

A Novel Multiphysics Tool to Assess CO<sub>2</sub> Storage and Re-migration Risks from Pore-scale to Regional-scale

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A DECHEMICAL INTERPRETATIO

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### **CO2MIG PROJECT MOTIVATION**

CO2MIG is a new technology Joint Industry Project (JIP) to understand how cap rock  $CO_2$  containment and plume migration function in subsurface injection projects. The CO2MIG tool is novel because it supports coupling between pore-scale geochemical reactions and large-scale dynamic fluid flow in a mathematically consistent way to enhance our understanding of the subsurface evolution of  $CO_2$  plumes.

Currently,  $CO_2$  migration monitoring tools used in Carbon Capture and Storage (CCS) focus on imaging the evolution of injected  $CO_2$ fluids in reservoirs and on Measurement, Monitoring and Verification (MMV) of surface emissions.

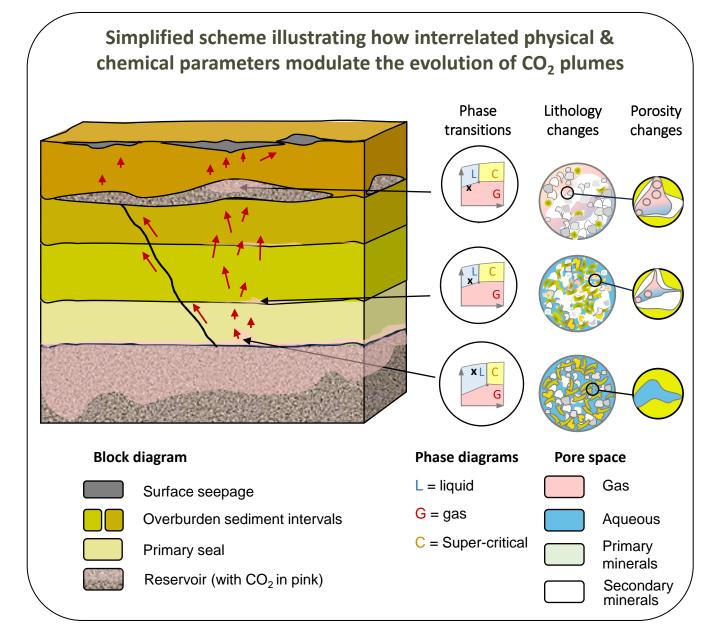
Our aim is to bridge the gap between the cost-intensive reservoir modelling and MMV surveys to optimize injection and monitoring strategies associated with the geological storage of CO<sub>2</sub>.

	•	customised to for plausible	specific AOI case scenarios		
Scenario 1		— () ———	Scenario n		
Surface monito	oring areas		Surface monitoring areas		
versus no or unreliable plume modelling					
implies somehow random surface MMV					
	Surface m	onitoring area?			
	Overburden Caprock Reservoir				
	Nesei voli				

# **CO2MIG MODELLING TOOL POTENTIAL**

The novel CO2MIG modelling tool is being developed using a sophisticated multiphysics reactive fluid flow model which can integrate local to large scale processes. The adaptation of this state-of-the-art numerical model to CO<sub>2</sub> migration in overburden formations enables enhanced simulations of the mechanisms controlling the evolution of the plumes in space and time. The capacities of the modelling workflow include:

- Understanding of multi-directional phase transitions within the plume.
- Understanding of the mechanisms of the multi-phase migration of leaked CO<sub>2</sub> in different lithological and structural settings.
- Testing of the model sensitivity to variations in model parameterization and for alternative scenarios.
- Customisation to multiphysics characteristics of the AOI, supporting a better identification of the mechanisms and risks of the CO<sub>2</sub> plume migration than possible with available multipurpose software can.



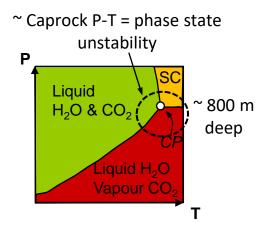
# MULTIPHYSICS MODEL TO PREDICT FLUID PHASES

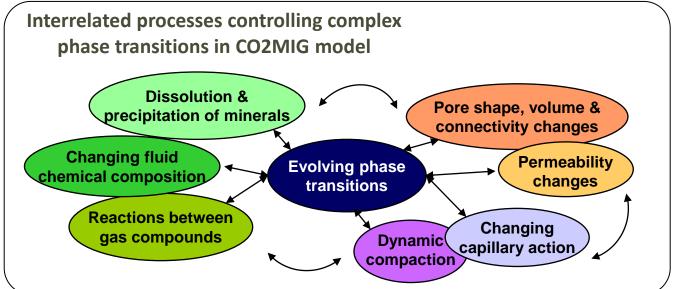
The flexible and highly versatile muti-component, multiphysics, non-isothermal reactive fluid flow software at the core of the CO2MIG modelling tool was built to model dynamic fluid flow in complex multiphysics frameworks.

