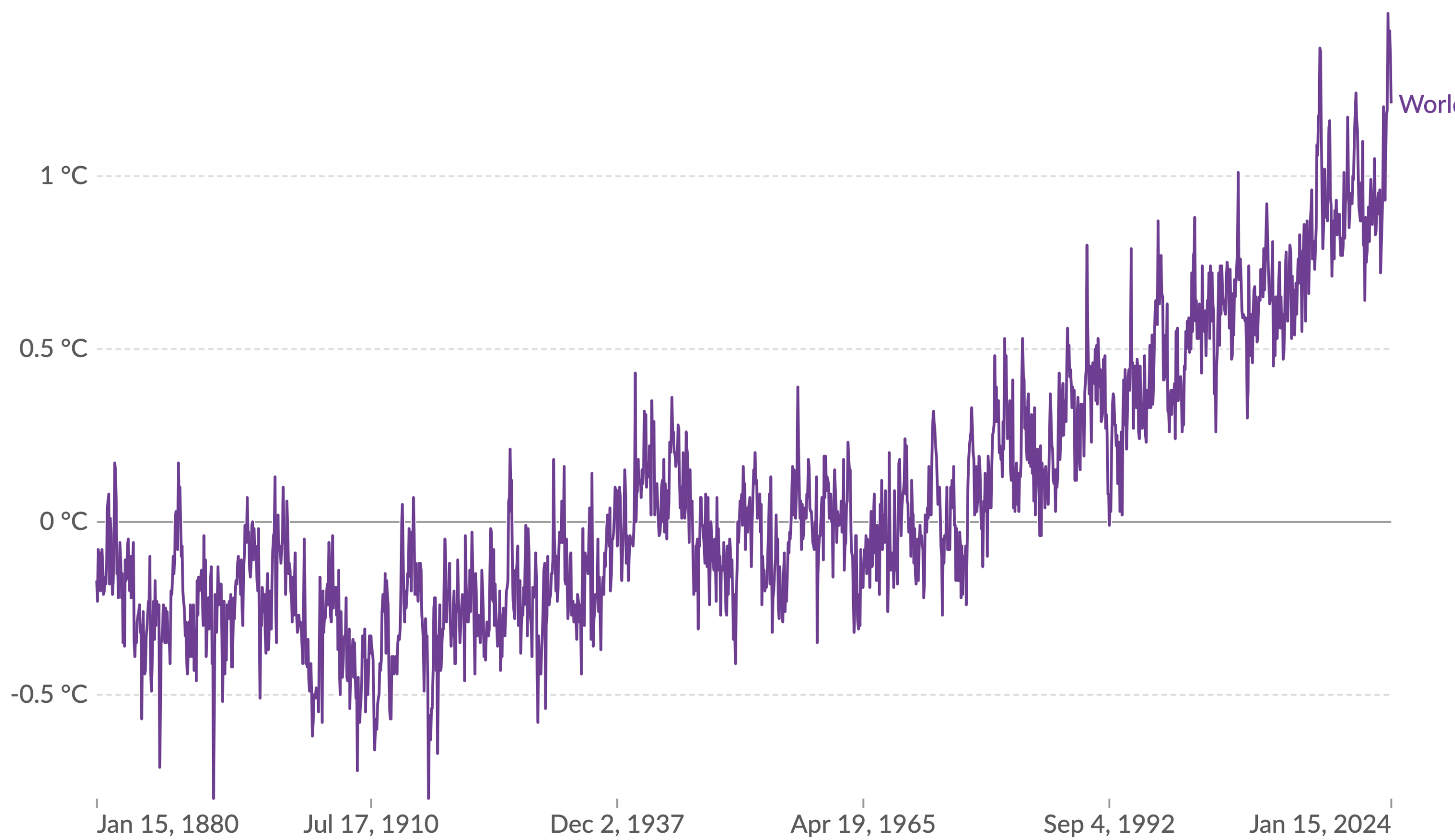
Companies

Airbus, Arcelor-Mittal Research

Global warming: monthly temperature anomaly

The combined land-surface air and sea-surface water temperature anomaly is given as the deviation from the 1951–1980 mean.

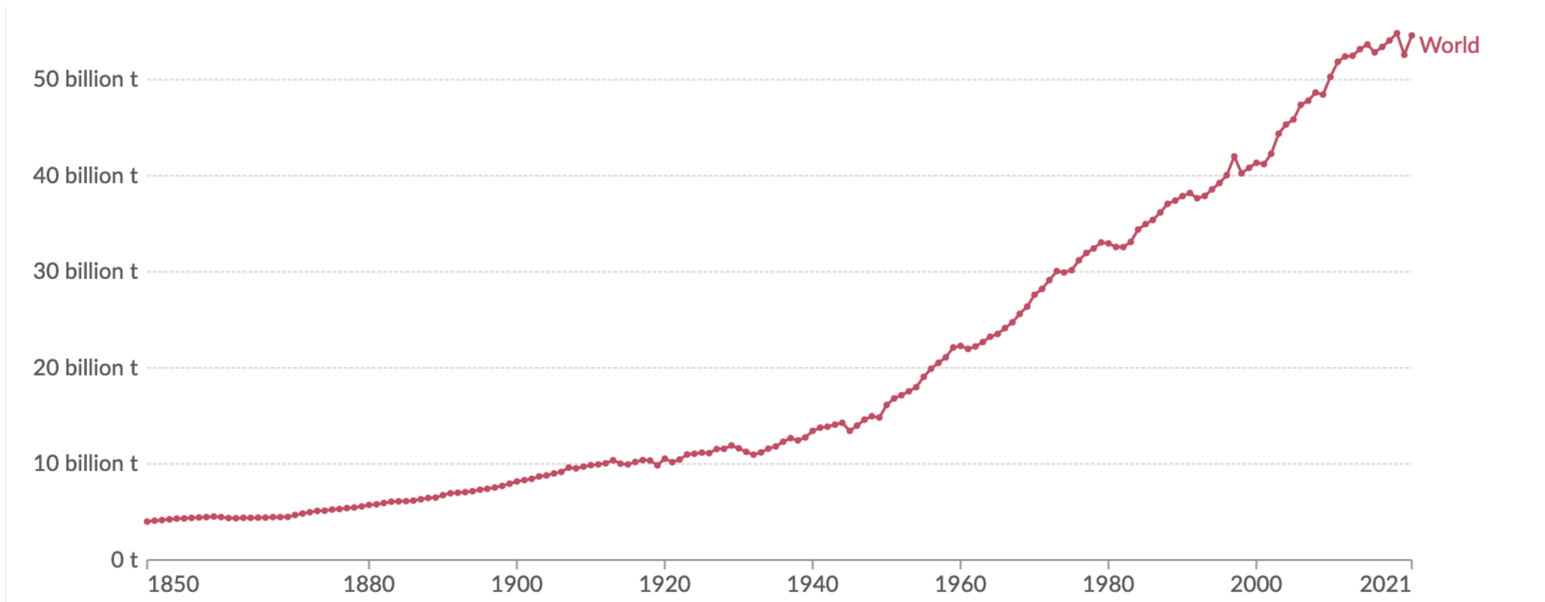
Our World in Data



Data source: NASA Goddard Institute for Space Studies - GISS Surface Temperature Analysis

Emissions de GES jusque en 2021

Greenhouse gas emissions until 2021



Focus on France

Focus on France

France is doing certain things well

PLANÈTE • POLLUTIONS

Climat : les émissions de gaz à effet de serre ont baissé en France sur les trois premiers trimestres de 2023

Selon le baromètre du Centre interprofessionnel technique d'études de la pollution atmosphérique, les trois grands contributeurs de cette baisse, estimée à 4,6 % par rapport à 2022, sont la production d'énergie, l'industrie et les bâtiments.

Par Stéphane Foucart

Publié le 26 décembre 2023 à 15h44, modifié le 27 décembre 2023 à 09h06 • Lecture 3 min. • Read in English

Offrir l'article

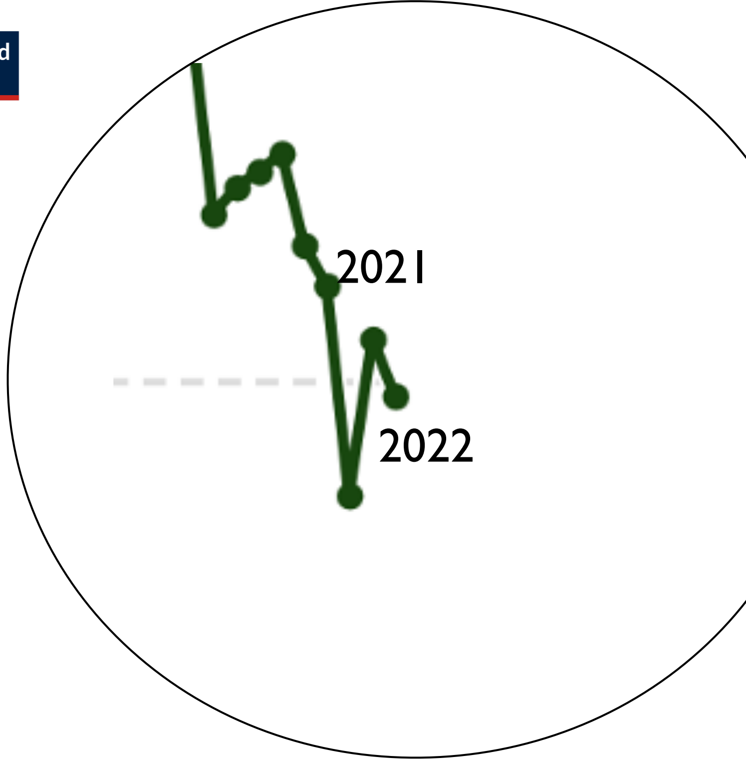
Article réservé aux abonnés

La centrale nucléaire EDF de Cattenom (Moselle), le 13 juin 2023. YVES HERMAN / REUTERS

Annual CO_2 emissions

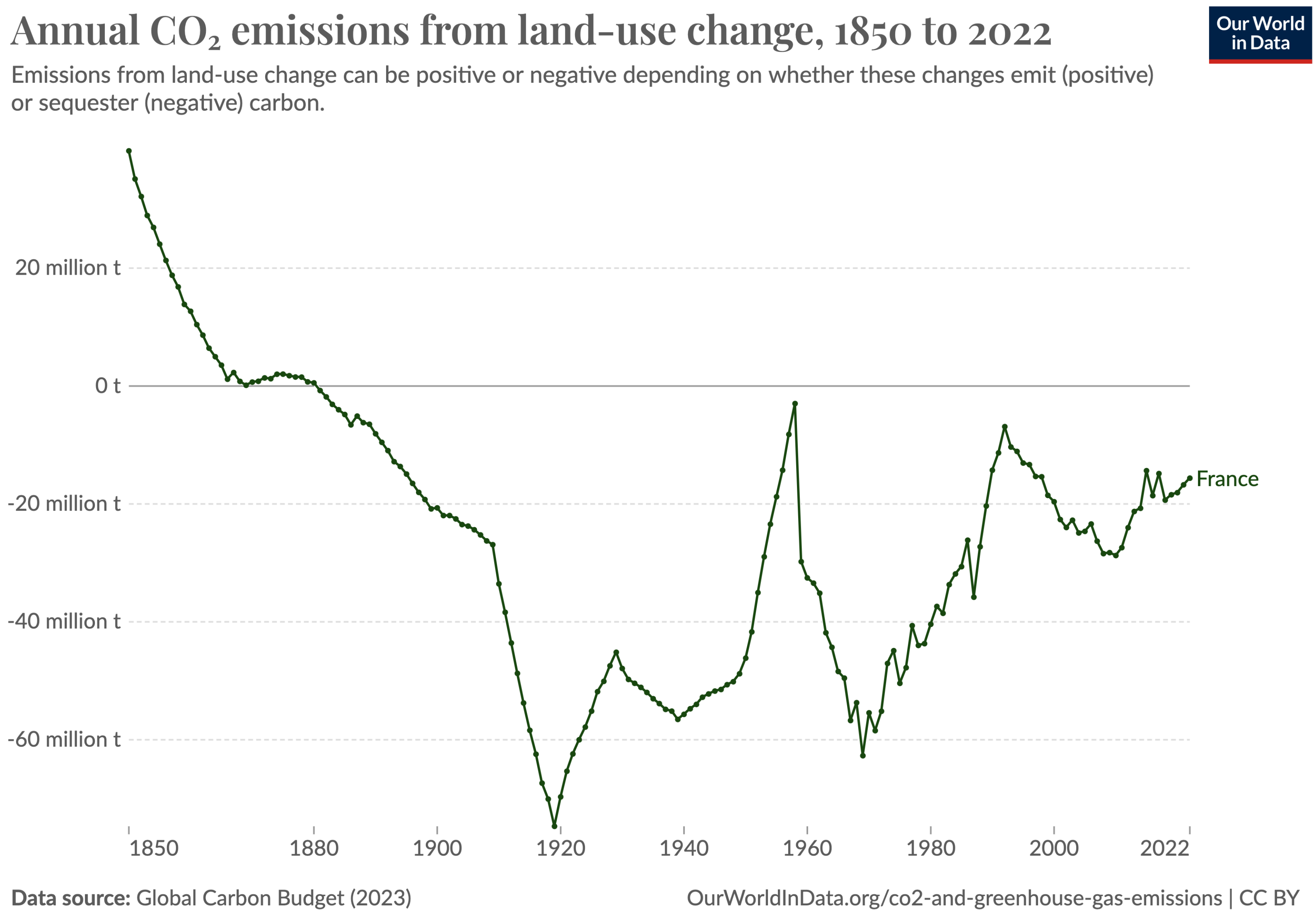
Our World in Data

Carbon dioxide (CO_2) emissions from fossil fuels and industry[1]. Land-use change is not included.



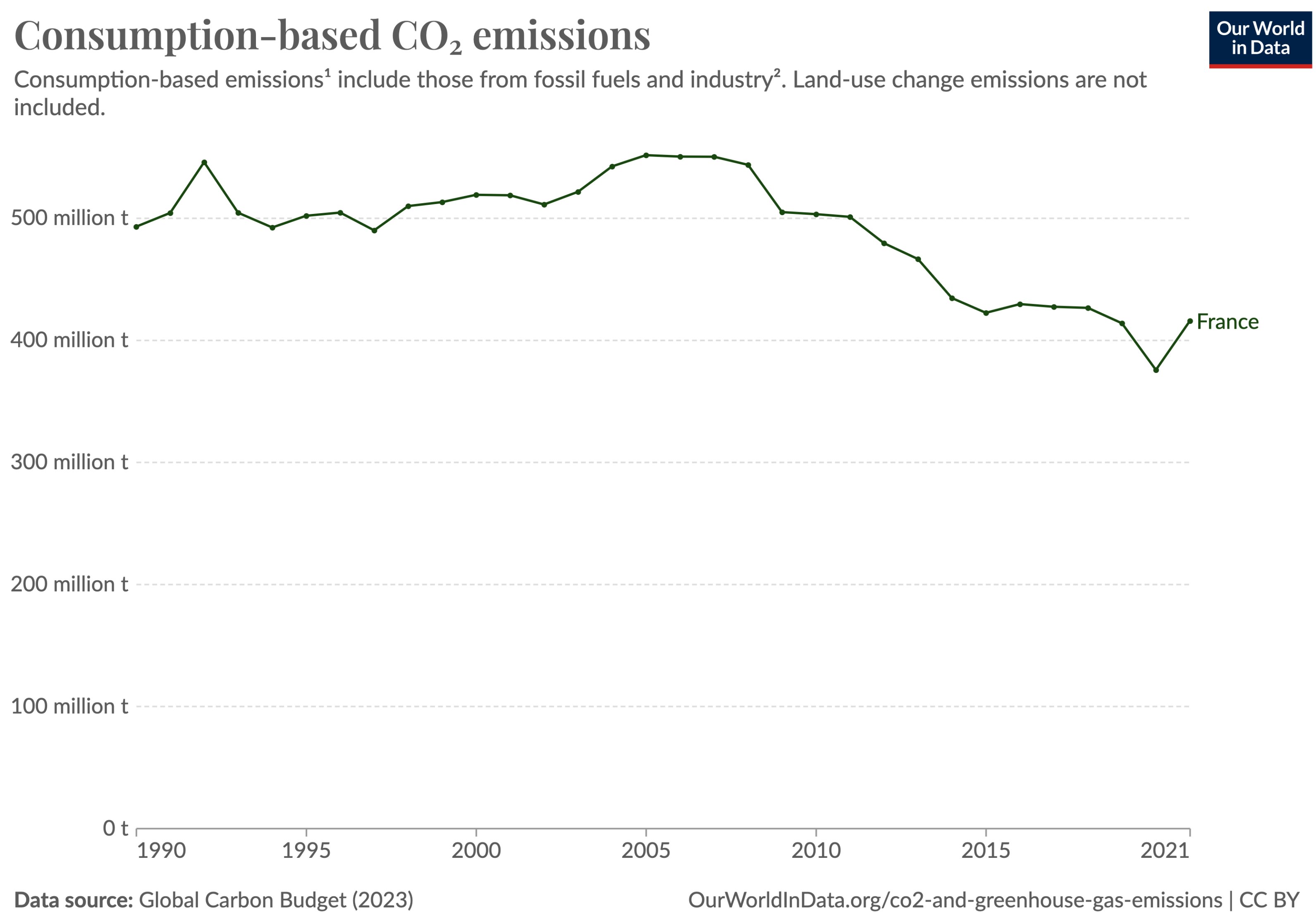
Data source: Global Carbon Budget (2023)

1. **Fossil emissions**: Fossil emissions measure the quantity of carbon dioxide (CO_2) emitted from the burning of fossil fuels, and directly from industrial processes such as cement and steel production. Fossil CO_2 includes emissions from coal, oil, gas, flaring, cement, steel, and other industrial processes. Fossil emissions do not include land use change, deforestation, soils, or vegetation.


