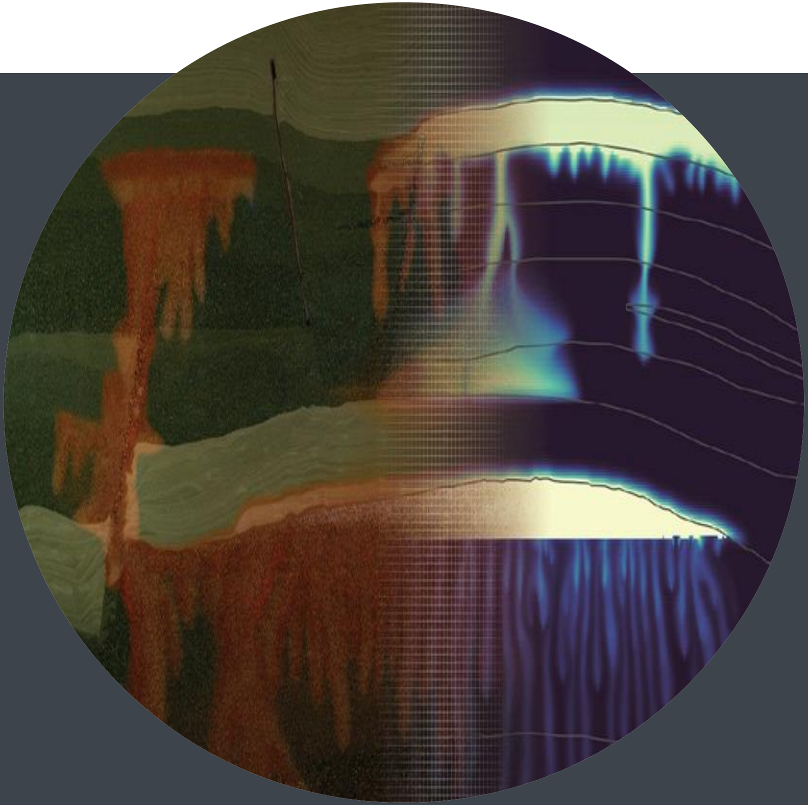
Universität Stuttgart
Institute for Modelling Hydraulic and Environmental Systems
Department of Hydromechanics and Modelling of Hydrosystems

Benchmarking Computational Models for GCS

Bernd Flemisch
Workshop "Mathematical and numerical modeling of CO_2 storage", Rueil-Malmaison, 01.02.2023



Outline

1. Motivation
2. Categorization
3. Selected GCS Benchmark Studies
    a. The Classic
    b. So Simple, Yet So Hard
    c. Reality Meets Modeling
    d. Back To Normal, But Bigger
4. Summary and Conclusion

Outline

1. **Motivation**
2. Categorization
3. Selected GCS Benchmark Studies
    a. The Classic
    b. So Simple, Yet So Hard
    c. Reality Meets Modeling
    d. Back To Normal, But Bigger
4. Summary and Conclusion

Essentially all models are wrong,
… but some are useful

George Box

One of the most influential statistician of the 20th century and a pioneer in the areas of quality control, time series analysis and design of experiments and Bayesian inference.

Motivation
Model Assessment

- Why do we even bother then?
- Because „Some are Useful“.
- But ... How do we know a model is „Useful“?
- We consider a model "useful" if it provides:
  - enhanced insight into a problem,
  - a means to test a theory/hypothesis.
- What are the approaches to determine if a model is "useful"?

Motivation
Model Assessment

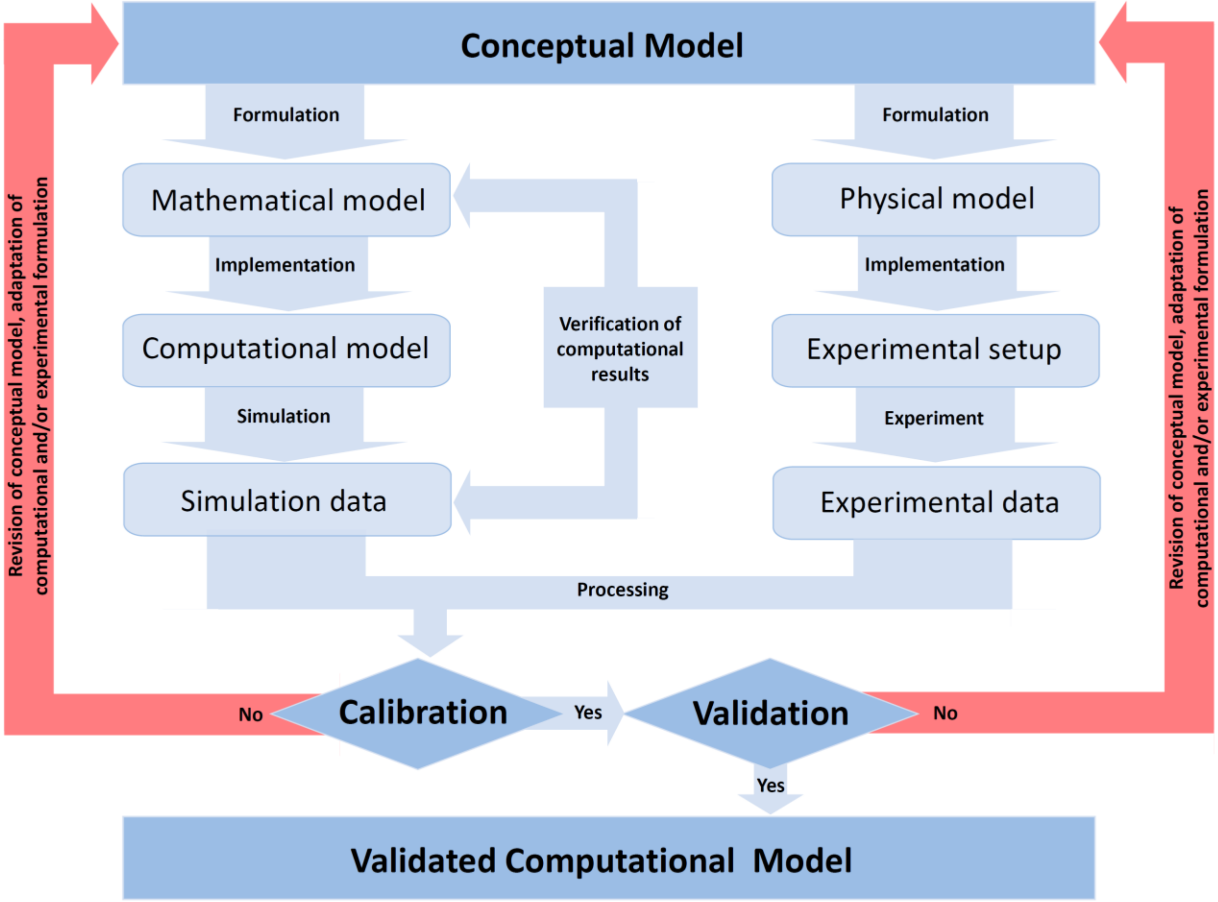
- Why do we even bother then?
- Because „Some are Useful“.
- But ... How do we know a model is „Useful“?
- We consider a model "useful" if it provides:
  - enhanced insight into a problem,
  - a means to test a theory/hypothesis.
- What are the approaches to determine if a model is "useful"?
  - **Common Methods: Verification and Validation.**

Outline

1. Motivation
2. **Categorization**
3. Selected GCS Benchmark Studies
   a. The Classic
   b. So Simple, Yet So Hard
   c. Reality Meets Modeling
   d. Back To Normal, But Bigger
4. Summary and Conclusion

Categorization

Process of Model Development



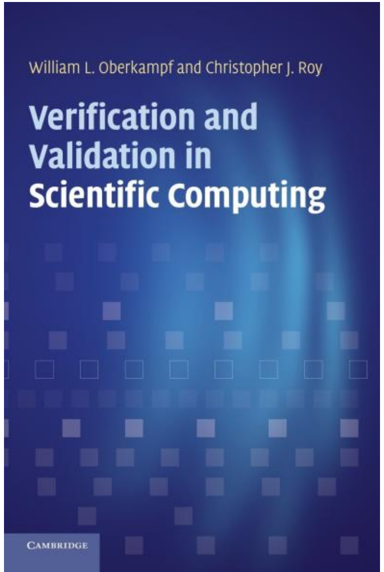
Terminology

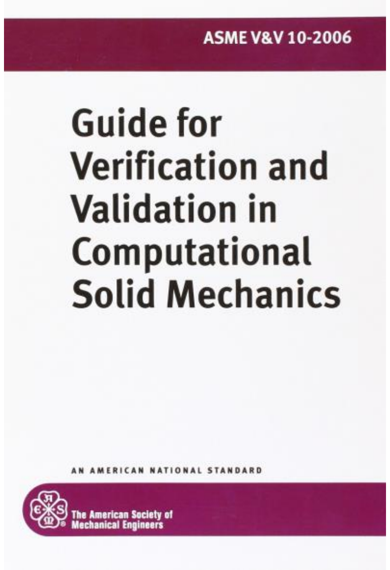
- ***Conceptual model:*** Idealized **representation of the physical behavior** of the reality of interest.
- ***Mathematical model:*** Mathematical description of the physical processes represented in this conceptual model.
- ***Computational model:*** Numerical implementation of the mathematical model that will be solved on a computer to yield the computational predictions of the system response.
- ***Verification:*** Examines whether the results of a **computational model** are close enough to given solutions of the underlying **mathematical model.**
- ***Calibration:*** Process of **adjusting parameters** in the computational model to improve **agreement with data.**
- ***Validation:*** Investigates how accurately a **computational model** describes the **reality.**

Categorization

Terminology

- ***System Response Quantity (SRQ):*** Quantity of interest to be compared. SRQs for one case ideally form a **hierarchy** ranging from globally integrated to local quantities.
- ***Comparison/Validation Metric:*** Difference in SRQs between the reference data and the computational results.





Categorization

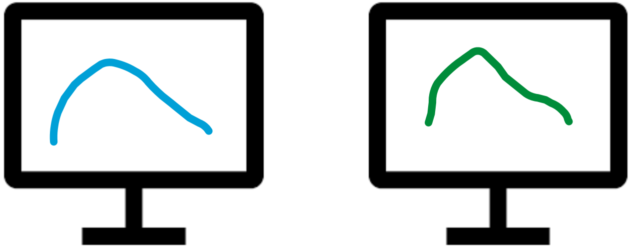
What is to be compared/verified/validated?

Type	Same	Different	Description granularity	Sanity check	Comparison metric
Code	ConcMod, MathMod, Disc	Imp	Finest	Solution match	Performance
Method	ConcMod, MathMod	Disc, Imp	Fine	Convergence	Diff to reference
Model	ConcMod	MathMod, Disc, Imp	Coarse	Calibration	Diff to (non-deterministic) reference

Categorization

Types of Reference Solutions

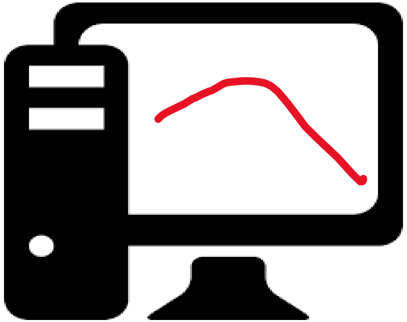
Code/Model/Method intercomparison



Analytical solution

$$y = f(t, x, \theta)$$

Numerical solution

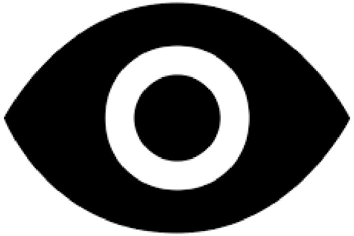


Experimental data

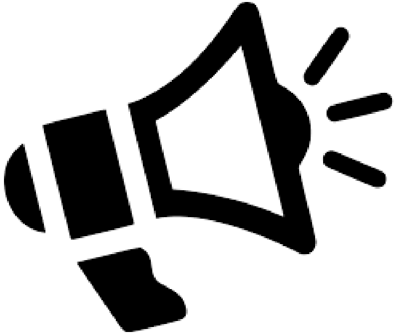
Categorization

Benchmarking Processes

Open or blind?



By invitation only or public call for participation?



Outline

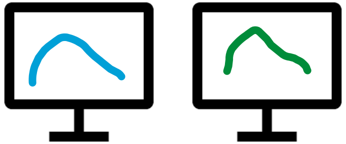
1. Motivation
2. Categorization
3. **Selected GCS Benchmark Studies**
    a. **The Classic**
    b. So Simple, Yet So Hard
    c. Reality Meets Modeling
    d. Back To Normal, But Bigger
4. Summary and Conclusion

Selected GCS Benchmark Studies

A benchmark study on problems related to CO_2 storage in geologic formations (2009)

- Code Comparison / Verification
- Public CFP
- First phase blind, second phase open process
- 14 groups, 14 simulators
- 3 Benchmark cases
- 1 case with semi-analytical solution, 2 without reference solution
- SRQs: Leakage rate / time, mass flux / time, arrival time, maximum leakage, saturation snapshots, performance
- Metrics: line plots

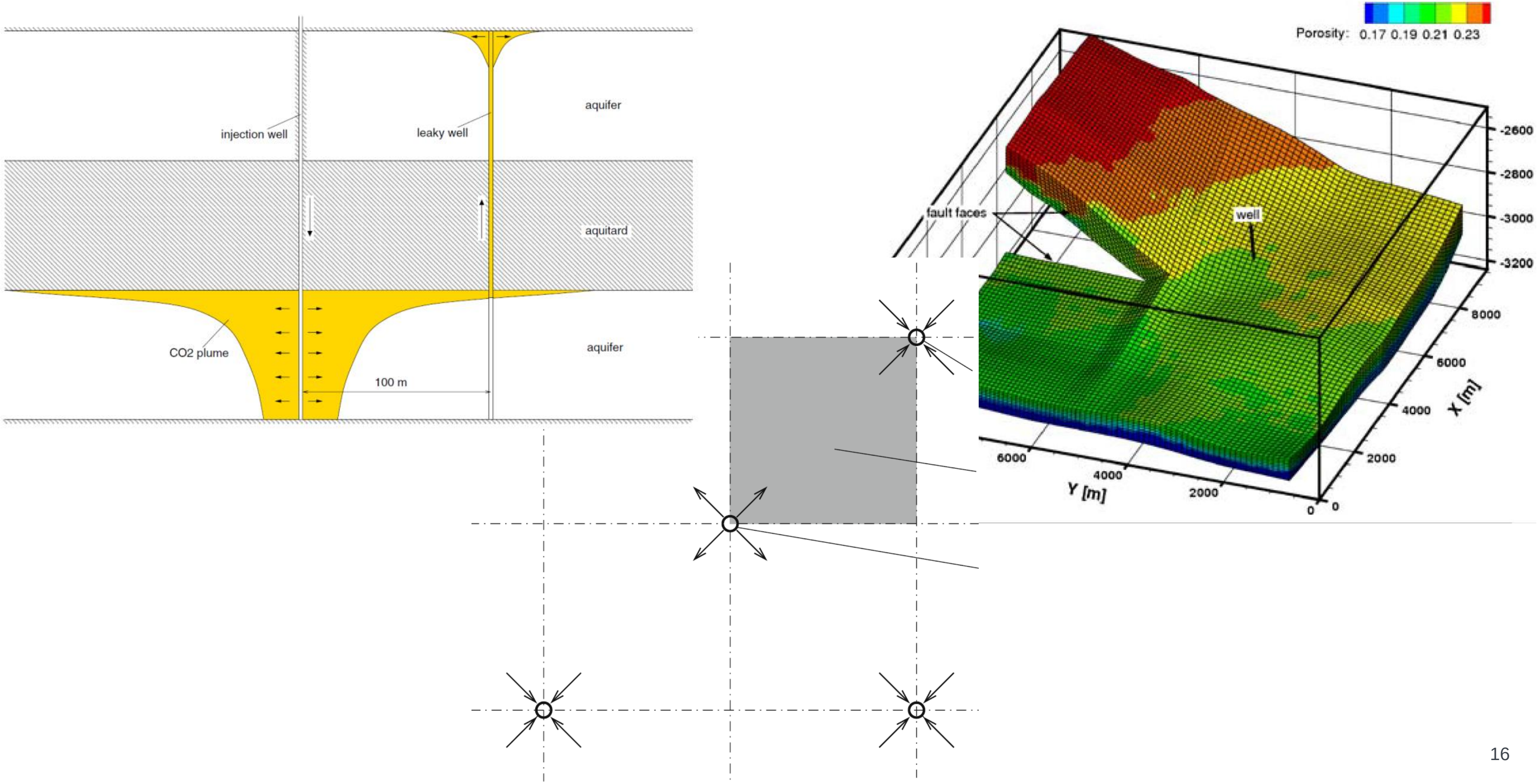
$$y = f(t, x, \theta)$$



H. Class, …, J. Nordbotten, …., B. Flemisch et al. (2009): “A benchmark study on problems related to CO2 storage in geologic formations“, *Computational Geosciences* 13, 409-434. DOI 10.1007/s10596-009-9146-x.

