Pacific Northwest NATIONAL LABORATORY

NATIONAL ENERGY TECHNOLOGY LABORATORY OIL & GAS

Carbon Management and Oil and Gas Research Project Review Meeting

# Coupled Hydrologic, Thermodynamic, and Geomechanical Processes of Natural Gas Hydrate Production (FWP-72688)

August 25, 2021

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U.S. DEPARTMENT OF ENERGY BATTELLE

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# Budget Period 1 Tasks

## BP1-Task 1.0 Project Management and Collaborative Research

Collaborative project with KIGAM via the Joint Korea-U.S. Gas Hydrate Project

KIGAM research directed at innovative production technologies for suboceanic deposits of gas hydrates, such as those found in the Ulleung Basin of the Korean East Sea

## BP1-Task 2.0 IGHCCS2

PNNL will participate in the 2nd International Gas Hydrate Code Comparison Study (IGHCCS2) as both participant (i.e., submitting solutions) and co-lead. The other co-leaders for this code comparison study will be Tim Kneafsey from Lawrence Berkeley National Laboratory and Yongkoo Seol from the National Energy Technology Laboratory. The study will be particularly focused on modeling coupled thermal, hydrological, and geomechanical processes and their effect on the production of methane gas from hydrate-bearing reservoirs. This study will build on the accomplishments of 1st International Hydrate Code Comparison Study (IHCCS-1), successfully executed from 2007 to 2009, and consider the expanded number of numerical simulators worldwide and advances in modeling capabilities of those analytical tools.

# Budget Period 2 Tasks

## BP2-Task 1.0 Project Management and Collaborative Research

Collaborative project with KIGAM via the Joint Korea-U.S. Gas Hydrate Project

KIGAM research directed at innovative production technologies for suboceanic deposits of gas hydrates, such as those found in the Ulleung Basin of the Korean East Sea

## BP2-Task 2.0 Simulations in Support of the Alaska North Slope Project

Numerical simulations to forecast the performance of the production test well of the joint NETL-JOGMEC-USGS-AIST Alaska North Slope (ANS) project, during a series of depressurizations, over the intrinsic permeability, relative permeability, and bound-water parameter space.

Additional simulations to forecast the response of the system to gas injection into the monitoring wells, following a period of depressurization.

## BP2-Task 3.0 Well Model Implementation in STOMP-HYDT-KE

Implementation of a well model similar to those developed for STOMP-CO2, STOMP-EOR, and STOMP-GT for deviated wells in STOMP-HYDT-KE.

# Budget Period 3 Tasks

## BP3-Task 1.0 Project Management and Collaborative Research

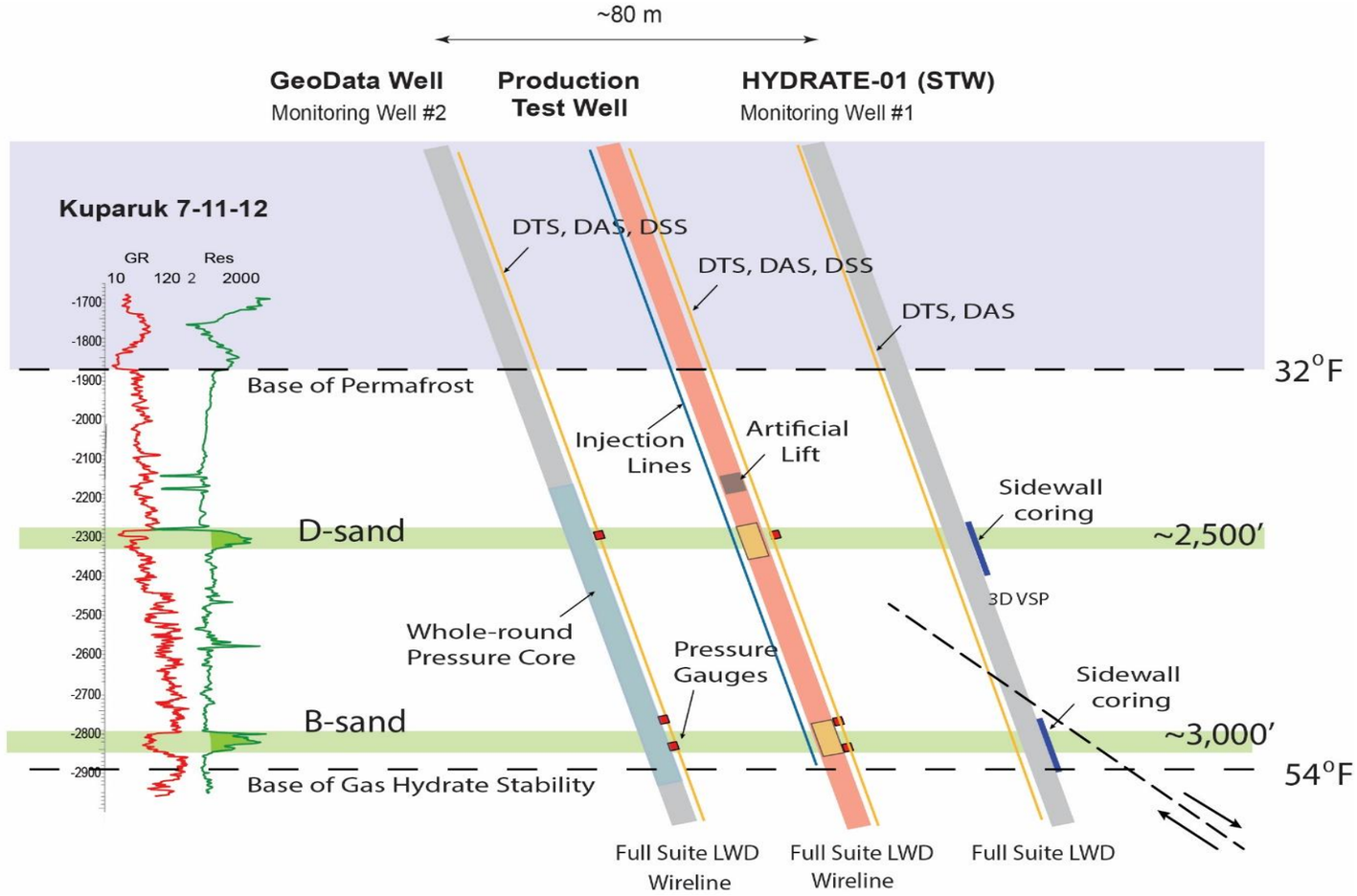
Collaborative project with KIGAM via the Joint Korea-U.S. Gas Hydrate Project

