VIRGINIA TECH

U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

2023 FECM / NETL Carbon Management Research Project Review Meeting

Resource Assessment of Geological Formations and Mine Waste for Carbon Dioxide Mineralization in the US Mid-Atlantic

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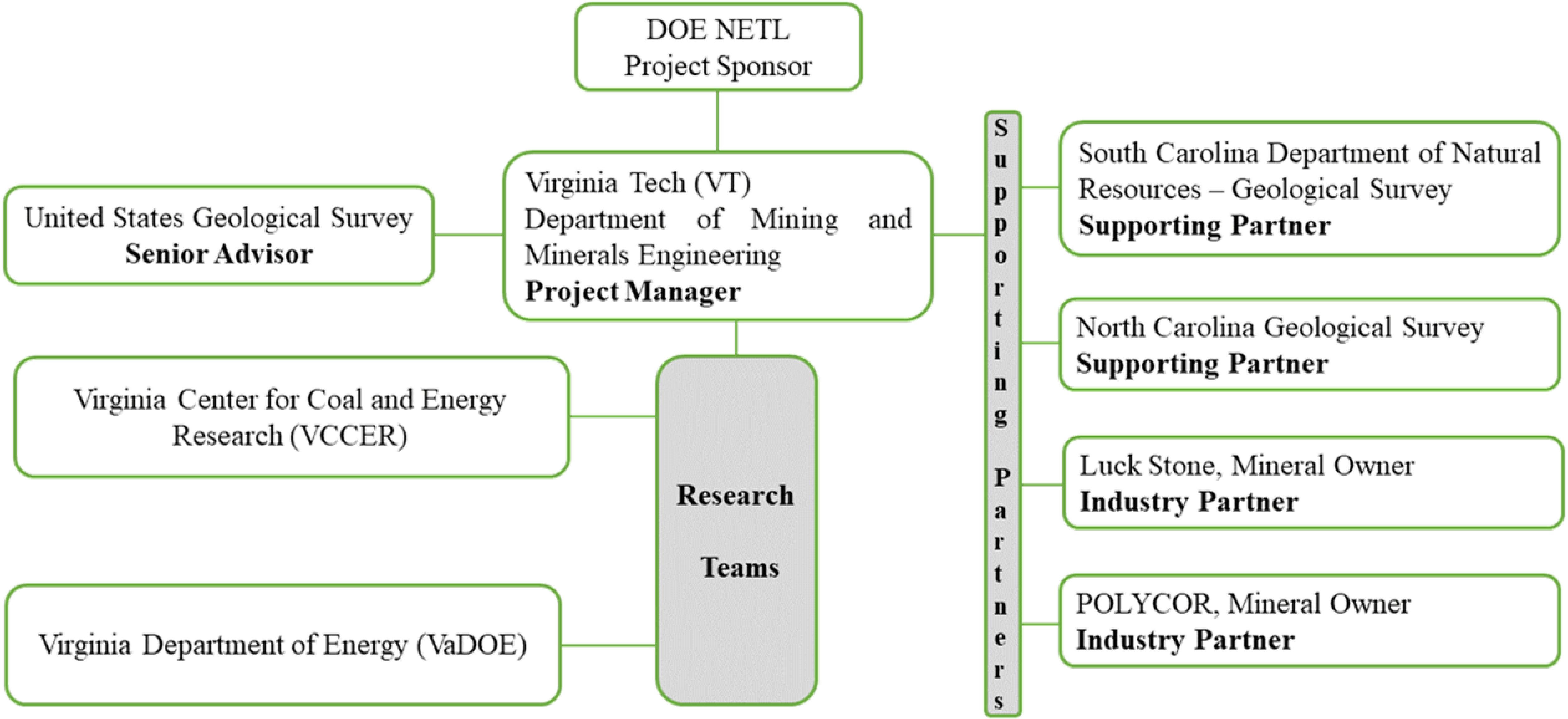
Research partner:
Virginia Department of Energy

2023 FECM / NETL Carbon Management Research Project Review Meeting
August 29, 2023

Outline

- Our team
- Project objectives
- Background information
- Our methodology and tasks
- Potential benefits

Our team


DOE NETL
Project Sponsor
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Department of Mining and Minerals Engineering
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Virginia Department of Energy (VaDOE)
Research Teams
Supporting Partners
South Carolina Department of Natural Resources – Geological Survey
Supporting Partner
North Carolina Geological Survey
Supporting Partner
Luck Stone, Mineral Owner
Industry Partner
POLYCOR, Mineral Owner
Industry Partner