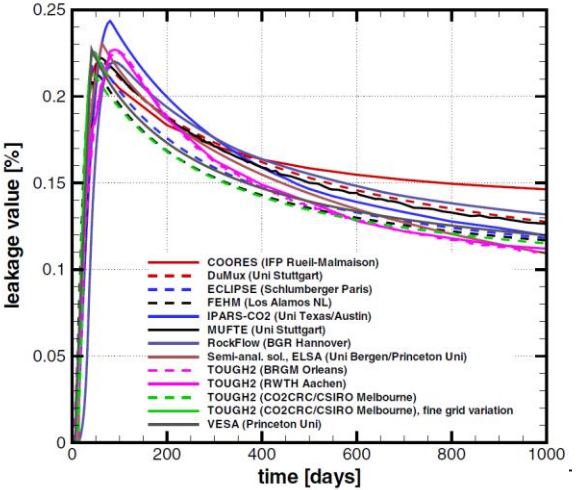
A benchmark study on problems related to CO_2 storage in geologic formations (2009)

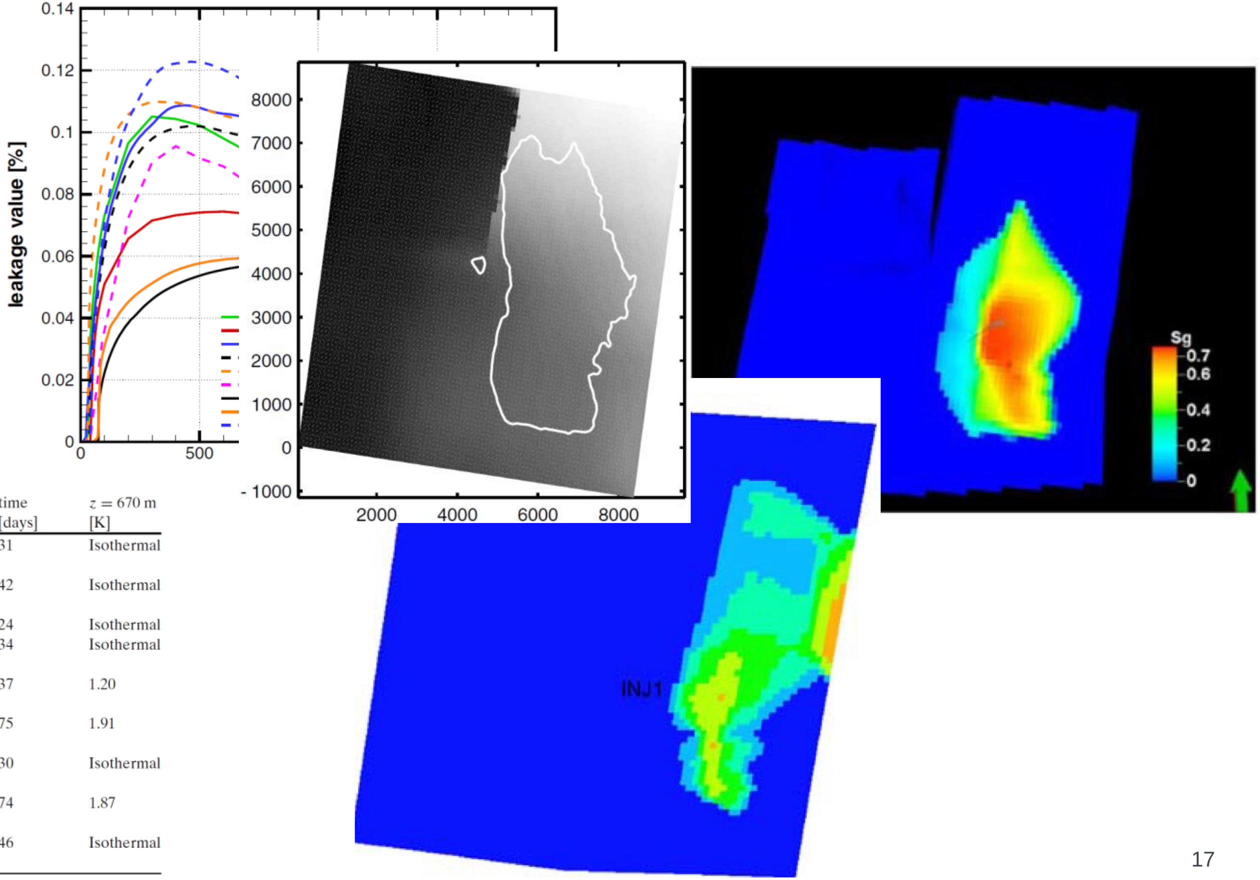
Benchmark Cases

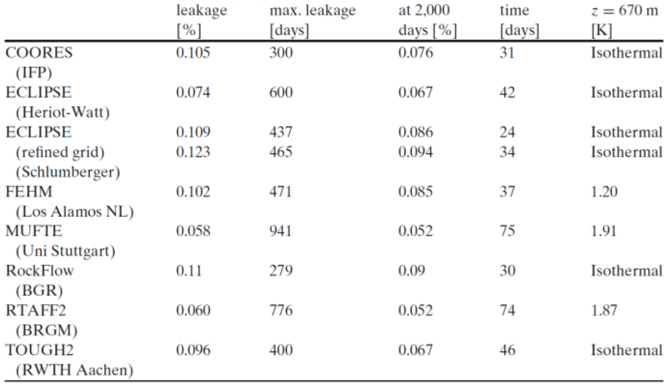


A benchmark study on problems related to CO_2 storage in geologic formations (2009)

SRQs, Measures and Metrics



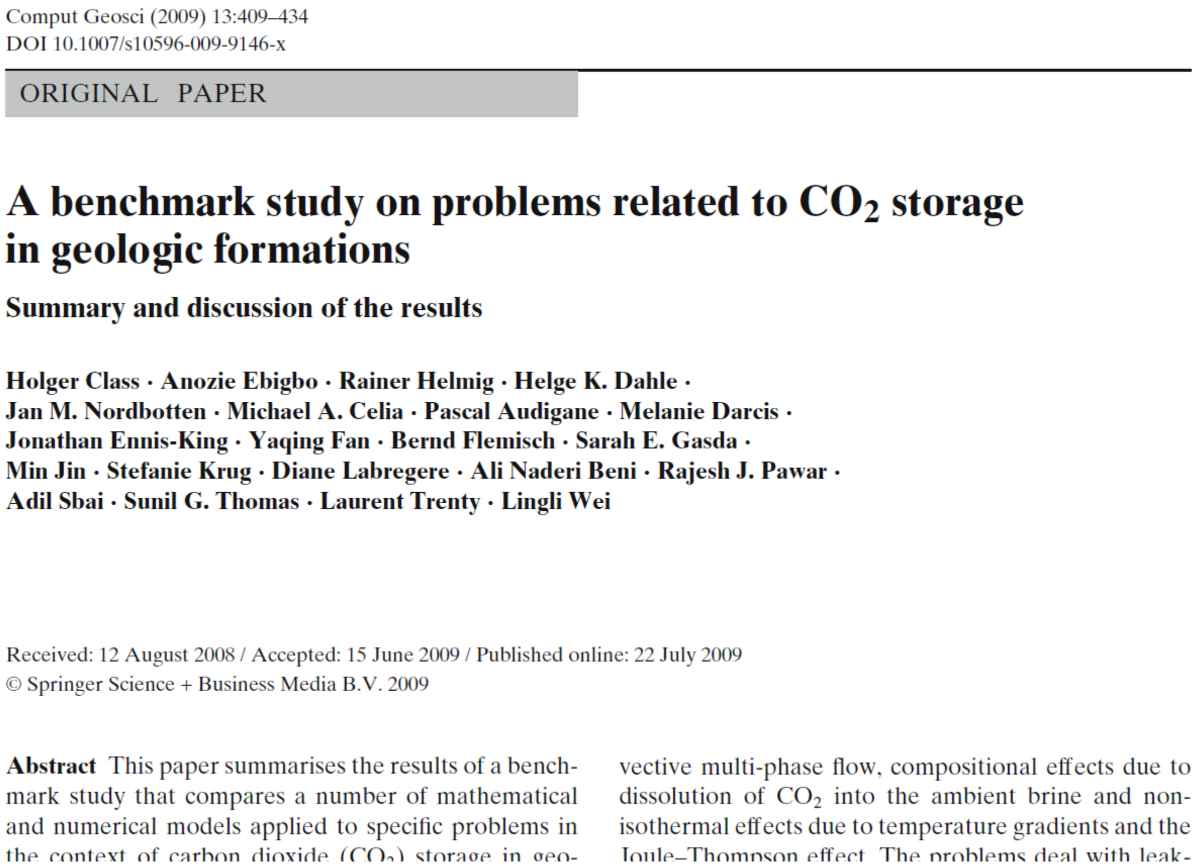




	leakage [%]	max. leakage [days]	at 2,000 days [%]	time [days]	$z = 670$ m [K]
COORES (IFP)	0.105	300	0.076	31	Isothermal
ECLIPSE (Heriot-Watt)	0.074	600	0.067	42	Isothermal
ECLIPSE	0.109	437	0.086	24	Isothermal
(refined grid) (Schlumberger)	0.123	465	0.094	34	Isothermal
FEHM (Los Alamos NL)	0.102	471	0.085	37	1.20
MUFTE (Uni Stuttgart)	0.058	941	0.052	75	1.91
RockFlow (BGR)	0.11	279	0.09	30	Isothermal
RTAFF2 (BRGM)	0.060	776	0.052	74	1.87
TOUGH2 (RWTH Aachen)	0.096	400	0.067	46	Isothermal

A benchmark study on problems related to CO_2 storage in geologic formations (2009)

Infrastructure for Comparison and Reproduction



Comput Geosci (2009) 13:409–434
DOI 10.1007/s10596-009-9146-x

ORIGINAL PAPER

A benchmark study on problems related to CO_2 storage in geologic formations

Summary and discussion of the results

**Holger Class · Anozie Ebigbo · Rainer Helmig · Helge K. Dahle ·
Jan M. Nordbotten · Michael A. Celia · Pascal Audigane · Melanie Darcis ·
Jonathan Ennis-King · Yaqing Fan · Bernd Flemisch · Sarah E. Gasda ·
Min Jin · Stefanie Krug · Diane Labregere · Ali Naderi Beni · Rajesh J. Pawar ·
Adil Sbai · Sunil G. Thomas · Laurent Trenty · Lingli Wei**

Received: 12 August 2008 / Accepted: 15 June 2009 / Published online: 22 July 2009

Abstract This paper summarises the results of a benchmark study that compares a number of mathematical and numerical models applied to specific problems in the context of carbon dioxide (CO_2) storage in geo-

vective multi-phase flow, compositional effects due to dissolution of CO_2 into the ambient brine and non-isothermal effects due to temperature gradients and the Joule–Thompson effect. The problems deal with leak-

Outline

1. Motivation
2. Categorization
3. **Selected GCS Benchmark Studies**
    a. The Classic
    b. **So Simple, Yet So Hard**
    c. Reality Meets Modeling
    d. Back To Normal, But Bigger
4. Summary and Conclusion

Selected GCS Benchmark Studies

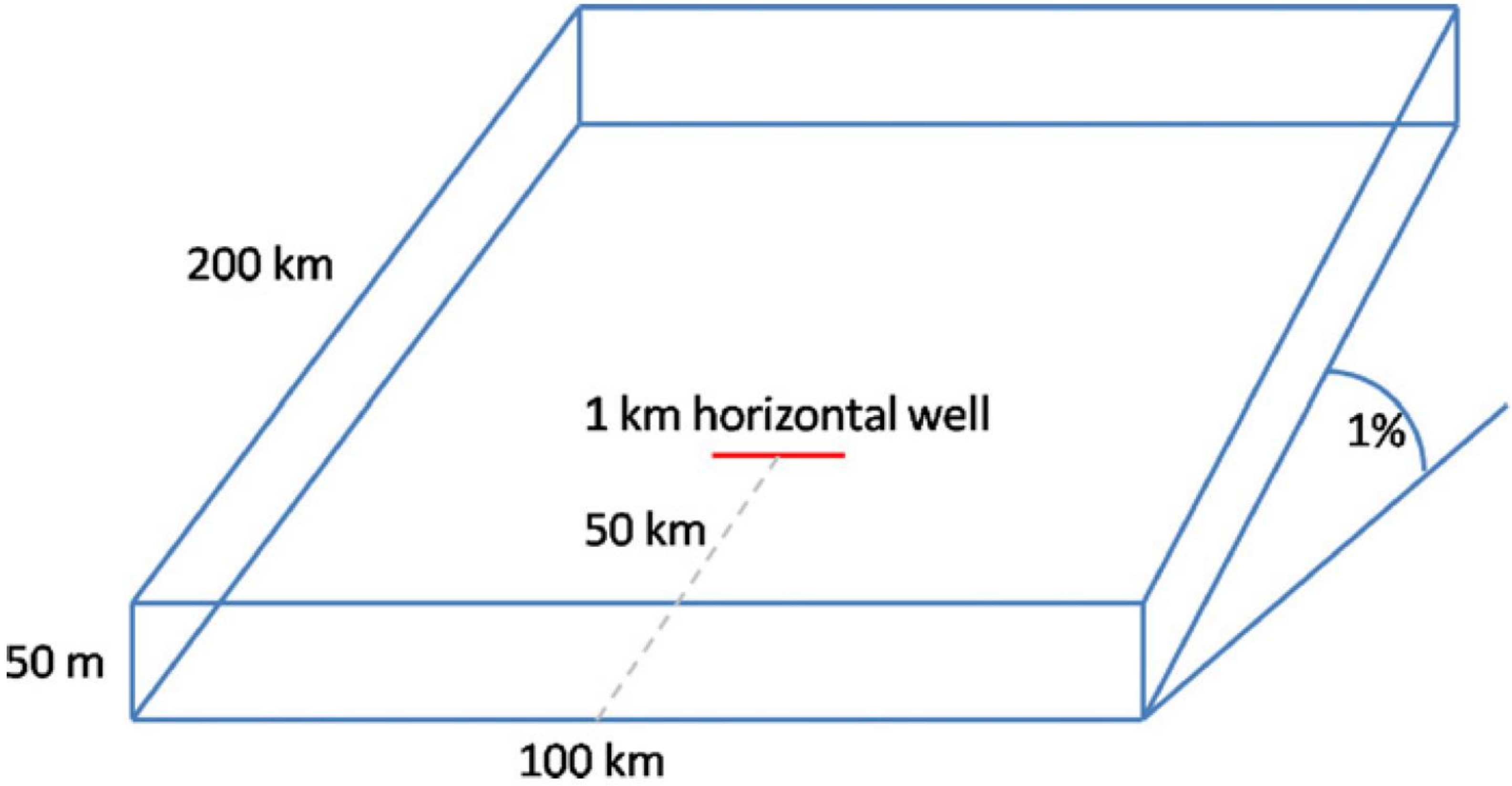
Uncertainties in practical simulation of CO_2 storage (2012)

- Model / code comparison
- By invitation, open process
- 6 groups, 6 simulators
- 1 Benchmark case
- No reference solution
- SRQs: phase partitioning, furthest updip plume extent, mean and variance of the location of the CO_2 phase, all over time
- Metrics: Line plots

J.M. Nordbotten, B. Flemisch, S.E. Gasda, H.M. Nilsen, Y. Fan, G.E. Pickup, B. Wiese, M.A. Celia, H.K. Dahle, G.T. Eigestad, K. Pruess (2012): “Uncertainties in practical simulation of CO2 storage“, *International Journal of Greenhouse Gas Control* 9, 234-242. DOI 10.1016/j.ijggc.2012.03.007.

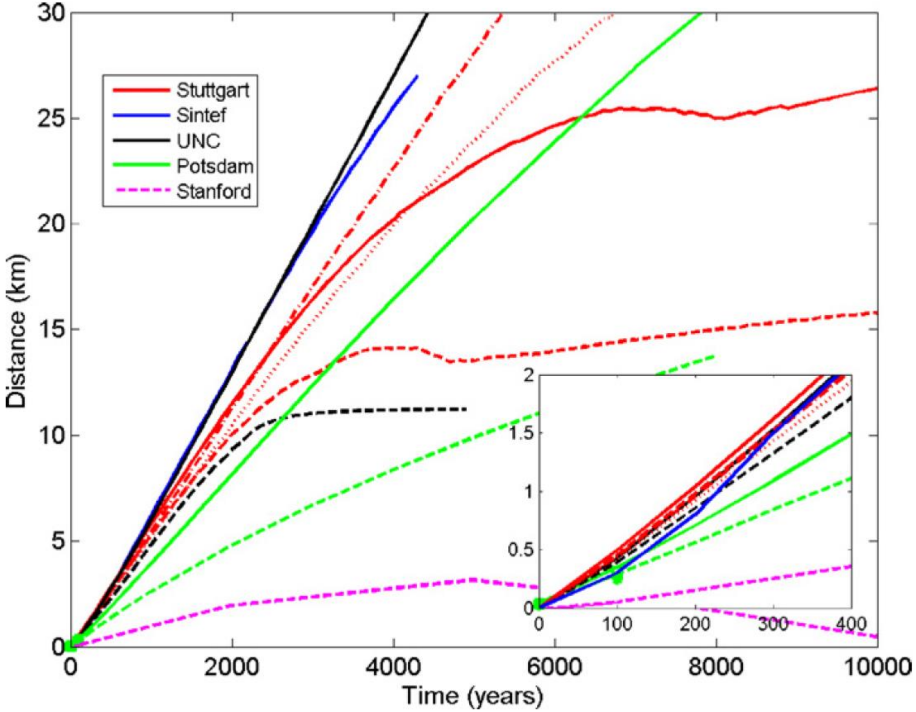
Uncertainties in practical simulation of CO2 storage (2012)

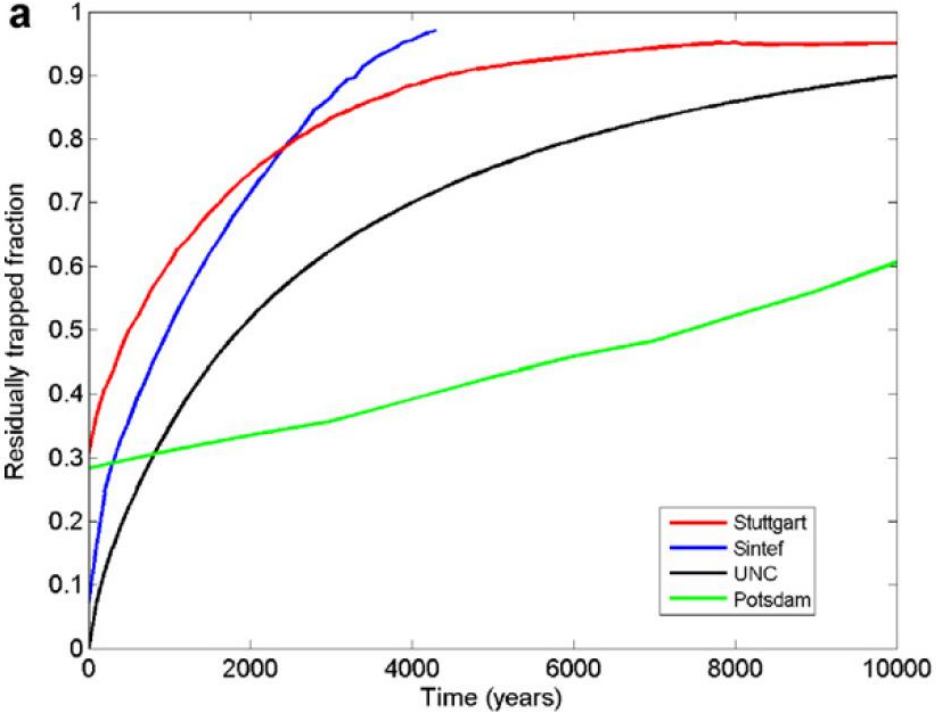
Benchmark Case



Uncertainties in practical simulation of CO2 storage (2012)

SRQs, Measures and Metrics





Uncertainties in practical simulation of CO2 storage (2012)

Infrastructure for Comparison and Reproduction

International Journal of Greenhouse Gas Control 9 (2012) 234–242

Contents lists available at SciVerse ScienceDirect

International Journal of Greenhouse Gas Control

journal homepage: www.elsevier.com/locate/ijggc

Uncertainties in practical simulation of CO_2 storage

J.M. Nordbotten*, B. Flemisch, S.E. Gasda, H.M. Nilsen, Y. Fan, G.E. Pickup, B. Wiese, M.A. Celia,
H.K. Dahle, G.T. Eigestad, K. Pruess

University of Bergen, Department of Mathematics, PB 7800, 5020 Bergen, Norway

ARTICLE INFO

Article history:
Received 27 October 2011
Received in revised form 15 March 2012
Accepted 16 March 2012
Available online 26 April 2012

ABSTRACT

Practical simulation of CO_2 storage in geological formations inherently involves decisions concerning relevant physics, upscaling, and numerical modeling. These decisions are unavoidable, since the full problem cannot be resolved by existing numerical approaches. Here, we report on the impact of three distinct approaches to make the problem computationally tractable: reduced physics, upscaling, and non-converged discretizations. Compounding these different strategies, we have used a benchmark study to

Outline

1. Motivation
2. Categorization
3. **Selected GCS Benchmark Studies**
    1. The Classic
    2. So Simple, Yet So Hard
    3. **Reality Meets Modeling**
    4. Back To Normal, But Bigger
4. Summary and Conclusion

Selected GCS Benchmark Studies

FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

- Validation / Model comparison
- Invitation-only, multi-stage blind/open process
- 9 groups, 9 models
- Data from **5 experimental runs**
- SRQs:
  - Saturation and concentration fields at selected time steps
  - Integrated phase composition … over time
  - **Mean and std dev** for various quantities
- Metrics: Multiple, e.g., Wasserstein distance
- Other reported characteristics: Model assumptions, implementation details, …