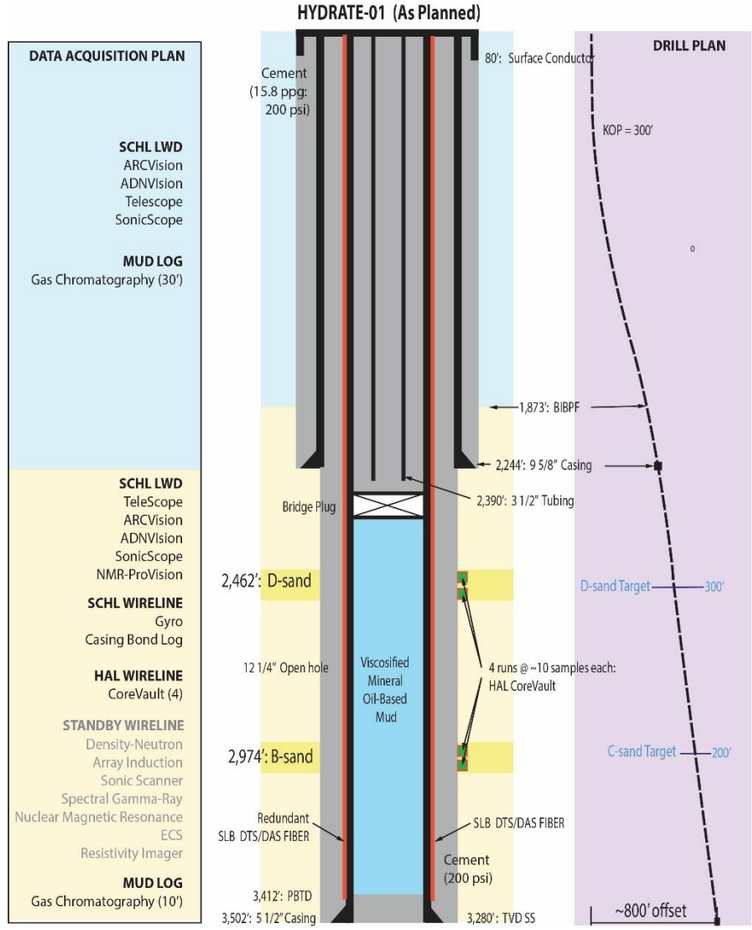
KIGAM research directed at innovative production technologies for suboceanic deposits of gas hydrates, such as those found in the Ulleung Basin of the Korean East Sea

## BP3-Task 3.0 STOMP-HYDT-KE Parallelization

PNNL will develop a parallel implementation of STOMP-HYDT-KE using MPI. MPI allows for parallel processing on shared memory (i.e., single nodes with multiple processors) and distributed memory computers (i.e., multiple nodes with multiple processors per node). The development involves converting the existing sequential implementation (i.e., single-processor) computer code into a parallel implementation. Ghost cells will be used to transfer information across processors and call parallel processing calls will be MPI based. This conversion will follow the framework and processes proven successful for developing parallel implementations of STOMP-GT and STOMP-CO2, but will not use Global Arrays calls. Those calls will instead be converted to MPI calls. To take full advantage of this implementation, STOMP-HYDT-KE will be linked to PETSc, the modern standard for parallel linear system solvers.

# Simulations in Support of the Alaska North Slope Project




Boswell, R., N. Okinaka, T. Collett. 2019. "Alaska North Slope Project Status." MHFAC Meeting, Houston, TX, April 23, 2019.

# Simulations in Support of the Alaska North Slope Project

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Cylindrical Domain
107 x 316
0.07 – 800 m
825.84 - 870.88 m

Simulation Time
540 days

Initial Conditions
51.447˚F, -0.061 ˚F/m
9.108 MPa, -9793 Pa/m

Well Pressure
4.8 MPa, -9793 Pa/m

Flowing Outer Boundary
51.447˚F, -0.061 ˚F/m
9.108 MPa, -9793 Pa/m
dissolved $CH_4$