The numerical model was produced to simulate gas hydrates dynamics, which involve intricate gas-liquid-solid phase changes (Gupta et al., 2020, 2022, 2023). It is unique in its capacity to support coupling between geochemical reactions at the pore-scale (i.e., small-time steps) and large-scale dynamic fluid flow (i.e., large time-steps) in a mathematically consistent manner. The model, which is not limited by the characteristics and amounts of reactions included, accounts for the interrelation of changes in geochemical reactions, sediment properties and permeability, and provides novel insight on how they control the evolution of  $CO_2$  plumes in the reservoir caprock and overburden, for instance:

Chemical changes of the porewater composition - The addition of CO<sub>2</sub> in pore fluids leads to chemical reactions between (1) solutes in water; (2) solutes and matrix minerals; and (3) aqueous solution and gas phase components. With an unlimited number of reactions in the reaction network, the complexity of the chemical processes can be user-defined.

Dynamic Pressure-Temperature-Composition conditions (P-T-X) - The model computes P-T-X variations resulting from physical-chemical changes induced by fluids migration. It enables enhanced plume migration prediction accuracy, crucial in CO<sub>2</sub> storage caprock & overburden conditions due to rapid & difficult to predict phase transitions.



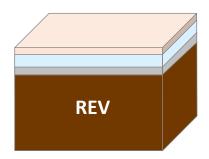


## STATE-OF-THE-ART NUMERICAL MODEL

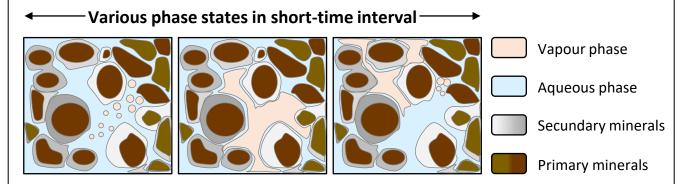
Customised multiphysics modules can be created because the model is built using flexible numerical approaches, yielding simulators able to model complex multiphysics settings when existing multipurpose software capacities are seriously limited.

Simulators with flexible numerical approaches involve the implementation of advanced numerical tools and of novel decoupling strategies that support the customisation of the model. An example is the use of advanced numerical methods to include complex pore-scale phase transitions, which cannot be modeled in a robust manner in most software for reasons schematically depicted below.

Phase states at the REV scale are difficult to estimate due to rapid local "back and forth" phase transitions caused by pore pressure changes, which are driven by non-linearity coupled processes such as (1) increasing  $CO_2$  concentration and (2) pore volume & connectivity changes due to precipitation/dissolution of minerals.

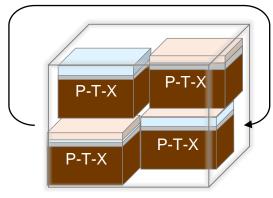


Min volume in which the porous media is considered homogeneous  $\, \smallsetminus \,$ 



The iterative resolution of mass, energy, and momentum conservation equations in the REVs is problematic, leading to model degeneracy

# Iterative runs in discretized model



**REV** = Representative Elementary Volume in finite volume discretization process

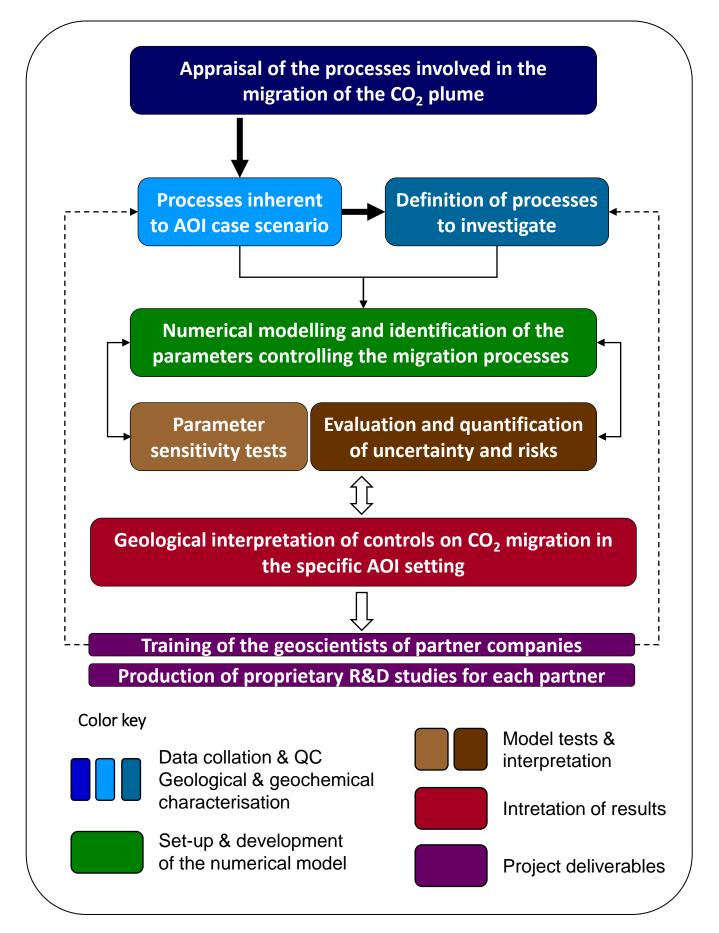
- Multipurpose modelling software, which rely on standard discretization<sup>1</sup> and numerical<sup>2</sup> methods (PVS<sup>2</sup>), cannot converge (i.e., model degeneracy).
- ✓ Advanced discretization methods<sup>3</sup>, integration of novel decoupling strategies<sup>4</sup>, and more general nonlinear solvers<sup>5</sup> used in the CO2MIG numerical model enable the customisation of the simulator leading to the convergence of the model (it is a more robust model).