Research team

- **Bahareh Nojabaei (PI)**

Mining and Minerals Engineering, multiphase multicomponent flow simulation, molecular simulation, machine learning and data analysis

- **Rohit Pandey (Co-PI)**

Virginia Tech Mining and Minerals Engineering,

- **Ryan Pollyea (Co-PI)**

Virginia Tech Geosciences and VCCER,

- **Nino Ripepi (Co-PI)**

Virginia Tech Mining and Minerals Engineering and VCCER,

- **Wencai Zhang (Co-PI)**

Virginia Tech Mining and Minerals Engineering,

- **Jenny Meng**

Virginia Department of Energy

- **Madalyn Blondes**

United States Geologic Survey

Primary objectives

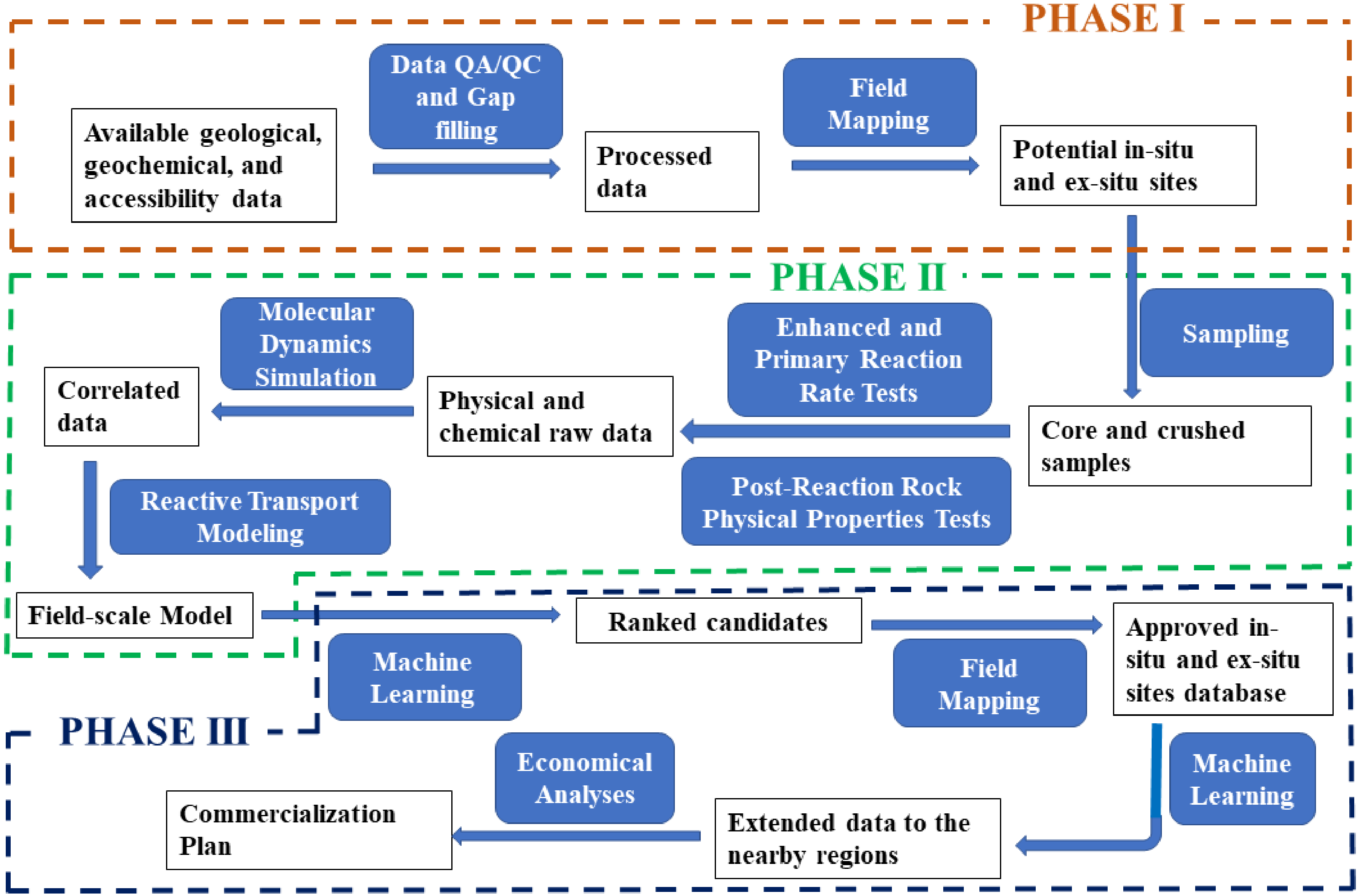
- Analyze the geological data in the US Mid-Atlantic region, and search for potentially suitable rock types.
- Assess the suitability of target formations and rocks for efficient and timely reactions through performing laboratory scale CO_2 mineralization reaction tests.
- Assess the post-mineralization properties of rocks through laboratory scale tests and molecular scale simulations.
- Upscale the laboratory scale assessments to the field scale, through reactive transport modeling and simulation, and regression analysis.
- Rank the candidates in terms of their suitability for carbon storage, through using machine learning and inclusion of multiple factors such as reaction rates, rock properties, accessibility, and mineralization associated costs.
- Extend and extrapolate our understanding to nearby regions, through using machine learning.
- Provide a database and map the carbon storage resources.