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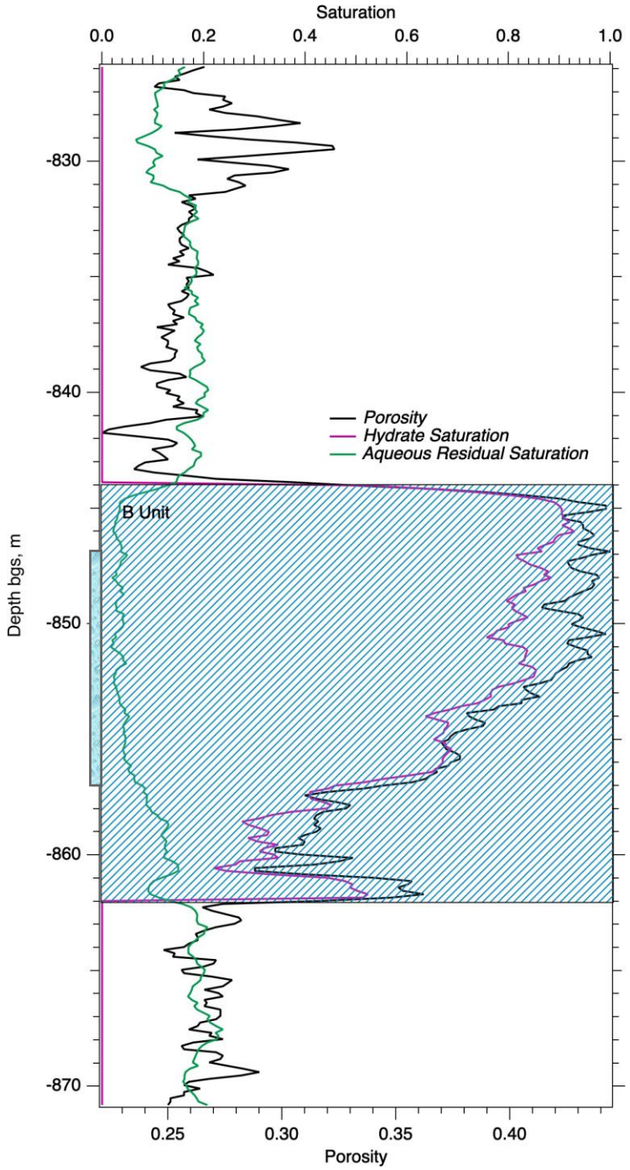