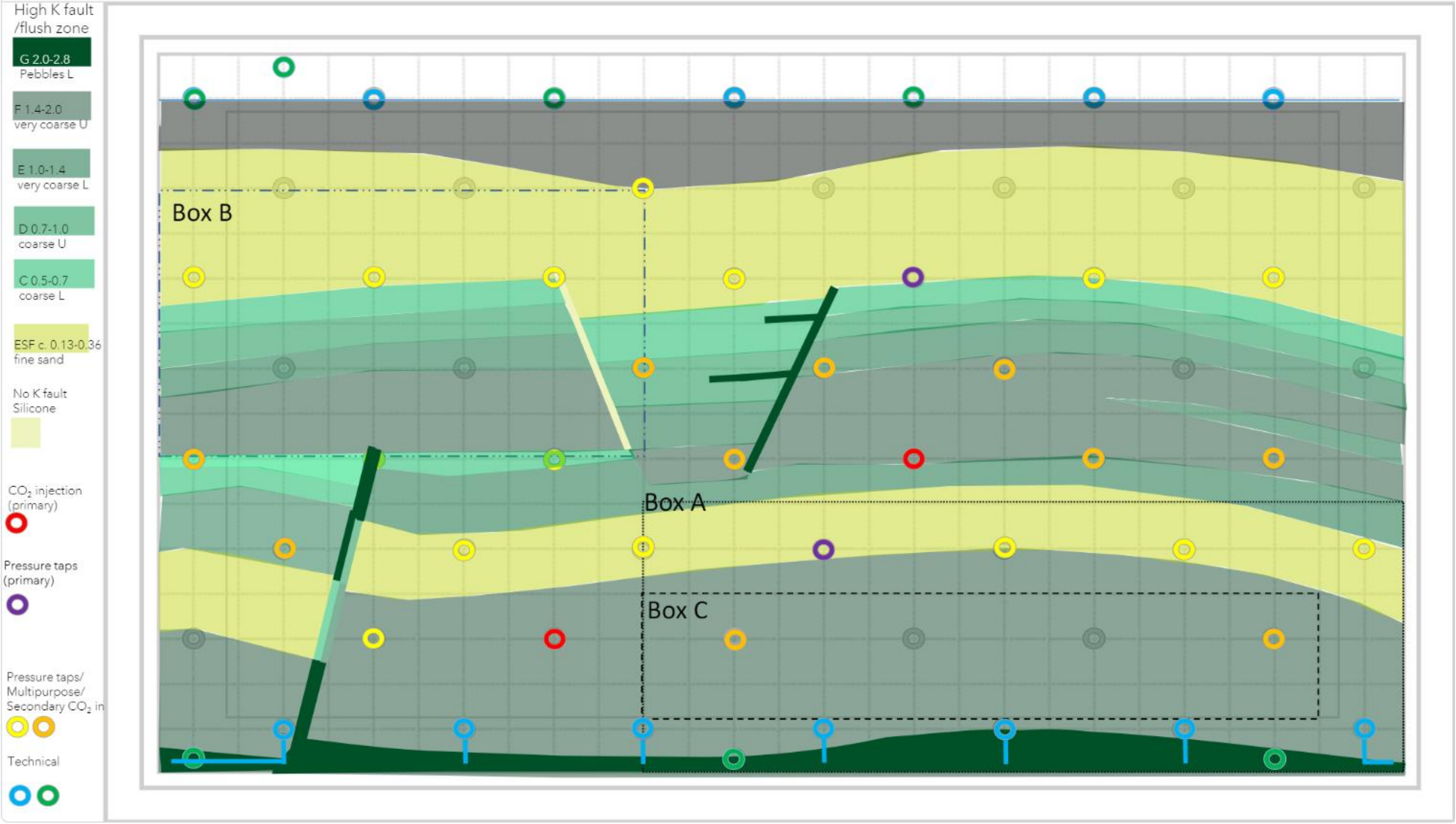
J. Nordbotten, M. Fernø, B. Flemisch, R. Juanes (eds.) (2024): “FluidFlower: A Meter-scale Experimental Laboratory for Geological CO2 Storage“, *TiPM Special Issue (in production)*.

FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Experimental Rig

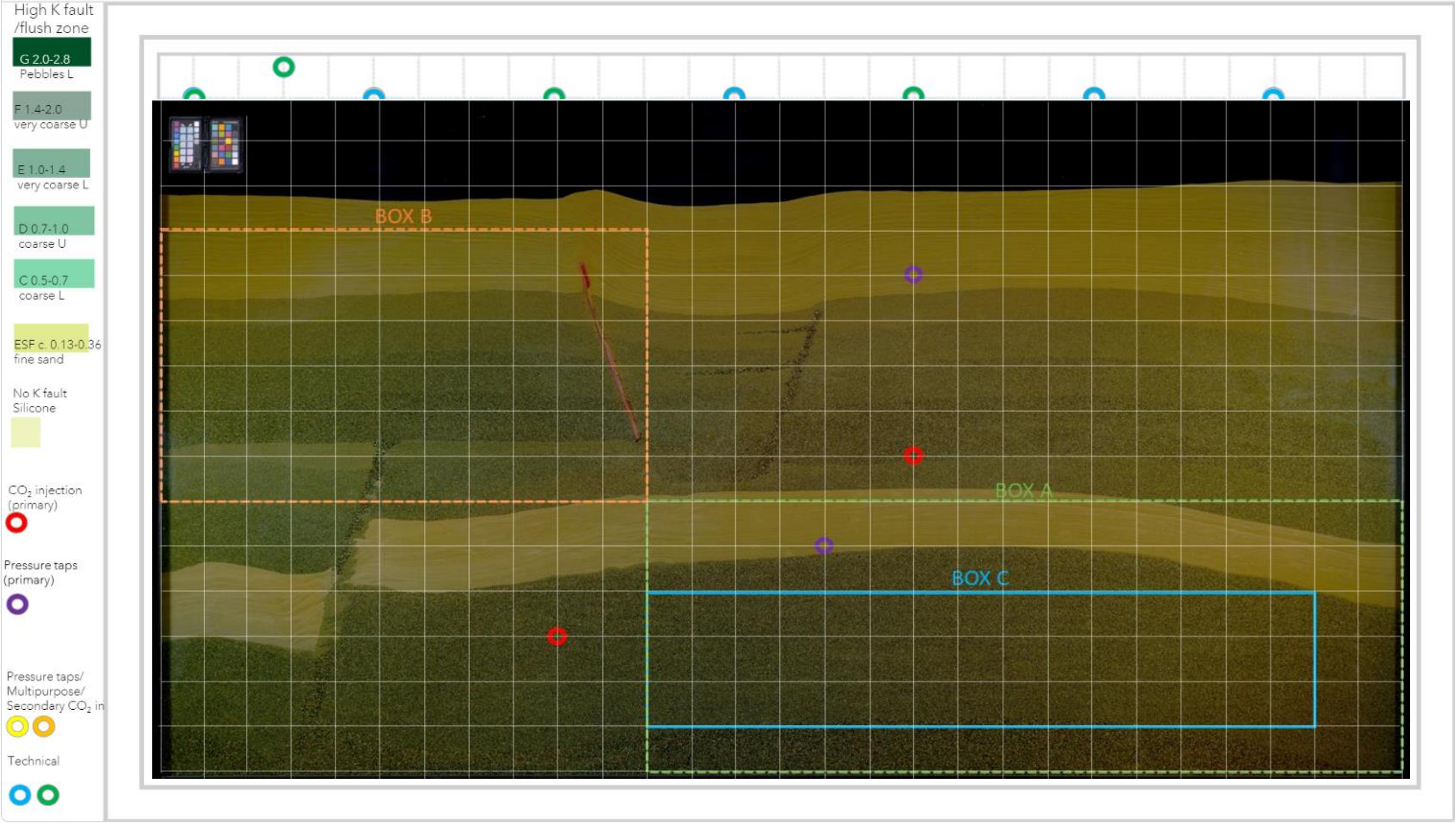
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Intended Geometry



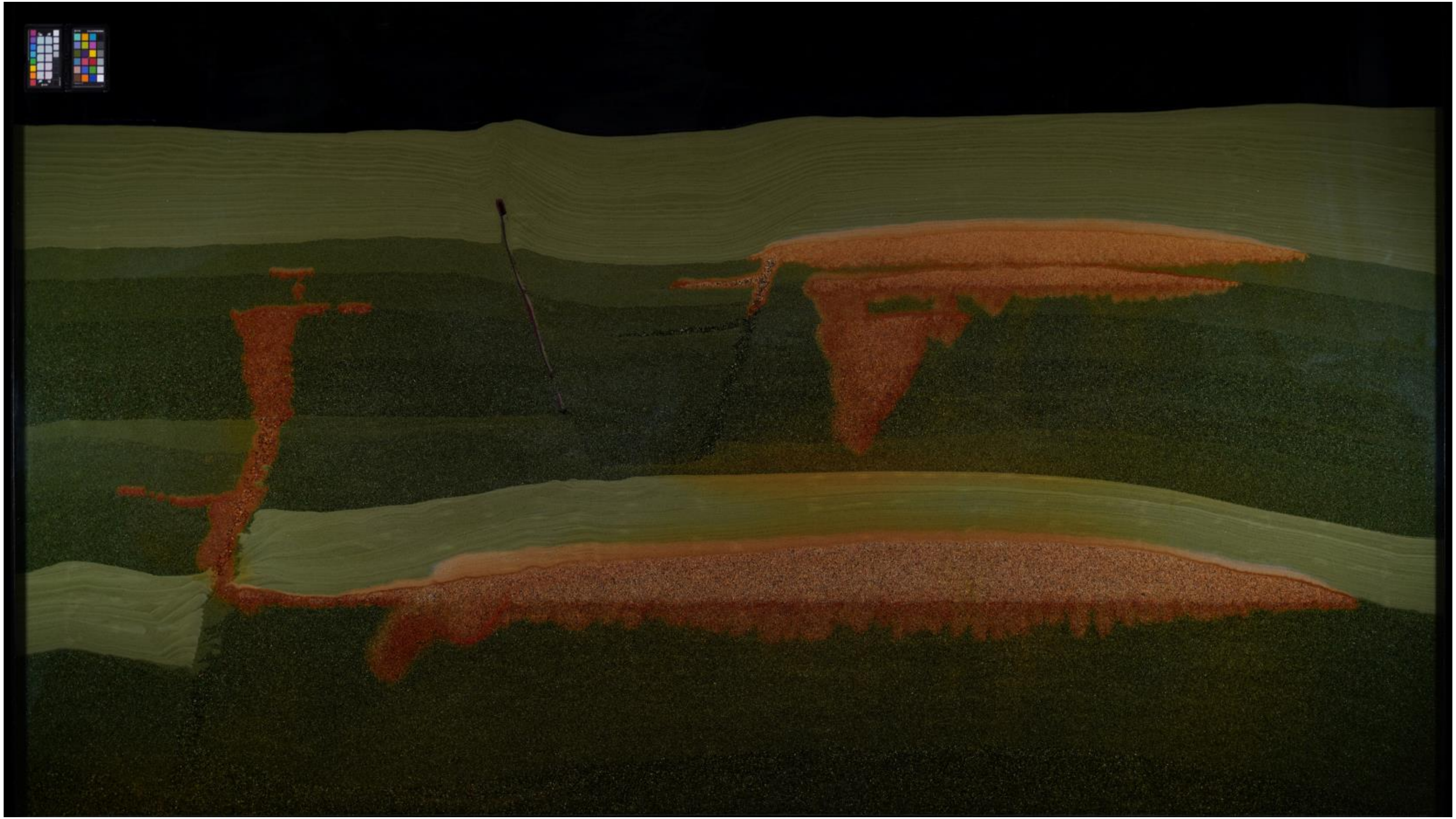
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Implemented Geometry



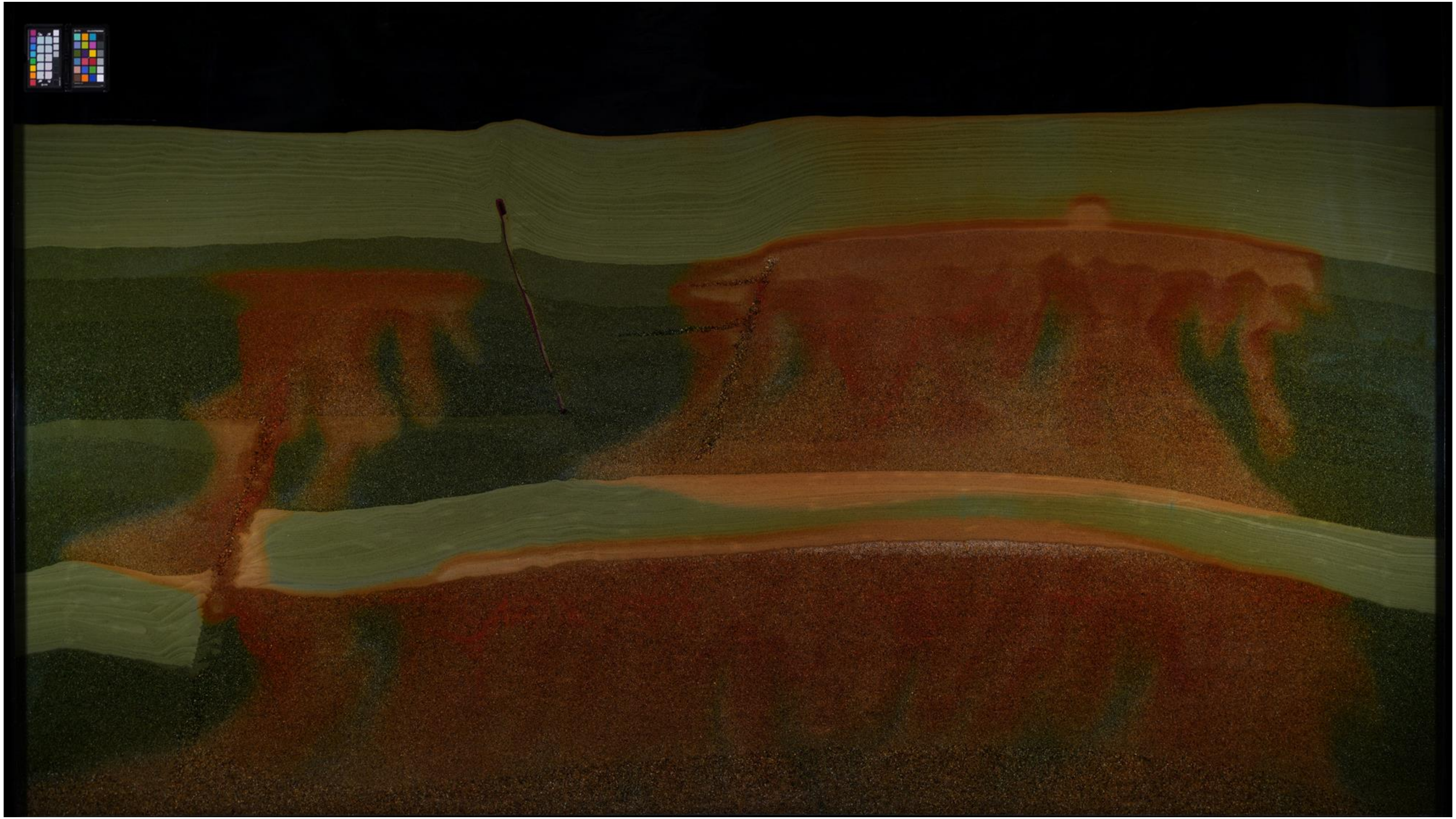
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Snapshot after 240 Minutes = 4 Hours



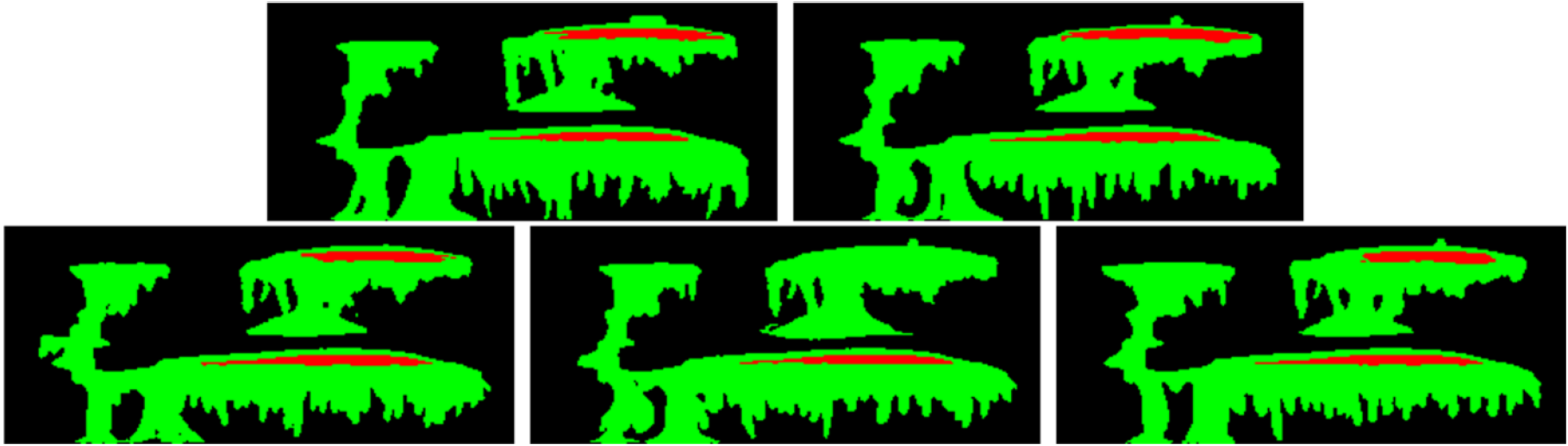
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Snapshot after 4320 Minutes = 72 Hours



FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

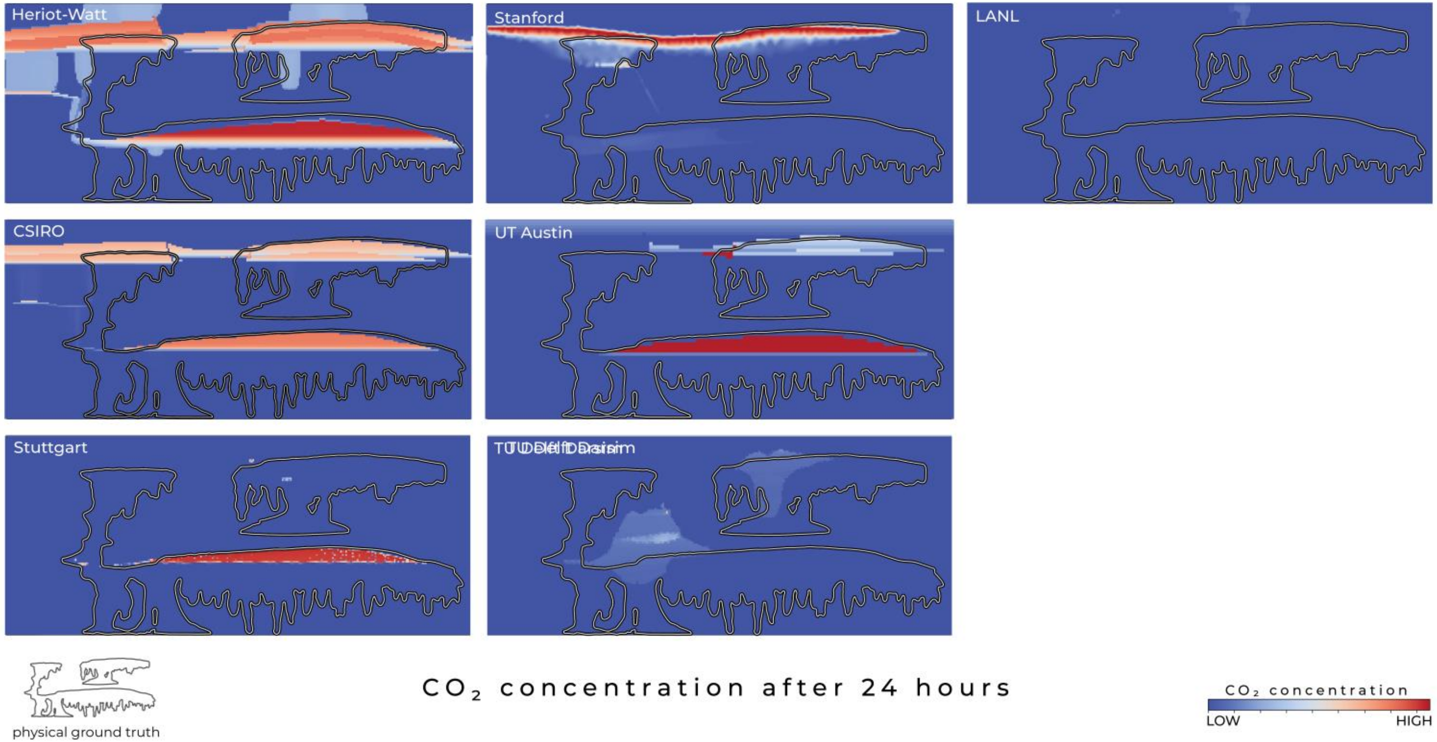
Five Operationally Identical Experimental Runs



Segmentation data after 24 hours.

FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

This experiment is hard to forecast independently

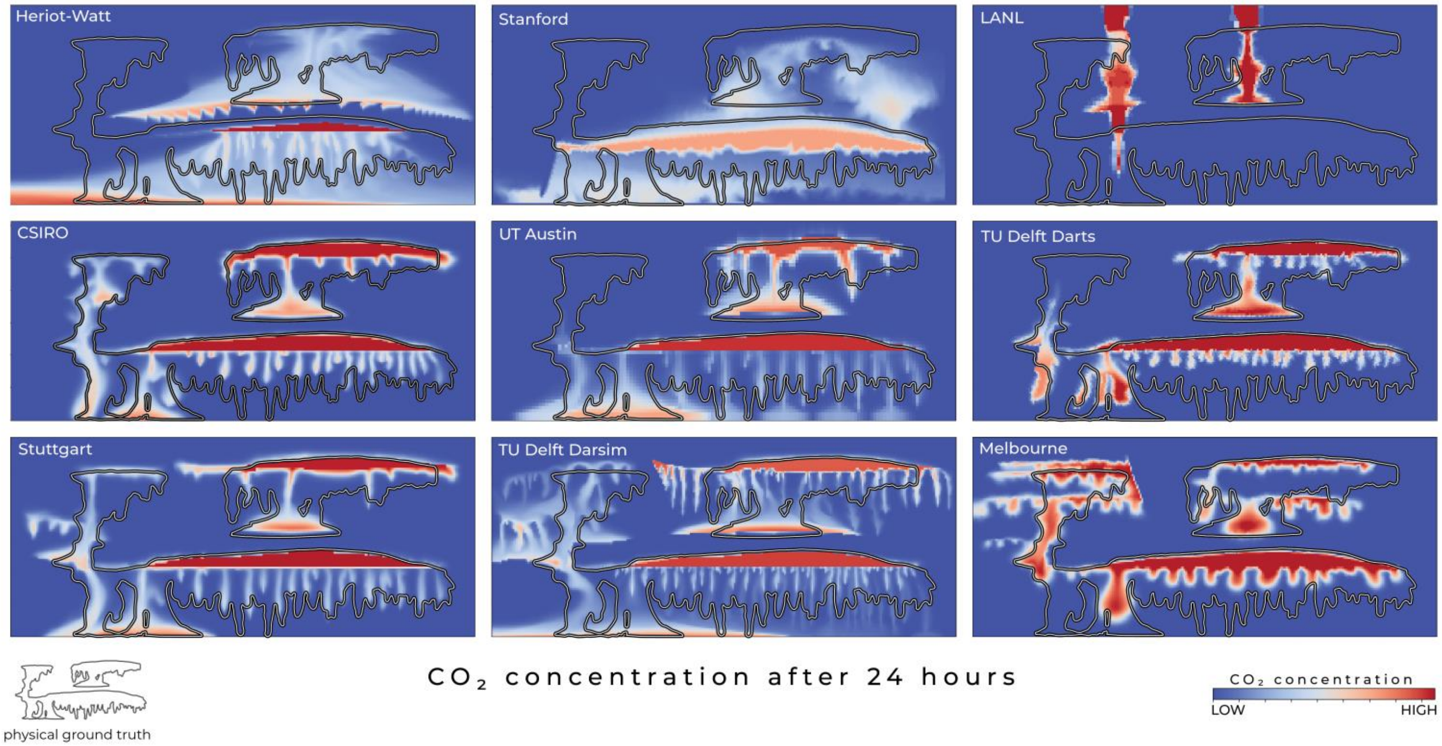


CO_2 concentration after 24 hours

Flemisch et al., https://github.com/fluidflower

FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

This experiment is hard to forecast collaboratively



Flemisch et al., 2023. Simulations show CO_2 concentration

FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Can We Quantify the Difference?

- Apply the **Wasserstein metric,** working on distributions of equal mass.
- Measures "the **minimal effort required to reconfigure the mass** of one distribution in order to recover the other distribution".
- Approximate roughly the **CO_2 mass density in each cell** by

$$\widetilde{m} = \varrho_{\mathrm{g}} s + c(1 - s)$$

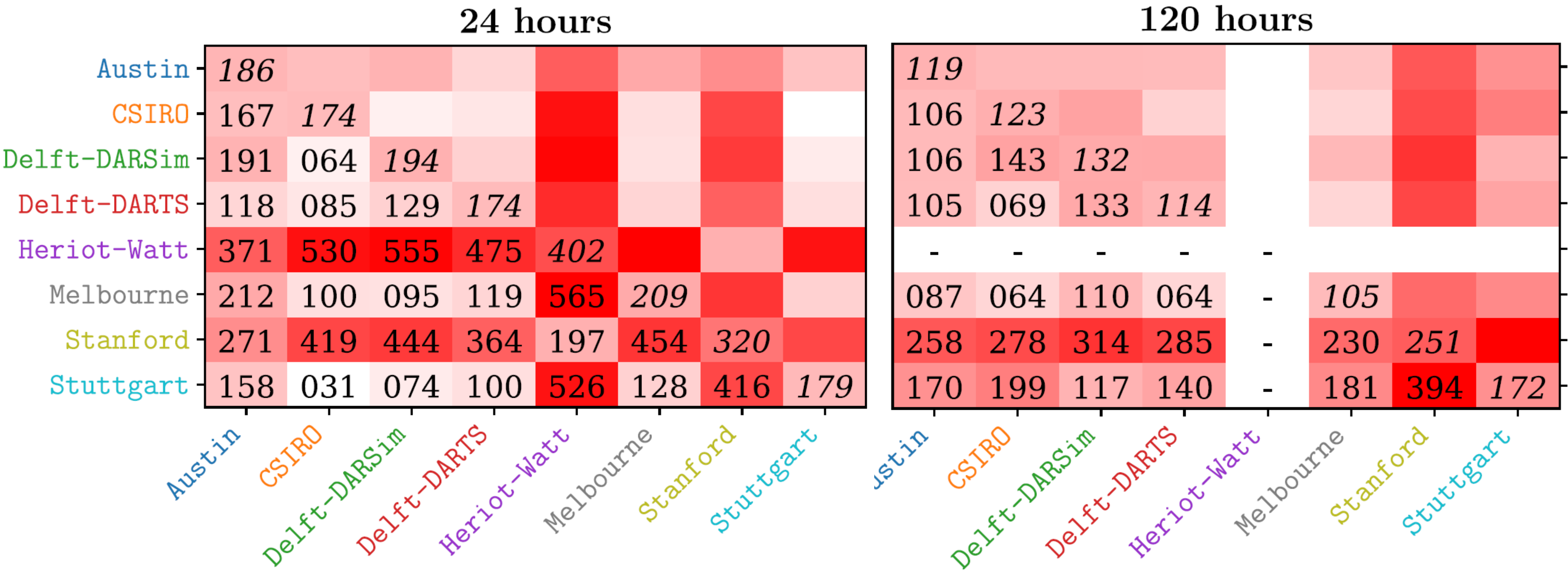
- **Normalize** these values to two-dimensional probability distributions.
- Apply the Python library **POT** to calculate the Wasserstein distances.
- **Rescaling** to the injected CO_2 mass yields distances of dimension **mass times length.**

V. Panaretos, Y. Zemel (2019): "Statistical aspects of Wasserstein distances", *Ann. Rev. Stat. Appl.* 1, 405–431.
DOI [10.1146/annurev-statistics-030718-104938J](https://doi.org/10.1146/annurev-statistics-030718-104938J).

R. Flamary et al. (2021): „POT: python optimal transport", *J. Mach. Learn. Res.* 22, 1–8. Repo at github.com/PythonOT/POT.

FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Wasserstein Distances Between Forecasts



24 hours

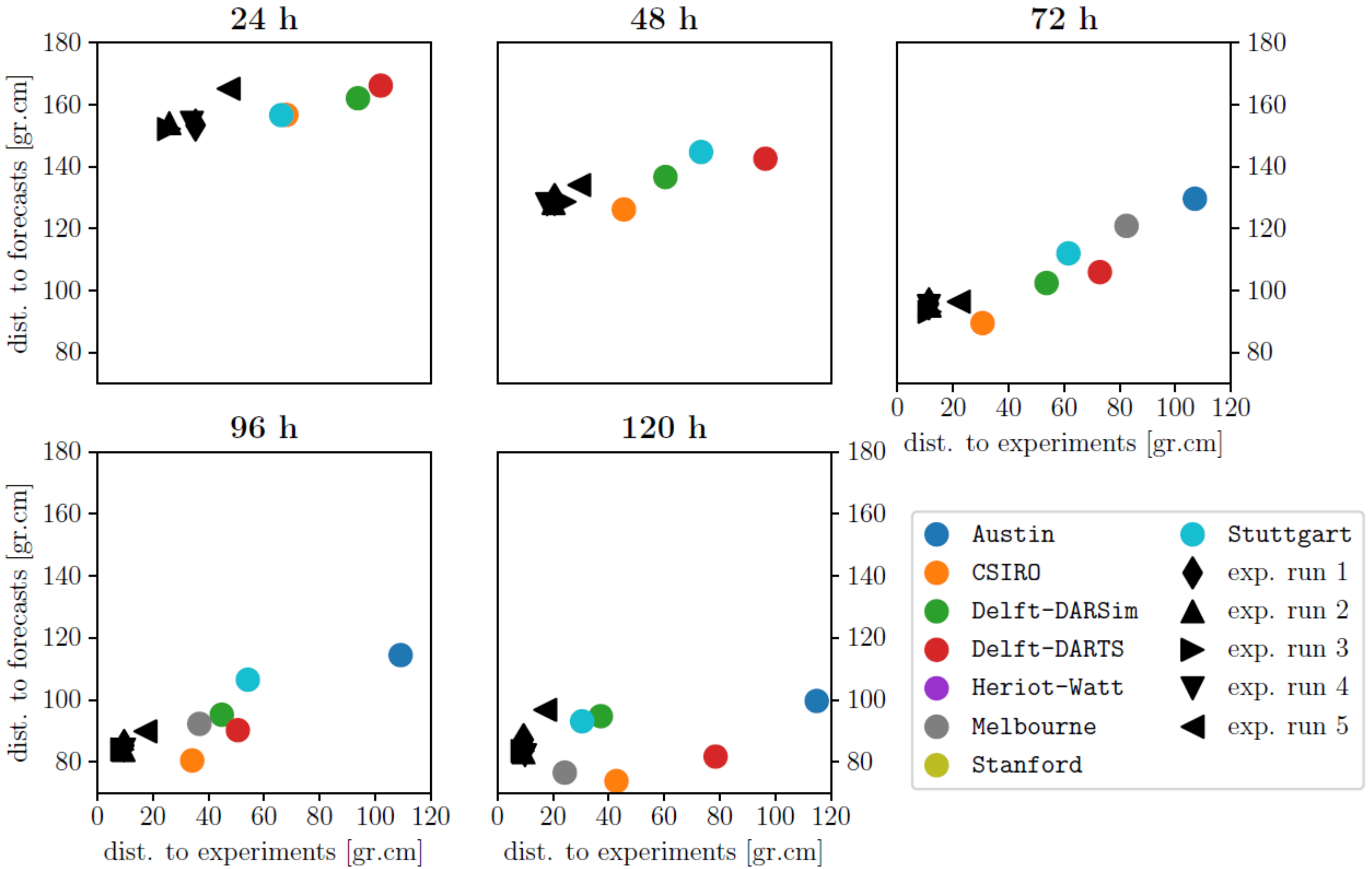
	Austin	CSIRO	Delft-DARSim	Delft-DARTS	Heriot-Watt	Melbourne	Stanford	Stuttgart
Austin	*186*							
CSIRO	167	*174*						
Delft-DARSim	191	064	*194*					
Delft-DARTS	118	085	129	*174*				
Heriot-Watt	371	530	555	475	*402*			
Melbourne	212	100	095	119	565	*209*		
Stanford	271	419	444	364	197	454	*320*	
Stuttgart	158	031	074	100	526	128	416	*179*

120 hours

	stin	CSIRO	Delft-DARSim	Delft-DARTS	Heriot-Watt	Melbourne	Stanford	Stuttgart
Austin	*119*							
CSIRO	106	*123*						
Delft-DARSim	106	143	*132*					
Delft-DARTS	105	069	133	*114*				
Heriot-Watt	-	-	-	-	-			
Melbourne	087	064	110	064	-	*105*		
Stanford	258	278	314	285	-	230	*251*	
Stuttgart	170	199	117	140	-	181	394	*172*

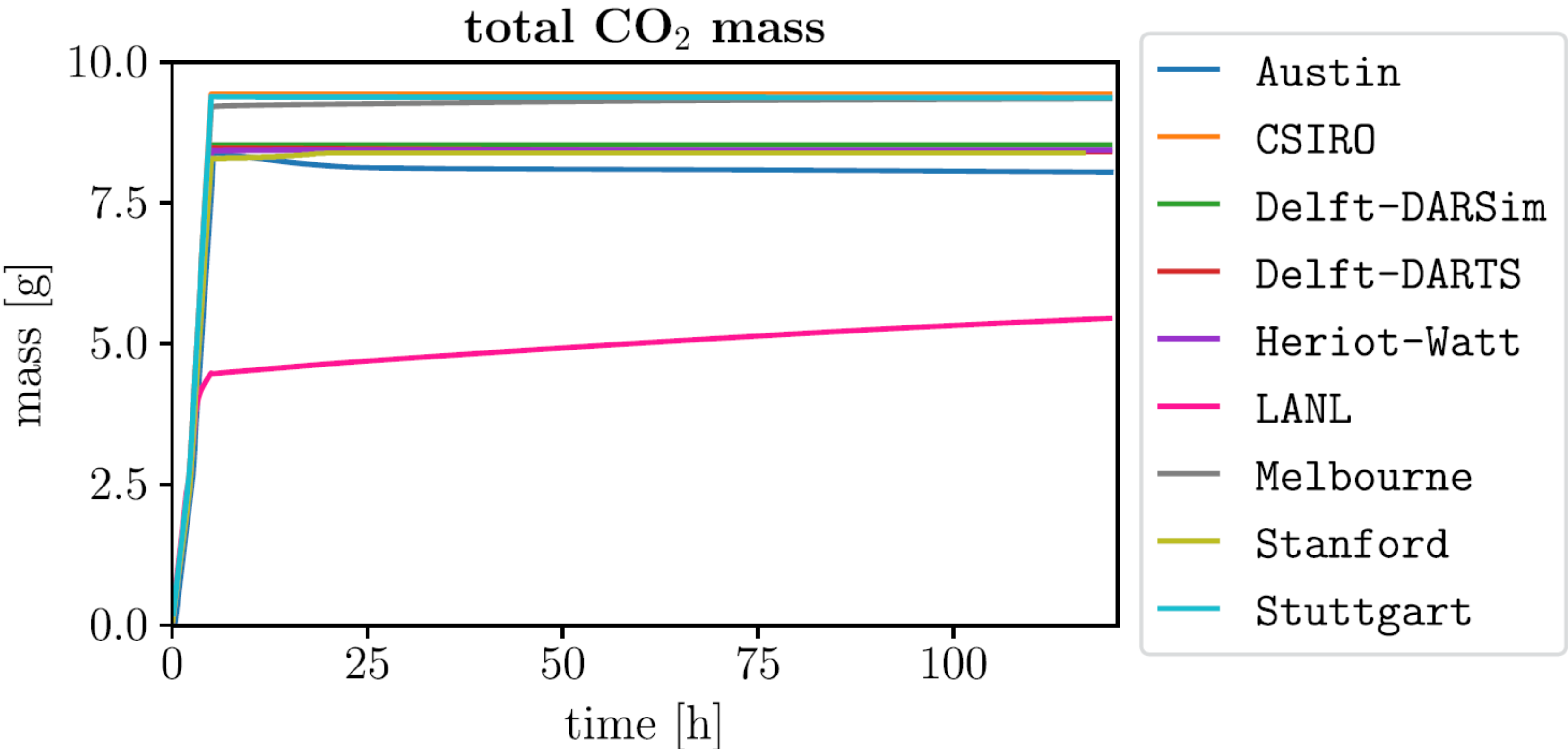
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Mean Wasserstein Distances To Forecasts and Experiments



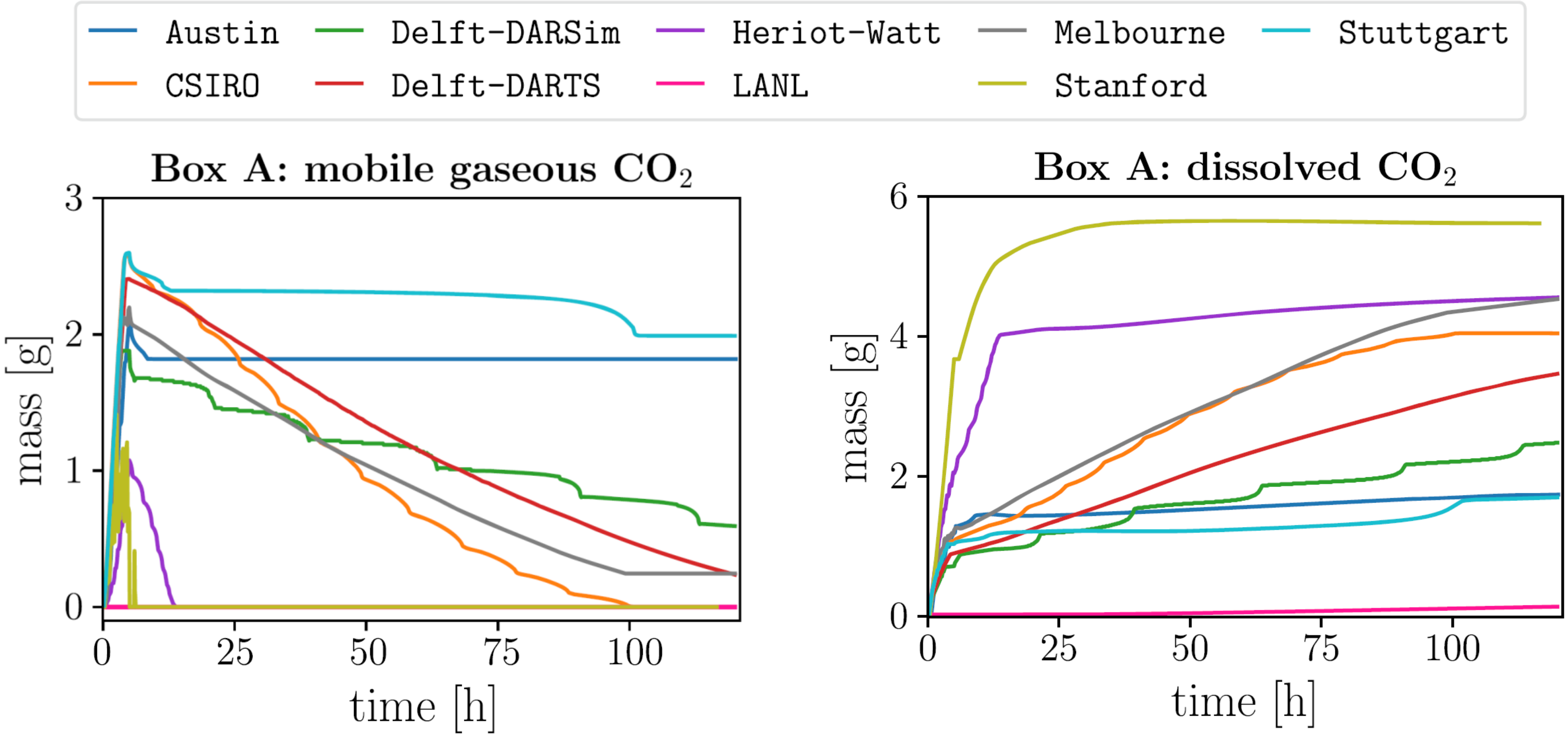
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Temporal Evolution of Total CO_2 mass in the computational domain