Multiscale data-driven framework

Phase I: Geological pre-study assessment, mapping, and data filtering

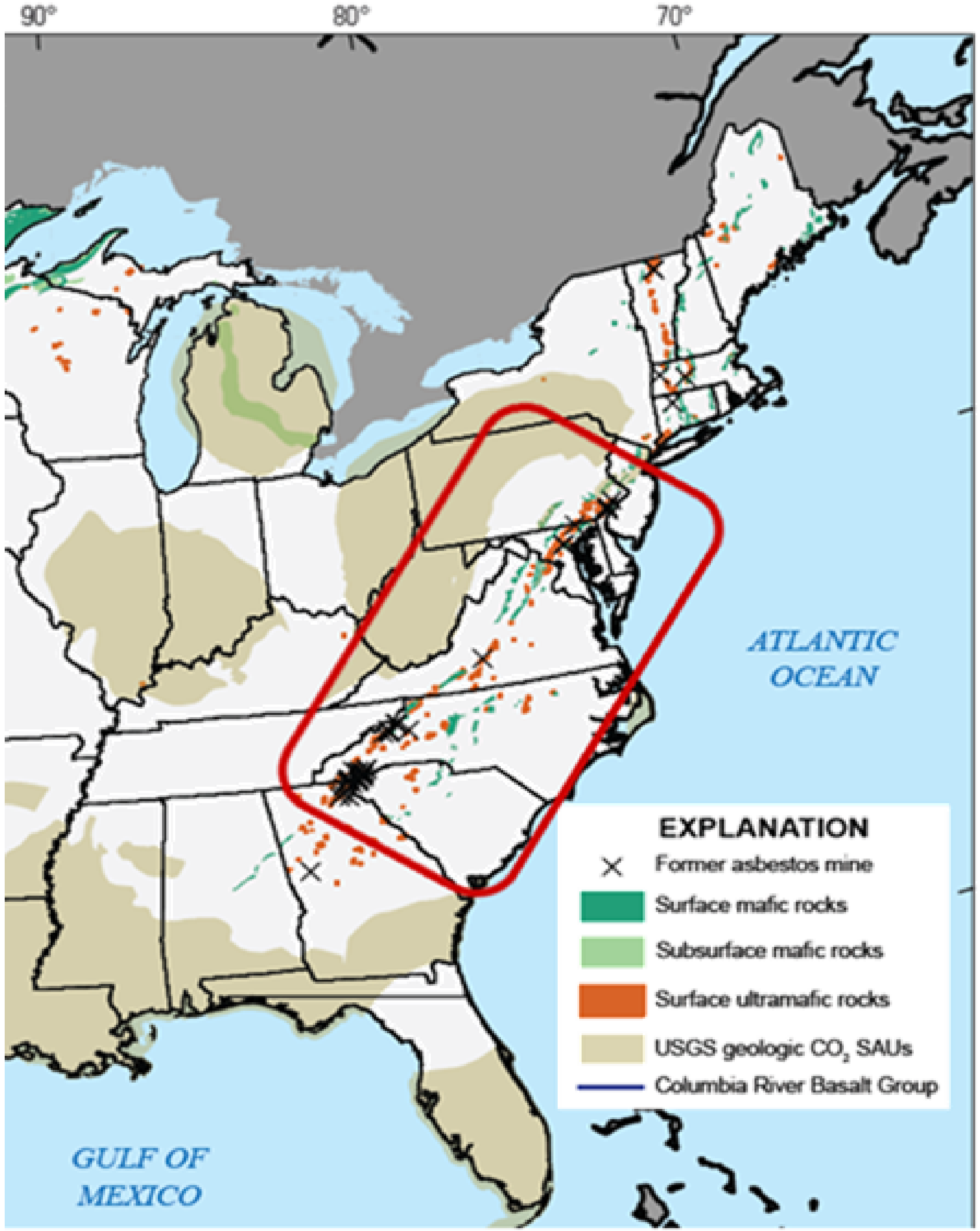
Phase II: Multiscale CO_2 mineralization characterization