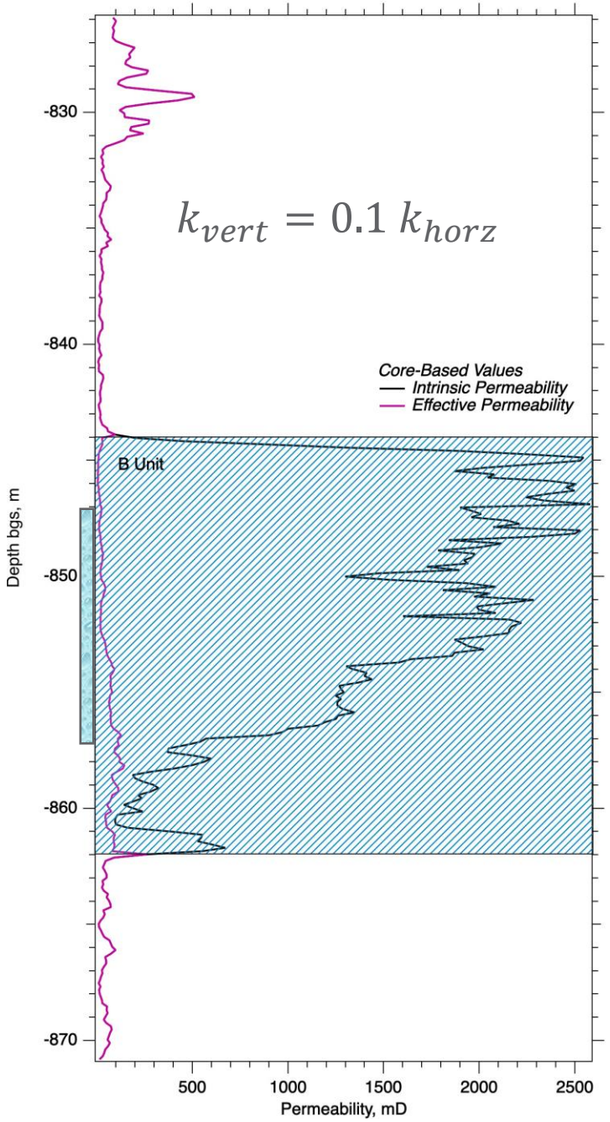


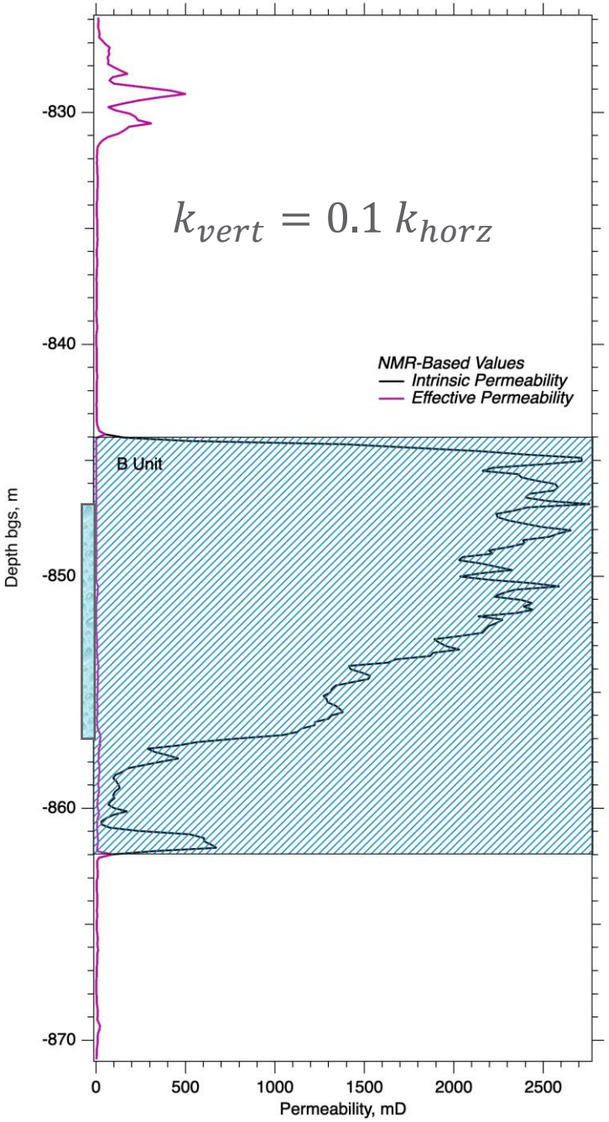

# Simulations in Support of the Alaska North Slope Project: Core-Based Scenario

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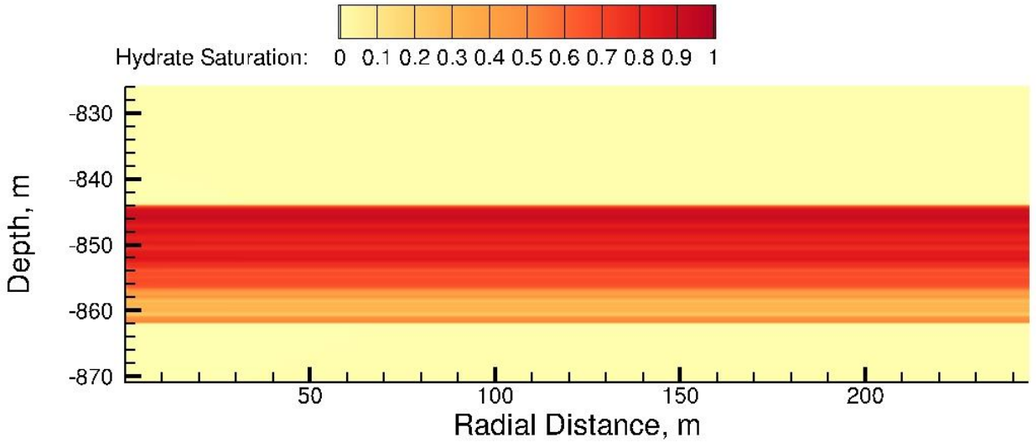