Annual CO_2 emissions from land-use change, 1850 to 2022
Our World in Data
Emissions from land-use change can be positive or negative depending on whether these changes emit (positive) or sequester (negative) carbon.
20 million t
0 t
-20 million t
-40 million t
-60 million t
1850
1880
1900
1920
1940
1960
1980
2000
2022
France
Data source: Global Carbon Budget (2023)
OurWorldInData.org/co2-and-greenhouse-gas-emissions | CC BY

Other things not so well

Add emissions embedded in imported products and services.
Remove emissions embedded in exported products and services.



ipcc

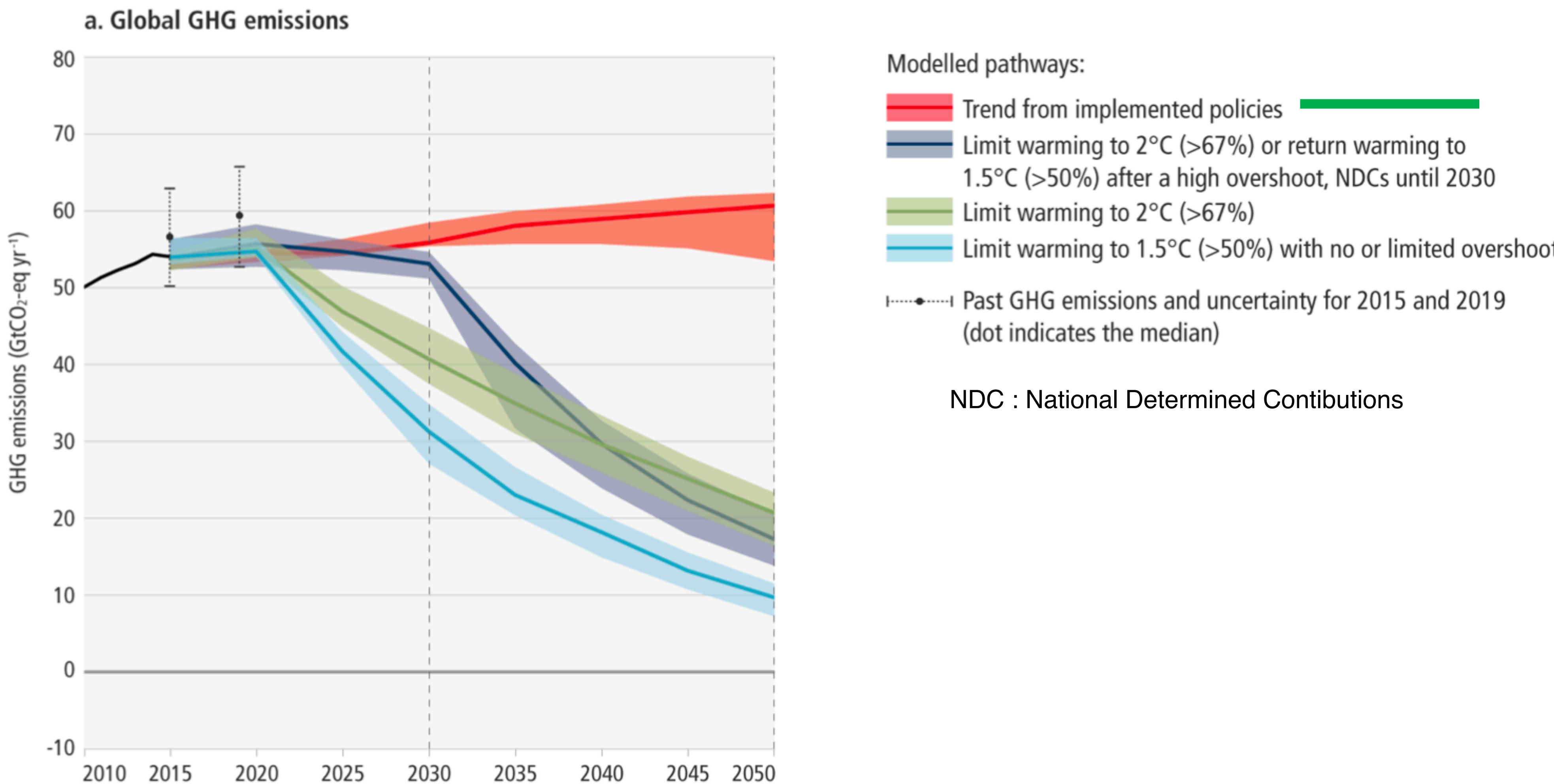
INTERGOVERNMENTAL PANEL ON climate change

Climate Change 2022

Mitigation of Climate Change

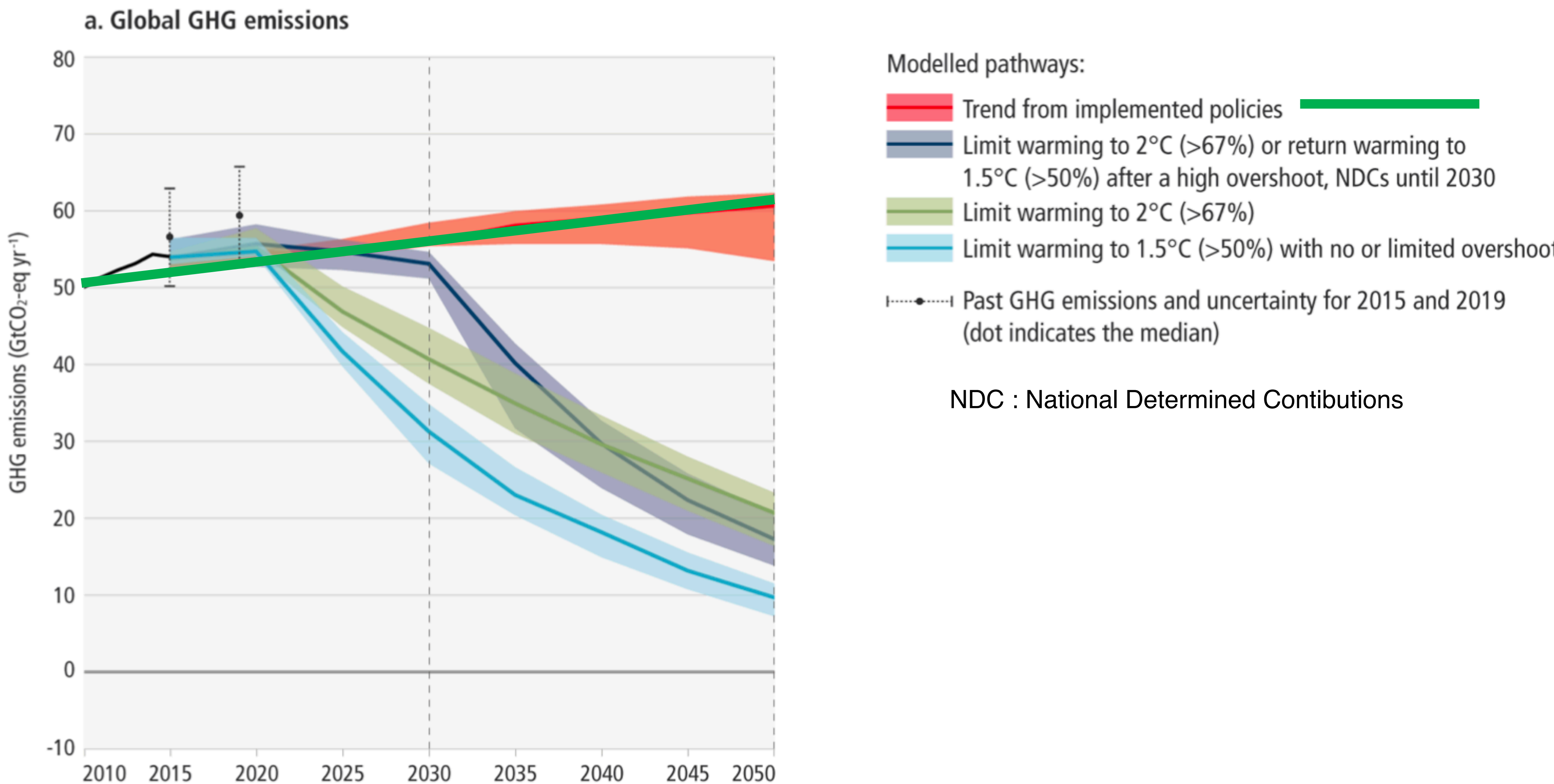
Summary for Policymakers

Pathways



NDC : National Determined Contibutions

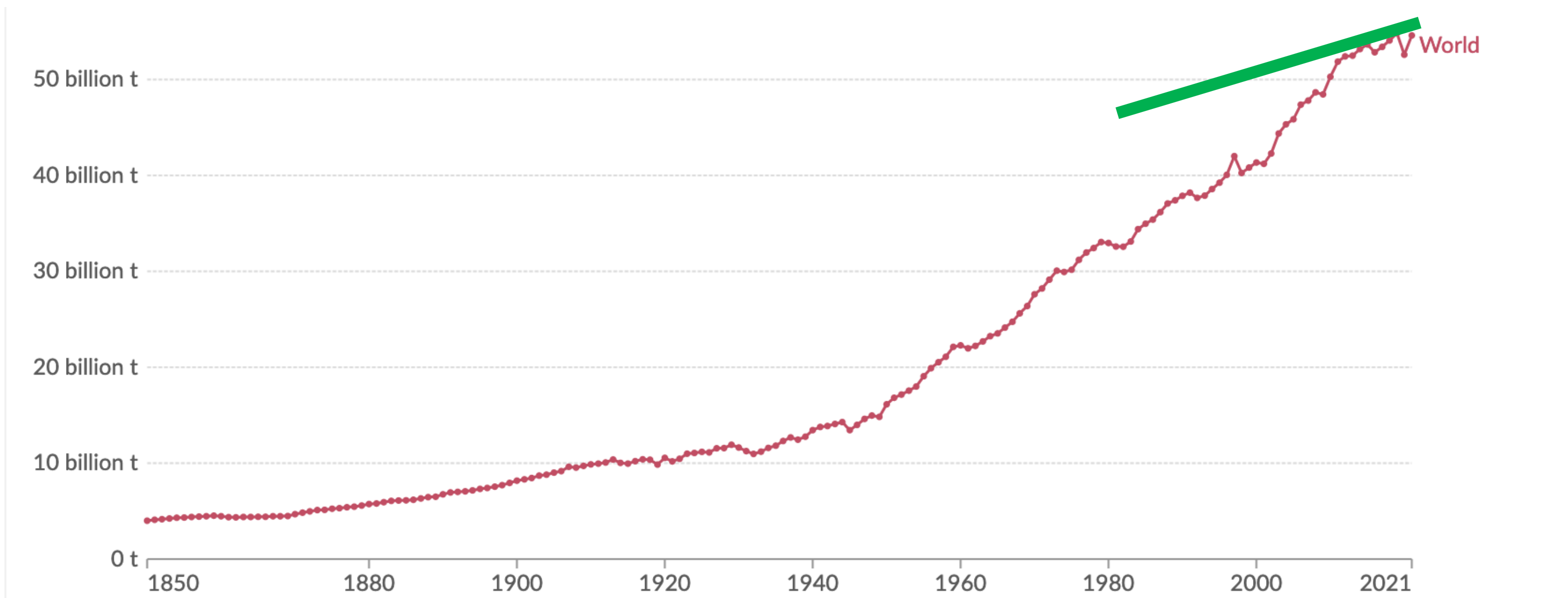
Pathways



NDC : National Determined Contibutions

Emissions de GES jusque en 2021

Trend from implemented policies



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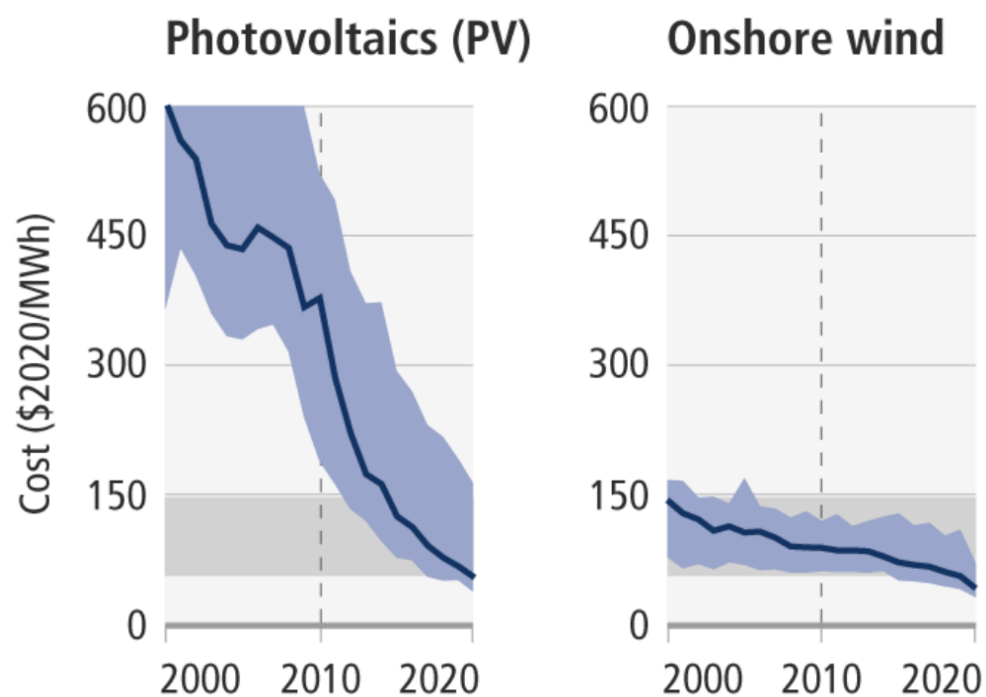
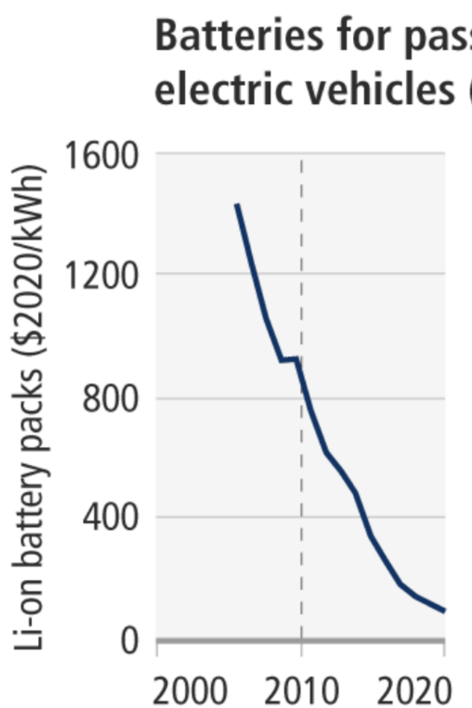
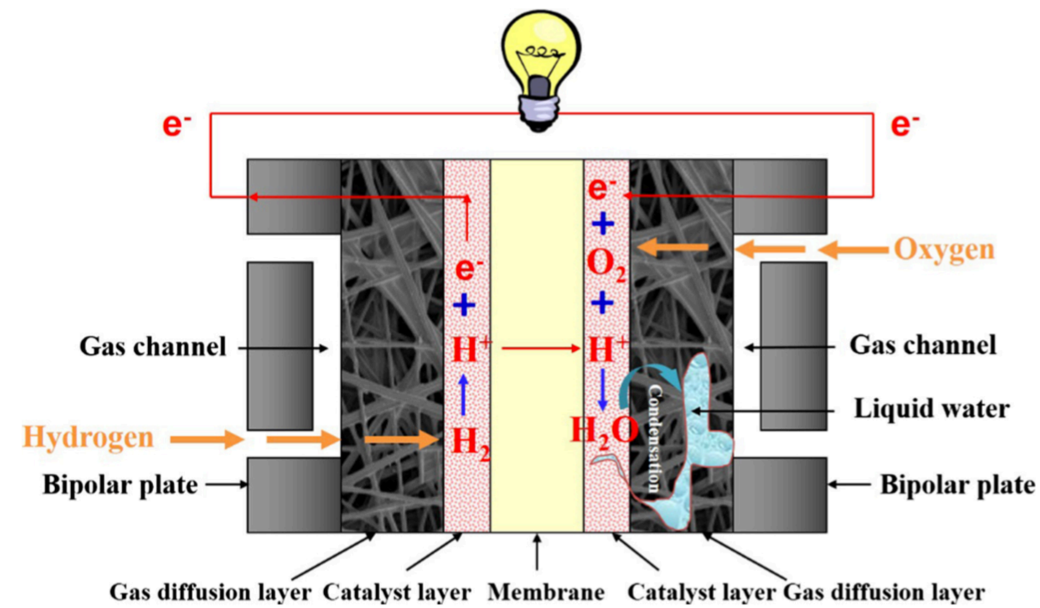
Soilutions are available: wind and solar have become much cheaper