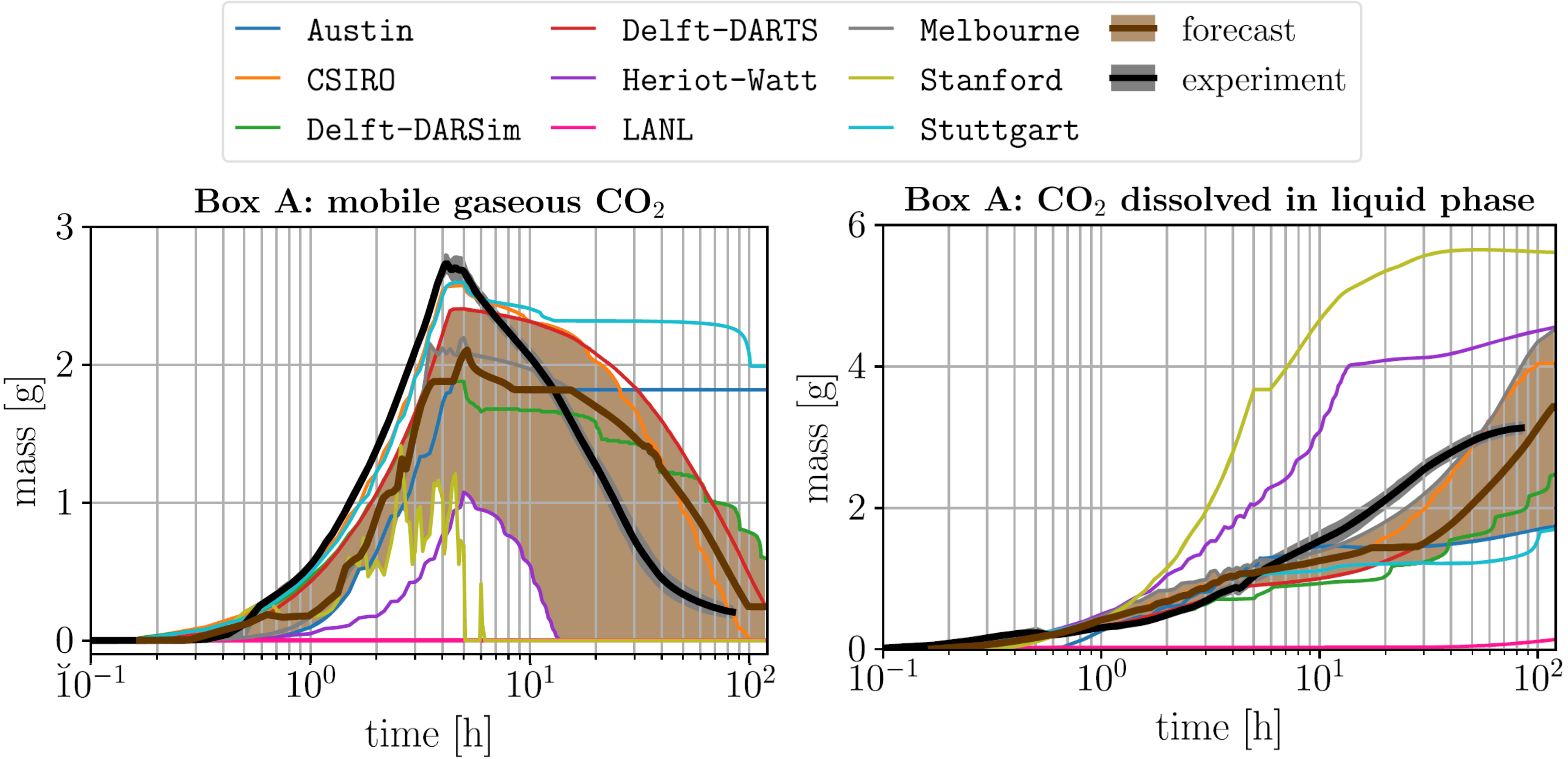
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

CO_2 Phase Distribution in Box A: Forecasts



FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

CO_2 Phase Distribution in Box A: Comparison



FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Sparse Data: SRQs

1. *As a proxy for assessing **risk of mechanical disturbance** of the overburden*:
   Maximum pressure at sensor number 1 and 2.
2. *As a proxy for when **leakage risk** starts declining*:
   Time of maximum mobile free phase in Box A.
3. *As a proxy for our ability to accurately predict **near well phase partitioning***:
   CO_2 phase distribution in Box A at 72 hours after injection starts.
4. *As a proxy for our ability to **handle uncertain geological features***:
   CO_2 phase distribution in Box B at 72 hours after injection starts.
5. *As a proxy for our ability to capture **onset of convective mixing***:
   Time for which a measure for finger length first exceeds 110% of the width of Box C.
6. *As a proxy for our ability to capture **migration into low-permeable seals***:
   Total mass of CO_2 in the top seal facies at final time.

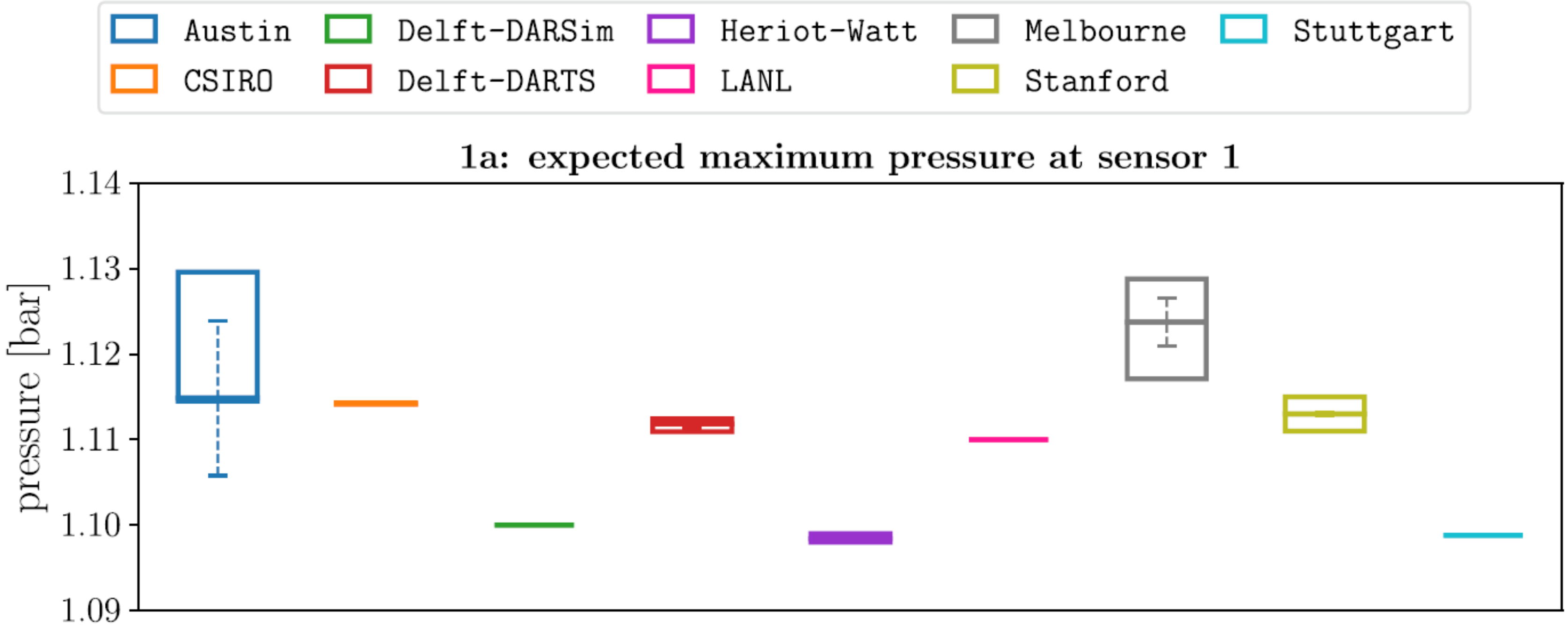
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Sparse Data: Reporting

- Each item had to be reported as **six numbers:**
  - prediction of the **mean** (stated as P10, P50 and P90)
  - prediction of the **standard deviation** (again as P10, P50, P90)
- **Any preferred methodology** could be chosen
  - ensemble runs
  - formal methods of uncertainty quantification
  - human intuition from experience
  - …
- Most groups **did not report** P10 and P90 for the standard deviations.

FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

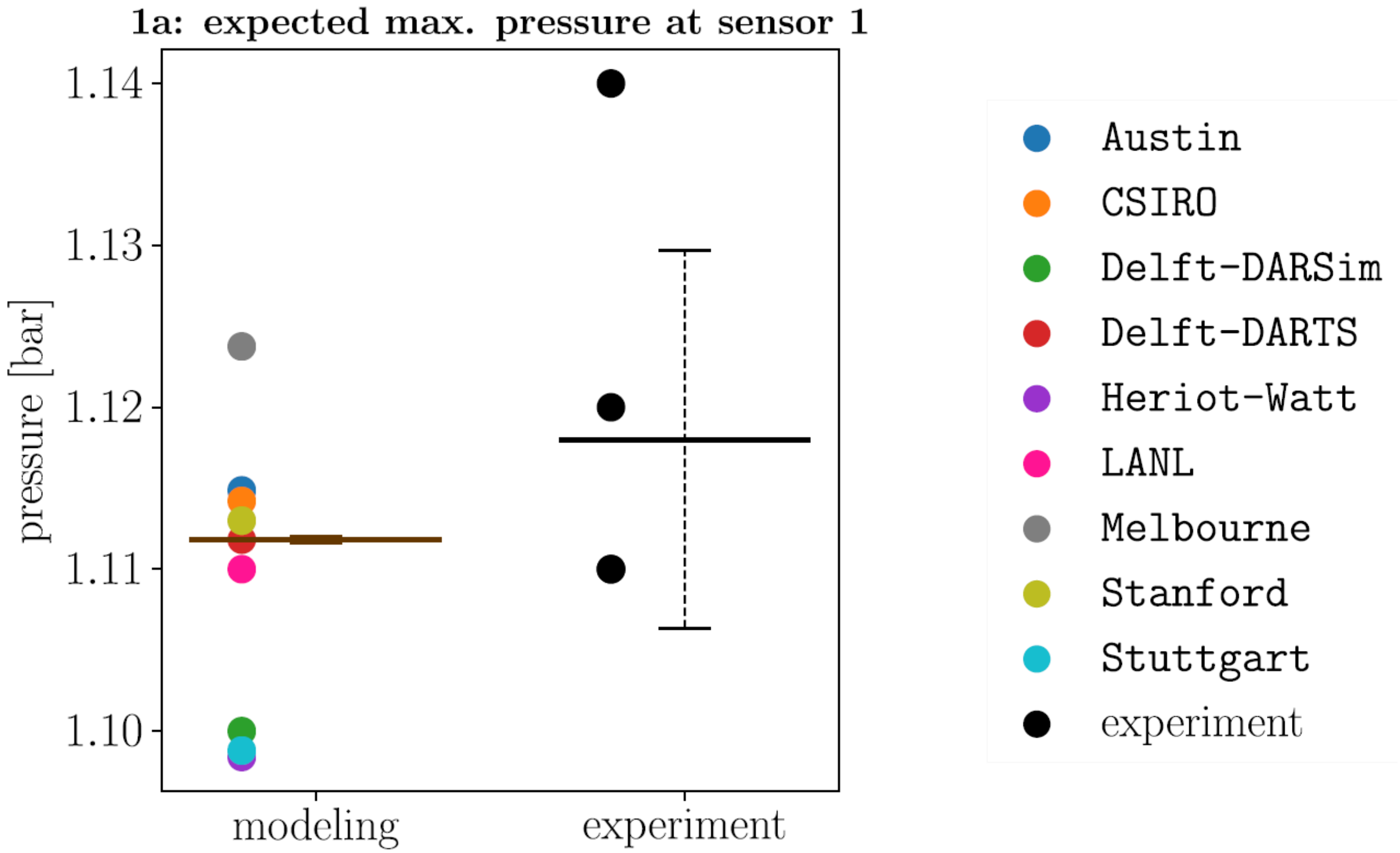
Sparse Data: Forecasts of Pressure at Sensor 1



Typical pressure variation in Bergen during experim. timespan

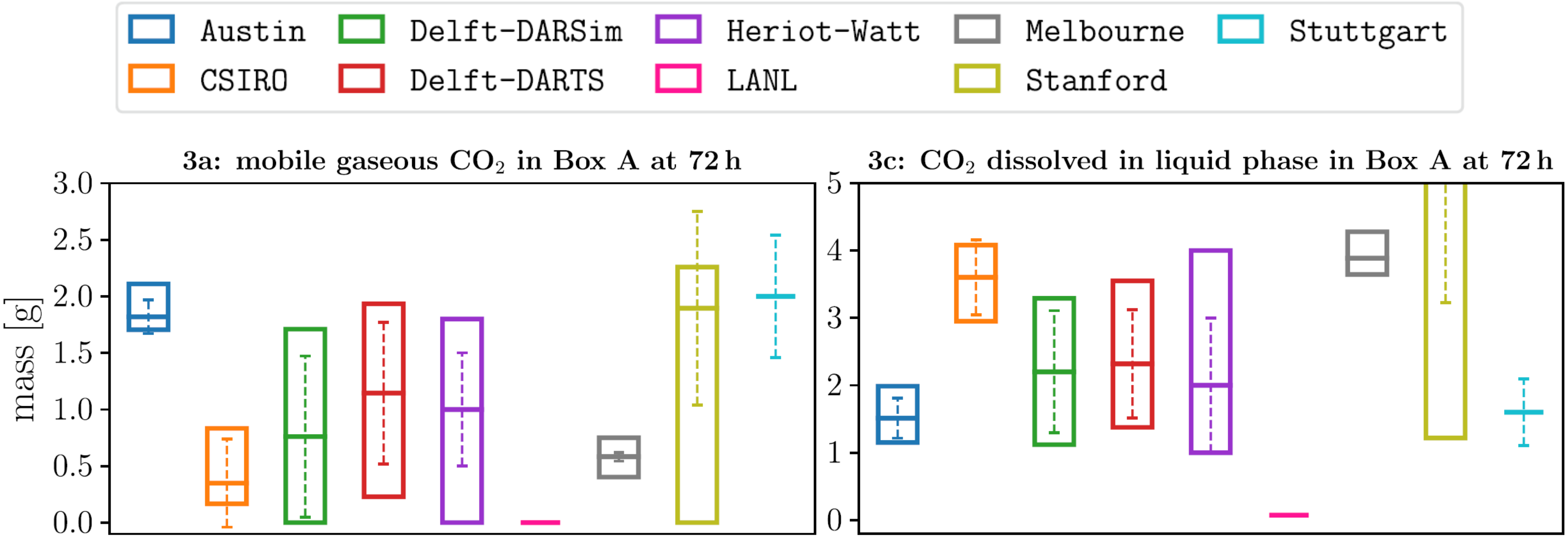
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Sparse Data: Comparison of Pressure at Sensor 1



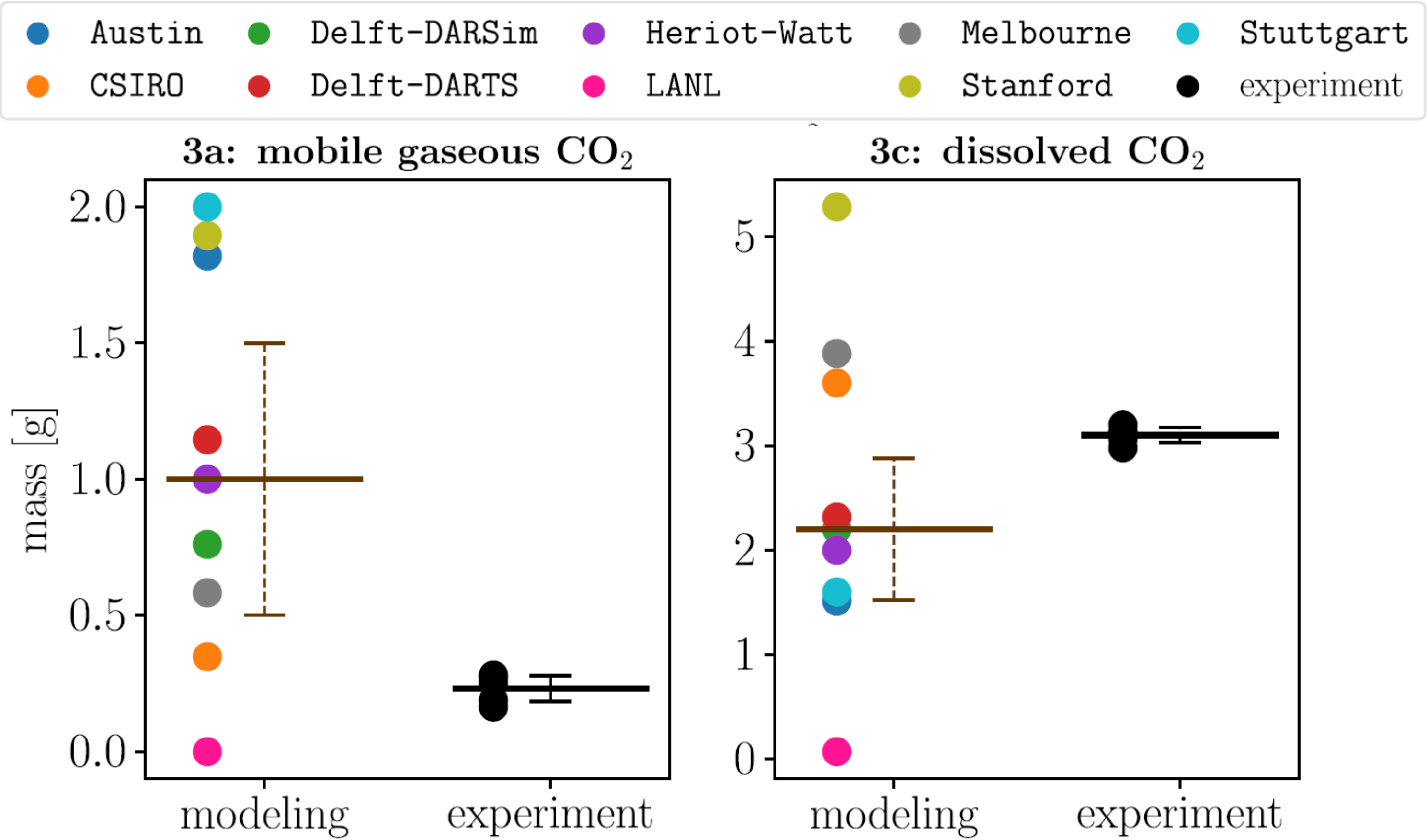
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Sparse Data: Forecasts of CO_2 Phase Composition in Box A at 72 hours