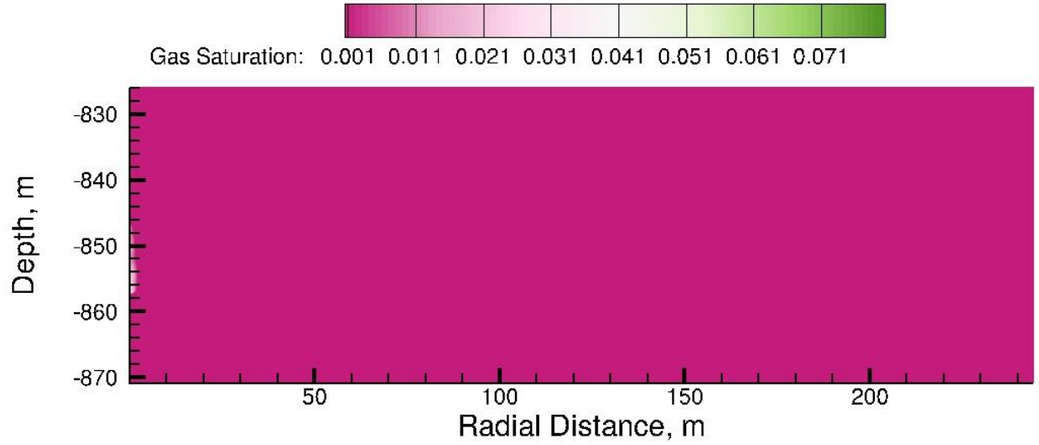


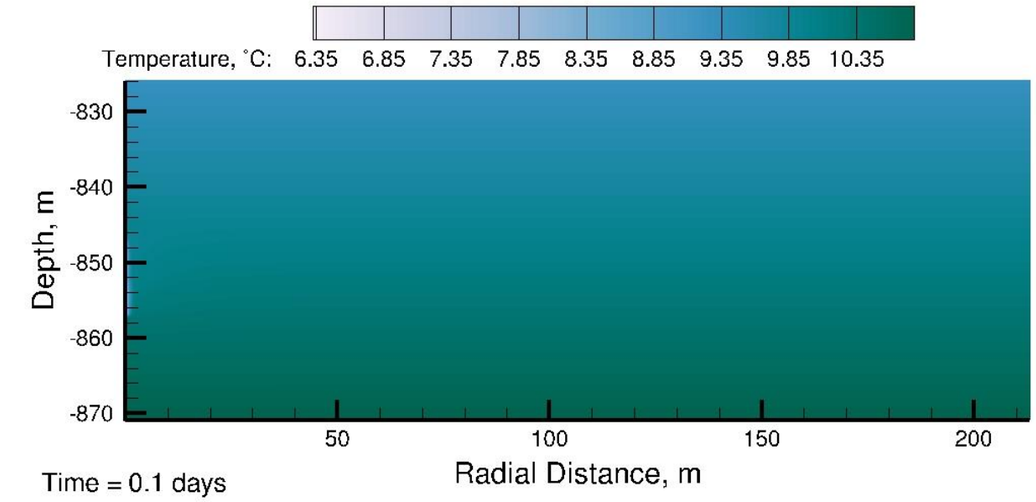


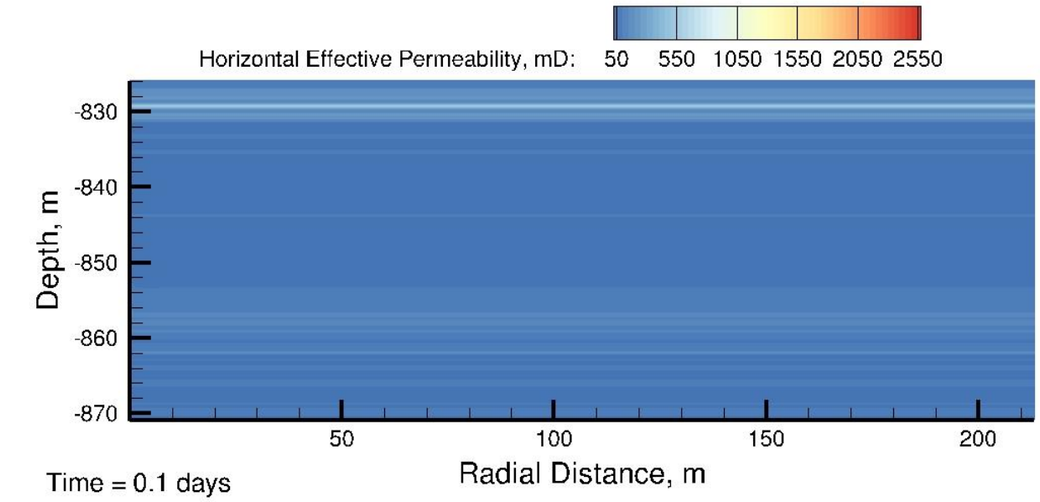

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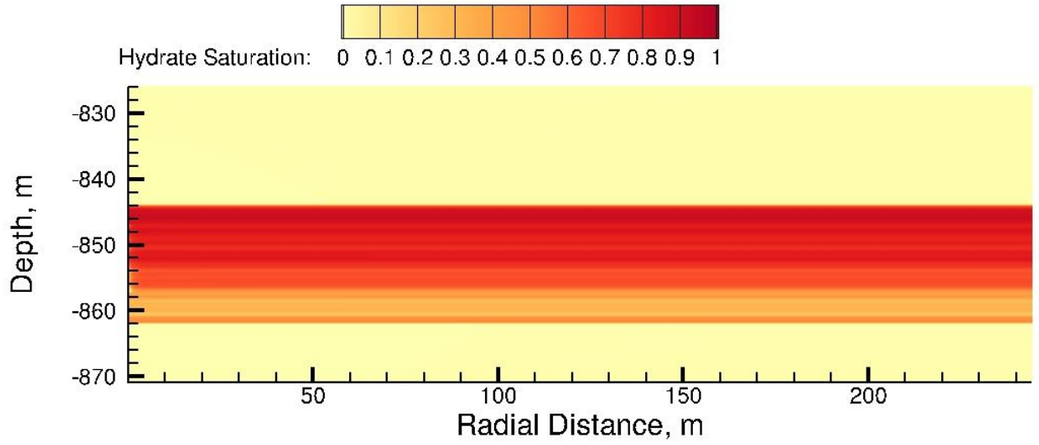