But energy storage remains a big issue





Fuel cell

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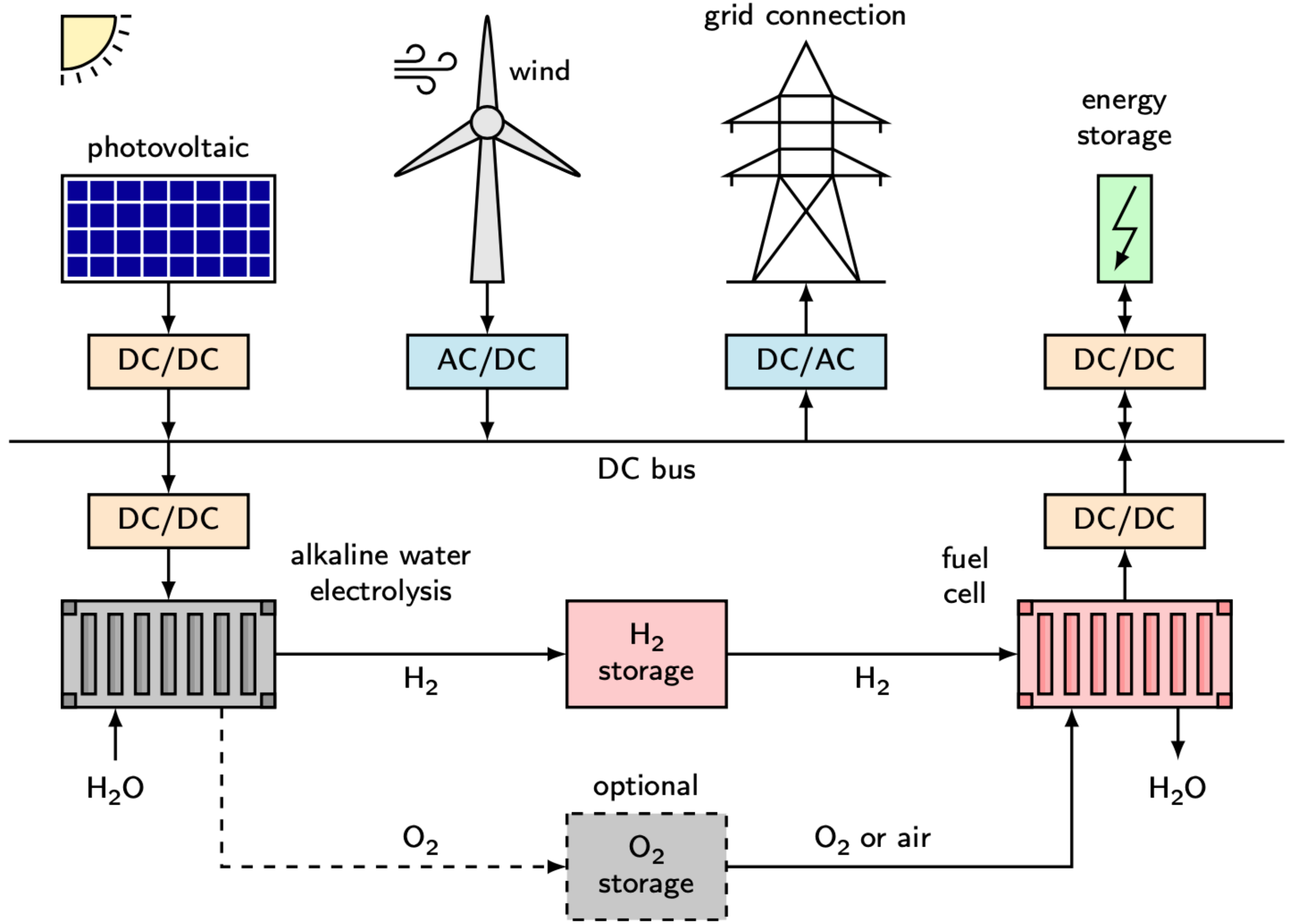
Hydrogen economy ?

Electric / Hydrogen energy system.



Colors of Hydrogen

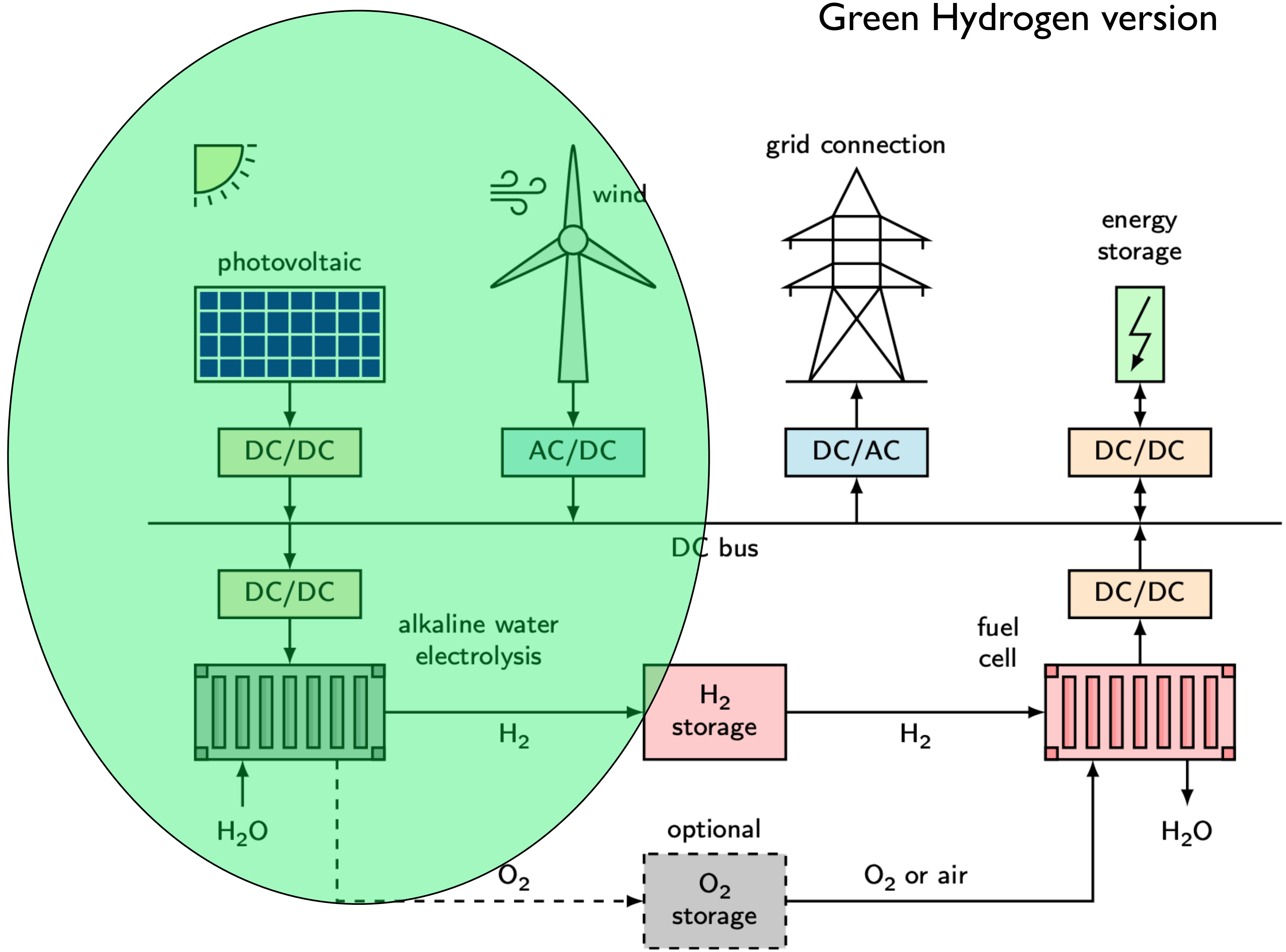
Green hydrogen: wind or solar electricity + electrolysis

Pink hydrogen: nuclear electricity + electrolysis

White hydrogen: native, from underground geological sources

Turquoise hydrogen: from pyrolisis of methane

Green Hydrogen version



Colors of Hydrogen

Green hydrogen: wind or solar electricity + electrolysis

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White hydrogen: native, from underground geological sources

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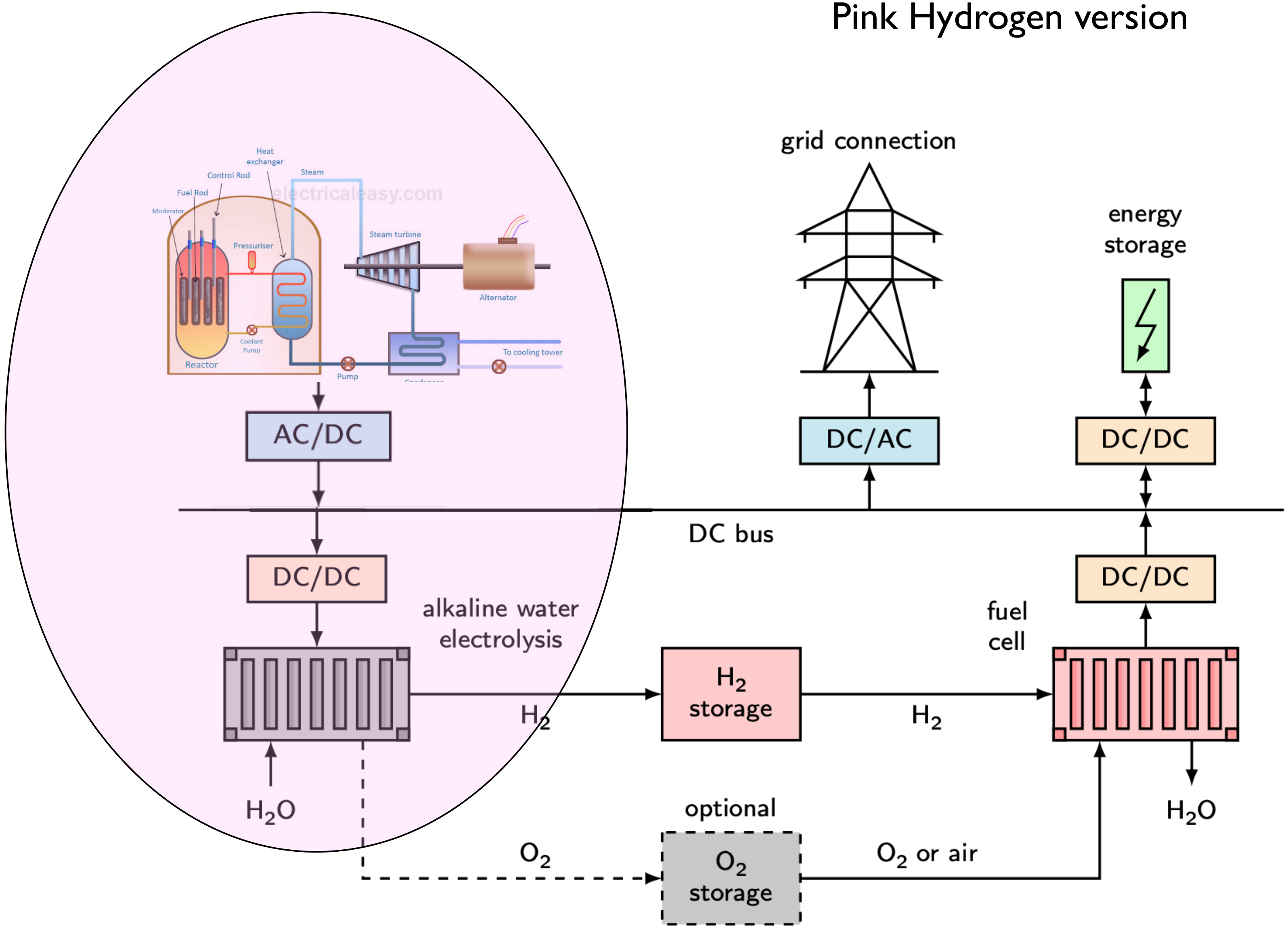
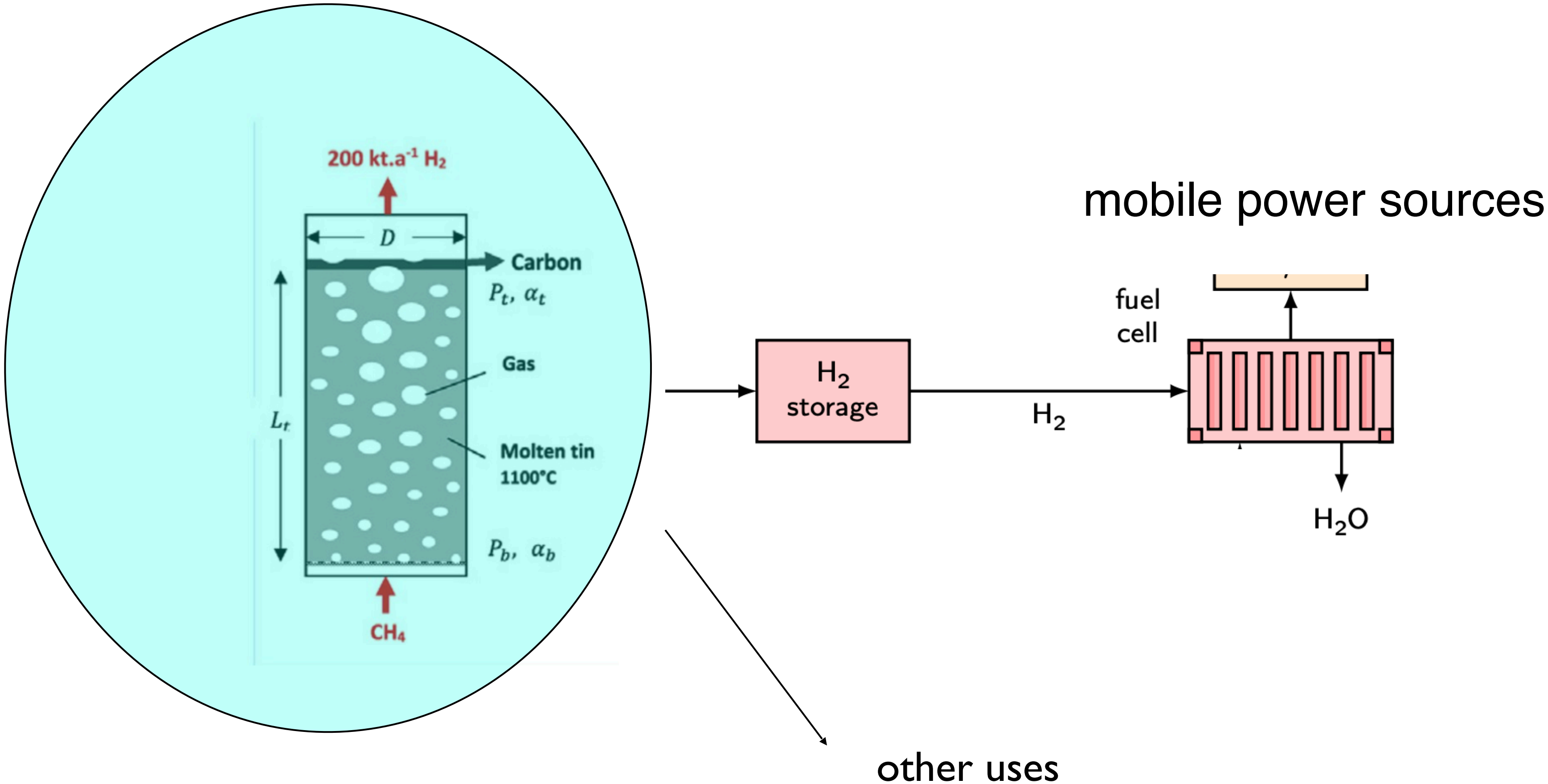
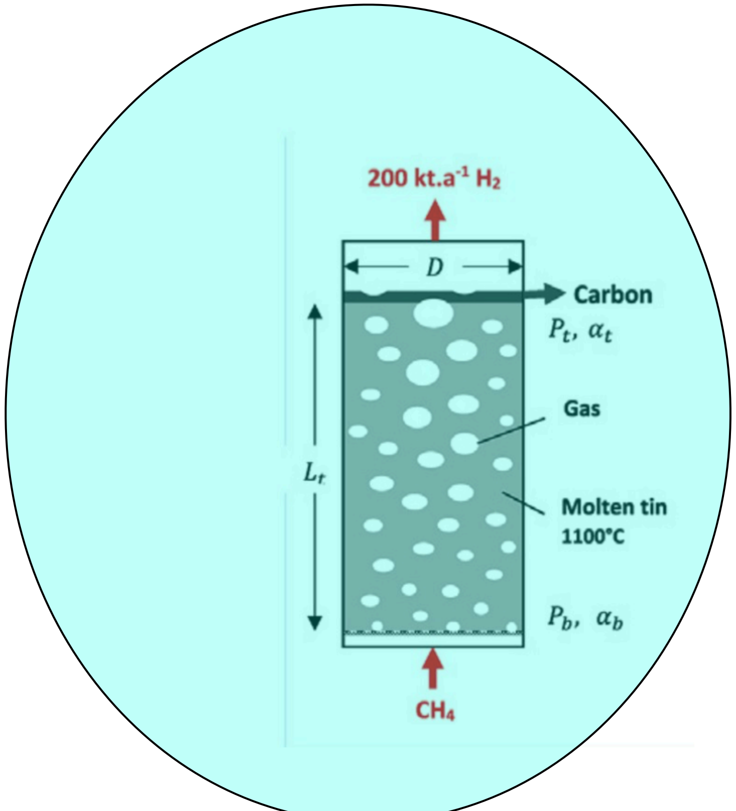
Pink Hydrogen version