Phase III: Post-study mapping, database development, and commercialization



Background information

- The Central Atlantic Magmatic Province (CAMP) is an expansive continental large igneous province that was emplaced ~201M years ago, prior to the breakup of Pangea.
- CAMP deposits are characterized by basalt rocks that were emplaced relatively quickly over a 1M year time period as lava flows, dike swarms and sills.
- Within the U.S. Mid-Atlantic region, CAMP deposits are associated with the Triassic rift basins that trend northeast throughout Georgia, South Carolina, North Carolina, Virginia, Maryland, and Pennsylvania.
- CAMP deposits are characterized by radiating dike swarms with sills that interbed the country rock and may comprise morphological features that are typical of flood basalt, specifically brecciated, high-permeability basalt flow margins separated by low-permeability flow interior.



Carbon mineralization potential

- Mafic rocks such as basalt have been shown to be suitable for carbon mineralization because they dissolve much faster than in more silica rich rocks.
- The CAMP deposits within the US Mid-Atlantic States contain both mafic and ultramafic rocks with high concentrations of desired cations (e.g. Mg^{2+}, Fe^{2+}, or Ca^{2+}) for carbon mineralization.
- The Mesozoic rift basins in the Eastern United States consists of extrusive igneous and metaigneous rift basalts, as well as mafic dikes and sills that intrude those deposits and surrounding rocks.
- Greenstone is metamorphosed basalt and ***a major rock for construction aggregate*** of the Blue Ridge Province from central Pennsylvania in a southwesterly direction through the central part of Virginia. ***Mining waste resources (fines) are available in the area*** as greenstone is an industrial construction aggregate in Mid-Atlantic States.
- The Mid-Atlantic States also have resources of ultramafic rocks in sparse outcrops in Virginia and Maryland, as well as peridotite and serpentinites.

Our hypothesis

- A working hypothesis being employed by the project team is that Mid-Atlantic States contain mafic and ultramafic storage resources that are suitable for both in situ and ex situ CO_2 mineralization with a potential for greater than 20 million tons of CO_2 stored per year via mineralization.
- Five target geologic units for the in-situ mineralization storage are selected by our team, and the areal extent of this units in Virginia are calculated. Among them are:
    - The Catoctin Formation meta-basalt at the Blue Ridge geological province with the total areal extent of ~1900 km^2, and an estimated thickness is ~915 m,
    - The soapstone belt at Albemarle-Nelson area with the areal extent of ~150 $km^{2,}$
    - The Diabase of Jurassic age at the Culpepper Basin with the areal extent of ~400 km^2,
    - Ultramafic komatiite at the Piedmont and Blue Ridge geological provinces with the areal extent of ~10 km^2.
- Our preliminary calculations with the assumption of 1% effective porosity, and that all the pore space fully mineralized with calcium carbonate, indicates that the Catoctin Formation can accept 20 million tons of CO_2 per year over a number of years.