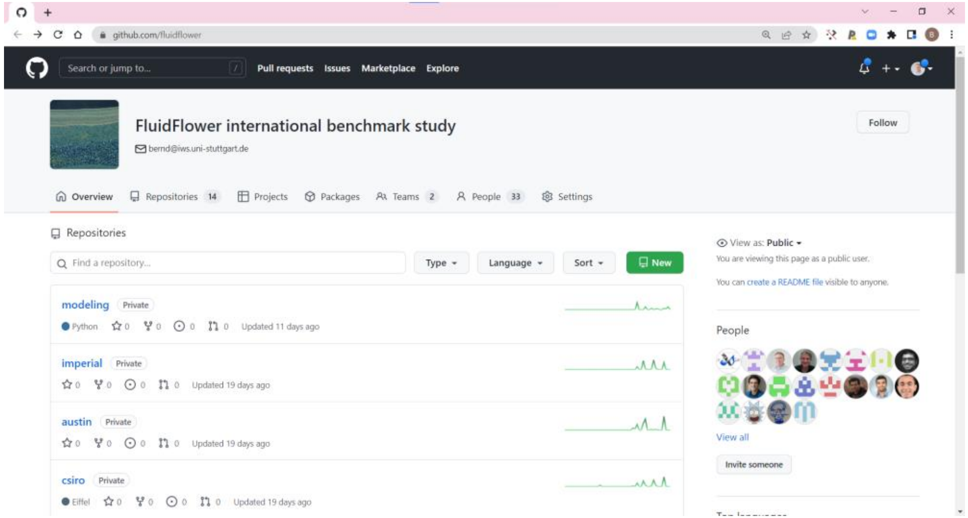
FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Sparse Data: Comparison of CO_2 Phase Composition in Box A at 72 hours



FluidFlower: A Meter-scale Experimental Laboratory for GCS (2024)

Infrastructure for Comparison and Reproduction



github.com/fluidflower

FluidFlower international benchmark study

bernd@iws.uni-stuttgart.de

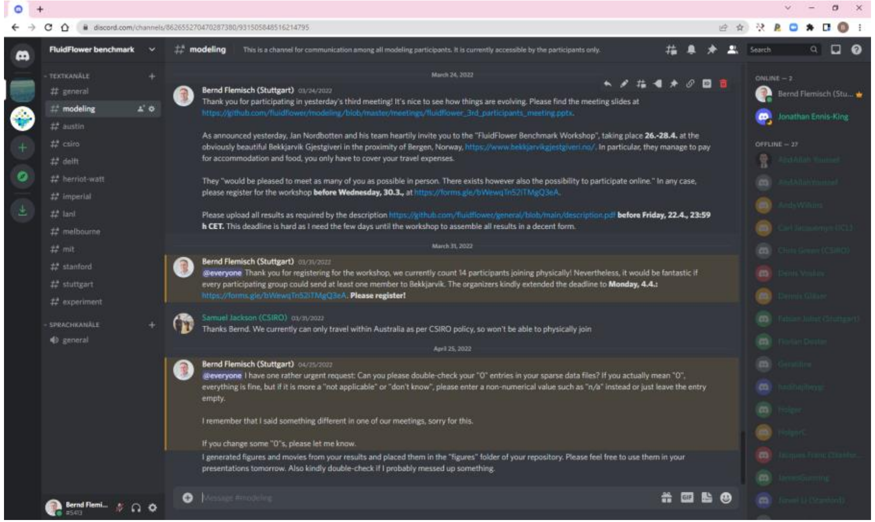
Repositories

Repository			Updated
modeling	Private	Python	Updated 11 days ago
imperial	Private		Updated 19 days ago
austin	Private		Updated 19 days ago
csiro	Private	Eiffel	Updated 19 days ago

View as: Public

You are viewing this page as a public user.

You can create a README file visible to anyone.



discord.com/channels/862655270470287380/931505848516214795

FluidFlower benchmark — # modeling: This is a channel for communication among all modeling participants. It is currently accessible by the participants only.

March 24, 2022

Bernd Flemisch (Stuttgart) 03/24/2022
Thank you for participating in yesterday's third meeting! It's nice to see how things are evolving. Please find the meeting slides at https://github.com/fluidflower/modeling/blob/master/meetings/fluidflower_3rd_participants_meeting.pptx.

As announced yesterday, Jan Nordbotten and his team heartily invite you to the "FluidFlower Benchmark Workshop", taking place **26.-28.4.** at the obviously beautiful Bekkjarvik Gjestgiveri in the proximity of Bergen, Norway, https://www.bekkjarvikgjestgiveri.no/. In particular, they manage to pay for accommodation and food, you only have to cover your travel expenses.

They "would be pleased to meet as many of you as possible in person. There exists however also the possibility to participate online." In any case, please register for the workshop **before Wednesday, 30.3.,** at https://forms.gle/bWewqTn52iTMgQ3eA.

Please upload all results as required by the description https://github.com/fluidflower/general/blob/main/description.pdf **before Friday, 22.4., 23:59 h CET.** This deadline is hard as I need the few days until the workshop to assemble all results in a decent form.

March 31, 2022

Bernd Flemisch (Stuttgart) 03/31/2022
@everyone Thank you for registering for the workshop, we currently count 14 participants joining physically! Nevertheless, it would be fantastic if every participating group could send at least one member to Bekkjarvik. The organizers kindly extended the deadline to **Monday, 4.4.:** https://forms.gle/bWewqTn52iTMgQ3eA. **Please register!**

Samuel Jackson (CSIRO) 03/31/2022
Thanks Bernd. We currently can only travel within Australia as per CSIRO policy, so won't be able to physically join

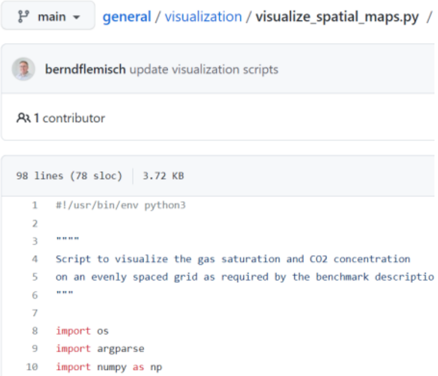
April 25, 2022

Bernd Flemisch (Stuttgart) 04/25/2022
@everyone I have one rather urgent request: Can you please double-check your "0" entries in your sparse data files? If you actually mean "0", everything is fine, but if it is more a "not applicable" or "don't know", please enter a non-numerical value such as "n/a" instead or just leave the entry empty.

I remember that I said something different in one of our meetings, sorry for this.

If you change some "0"s, please let me know.

I generated figures and movies from your results and placed them in the "figures" folder of your repository. Please feel free to use them in your presentations tomorrow. Also kindly double-check if I probably messed up something.



main / general / visualization / visualize_spatial_maps.py /

berndflemisch update visualization scripts

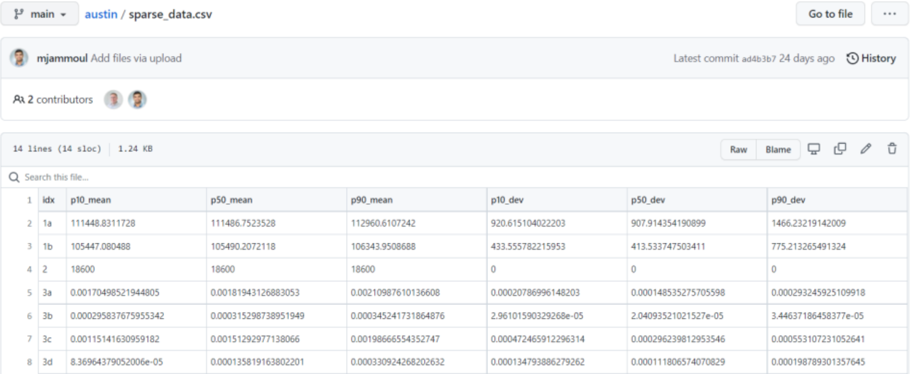
1 contributor

98 lines (78 sloc) | 3.72 KB

```
#!/usr/bin/env python3

"""
Script to visualize the gas saturation and CO2 concentration
on an evenly spaced grid as required by the benchmark descriptio
"""

import os
import argparse
import numpy as np
```



main / austin / sparse_data.csv

mjammoul Add files via upload — Latest commit ad4b3b7 24 days ago — History

2 contributors

14 lines (14 sloc) | 1.24 KB

idx	p10_mean	p50_mean	p90_mean	p10_dev	p50_dev	p90_dev
1a	111448.8311728	111486.7523528	112960.6107242	920.615104022203	907.914354190899	1466.23219142009
1b	105447.080488	105490.2072118	106343.9508688	433.555782215953	413.533747503411	775.213265491324
2	18600	18600	18600	0	0	0
3a	0.00170498521944805	0.00181943126883053	0.00210987610136608	0.000207869961482O3	0.000148535275705598	0.000293245925109918
3b	0.000295837675955342	0.000315298738951949	0.000345241731864876	2.96101590329268e-05	2.04093521021527e-05	3.44637186458377e-05
3c	0.00115141630959182	0.00151292977138066	0.00198666554352747	0.000472465912296314	0.000296239812953546	0.000553107231052641
3d	8.36964379052006e-05	0.000135819163802201	0.000330924268202632	0.000134793886279262	0.000111806574070829	0.000198789301357645

Outline

1. Motivation
2. Categorization
3. **Selected GCS Benchmark Studies**
    a. The Classic
    b. So Simple, Yet So Hard
    c. Reality Meets Modeling
    d. **Back To Normal, But Bigger**
4. Summary and Conclusion

Selected GCS Benchmark Studies

The 11th SPE Comparative Solution Project (2024)

- Code comparison / Verification
- Public CFP, multi-stage blind/open process
- More than 40 signed participation agreements
- 3 Benchmark cases
- No reference solutions (yet)
- SRQs:
  - Saturation and concentration fields at selected time steps
  - Integrated phase composition … over time
- Metrics: Multiple, e.g., Wasserstein distance
- Other reported characteristics: Implementation details, numerical performance

J. Nordbotten, M. Fernø, B. Flemisch, A. Kovscek, K.-A. Lie (2024): “The 11th Society of Petroleum Engineers Comparative Solution Project: Problem Definition“, *SPE Journal*. DOI 10.2118/218015-PA.

Challenges

- Simulations are highly sensitive to implementation of non-linear constitutive laws
- Simulations display strong sensitivity to grid types and refinement
- Non-linear solvers appear to be not robust and small timesteps are required even at moderate grid sizes
- Majority of computational difficulties are localized in (time-dependent) parts of the domain
- Grid convergence studies require physical diffusion or dispersion for reference solution to exist

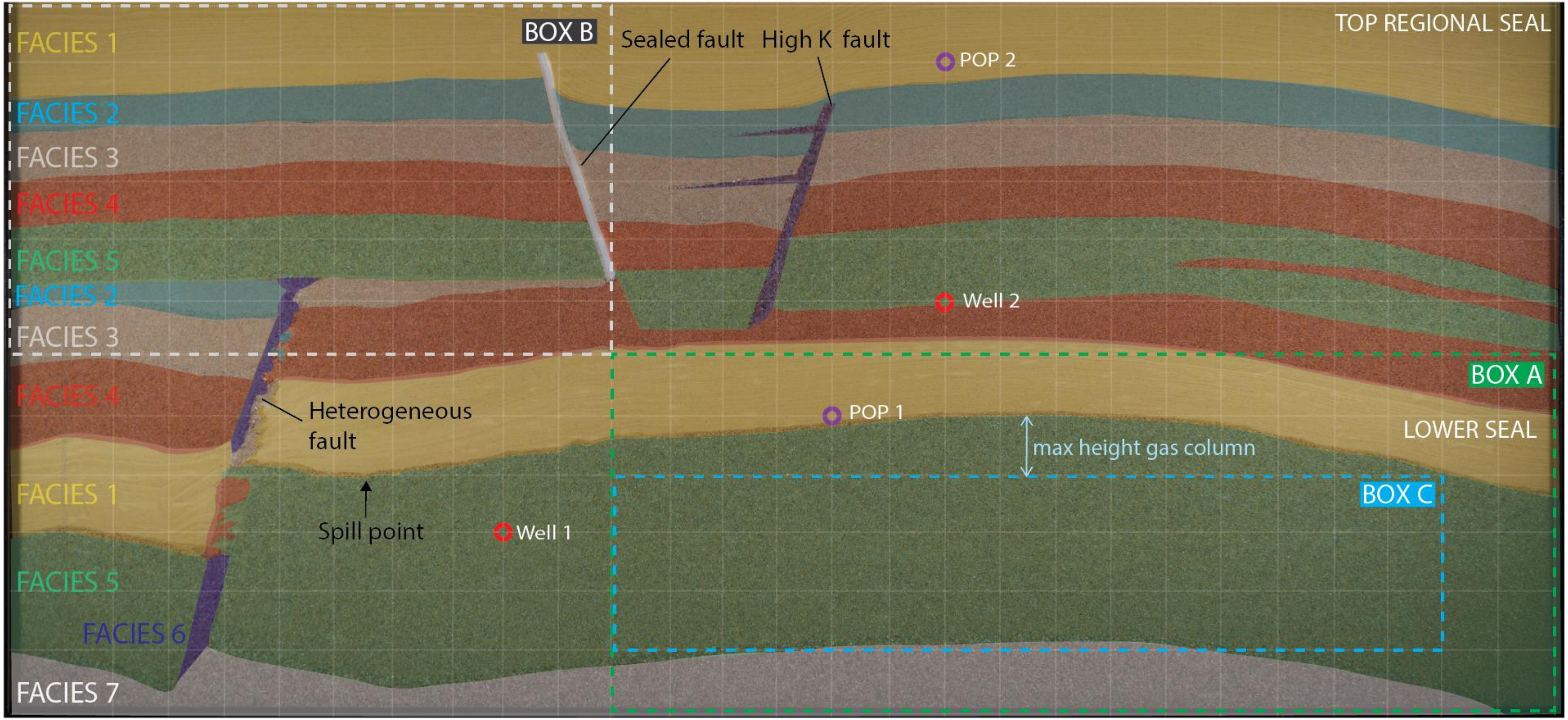
Claim: State-of-the-art is not sufficient for reliable forecasts

The 11th SPE Comparative Solution Project

Basic Setting

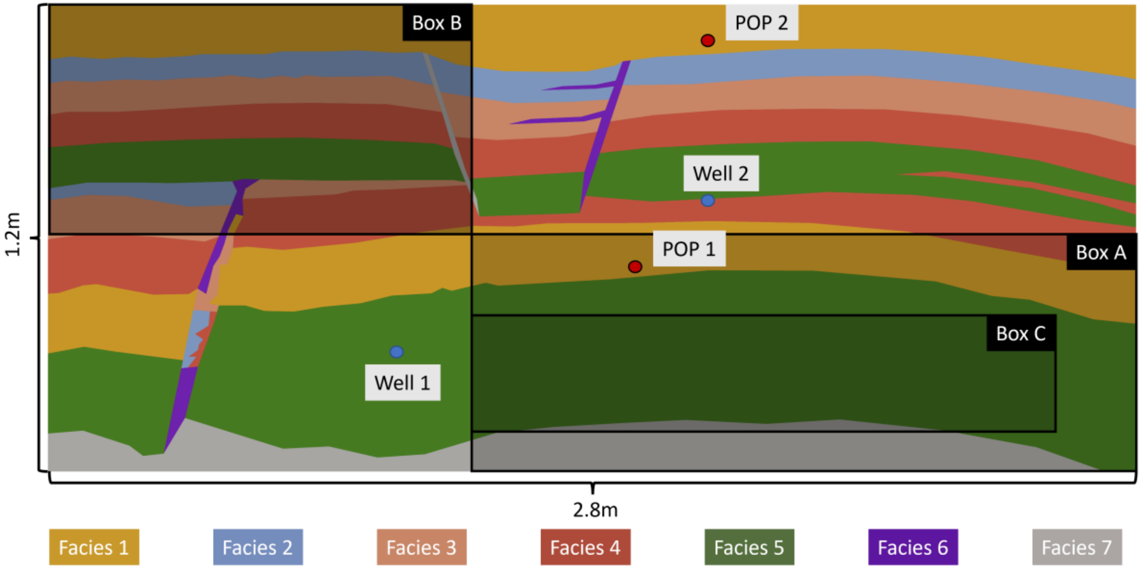
- Three **fully specified** simulation problems
  - Two-phase, two-component flows with thermal effects
  - All geometry and constitutive laws precisely defined
  - In principle, a unique solution should exist in the mathematical sense
  - No geomechanics, no geochemistry
- All three versions use the same baseline geometry as the original experimental validation study

Baseline Geometry



The 11th SPE Comparative Solution Project

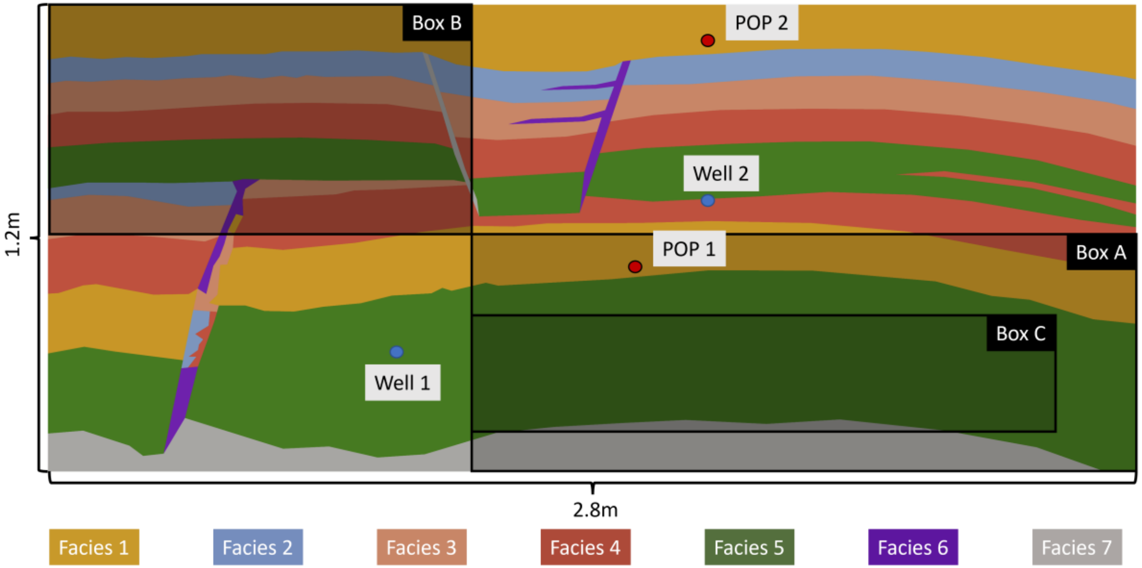
SPE11A – Lab Conditions



- Two-phase, two-component, isothermal
- 5 hour injection in Well 1, 2.5 hour injection in Well 2
- 120 hour total simulation time

The 11th SPE Comparative Solution Project

SPE11A – Lab Conditions

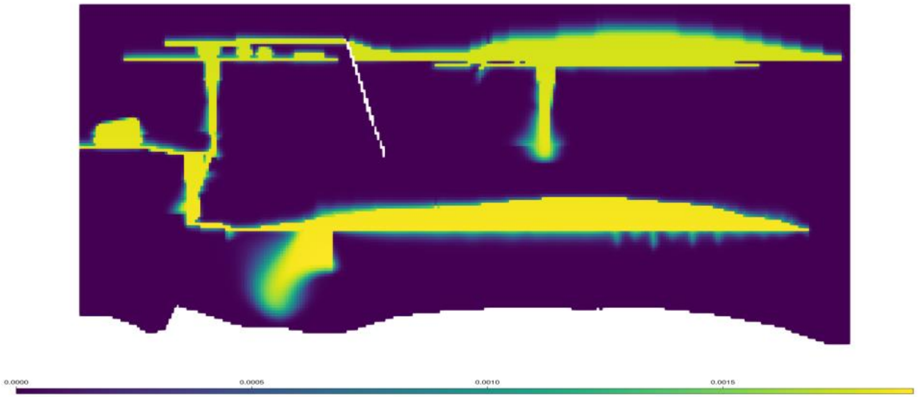


Reporting requirements

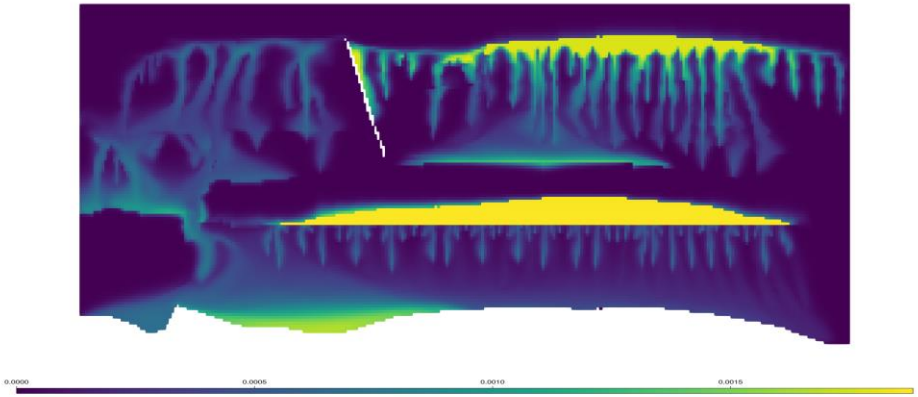
- Time-history of target quantities (proxies for storage safety)
- All field variables at 1 hour intervals on a 1 cm by 1 cm grid
- Various performance metrics