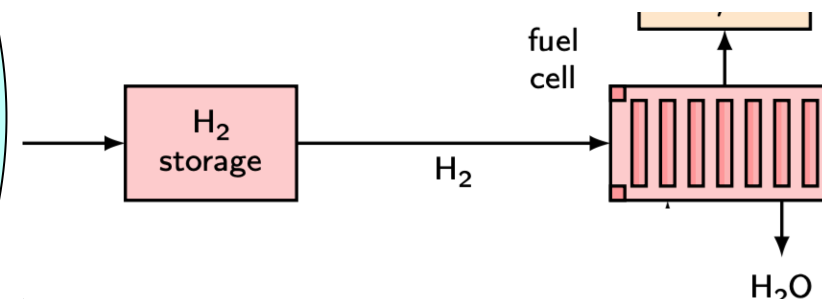
Turquoise Hydrogen version

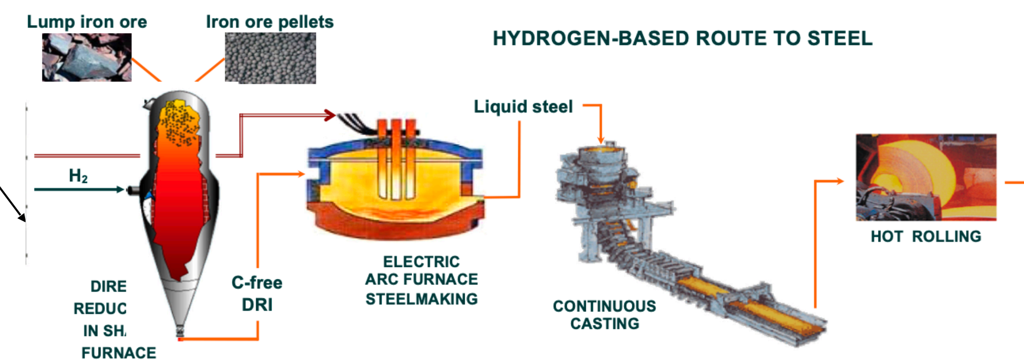


Turquoise Hydrogen version



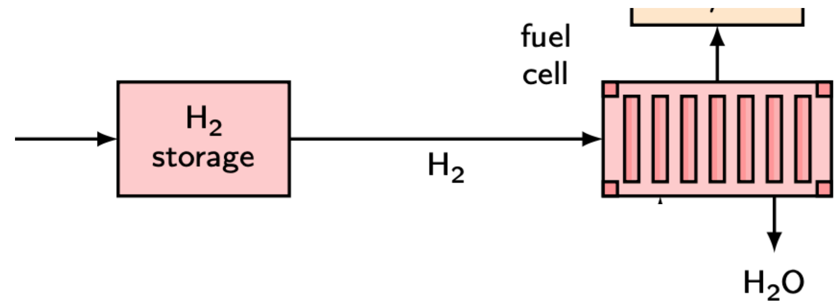
mobile power sources



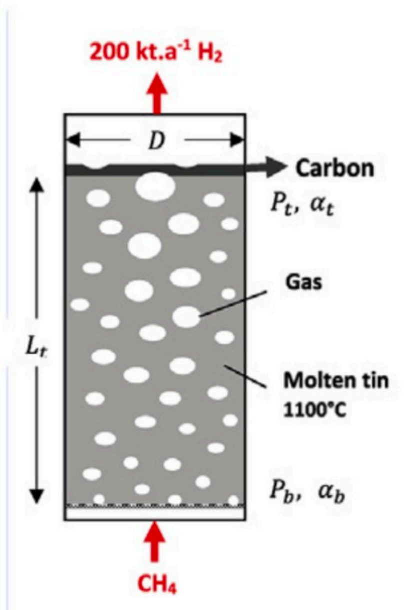


Jean Robin's PhD with AM

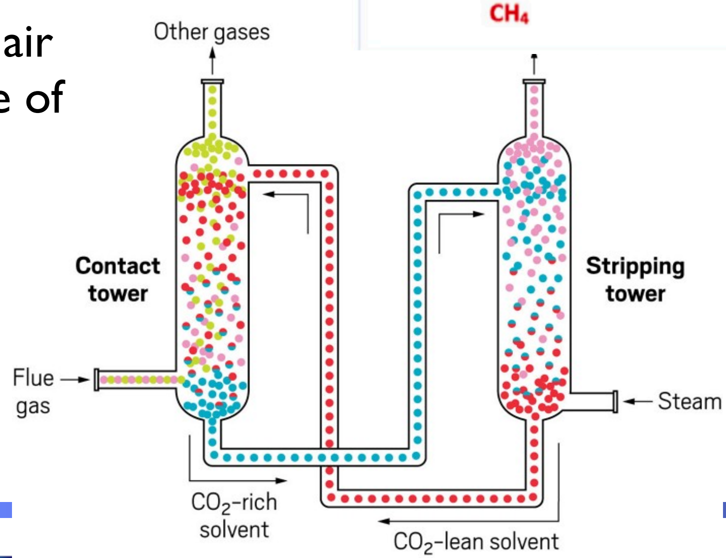
mobile power sources



Pyrolisis



Direct air capture of CO2



CO2 + H2 ⟶ "clean fuel, e-fuel"

Is Direct Air Capture realistic ?

- the price range is from 140 to 990 USD !!!

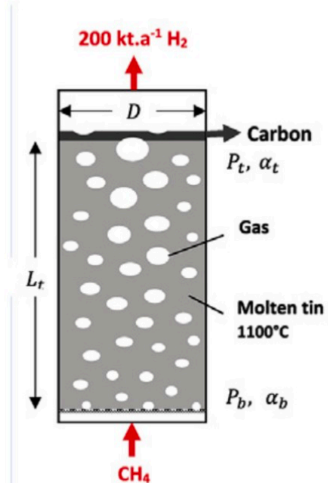
Is Direct Air Capture (DAC) realistic ?

- the price range is from 140 to 990 USD !!!
- The Inflation Reduction Act, passed in 2022, allocates subsidies of USD180 (€165) per tonne captured through DAC.
- Burning a ton of gasoline emits 3 tons of CO_2, so it would cost 3000 USD per ton of gasoline. But 1000 liters of gasoline cost 2200 USD at the gas station in France: same order of magnitude, but significantly more expensive.

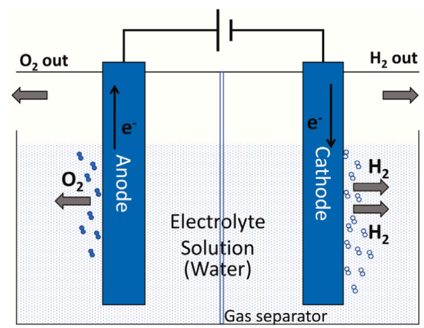
Techno-solutionism ?

Three topics

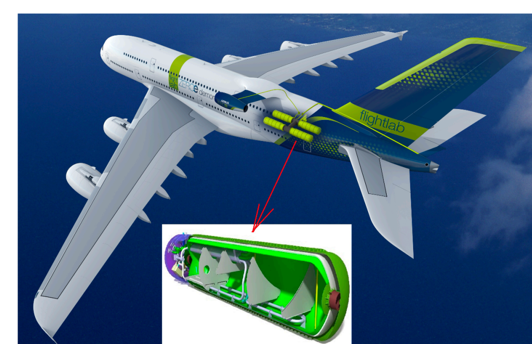
- Pyrolisis



- Electrolysis



- Hydrogen tank for aerospace



Pyrolisis

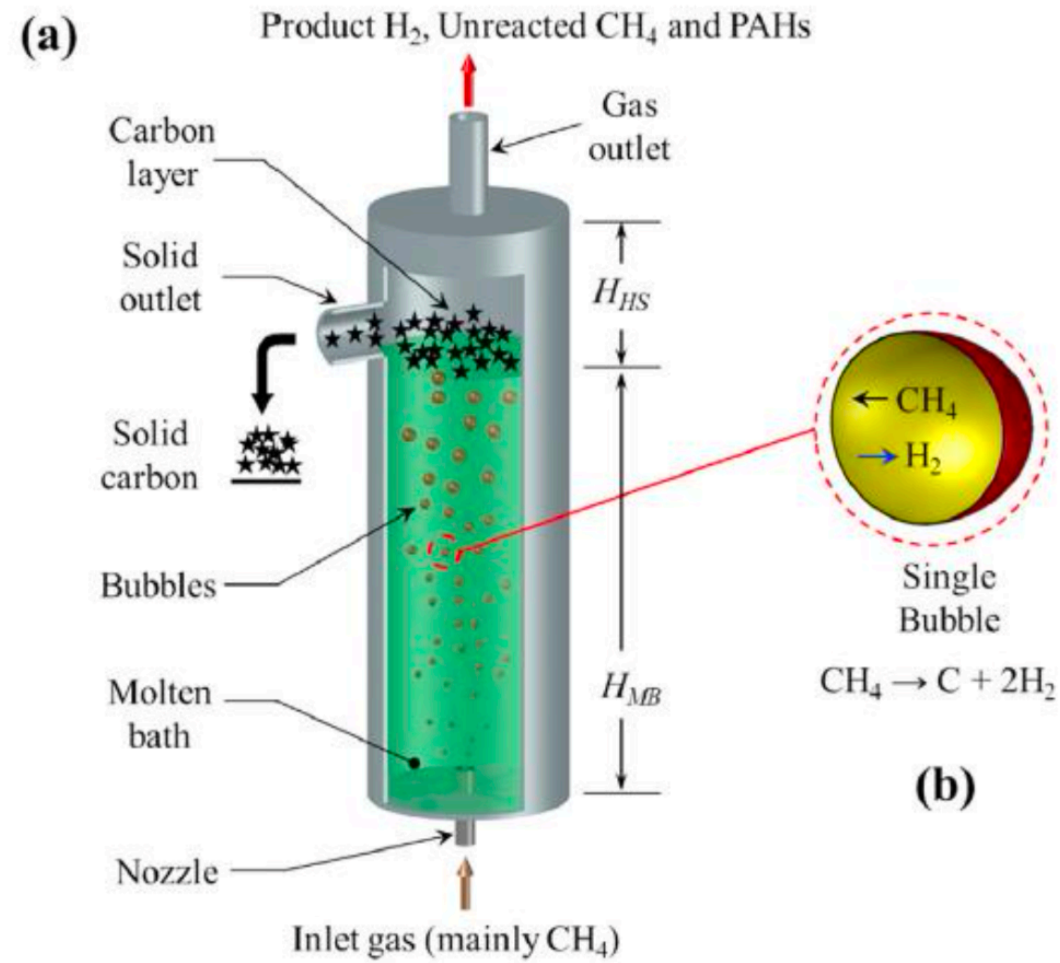
$$CH4 \rightleftharpoons 2\ H2 + (C)_S$$

- Non-catalytic
- Catalytic : steel, gallium, carbon

Two types of reactor: liquid metal or carbon bed.

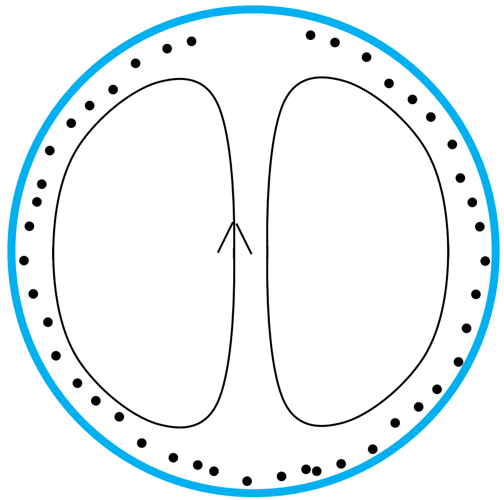
Liquid Metal Bubble Reactor

(LMBR)



Essential phenomena

- hydrodynamics (two phase)
- reaction on surface or in bulk
- soot formation
- radiative transfer.
- conductive and convective heat transfer.



Fluid equations: Navier--Stokes

$$\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{T} + \rho \mathbf{g} + \mathbf{F}_c;$$

Species transport is described by Fick's law

$$\partial_t(\rho x_i) + \nabla \cdot (\rho \mathbf{u} x_i) = \nabla \cdot \mathbf{j}_i$$

where x_i is the mass concentration and $\mathbf{j}$ is the Fickian diffusive transport of species i.

Heat transport is described by the energy equation.

$$\rho \frac{De}{Dt} + p \nabla \cdot \mathbf{u} = \Phi + \nabla \cdot \mathbf{q}.$$

$\mathbf{q}$ is the heat flux which may be decomposed into diffusive and radiative flux as follows

$$\mathbf{q} = \mathbf{q}_d + \mathbf{q}_r\,,$$

with

$$\mathbf{q}_d = -\lambda \nabla T,$$

where λ is Fourier's coefficient and $\mathbf{q}_r$ is the radiative flux. The opacity of the soot and any more compact carbon layer may affect the radiative transfer importantly, fortunately we have

Guillaume Legros and Raghavendra Raman

who are great experts of radiative heat transfer.

Can we do radiative transfer with Basilisk ?

JOURNAL OF COMPUTATIONAL PHYSICS **139**, 380–398 (1998)
ARTICLE NO. CP975870

An Adaptive Mesh Refinement Algorithm for the Radiative Transport Equation

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** Research and Development Division, Babcock & Wilcox, Alliance, Ohio 44601; †Center for Computational Sciences & Engineering, Lawrence Berkeley National Laboratory, Berkeley, California 94720*

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Anticipated difficulties:

- Narrow regions for reaction or surface reactions →combustion models.
- Marangoni (surface tension gradient) effects.
- Large density ratio, large surface tension effects.
- Thin chemical boundary layers.

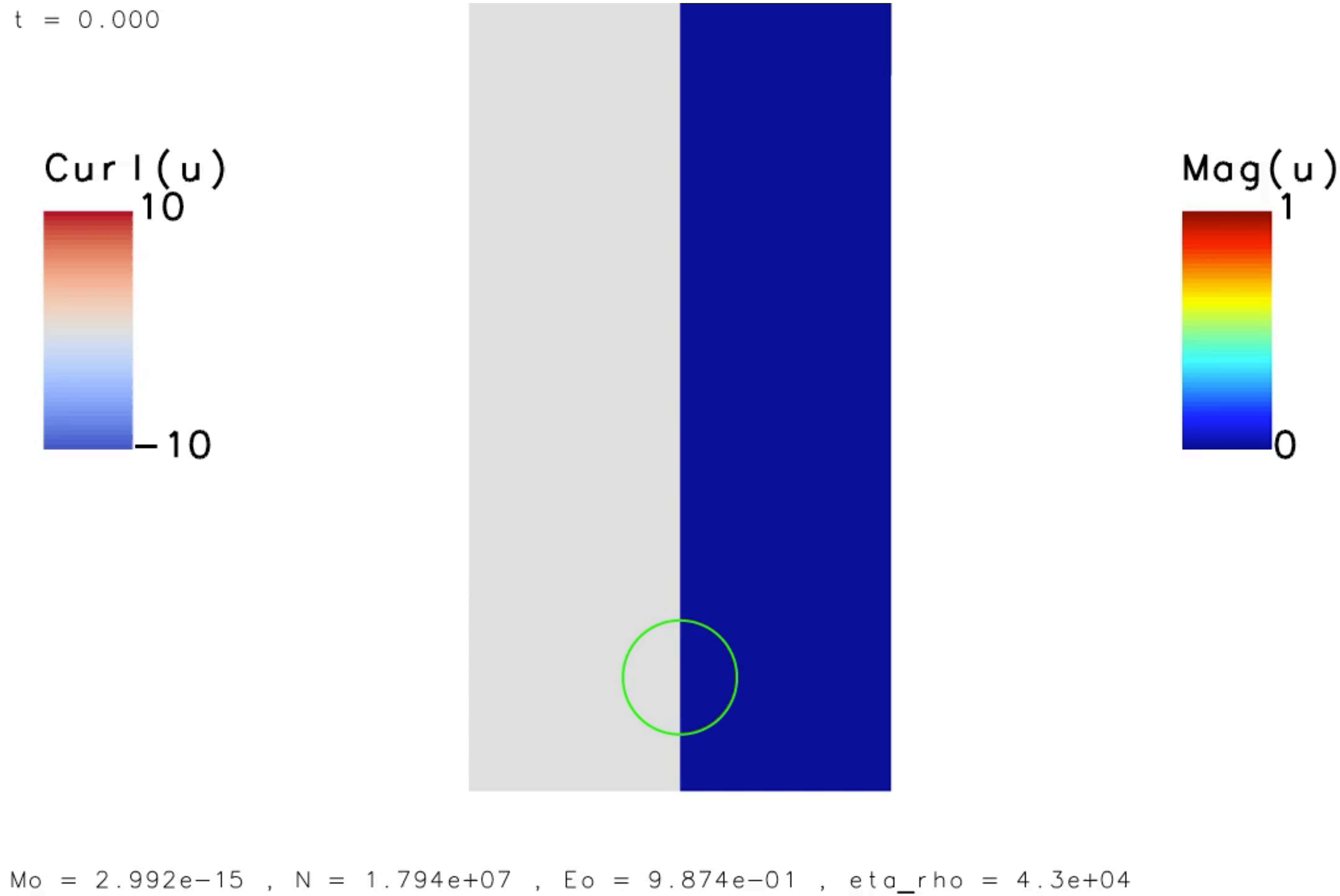
(In technical terms, small Morton number and large Schmidt numbers)

2.7mm bubble
in molten tin.