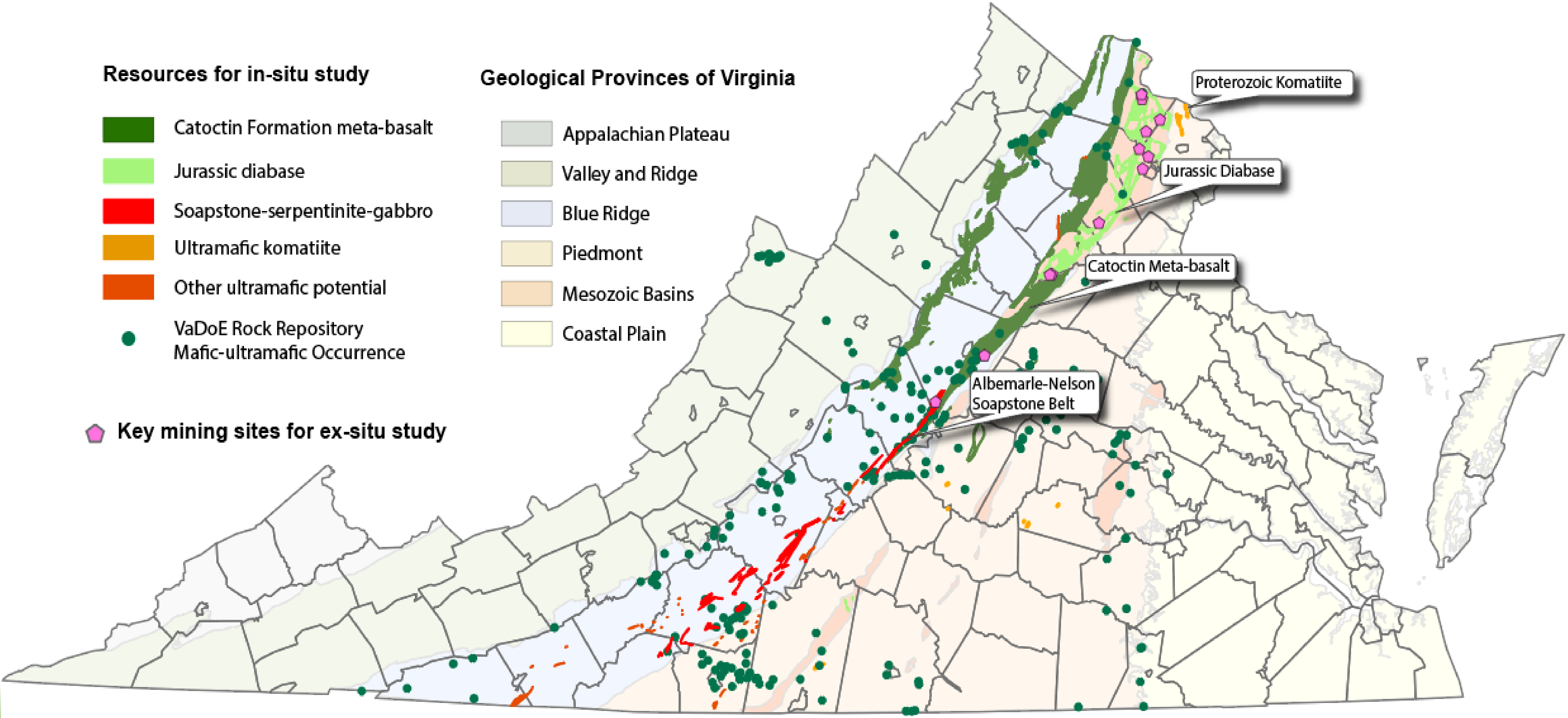
Ex situ and in situ mineralization

- *Ex situ* carbon mineralization refers to the process of reacting CO_2-charged aqueous solution with processed rocks in an engineered reactor vessel under controlled conditions.
    - Significant amounts of mine waste fines are available.
- *In situ* carbon mineralization refers to the process of injecting CO_2 into deep geological formations as either a supercritical fluid or a CO_2-charged aqueous solution.
- We envision that the ultramafic rocks are more suitable for in-situ, while the mafic mine wastes are better fits for ex-situ (or in-situ surface) carbon mineralization.

The mafic rocks are only good candidates for mineralization, if they are in the form of mine wastes and already crushed. Crushing the rocks in small pieces allows for a larger contact area with CO_2 and results in accelerating the mineralization process.

A broad range of potential resource types and formations, for both in-situ and ex-situ mineralization will be considered.

Potential carbon mineralization resources of Virginia



Tasks

Task 1.0 – Project Management and Planning

Task 2.0 – Geological Assessment

Task 3.0 – Prospective CO_2 Storage Resource Characterization

Task 4.0 – Post-Field Study Mapping

Task 5.0 – Future Commercialization and Mineralization Cost Assessment

Task 2.0 –Geological Assessment

Lead Researcher:

Jenny Meng, VaDOE

Subtask 2.1 – Geologic overview

- Defining the initial scope of the study at the beginning of the project, such as areas with suitable rock, sampling area, and qualified mine locations. The Recipient will characterize the current state of knowledge for suitable storage units within the study area.
- Assessments of mafic and ultramafic rock exposure through existing geologic database, including up-to-date geologic maps, results of petrological analysis, geochemical laboratory results, USGS topographic maps and other aerial and geophysical surveys.
- Gathering information on the ultramafic and mafic bedrock spatial extents, depth, key formations, petrology, accessibility, and existing physical and chemical properties.
- Selection of mining sites that associate with mafic and ultramafic rock production for conducting the industrial waste investigation.