The 11th SPE Comparative Solution Project

Example Simulation of SPE11A



Injection stop

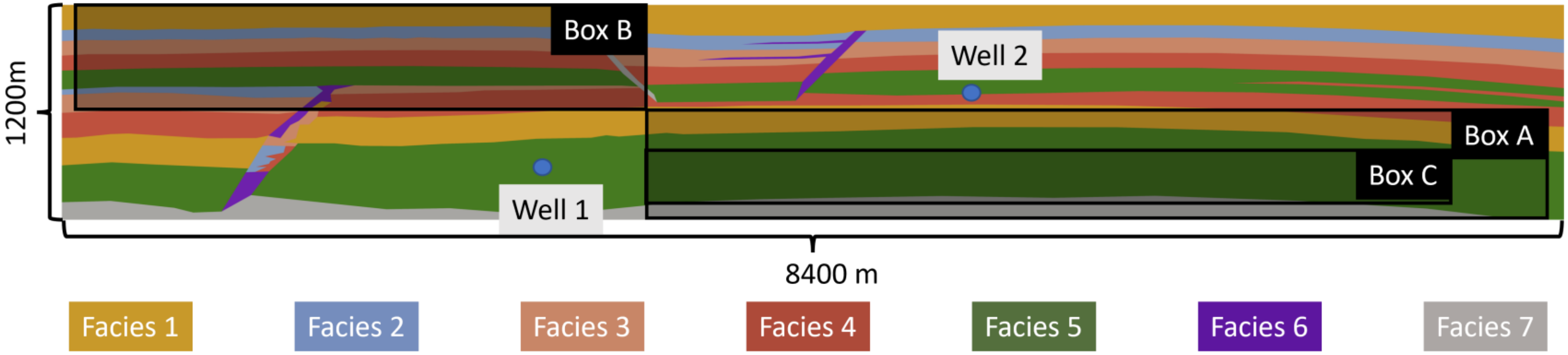


48 hours

SINTEF Digital/Matlab Reservoir Simulation Toolbox (MRST)

The 11th SPE Comparative Solution Project

SPE11B – 2D Field Transect

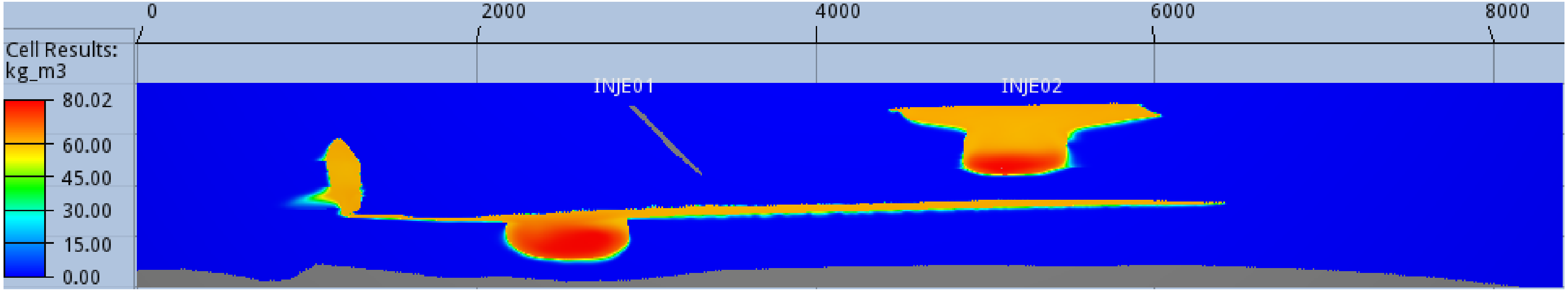


- Geometry from 11A stretched 3000:1 and 1000:1
- Two-phase, two-component, thermal
- 1000 year pre-injection equilibration
- 50 year injection in Well 1, 25 year injection in Well 2, at 10 degrees Celsius
- 2000 year total simulation time
- Reporting requirements as for 11A, but sparser in space and time

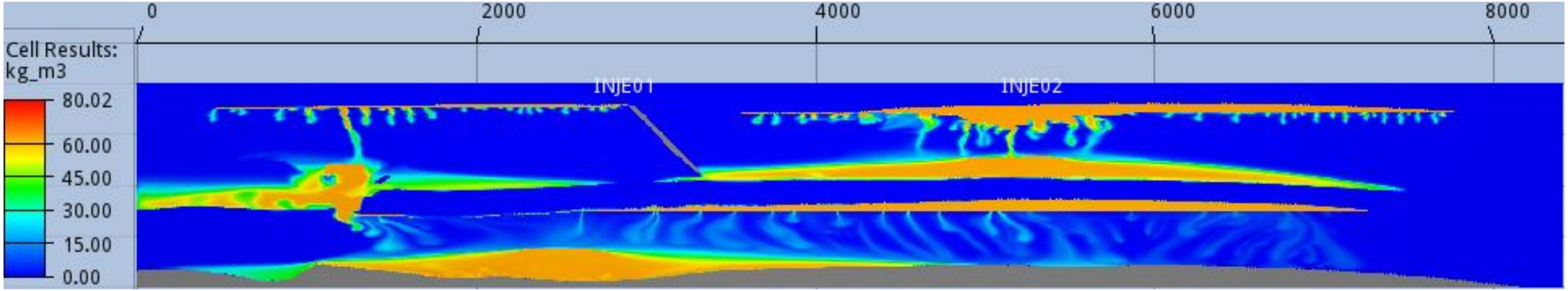
The 11th SPE Comparative Solution Project

Example Simulation of SPE11B

Injection stop



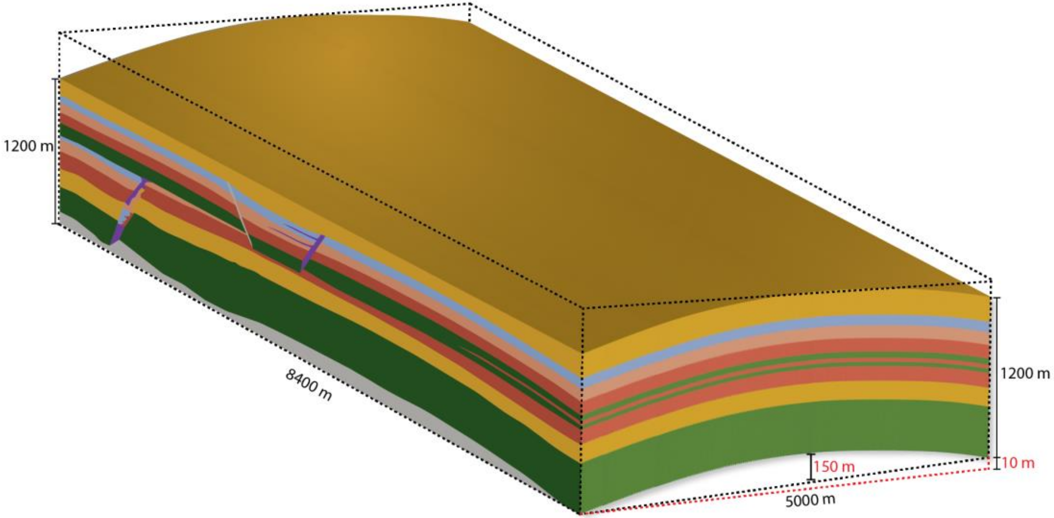
1000 years



NORCE/Open Porous Media simulator (OPM Flow)

The 11th SPE Comparative Solution Project

SPE11C – 3D Field

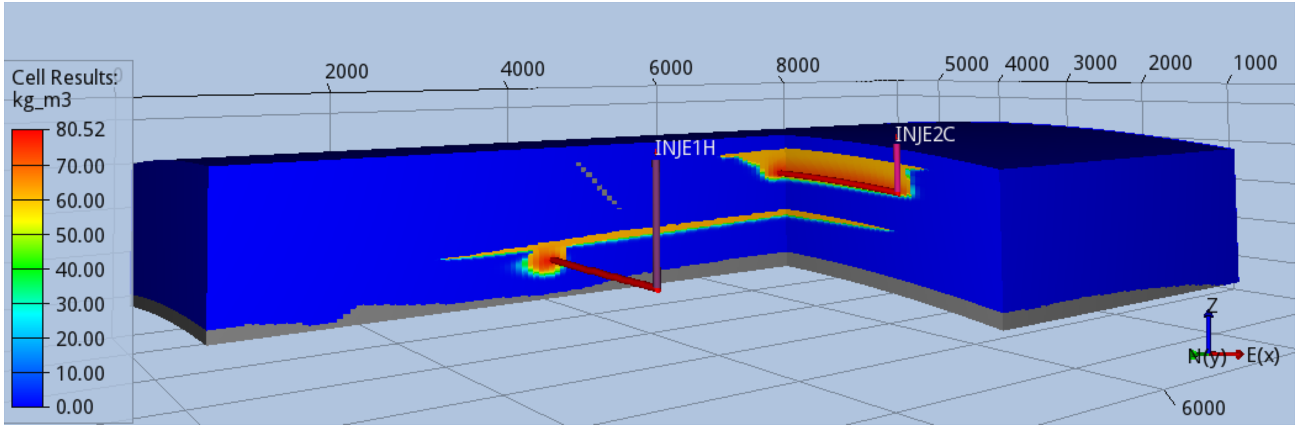


- Geometry from 11B stretched
  5000 meters along a parabola with slight skew
- All model equations and parameters as in 11B
- Well 1 is horizontal, Well 2 is arched following the layering
- Injection schedule and simulation time as for 11B
- Reporting requirements as for 11B, but yet sparser in space and time

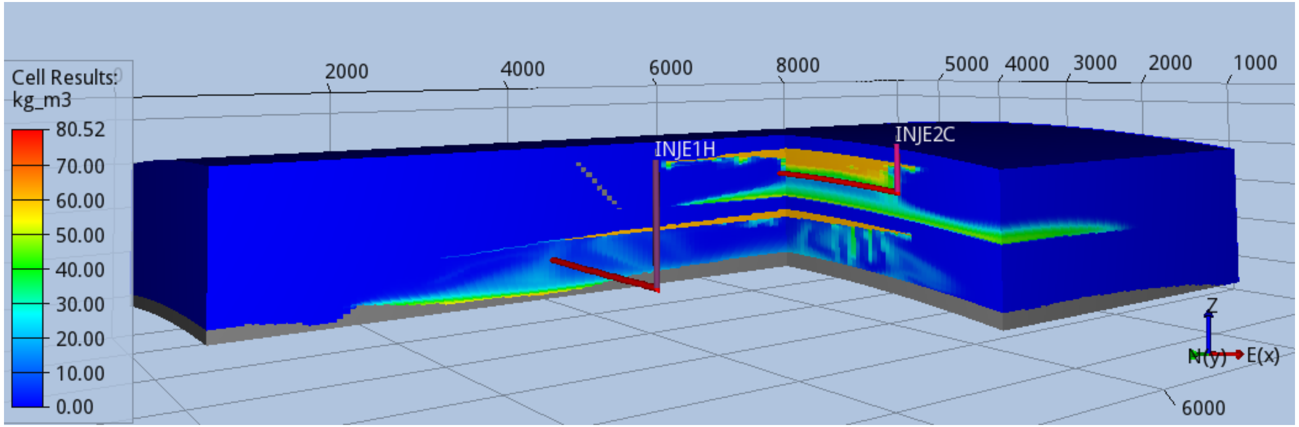
The 11th SPE Comparative Solution Project

Example simulation of SPE11C

Injection stop



1000 years



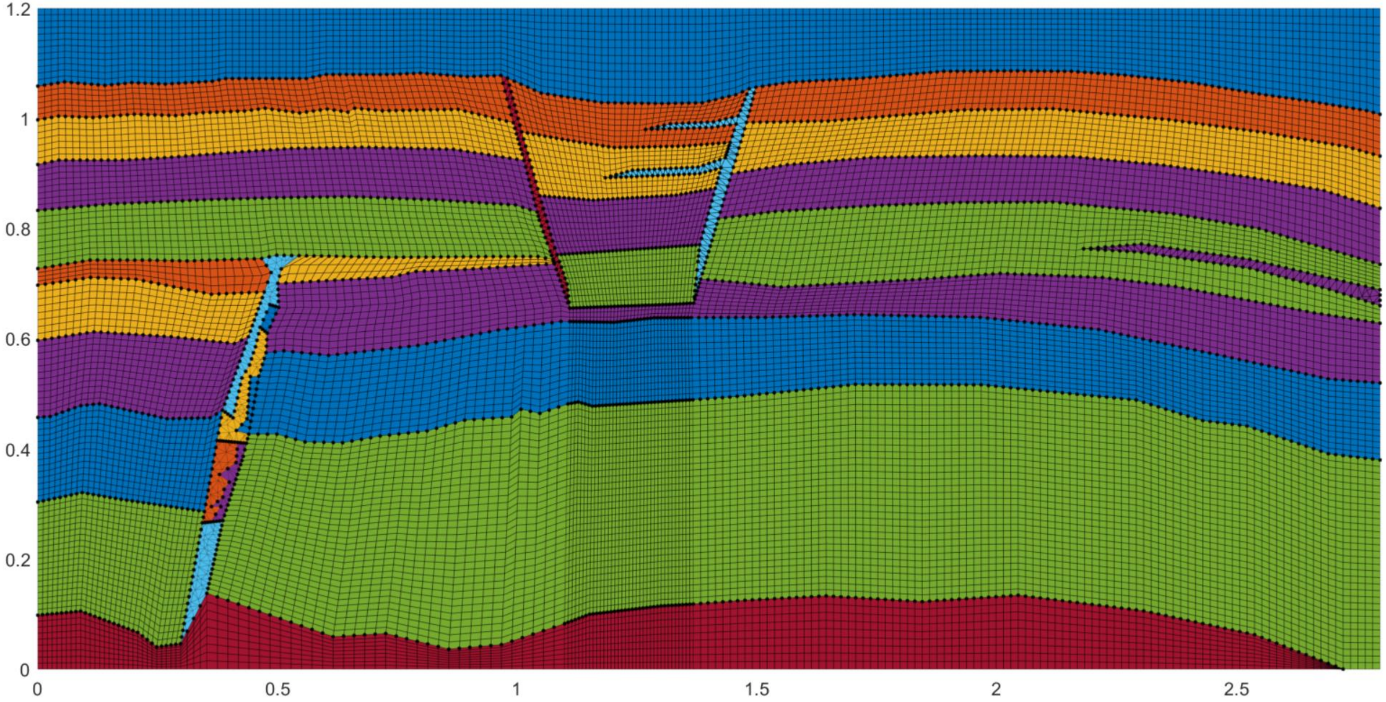
NORCE/OPM Flow

Some Known Challenges

- Common for all three versions:
  - Capillary entry pressure is a leading storage mechanism during injection
  - Injection of dry CO_2 leads to essentially immobile water saturation with very high capillary pressures
  - Convective mixing is the dominant physical process post-injection, but is difficult to resolve without an excessive number of grid cells
  - Cartesian grids tend to give unphysical “stair-case-like” dissolution rates post-injection.
  - Reporting metrics are sensitive to numerical errors
- SPE11A: Low density of CO_2 in gas phase leads to particularly strong non-linearities as gas “vanishes” into the water phase.
- SPE11B: Two-phase flow physics easier(?) than 11A, but thermal effects must be resolved.
- SPE11C:
  - The computational cost of three dimensions implies that properly resolving convective mixing is almost impossible on standard hardware.
  - Results will likely show strong grid dependence, or require upscaling methods.

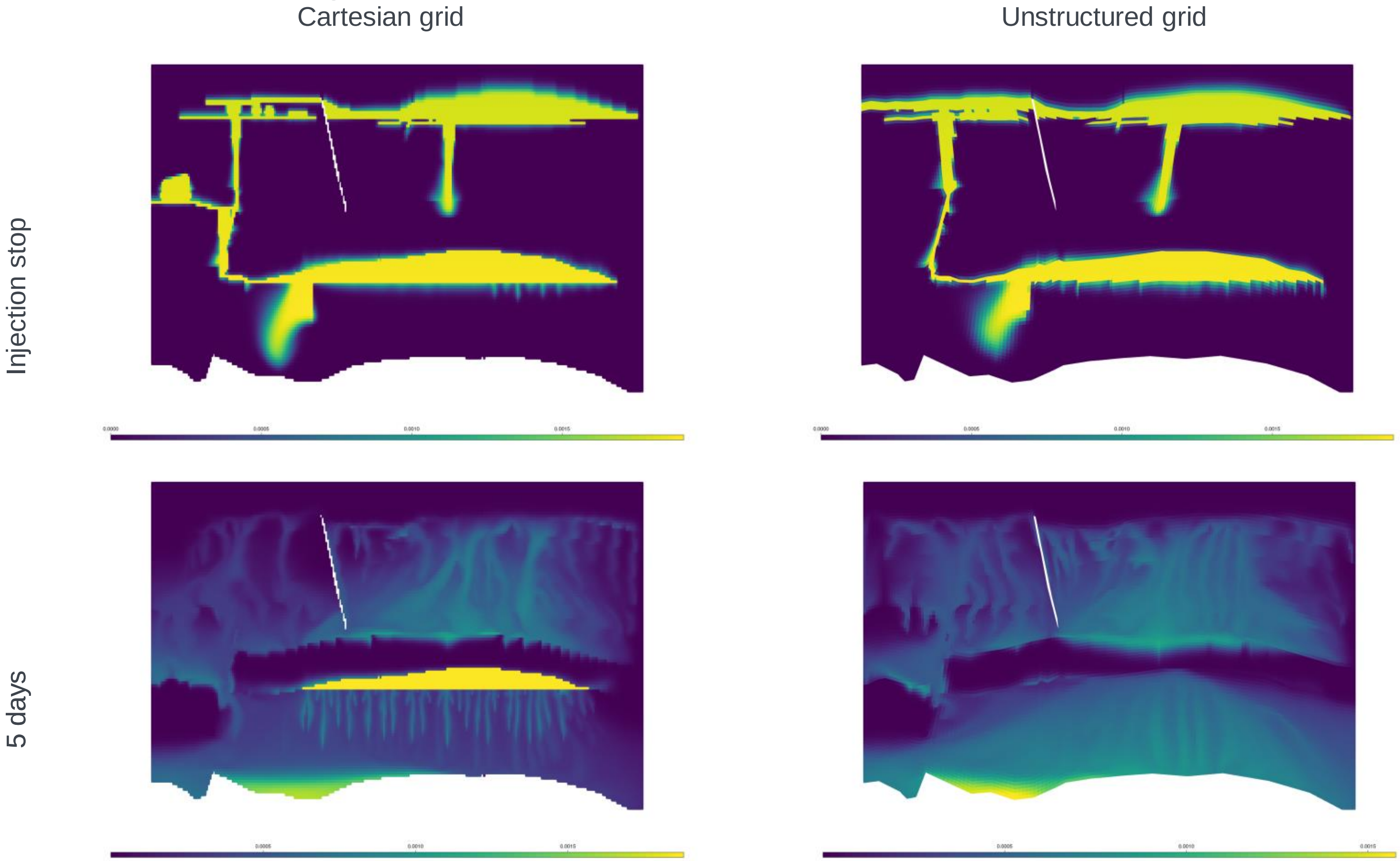
The 11th SPE Comparative Solution Project