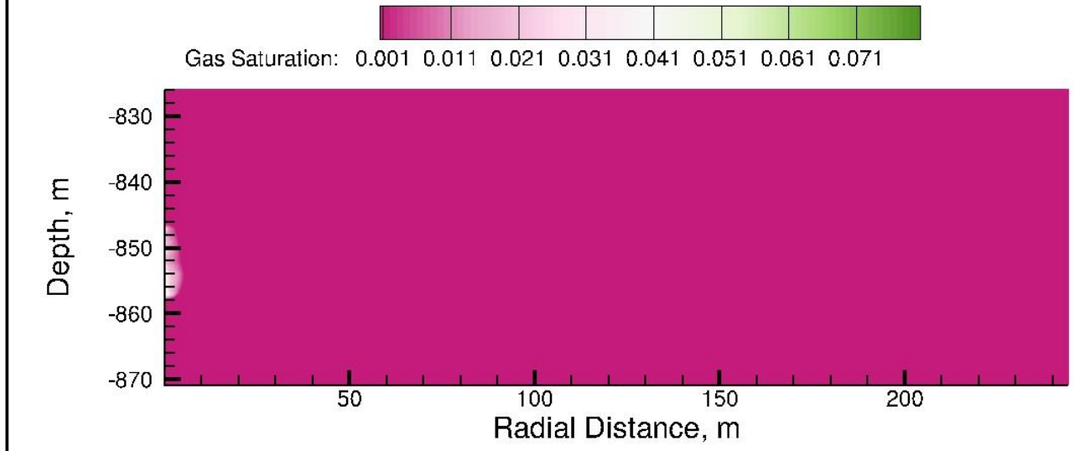


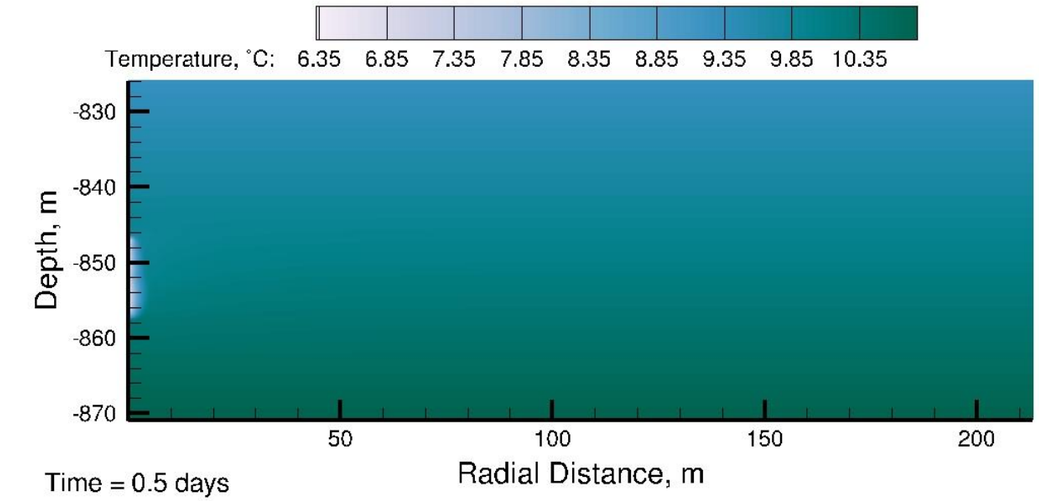


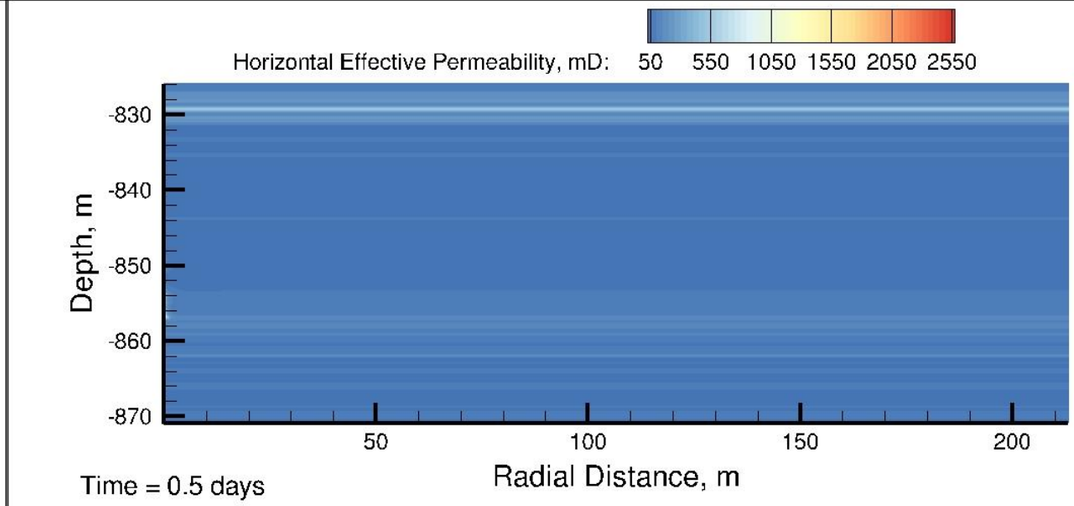

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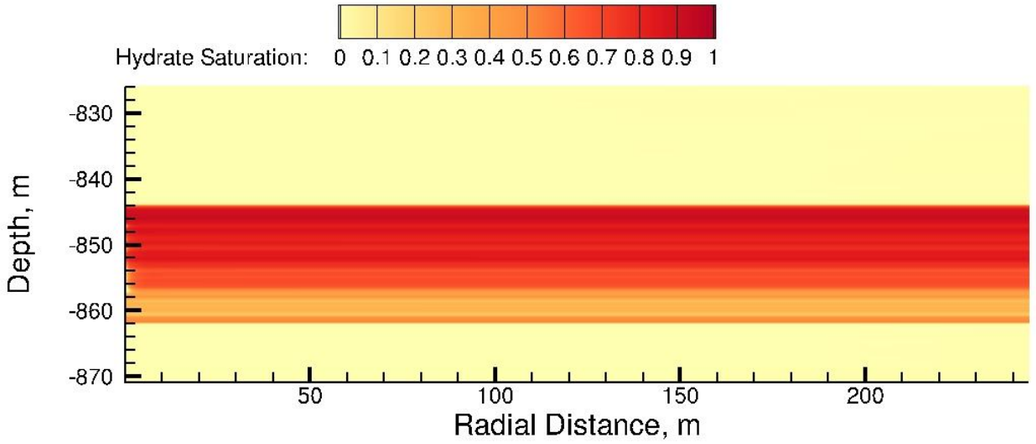