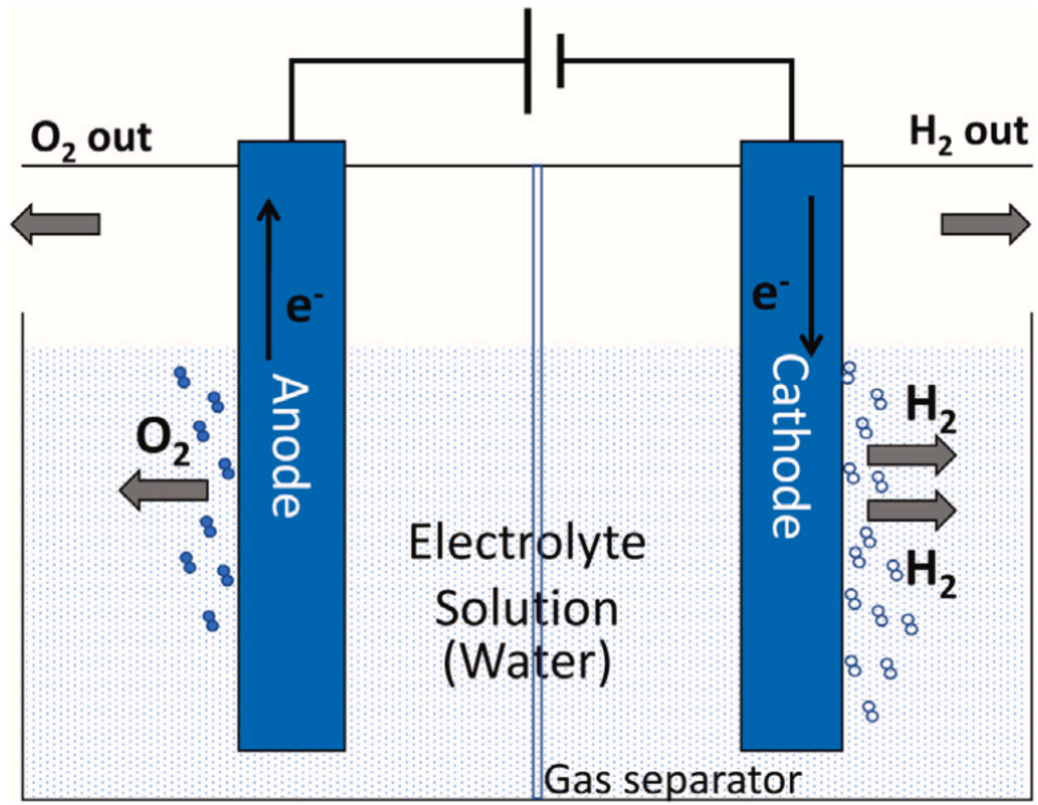
Video by
Mohammad
Taleghani

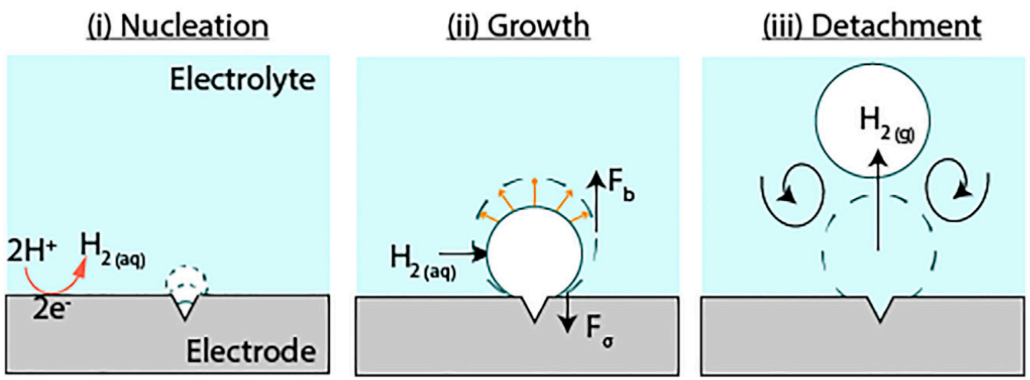
with the help
of Jieyun Pan

using Basilisk

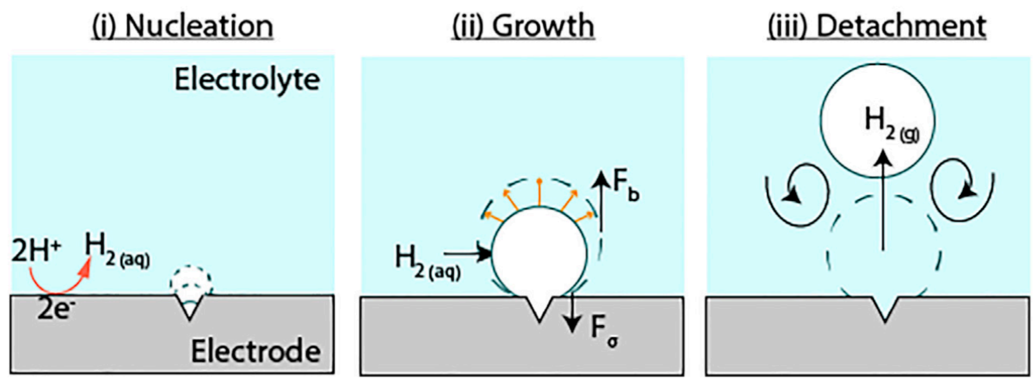


Elctrolisis

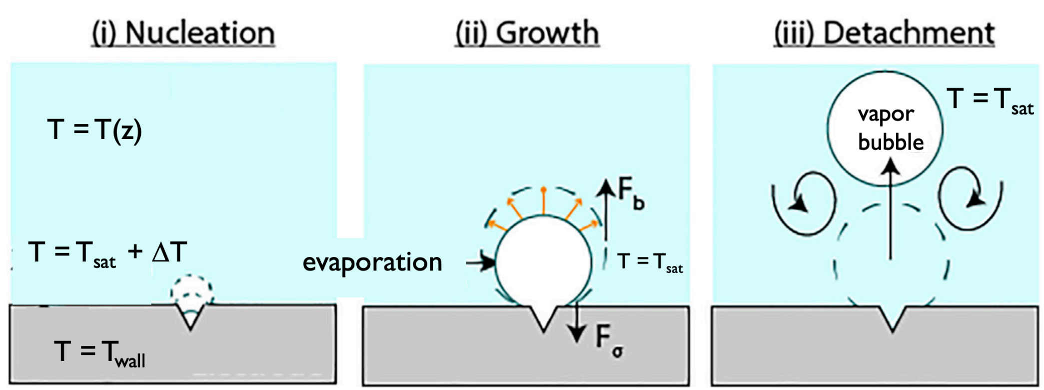




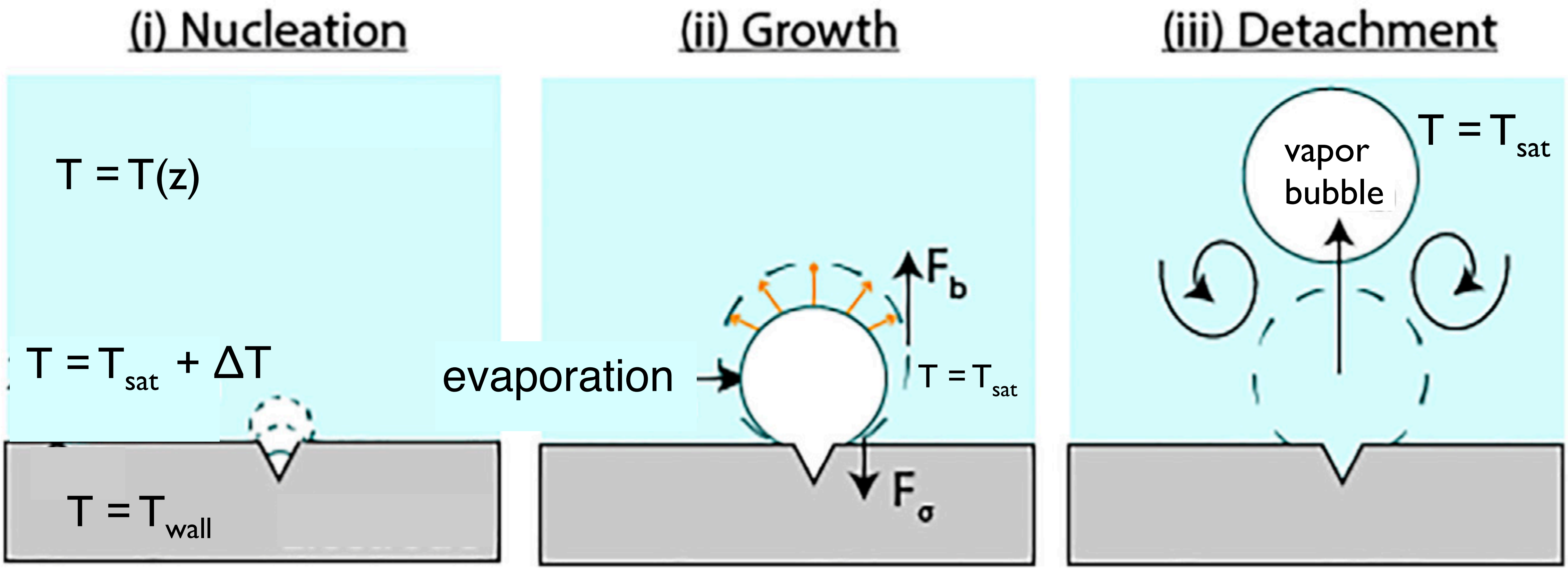
Evolution of an hydrogen bubble



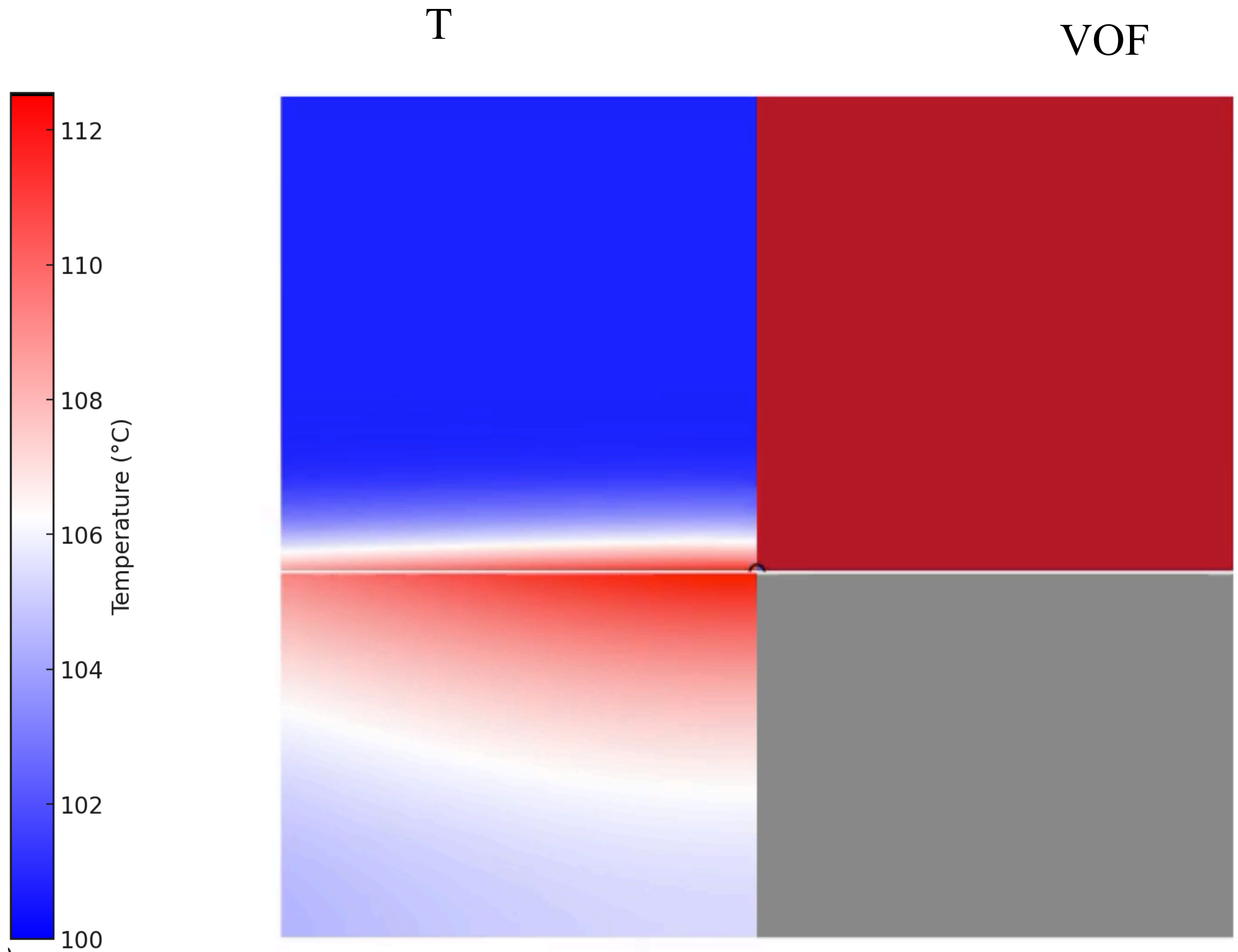
Evolution of an hydrogen bubble



Evolution of a vapor bubble


(i) Nucleation
(ii) Growth
(iii) Detachment
T = T(z)
T = T_sat + ΔT
T = T_wall
evaporation
F_b
F_σ
T = T_sat
vapor
bubble
T = T_sat

Level 12

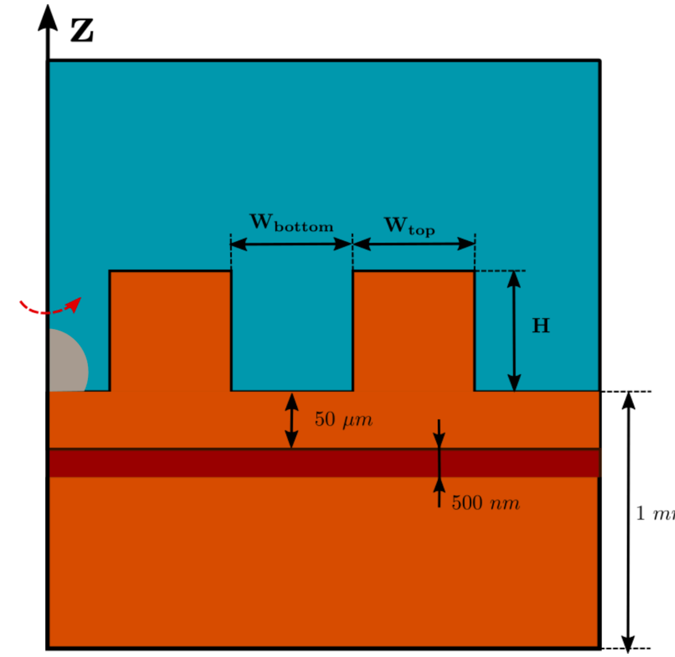


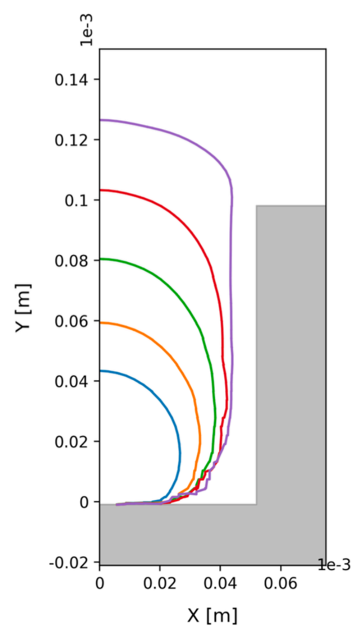
Simulation by
Tian Long

using Basilisk
(modified
for phase change
and heat transfer)