Example Challenge: Gridding



The 11th SPE Comparative Solution Project

Example Challenge: Grid-dependent solutions on 11A

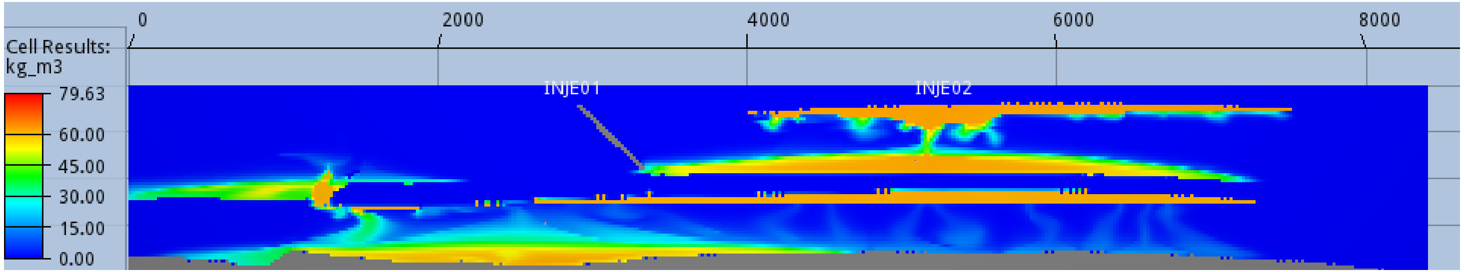

Cartesian grid
Unstructured grid

Injection stop
5 days

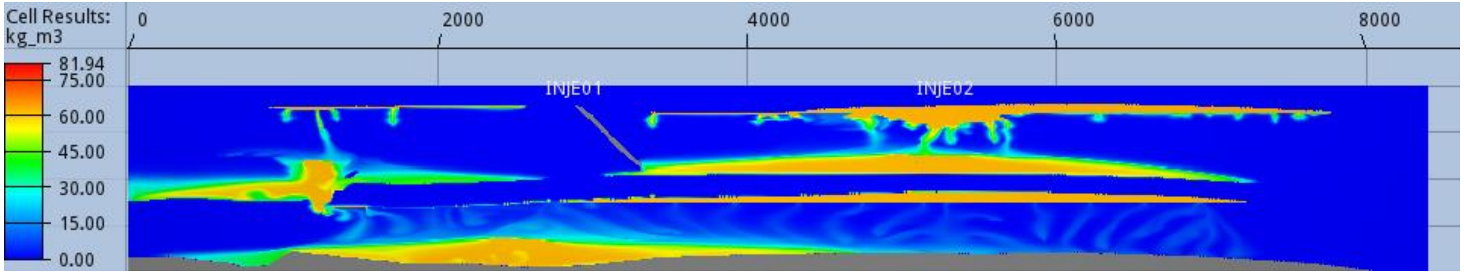
The 11th SPE Comparative Solution Project

Example challenge: Sensitivity to grid resolution for 11B

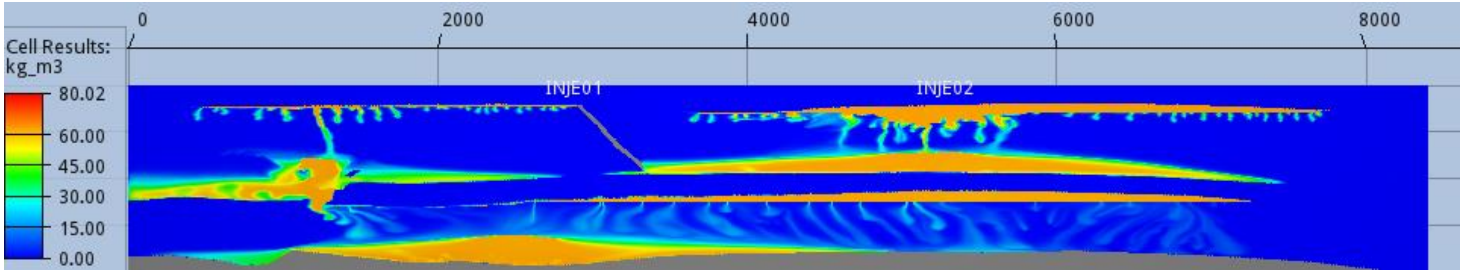
20m x 20m



10m x 10m



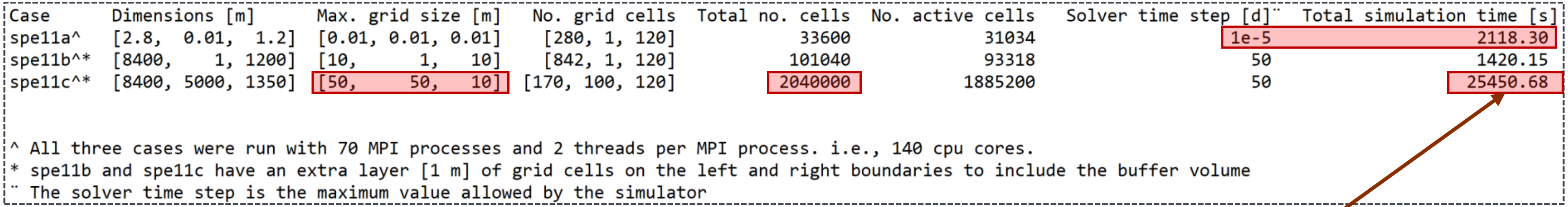
5m x 5m



NORCE/OPM Flow

The 11th SPE Comparative Solution Project

Example challenge: Computational times



```
Case       Dimensions [m]       Max. grid size [m]    No. grid cells  Total no. cells  No. active cells   Solver time step [d]¨  Total simulation time [s]
spe11a^    [2.8,   0.01,   1.2]  [0.01, 0.01, 0.01]    [280, 1, 120]            33600             31034                   1e-5                  2118.30
spe11b^*   [8400,     1, 1200]  [10,       1,    10]    [842, 1, 120]           101040             93318                     50                  1420.15
spe11c^*   [8400, 5000, 1350]  [50,      50,    10]  [170, 100, 120]          2040000           1885200                     50                 25450.68


^ All three cases were run with 70 MPI processes and 2 threads per MPI process. i.e., 140 cpu cores.
* spe11b and spe11c have an extra layer [1 m] of grid cells on the left and right boundaries to include the buffer volume
¨ The solver time step is the maximum value allowed by the simulator
```

CPU time used is over 50 days for the SPE11C at this resolution

Expected developments in the context of SPE11

- Development and verification of accurate and efficient discretization methods for multiphase, multicomponent flow and transport.
- Development and verification of space-time adaptive gridding and domain decomposition methods.
- Development of upscaling methods for convective mixing and dispersion of in the context of CO_2 dissolution into water.
- Development and verification of robust and efficient linear and non-linear solvers and solution and time-stepping strategies for 2D and 3D at laboratory and field conditions.
- Assessment of the importance of physical processes omitted from this study, including (but not limited to) geochemical reactions, mechanical response, and more realistic boundary conditions.

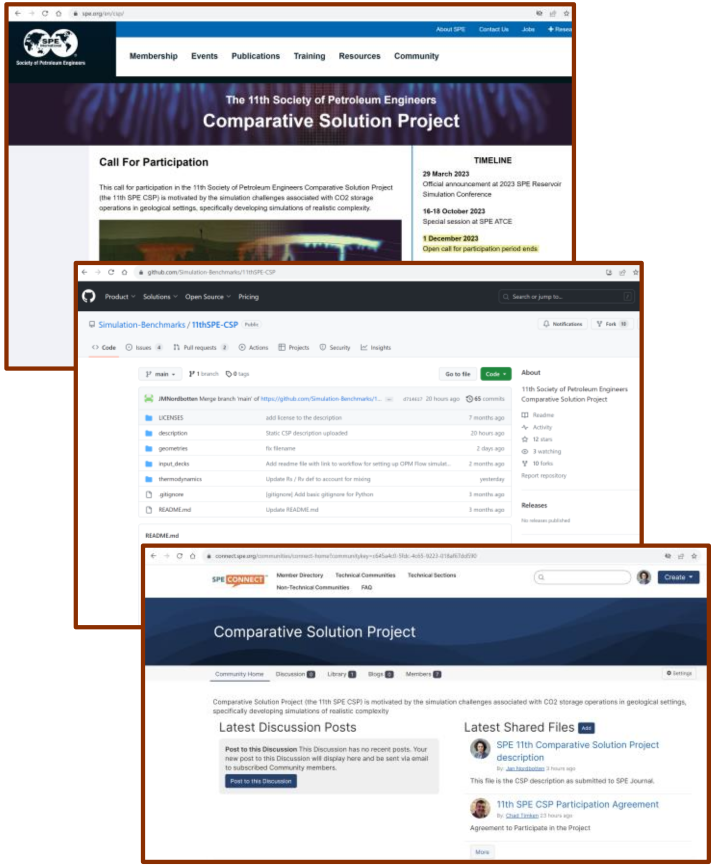
The 11th SPE Comparative Solution Project

Resources

Official webpage:
https://spe.org/csp

Community resources:
https://github.com/Simulation-Benchmarks/11thSPE-CSP

Discussion at SPE Connect:
https://connect.spe.org/home/memberhome



The 11th Society of Petroleum Engineers
Comparative Solution Project

Call For Participation

This call for participation in the 11th Society of Petroleum Engineers Comparative Solution Project (the 11th SPE CSP) is motivated by the simulation challenges associated with CO2 storage operations in geological settings, specifically developing simulations of realistic complexity.

TIMELINE

29 March 2023
Official announcement at 2023 SPE Reservoir Simulation Conference

16-18 October 2023
Special session at SPE ATCE

1 December 2023
Open call for participation period ends

JMNordbotten Merge branch 'main' of https://github.com/Simulation-Benchmarks/1... d714617 20 hours ago 65 commits

LICENSES	add license to the description	7 months ago
description	Static CSP description uploaded	20 hours ago
geometries	fix filename	2 days ago
input_decks	Add readme file with link to workflow for setting up OPM Flow simulat...	2 months ago
thermodynamics	Update Rs / Rv def to account for mixing	yesterday
.gitignore	[gitignore] Add basic gitignore for Python	3 months ago
README.md	Update README.md	3 months ago

README.md

About

11th Society of Petroleum Engineers Comparative Solution Project

Comparative Solution Project (the 11th SPE CSP) is motivated by the simulation challenges associated with CO2 storage operations in geological settings, specifically developing simulations of realistic complexity

Latest Discussion Posts

Post to this Discussion This Discussion has no recent posts. Your new post to this Discussion will display here and be sent via email to subscribed Community members.

Latest Shared Files

SPE 11th Comparative Solution Project description
By: Jan Nordbotten 3 hours ago
This file is the CSP description as submitted to SPE Journal.

11th SPE CSP Participation Agreement
By: Chad Timken 23 hours ago
Agreement to Participate in the Project

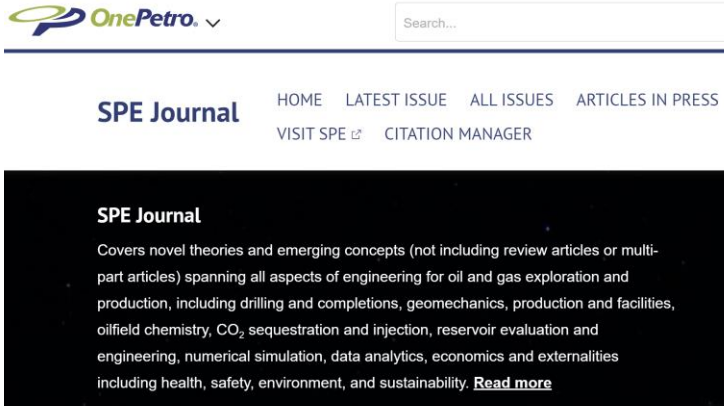
The 11th SPE Comparative Solution Project

Timeline

- March 29, 2023: First announcement at the 2023 SPE Reservoir Simulation Conference, Galveston, Texas.
- October 1, 2023: Final date for publication of corrections or amendments to the CSP description.
- October 16-18, 2023: Special session at SPE Annual Technical Conference and Exhibition (ATCE).
- December 1, 2023: Open call for participation period ends.
- **March 1, 2024: Deadline for submission of early CSP simulation results.**
- March, 2024: First intercomparison workshop for all CSP participants (virtual).
- **September 1, 2024: Deadline for submission of final CSP simulation results.**
- September, 2024: Final intercomparison workshop for all CSP participants (hybrid).
- December 2024: Completion of draft report on the results of the CSP.
- February 2025: Report on the results of the CSP finalized and submitted.
- **March, 2025: Special session at the 2025 SPE Reservoir Simulation Conference, Galveston, Texas.**

SPE Journal Special Issue

- SPE11 special issue already live!
- Two-year paper submission window.
- Continuous publication.
- Open for all CSP-related research papers!



SPE Journal

Covers novel theories and emerging concepts (not including review articles or multi-part articles) spanning all aspects of engineering for oil and gas exploration and production, including drilling and completions, geomechanics, production and facilities, oilfield chemistry, CO_2 sequestration and injection, reservoir evaluation and engineering, numerical simulation, data analytics, economics and externalities including health, safety, environment, and sustainability. **Read more**

The 11th Society of Petroleum Engineers Comparative Solution Project: Problem Definition

Jan M. Nordbotten[1]*, Martin A. Fernø[2], Bernd Flemisch[3], Anthony R. Kovscek[4], and Knut-Andreas Lie[5]

[1]Department of Mathematics, University of Bergen; Norwegian Research Center (NORCE)
[2]Department of Physics and Technology, University of Bergen; Norwegian Research Center (NORCE)
[3]Institute for Modelling Hydraulic and Environmental Systems, University of Stuttgart
[4]Energy Science & Engineering, Stanford University
[5]SINTEF Digital, Mathematics & Cybernetics

Summary

This article contains the description of, and call for participation in, the 11th Society of Petroleum Engineers Comparative Solution Project (the 11th SPE CSP, https://spe.org/csp). It is motivated by the simulation challenges associated with CO_2 storage operations in geological settings of realistic complexity. The 11th SPE CSP contains three versions: Version 11A is a 2D geometry at the laboratory scale, inspired by a recent CO_2 storage forecasting and validation study. For Version 11B, the 2D geometry and operational conditions from 11A are rescaled to field conditions characteristic of the Norwegian Continental Shelf. Finally, for Version 11C, the geometry of Version 11B is extruded to a full 3D field model. The CSP has a two-year timeline, being launched at the 2023 SPE Reservoir Simulation Conference and culminating at the 2025 SPE Reservoir Simulation Conference. A community effort is run in parallel to develop utility scripts and input files for common simulators to lower the threshold of participation; see the link to supplementary material on the CSP website. At the time of writing, complete input decks for one simulator are already ready for all three versions.

Introduction

Safe and efficient implementation of geological carbon storage (GCS) necessarily relies on reservoir simulators applied to uncertain geological data. While the strengths and limitations of reservoir simulation are well appreciated within petroleum production, GCS raises new challenges both in terms of physical processes and timescales. As an example, the enhancement of dissolution from a CO_2-rich supercritical phase to the aqueous phase through convective mixing ensures important long-term storage security, relevant on timescales from decades to centuries.

One consequence of the relative youth of the GCS industry, combined with the long timescales and new physical processes of interest, is that available field data for validation of simulation technology is still rare. This increases the importance of validation against proxy systems and code verification through comprehensive benchmarking efforts among simulators.

Background and Motivation. During 2021–22, three of the present organizers led a forecasting and validation study within the academic GCS community (Nordbotten et al. 2022; Flemisch et al. 2023), as illustrated in **Fig. 1.** The primary intent was to validate the long-term performance of numerical simulators for GCS, with particular emphasis on the post-injection period, and to assess the ability to state accurately well-calibrated forecasting intervals. The study also revealed several numerical challenges, both in terms of numerical accuracy when resolving the reservoir dynamics and in terms of obtaining good solver performance (see, e.g., Flemisch et al. (2023); Saló-Salgado et al. (2023); Wapperom et al. (2023)).

Separately, the development of numerical simulation capabilities for subsurface applications has historically benefited substantially from common reference simulation cases, notably the series of 10 CSPs organized within the SPE between 1981 and 2001 [see Islam and Sepehrnoori (2013) for a review]. These observations provided the initial motivation for developing a set of benchmark cases for CO_2 storage within the concept of a new SPE CSP.

In developing this 11th SPE CSP (https://spe.org/csp), we hope to provide a common platform and reference case for numerical simulation of GCS. Specifically, we anticipate that the following topics will be discussed relative to this baseline:

- Development and verification of accurate and efficient discretization methods for multiphase, multicomponent flow and transport.
- Development and verification of space–time adaptive gridding and domain decomposition methods.
- Development of upscaling methods for convective mixing and dispersion in the context of CO_2 dissolution into water.
- Development and verification of robust and efficient linear and nonlinear solvers and solution and timestepping strategies for 2D and 3D at laboratory and field conditions and well models.
- Assessment of the importance of physical processes omitted from this study, including (but not limited to) geochemical reactions, mechanical response, and more realistic boundary conditions.

Furthermore, as of the date of launching this CSP, we do not anticipate that a fully converged solution (in the sense of grid refinement) will be achievable for any of the three versions of the CSP by means of standard numerical methods on desktop hardware. This anticipation is justified in part based on the experiences from the previous academic benchmark cited above and in part due to the known challenges associated with accurately simulating the dissolution and convective mixing of CO_2 into water, in particular outside the context of

---

*Corresponding author; email: jan.nordbotten@math.uib.no

Original SPE manuscript received for review 15 June 2023. Revised manuscript received for review 12 October 2023. Paper (SPE 218015) peer approved 17 October 2023. This paper is published as part of the 11th Comparative Solution Project Special Issue.

Outline

1. Motivation
2. Categorization
3. Selected GCS Benchmark Studies
   a. The Classic
   b. So Simple, Yet So Hard
   c. Reality Meets Modeling
   d. Back To Normal, But Bigger
4. **Summary and Conclusion**

Summary and Conclusion

Take-Home Messages

- Verification and validation are **indispensable** for computational model development.
- Available benchmarks **facilitate** V&V tasks.
- Conducting benchmark studies helps to **bond/build/grow** communities.
- **No standardized V&V protocols** for the “GCS modeling community” exist.
- Standard models capture the **physical processes correctly.**
- Modelers tend to be **overconfident** in their own predictions.
- Predicted confidence intervals are typically **too narrow.**

Universität Stuttgart
Institute for Modelling Hydraulic and Environmental Systems
Department of Hydromechanics and Modelling of Hydrosystems

Thank you!

Bernd Flemisch

E-Mail bernd@iws.uni-stuttgart.de
Phone +49 (0) 711 685-69162
www.iws.uni-stuttgart.de/lh2

University of Stuttgart
IWS-LH2
Pfaffenwaldring 61, 70569 Stuttgart

- **FluidFlower benchmark:**
  J. Nordbotten, M. Fernø, M. Jørgensen, R. Juanes
  + co-workers
  + all participants
- **11th SPE CSP:**
  J. Nordbotten, M. Fernø, A. Kovscek, K.-A. Lie
  T. H. Sandve, D. Landa Marban
  H. Nilsen, O. Andersen, O. Møyner, V. Nevland
  M.A. Giddins, J. Haukås
  H. Class, D. Gläser, K. Wendel