Examples of numerical methods: <sup>1</sup>Cell-centered finite volume; <sup>2</sup>Primary Variable Switching; <sup>3</sup>Discontinuous Galerkin FEM; <sup>4</sup>Non-linear Complementarity Problem; <sup>5</sup>Semi-smooth methods

# **PROJECT STRATEGY & WORKFLOW**

# The technology development project is structured in a succession of stages involving:

- Analysis and interpretation of geological and geochemical data.
- Modelling of the controls on CO<sub>2</sub> migration in the customised multiphysics framework.
- Sensitivity analysis and evaluation/quantification of the uncertainty and risks associated with the different case scenarios specific to the AOIs.



#### **PROJECT SCHEDULE**

The multi-physics CO<sub>2</sub> migration modeling workflow research and development project will have a duration of two years.

- The main stages of the project comprise:
  - The characterization of the geological/geochemical setting.
  - Definition of the objectives, elaboration of case scenarios and identification of the requirements of the migration model.
  - Development of the numerical model and testing of different case scenarios.
  - Risk and uncertainty analysis specific to the different case scenarios.
  - Project completion and presentation.
  - Several workshops will be organized to support a fruitful collaboration between project researchers and partner geoscientist as well as for the training of the latter in the interpretation of the model results.

Project phase	Year 1	Year 2
Geological & geochemical characterisation; Case scenarios conception		
Software deployment and development		
Migration model; Risk & uncertainty analyses		
Highly documented proprietary report of the R&D study		
Contribution to the elaboration of surface leakage risk maps		
Surface leakage risk maps; MMV guidelines		
Workshops and meetings		

### Scheduled phases of the R&D CO<sub>2</sub> migration modeling project

## **BENEFITS AND COMMITMENTS**

The partner companies in this project will gain:

- The application and customisation of the novel CO<sub>2</sub> migration modelling tool to their defined Area-Of-Interest (AOI), including:
  - ✓ A fully documented proprietary report of the migration modelling workflow research performed in, and specifically for, their AOI.
  - ✓ The identification and characterization of factors that are determinant for the evolution of CO₂ plumes from potential reservoir caprock leak to the surface.
  - ✓ Surface leakage risk maps in a range of scenarios applicable to the partner's AOI.
  - ✓ Monitoring strategy guidelines for the AOI.
  - ✓ Advice on key follow-up activities and data acquisition.
- Training of the partner's geoscientists in the interpretation of the outcomes of the CO2MIG modelling workflow via in-person and online workshops:
  - Collaborative evaluation of key aspects to be investigated in the AOI during the R&D project.
  - Explanation of the science, potential and limitations on what can be inferred from the outcomes of the migration model workflow.

The companies should provide all relevant data in their AOI to support the research and development of the modelling workflow.

The companies that sign up for this project will commit to a twoyears partnership with the following fees (in GBP):

- One company/operator £45K/year
- One operator and one or two partners:
  - Main operator £35K/year
  - **\*** Each partner £15K/year
- One operator and three or more partners:
  - Main operator £25K/year
  - **\*** Each partner £10K/year

The costs include a 2-3 day in-person workshop for 2 instructors per year and may include visits to different companies depending on location.

## THE PROJECT TEAM

The multi-disciplinary project team encompasses experts from the fields of geology, geochemistry, modelling and statistical modelling.



Dr Marianne Nuzzo, is the Project Leader and the lead geochemist at IGI. Marianne holds a Ph.D. in biogeochemistry from the University of Bristol (UK), followed by 6 years of research in seep geochemistry. She has been working as an oil & gas geochemist for the industry since she joined IGI in 2013.



Dr Tiago Cunha is a geologist, marine geophysicist and modeller with over 20 years of experience in Basin and Petroleum Systems modelling (BPSM). Tiago holds a Ph.D. in marine geophysics from the University of Oxford (UK), followed by 5+ years of research in rift basins and neotectonics.



Dr Dan Cornford is a mathematician and IGI's director. Dan holds a Ph.D. in spatial statistics and climatology from the University of Birmingham (UK), with 20+ years of research in statistical modelling. He has since been leading IGI's software development and ML activities for 12+ years.

The IGI Team will interact with our two university consultants: Dr Shubhangi Gupta, who produced the software, and Dr Ewa Burwicz-Galerne, who tested initial versions, to adapt the model and advise on its usage according to the specificities of the AOIs.

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