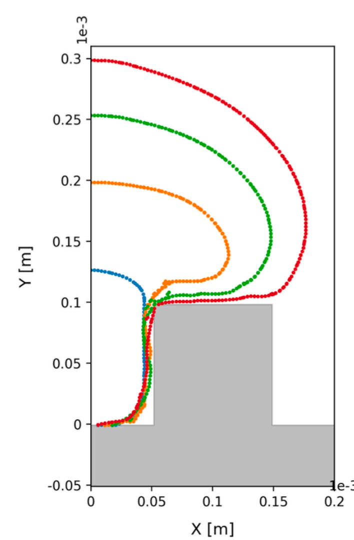
Simulations by Xiangbin Chen,
(modified for phase change and heat transfer)

Using Basilisk with contact-embed (modified)

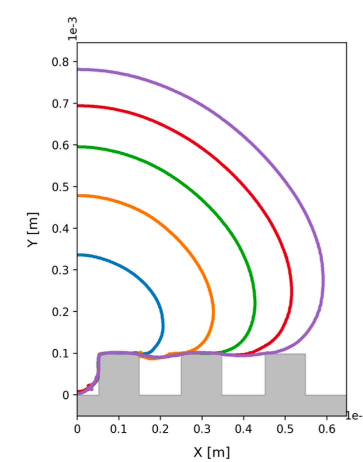




0 ~ 8µs



20 ~ 80µs



100 ~ 500µs

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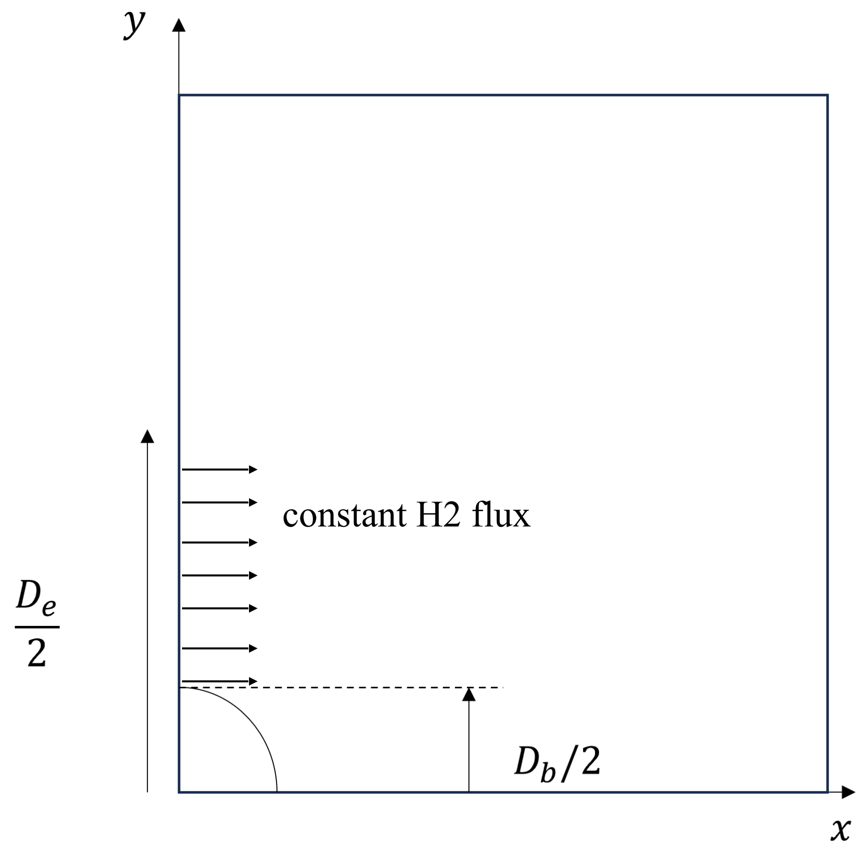
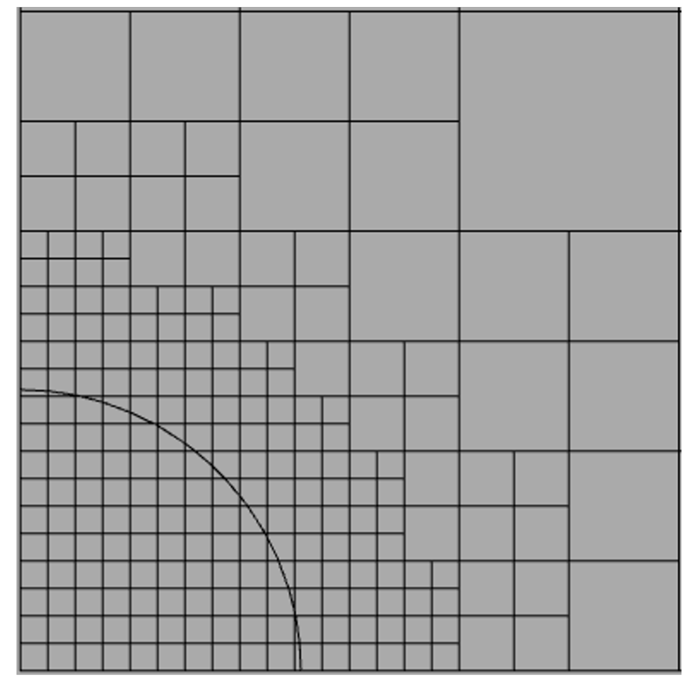
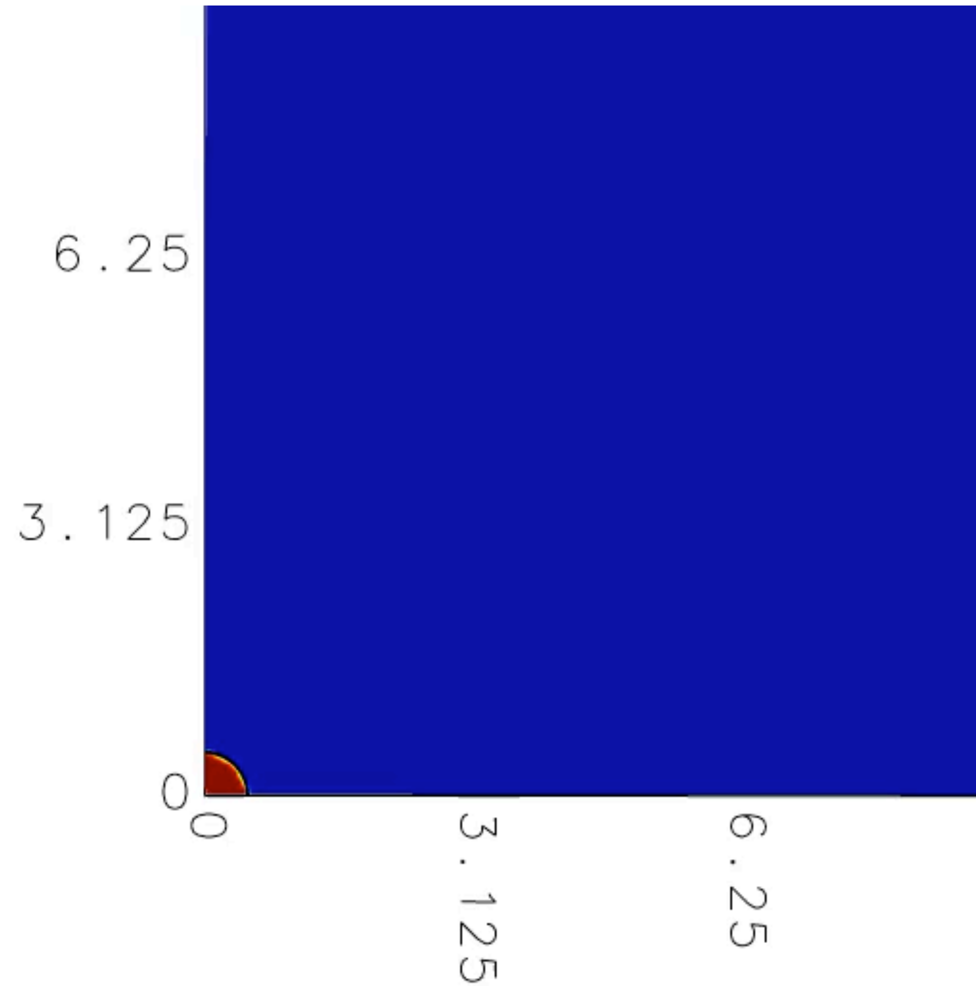
Electrolysis simulation by Wei Qin and Tian Long

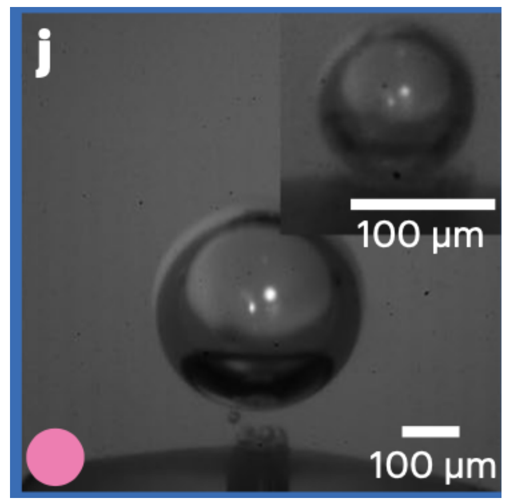


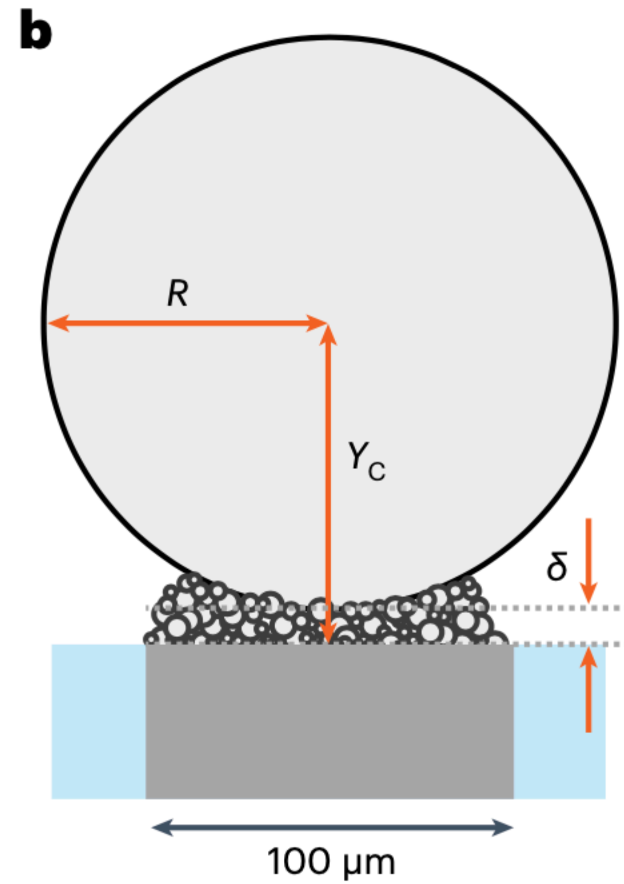


Electrolysis simulation
by Wei Qin
and Tian Long



interaction
of many small bubbles
with large detaching
bubbles.

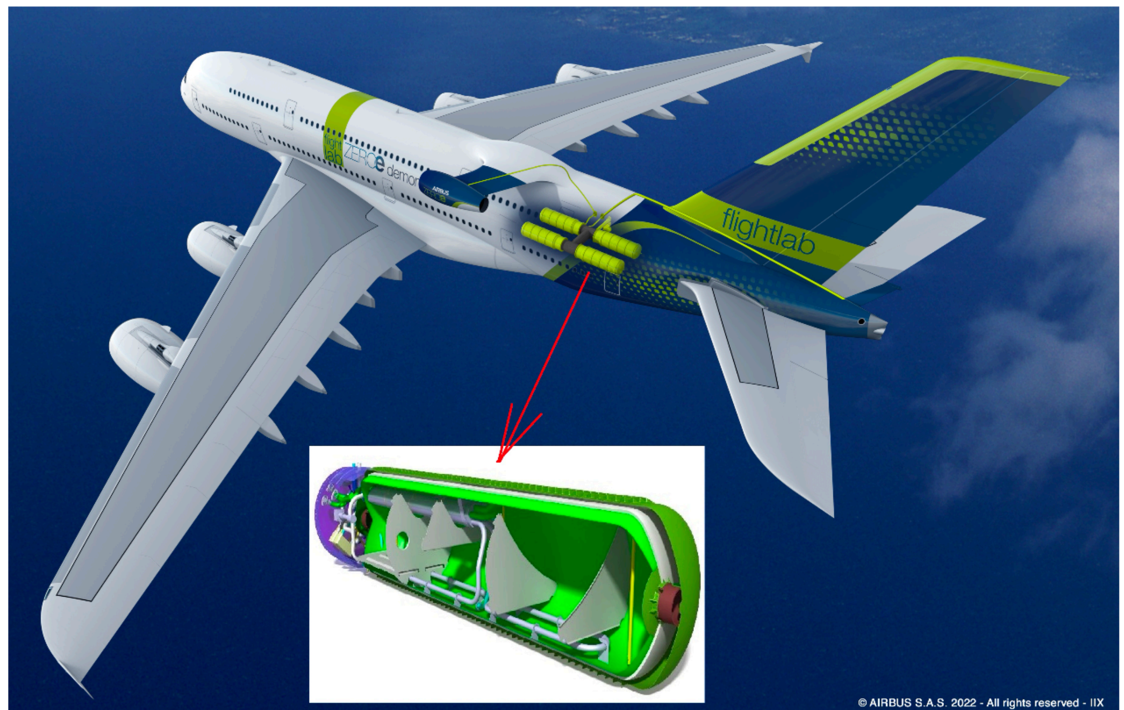




Difficulties

- Physical understanding : why so many small bubbles ?
- Marangoni effects
- Large density ratios.
- Thin chemical boundary layers.

The Hydrogen Aircraft Sloshing Tank Advancement (HASTA) project



Universities

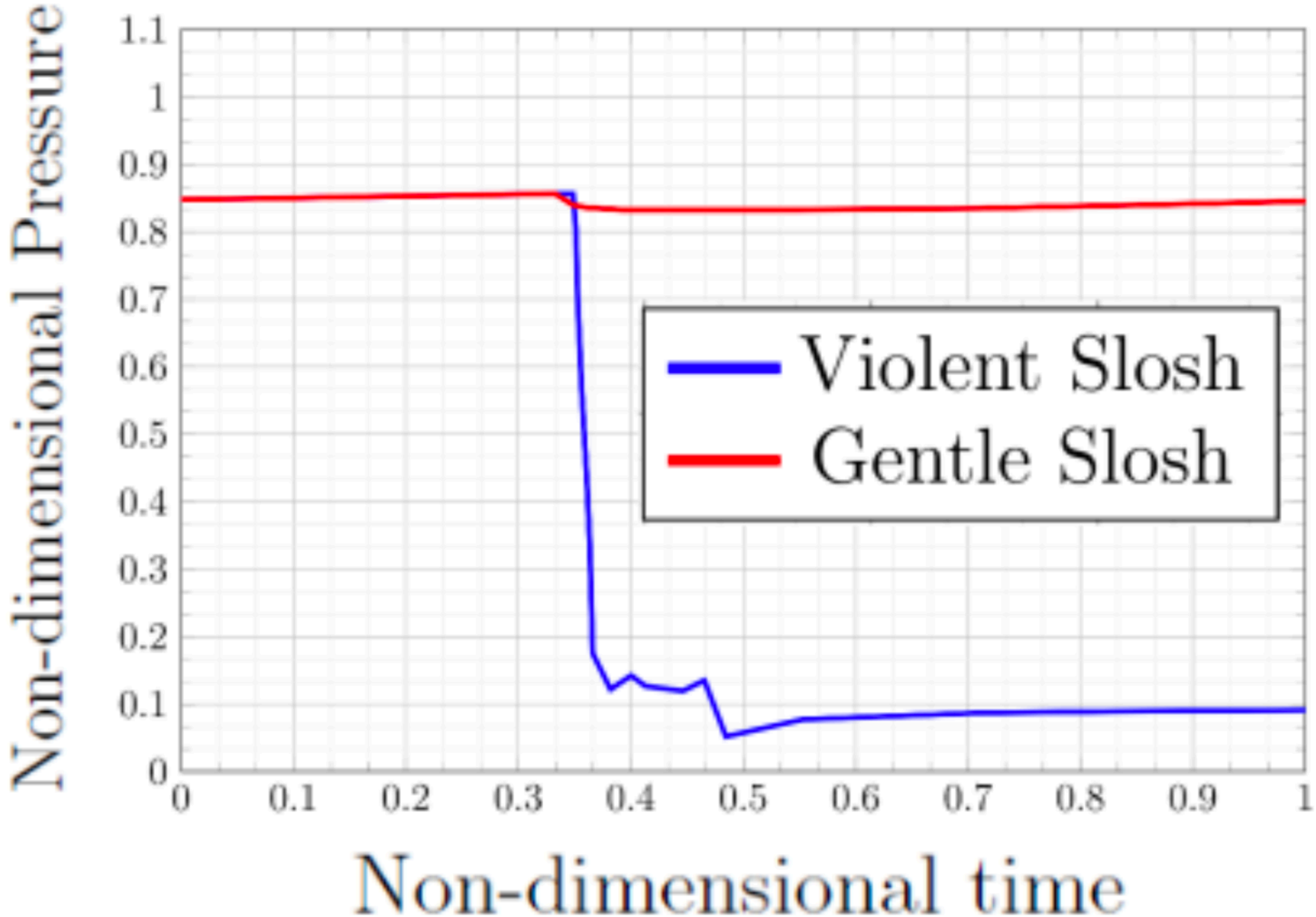
Le Cap (Arnaud Malan, Yusufali Omar)
Bristol
Roma La Sapienza
Roma Niccolo Cusano
∂'Alembert and SU

Public and private agencies

Von Karman Institute
UK Research and Innovation (UKRI)
CNR (Italie)
Military Technical Academy Ferdinand I
DLR

Industrial partners

Airbus
ArianeGroup


Non-dimensional Pressure
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Violent Slosh
Gentle Slosh
Non-dimensional time

plan: use VOF and phase change models to simulate sloshing with heat and mass transfer.