Subtask 2.2 – Pre-field Study mapping and sampling

- Performing geologic field investigation to assess the suitable geologic exposure in Virginia. Suitable natural materials including mafic and ultramafic rocks will be outlined.
- Sample collections for lab testing effort from Virginia and other nearby states. Rock samples will be collected during the field work and existing mapping activities. Samples will be selected and submitted to commercial laboratories for whole rock plus trace element, quantitative mineralogical, and geotechnical analyses.

Task 3.0 – Prospective CO_2 Storage Resource Characterization

Lead Researchers:

Rohit Pandey, VT

Wencai Zhang, VT

Ryan Pollyea, VT

Bahareh Nojabaei, VT

Subtask 3.1 –Laboratory analyses of rock physical properties

The laboratory analysis of flow-coupled-geomechanical properties of reservoir rock will be assessed to evaluate:

a) Effect of CO_2 mineralization on the structural/textural properties of the rock type;
b) Dynamic evolution of permeability of reservoir rock with continued CO_2 mineralization.

- Determination of strength, shear/bulk modulus and failure envelope of samples pre- and post-mineralization for representative samples from the Central Atlantic Magmatic Province CAMP region.

- Using flow-through permeameter, both artificially fractured plugs and intact cores plugs will be evaluated to understand the effect of reactive surface area on mineral dissolution and carbonate precipitation rates at multiple timepoints. The change in permeability will also be measured.

- Using a scanning electron microscope and a micro-CT, providing high resolution understanding of the effect of CO_2 mineralization on the flow and structural properties of reservoir rocks.

Subtask 3.2 –Laboratory Analyses of reactions and product evaluation

- Representative slurry samples will be collected during the carbon mineralization process to evaluate carbon mineralization efficiency, dissolution of various species, and the kinetics of the reactions occurring in the process will be calculated.
- The carbon mineralization tests will be carried out under different conditions to evaluate the effect of different parameters, such as pressure, temperature, and solution matrix.
- Mineral dissolution tests will also be performed on the samples to evaluate the extractability of critical elements, i.e Rare Earth Elements.
- Results from the mineral dissolution tests will be analyzed to determine the underlying metabolic pathways in order to identify the microbial communities potentially catalyzing host-rock dissolution.

Subtask 3.2 –Laboratory Analyses of reactions and product evaluation

Feed particle size
Feed porosity
Feed surface area
Feed mineralogy
Reaction pressure
Reaction temperature
Reaction solids content
Reaction time
Solution chemistry
Etc.

<u>Carbon Mineralization</u>

Carbon mineralization efficiency;
Carbon mineralization kinetics;
Carbon mineralization mechanisms;
Dissolution behavior;
Product characteristics

<u>CM Recovery</u>

Leaching kinetics & thermodynamics of CMs and carbon-reactive species;
Metabolic pathways