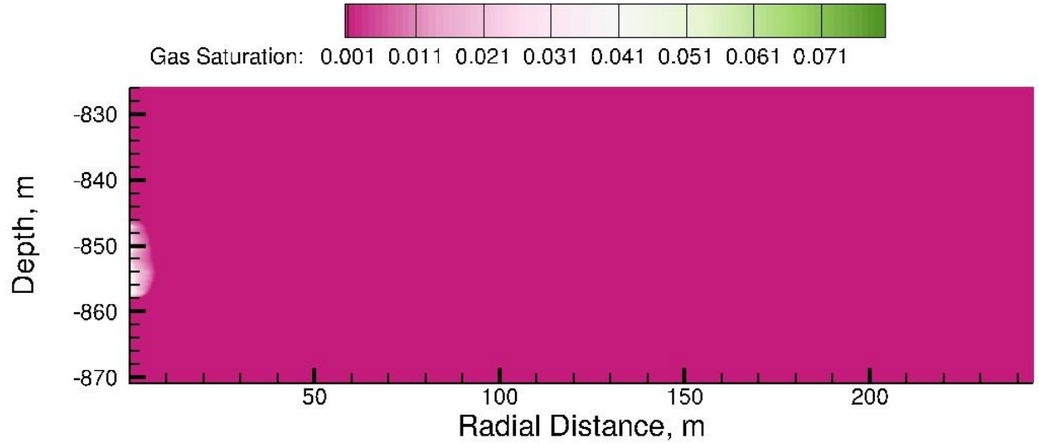


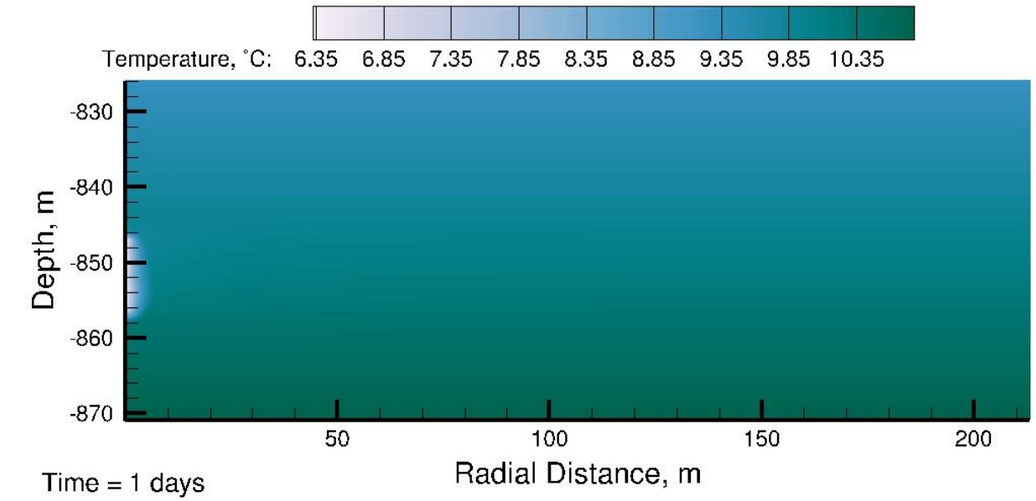


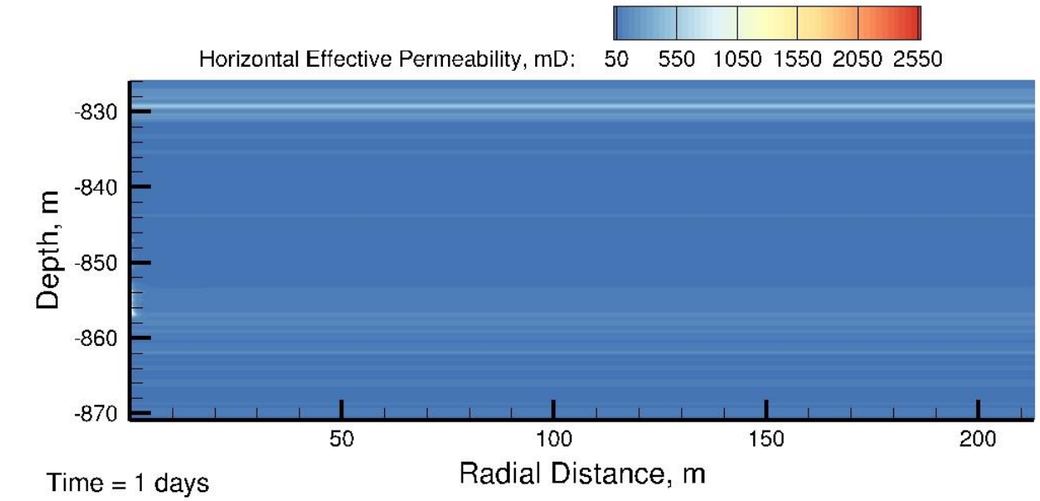

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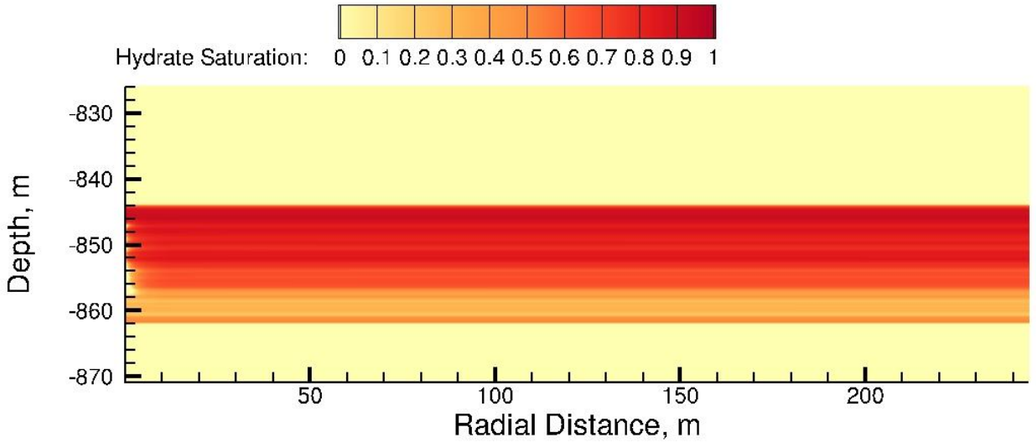