Project start September 1, 2024.

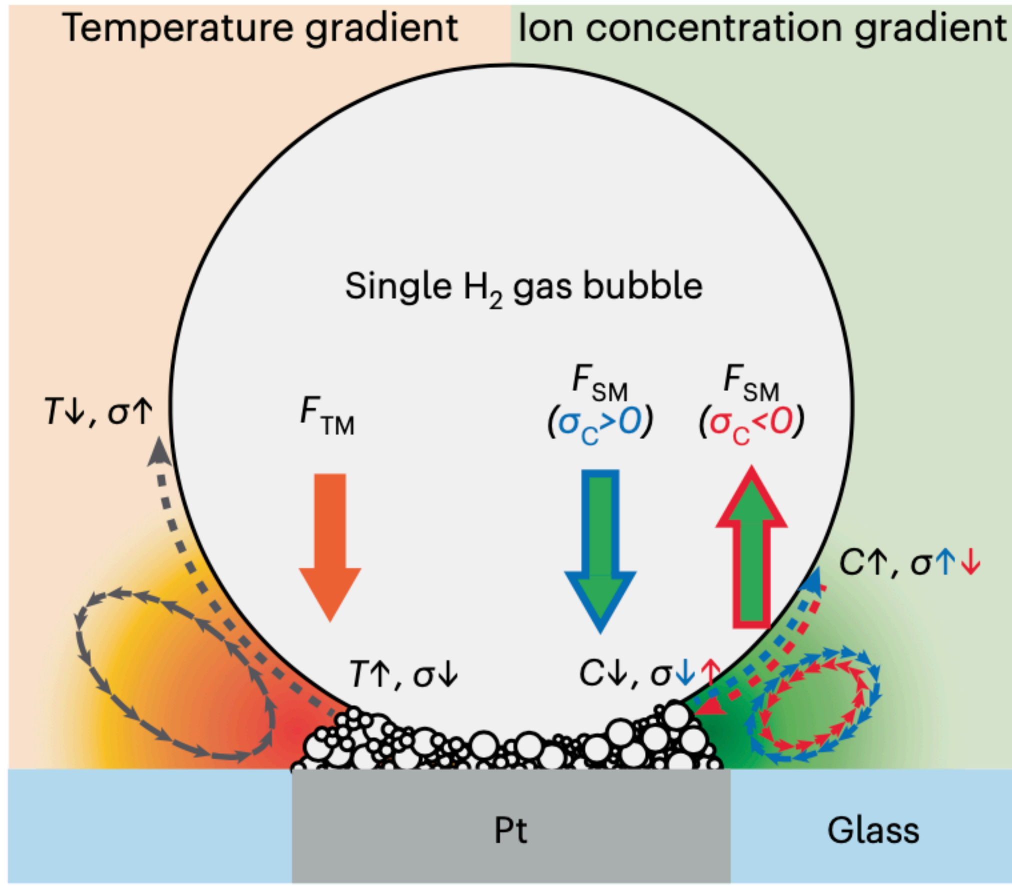
The end

Morton number $$\mathrm{Mo} = \frac{\Delta\rho\, g\mu^4}{\rho^2\sigma^3}$$

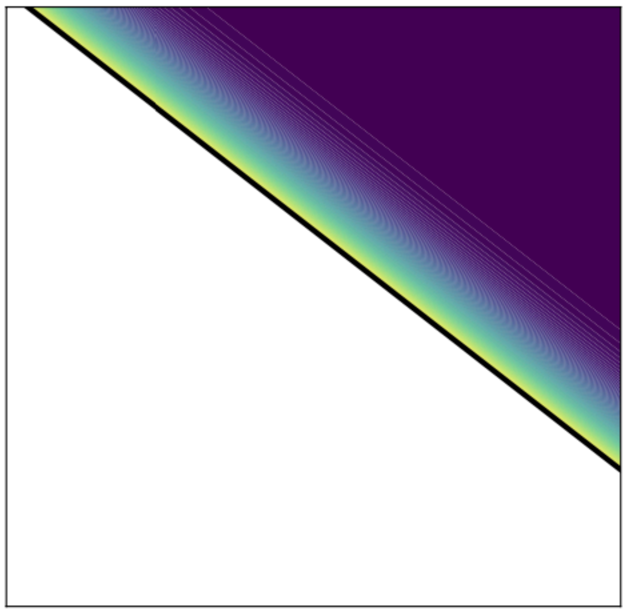
Schmidt number $$\mathrm{Sc} = \frac{\nu}{D}$$

Galileo number $$N = \frac{g\rho\Delta\rho L^3}{\mu^2}$$

Eötvös number $$\mathrm{Eo} = \frac{\Delta\rho g L^2}{\sigma}$$


Temperature gradient
Ion concentration gradient
Single H_2 gas bubble
$T\downarrow$, $\sigma\uparrow$
F_{TM}
F_{SM} ($\sigma_C>0$)
F_{SM} ($\sigma_C<0$)
$C\uparrow$, $\sigma\uparrow\downarrow$
$T\uparrow$, $\sigma\downarrow$
$C\downarrow$, $\sigma\downarrow\uparrow$
Pt
Glass

Subgrid method



Fit a boundary layer distribution of concentration above the interface.

Boundary layer shape solution of

$$[u_I + \omega(z - z_{ow})]\partial_r C = D_w \partial^2_{zz} C$$

Allows to deal with super thin boundary layers.

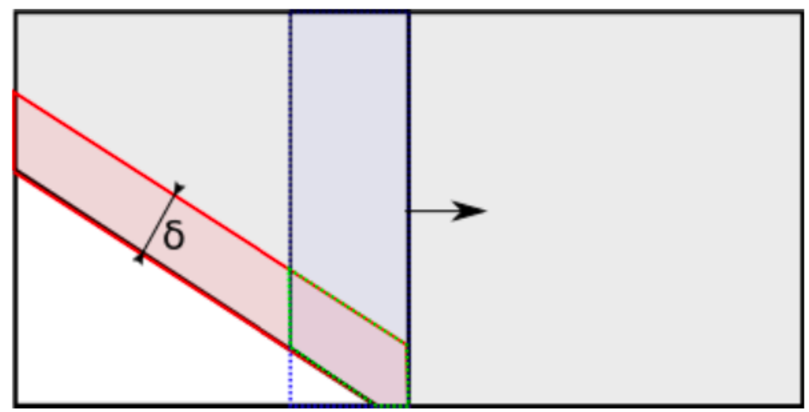
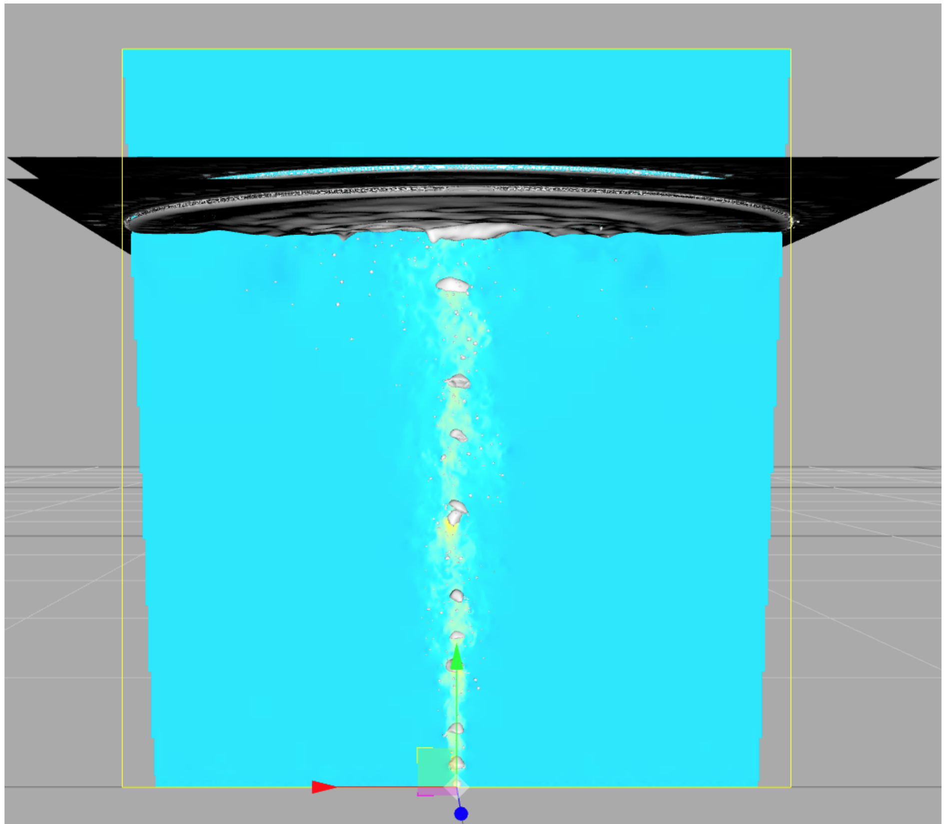
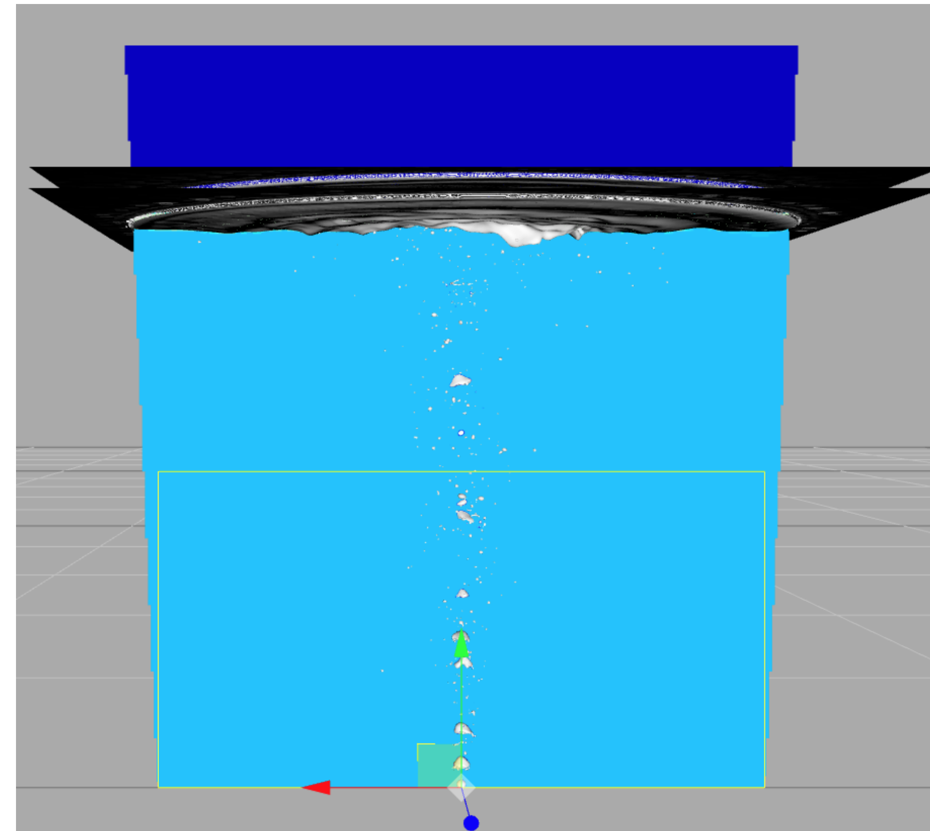
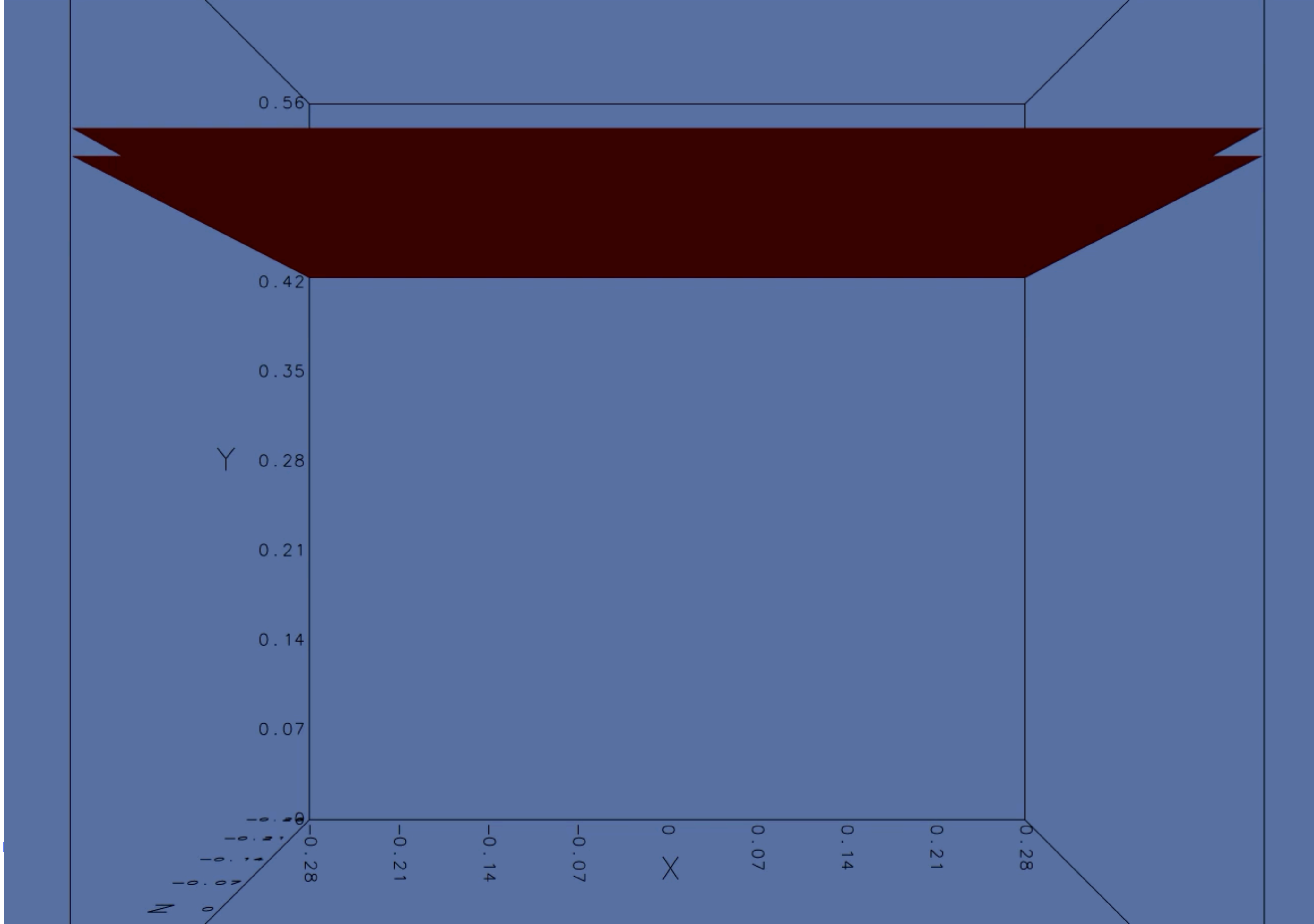


Figure: Visualization of Advection Correction: The green region represents the SGS tracer flux