CO_2

Input for other tasks

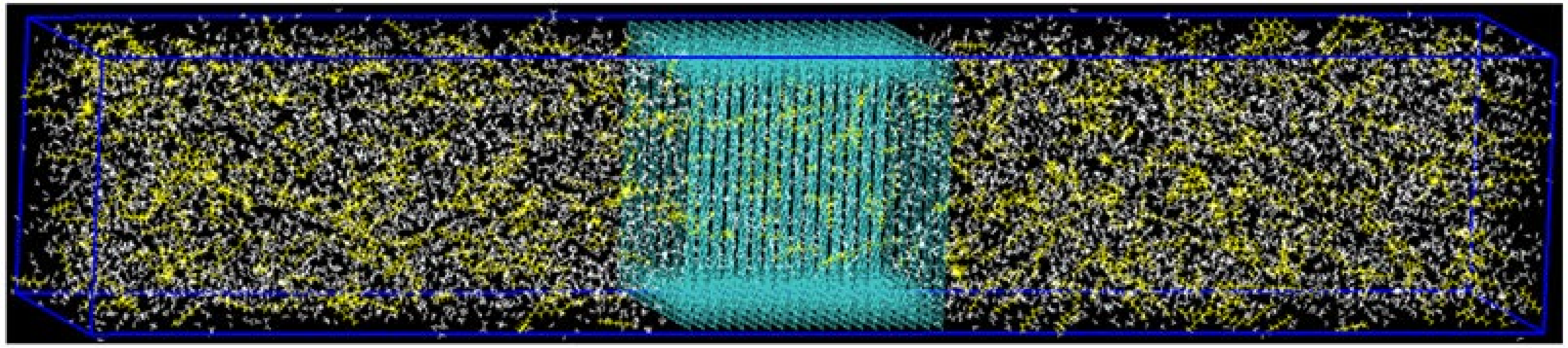
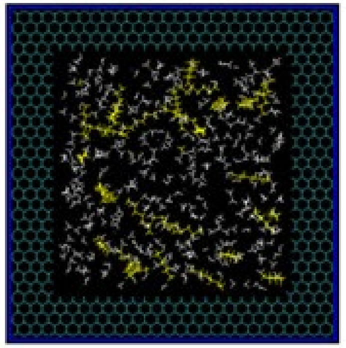
Equipment available at VT: Nikon X-Ray CT System; Tescan Automated SEM; CoreLab Permeability Equipment;

Subtask 3.3 – Molecular scale simulation

- Translation of the characterization results into simplified and quantified physical and chemical processes to develop the large-scale reactive simulation model (next task).
- Molecular dynamics simulations to determine:

1) If carbon mineralization affect reactive surface area and the reaction rate.
2) If mineralization occurrences uniformly across the rock surface and the pore network
3) Mineralization effect on hydraulic properties, permeability and porosity.
4) Time scale for changes.
5) Reactivity and hydraulic properties with respect to flow rate.

- The results from the molecular dynamics simulations will be integrated with the outcomes of experimental analyses of Subtasks 3.1 and 3.2 and will be used in the form of analytical expressions and numerical correlations as a feed to the field-scale reactive transport model (Subtask 3.4).

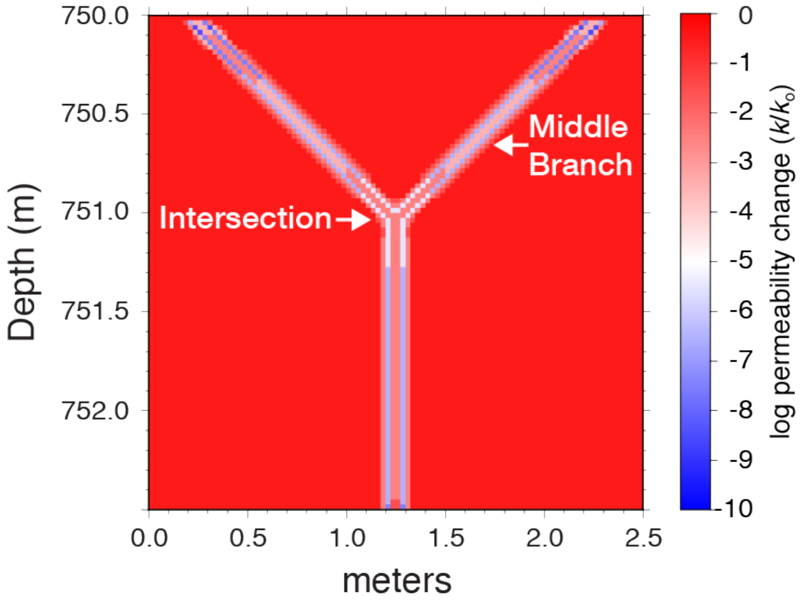



Subtask 3.3 – Upscaling and identification of target development areas

- Performing individual reservoir models for sites within the study area to assess *site-scale* carbon mineralization throughout the study area.
  -The results from each site-scale simulation will yield a time-dependent and uncertainty-bounded estimate of the CO_2 mineralization potential for various mafic terrains throughout the U.S. Mid-Atlantic region.

- Performing a set of numerical simulations that model flow-through reactor vessels to assess the *ex-situ* carbon mineralization potential for mafic waste rock.

> ➢ To identify the optimal fluid chemistry and grain-size distribution, a set of individual simulations will be performed for each rock type.
>
> ➢ Mineralization efficiency per unit time will be quantified as the ratio of mass of carbon sequestered in mineral phases to the mass of carbon injected into the reactor vessel.