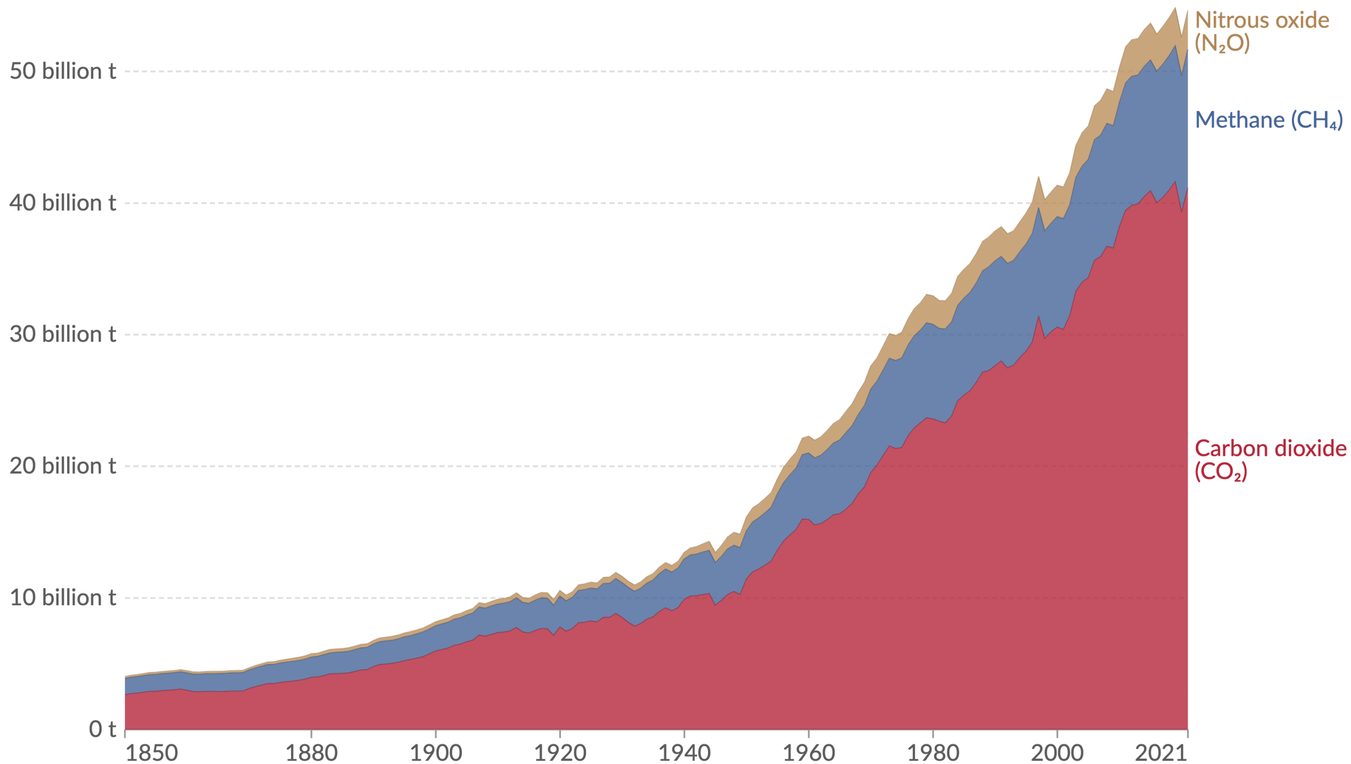




0.56
0.42
0.35
Y
0.28
0.21
0.14
0.07
0
-0.28
-0.21
-0.14
-0.07
0
X
0.07
0.14
0.21
0.28

Greenhouse gas emissions by gas, World, 1850 to 2021

Greenhouse gas emissions[1] from all sources, including agriculture and land-use change. They are measured in tonnes of carbon dioxide-equivalents[2] over a 100-year timescale.



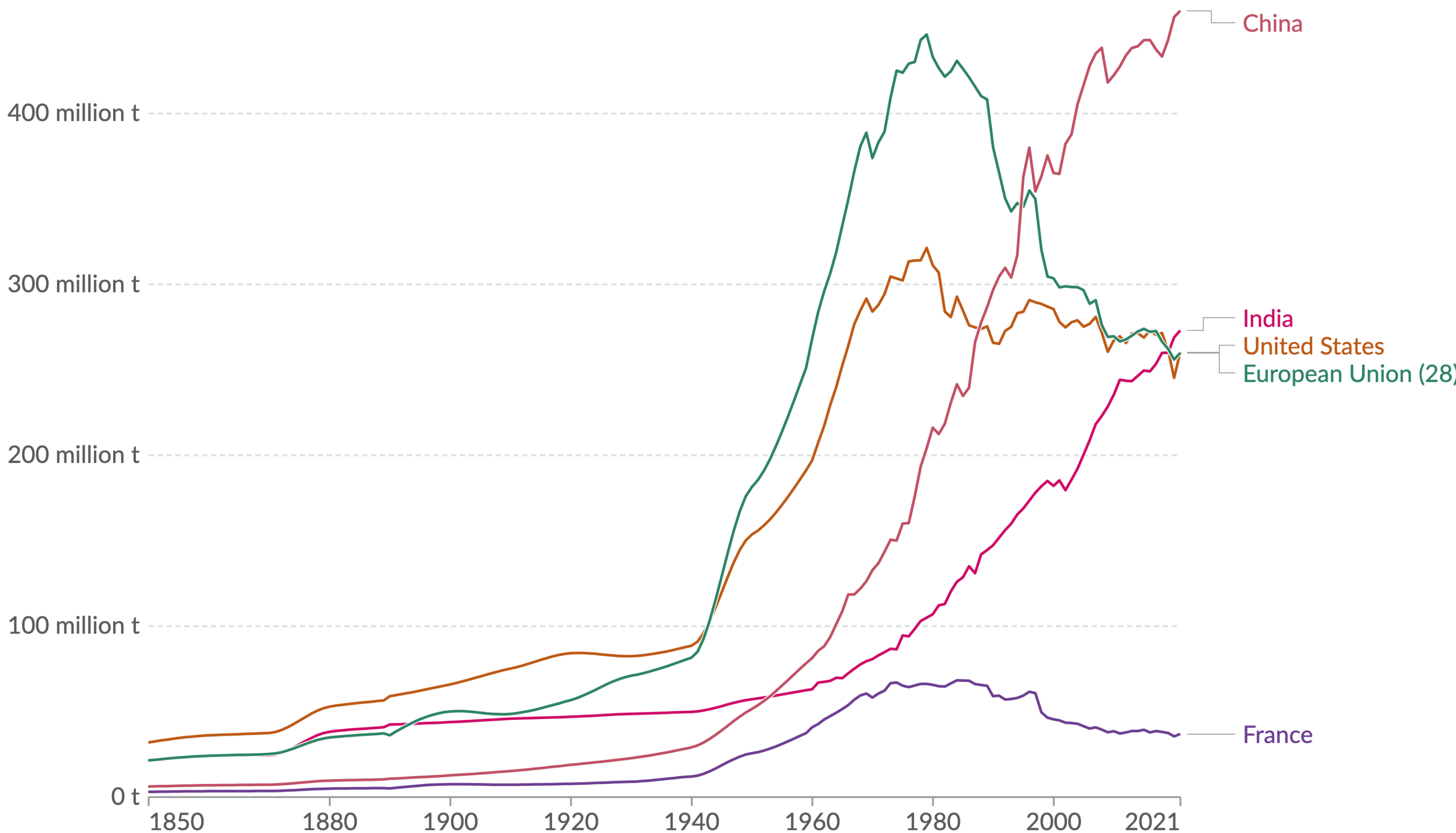
Data source: Jones et al. (2023)

1. Greenhouse gas emissions: A greenhouse gas (GHG) is a gas that causes the atmosphere to warm by absorbing and emitting radiant energy. Greenhouse gases absorb radiation that is radiated by Earth, preventing this heat from escaping to space. Carbon dioxide (CO_2) is the most well-known greenhouse gas, but there are others including methane, nitrous oxide, and in fact, water vapor. Human-made emissions of greenhouse gases from fossil fuels, industry, and agriculture are the leading cause of global climate change. Greenhouse gas emissions measure the total amount of all greenhouse gases that are emitted. These are often quantified in carbon dioxide equivalents (CO_2eq) which take account of the amount of warming that each molecule of different gases creates.

2. Carbon dioxide equivalents (CO_2eq): Carbon dioxide is the most important greenhouse gas, but not the only one. To capture all greenhouse gas emissions, researchers express them in “carbon dioxide equivalents” (CO_2eq). This takes all greenhouse gases into account, not just CO_2. To express all greenhouse gases in carbon dioxide equivalents (CO_2eq), each one is weighted by its global warming potential (GWP) value. GWP measures the amount of warming a gas creates compared to CO_2. CO_2 is given a GWP value of one. If a gas had a GWP of 10 then one kilogram of that gas would generate ten times the warming effect as one kilogram of CO_2. Carbon dioxide equivalents are calculated for each gas by multiplying the mass of emissions of a specific greenhouse gas by its GWP factor. This warming can be stated over different timescales. To calculate CO_2eq over 100 years, we’d multiply each gas by its GWP over a 100-year timescale (GWP100). Total greenhouse gas emissions – measured in CO_2eq – are then calculated by summing each gas’ CO_2eq value.

Nitrous oxide emissions

Nitrous oxide (N_2O) emissions are measured in tonnes of carbon dioxide-equivalents[1].



Data source: Jones et al. (2023)

1. **Carbon dioxide equivalents (CO_2eq)**: Carbon dioxide is the most important greenhouse gas, but not the only one. To capture all greenhouse gas emissions, researchers express them in "carbon dioxide equivalents" (CO_2eq). This takes all greenhouse gases into account, not just CO_2. To express all greenhouse gases in carbon dioxide equivalents (CO_2eq), each one is weighted by its global warming potential (GWP) value. GWP measures the amount of warming a gas creates compared to CO_2. CO_2 is given a GWP value of one. If a gas had a GWP of 10 then one kilogram of that gas would generate ten times the warming effect as one kilogram of CO_2. Carbon dioxide equivalents are calculated for each gas by multiplying the mass of emissions of a specific greenhouse gas by its GWP factor. This warming can be stated over different timescales. To calculate CO_2eq over 100 years, we'd multiply each gas by its GWP over a 100-year timescale (GWP100). Total greenhouse gas emissions – measured in CO_2eq – are then calculated by summing each gas' CO_2eq value.

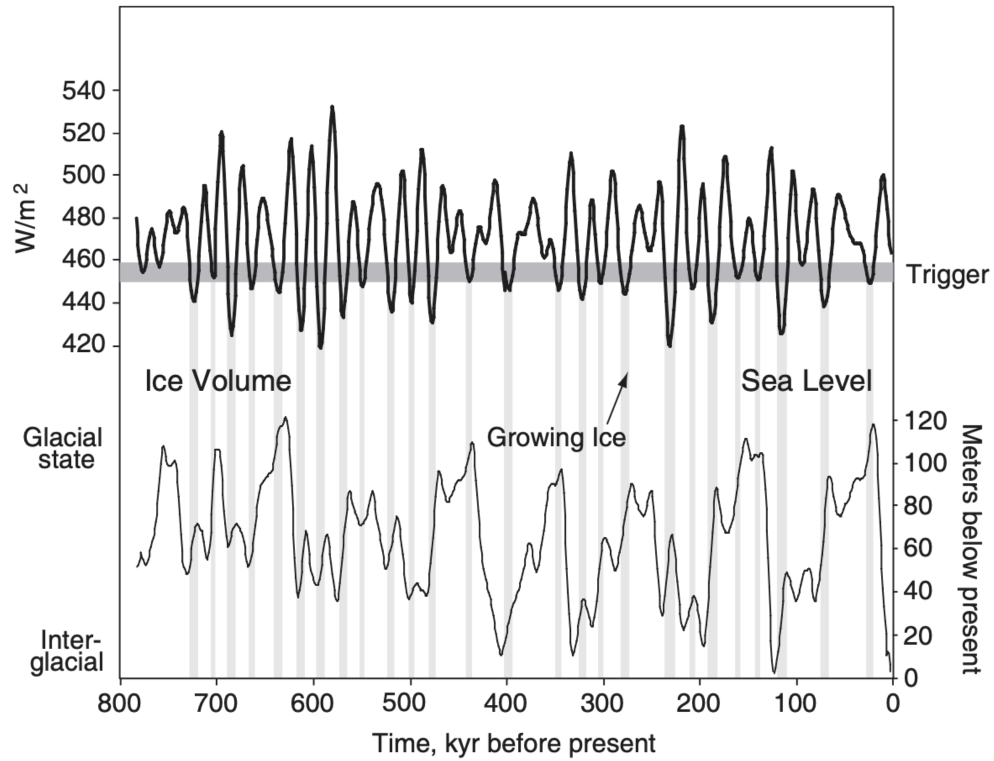
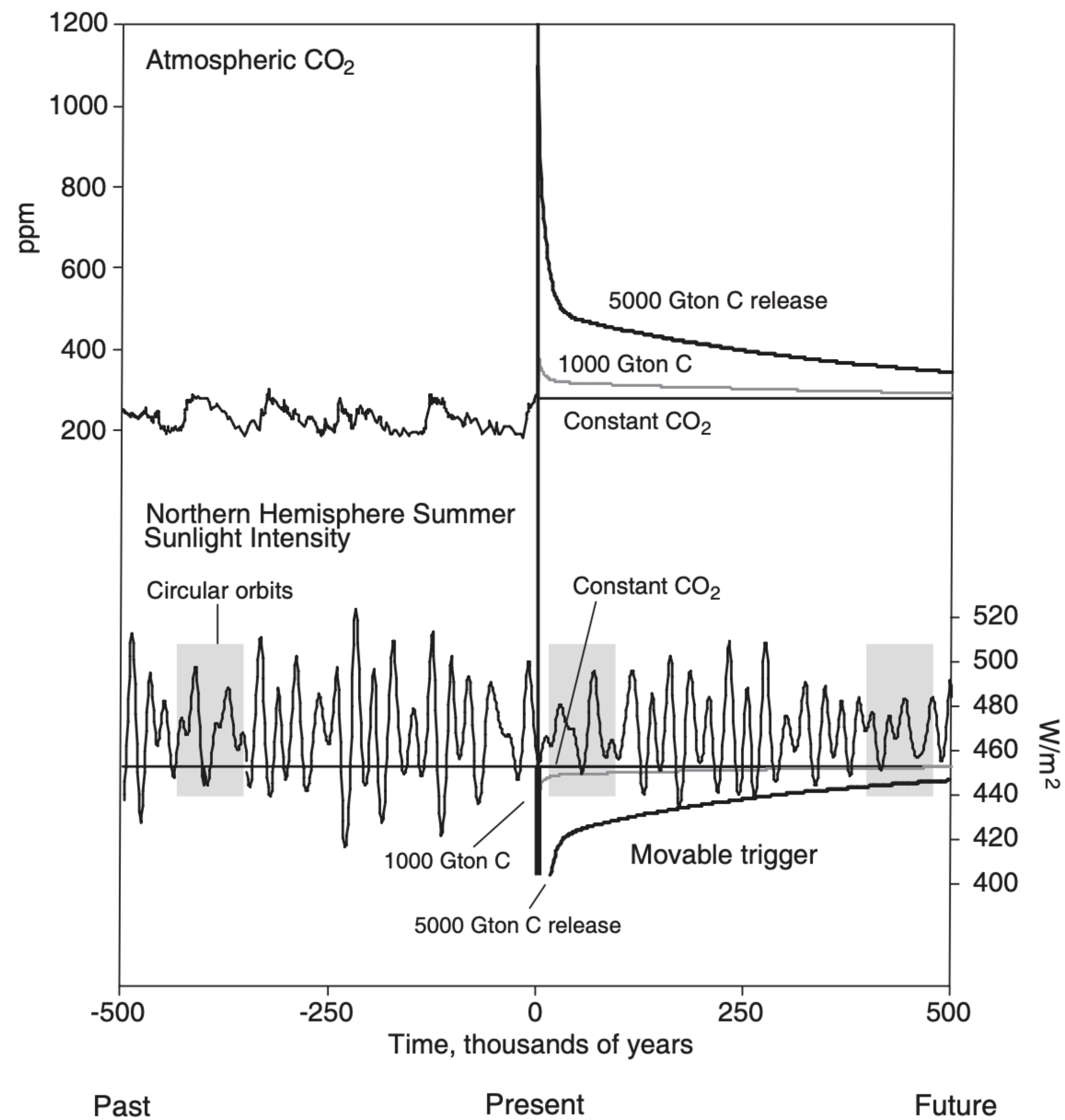


FIGURE 19. Top: Northern hemisphere summer sunshine intensity as modulated by orbital variation. Bottom: ice volume. Vertical bars are times when summer sunlight drops below a Trigger value. In those times, ice grows.

David Archer, The Long Thaw, 2009, Princeton University Press


Atmospheric CO_2
ppm
1200
1000
800
600
400
200
5000 Gton C release
1000 Gton C
Constant CO_2
Northern Hemisphere Summer Sunlight Intensity
Circular orbits
Constant CO_2
520
500
480
460
440
420
400
W/m^2
1000 Gton C
Movable trigger
5000 Gton C release
-500
-250
0
250
500
Time, thousands of years
Past
Present
Future