Simulation results showing patterns of permeability change caused by CO_2 mineralization in a basalt fracture for a moderate permeability-porosity coupling

Task 4.0 – Post-Field Study Mapping

Lead Researcher:

Jenny Meng

Bahareh Nojabaei

Subtask 4.1 – Ranking targets through using machine learning

- Machine learning will be used to scan through all the influential factors, to rank the CO_2 mineralization site candidates and locate the most prospective active regions.

➢ There are multiple sources of uncertainties and simplifying assumptions associated with our geological and physical data, and the state-of-the-art physics-based simulation models.

➢ The degree of suitability of a potential site is affected by multiple geological, chemical, physical, and economical factors.

Subtask 4.2 – Database development for potential site candidates

- Storage resource data for the Mid-Atlantic areas will be provided to DOE/NETL for inclusion in the Energy Data Exchange (EDX) System.
- Based on the stratigraphic markers, structure, physical and chemical property, and volumetric storage potential the we evaluate the influential factors that affect the prioritizing of carbon-mineralization sites.
- High-resolution geologic maps for prioritized locations will be constructed.

Subtask 4.3 – Data analyses and extension to nearby regions

- Extension of the resource assessment to the nearby regions with limited geological data, through machine learning regression approaches.

- Development of a map for the Mid-Atlantic region and beyond, by fitting regression models to the predicted storage potentials. (The experiments and reactive transport modeling will be performed for the Mid-Atlantic region.)

- Ranking the mineralization candidates

➢ The Recipient will provide for a broader area within the Eastern U.S. from the data analyses, and machine learning.

➢ We will apply XGBoost and Random Forest, tree-based machine learning algorithms that have been successfully applied in geosciences and widely used in classification and regression problems.

Task 5.0 – Future Commercialization and Mineralization Cost Assessment

Lead Researcher:

Bahareh Nojabaei

Nino Ripepi

Task 5.0 – Future Commercialization and Mineralization Cost Assessment

- Assessment of the cost of mineralization for both potential in-situ and ex-situ resources,
- Development of site-specific commercialization plans.
- Comprehensively analyses and communication of the outcome of our analyses with the relevant stakeholders.

Project timeline

Task Name	Assigned Resources	Year 1				Year 2			
		Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4
Task 1.0 – Project Management and Planning	B. Nojabaei and N. Ripepi, VT								
Task 2.0 – Task 2.0 - Geological Assessment	VaDOE & VT								
Subtask 2.1 – Geologic overview	VaDOE	A							
Subtask 2.2 – Pre-field Study mapping	VaDOE		B						
Subtask 2.3 – Suitable industrial waste sites investigation	VaDOE & VT	C							
Task 3.0 - Prospective CO2 Storage Resource Characterization	VT								
Subtask 3.1 – Laboratory analyses of rock physical properties	R. Pandey, VT					D			
Subtask 3.2 – Laboratory Analyses of reactions and product evaluation	Wencai Zhang, VT					E			
Subtask 3.3 – Molecular scale simulation	B. Nojabaei, VT					F			
Subtask 3.4 – Upscaling and identification of target development areas	R. Pollyea, VT						G		
Task 4.0 – Post-Field Study Mapping	VaDOE & VT								
Subtask 4.1 – Ranking targets through using machine learning	B. Nojabaei, VT							H	
Subtask 4.2 – Database development for potential site candidates	VaDOE								I
Subtask 4.3 – Data analyses and extension to nearby regions	B. Nojabaei, VT								J
Task 5.0 – Future Commercialization and Mineralization Cost Assessment	B. Nojabaei and N. Ripepi, VT								K

Potential project benefits

- The results of this proposed project will help the local and national communities meet the national decarbonization goals.
- Could help mining companies reduce waste fines and create a new product.
- The resource assessment and characterization of mineralization sites in the U.S. Mid-Atlantic empowers businesses to lead this carbon management effort in regional and global scales.
- To help the U.S. achieve its climate and environmental ambitions, these procedures should be cost-effective. Throughout this project, we provide insight on how to proceed with the most suitable mineralization approach and location, that is not only environmentally viable, but also is it economic in long term.
- Therefore, in addition to carbon storage capacity assessment, the extractability of critical elements will be evaluated. This will contribute to the development of concurrent carbon mineralization and critical elements recovery strategies in the future.