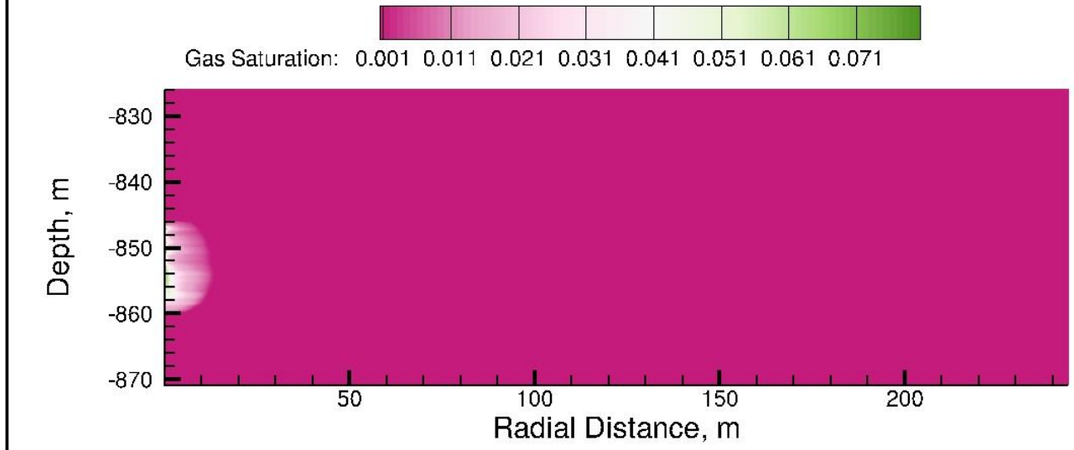


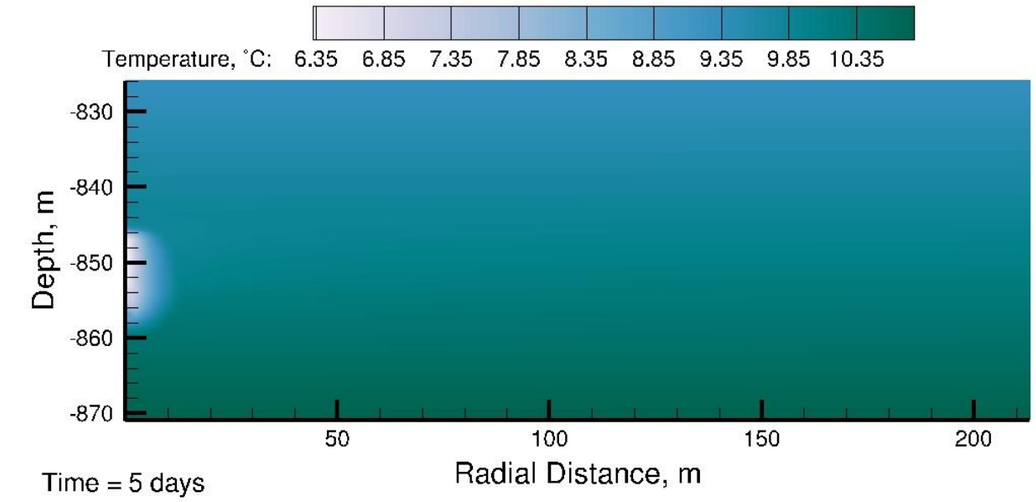


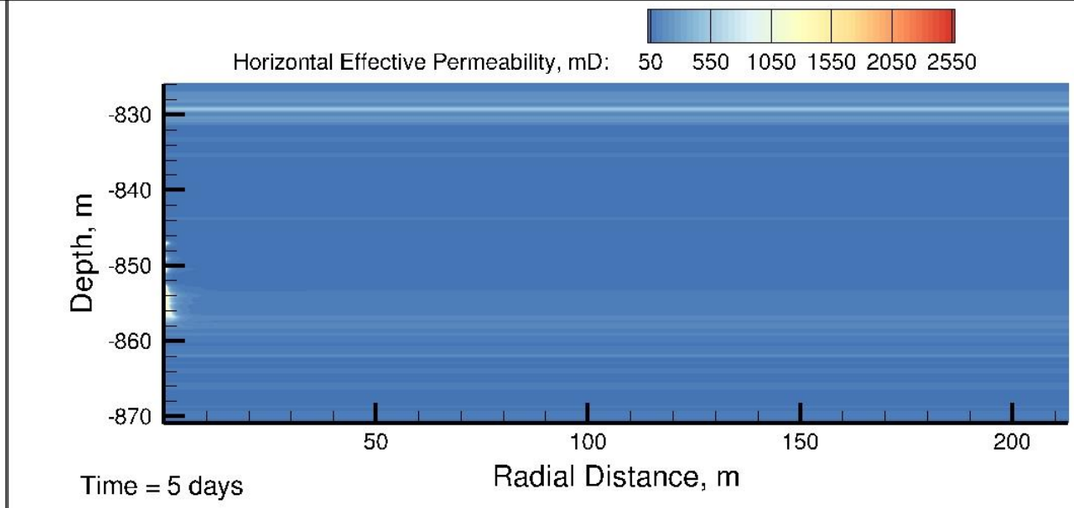

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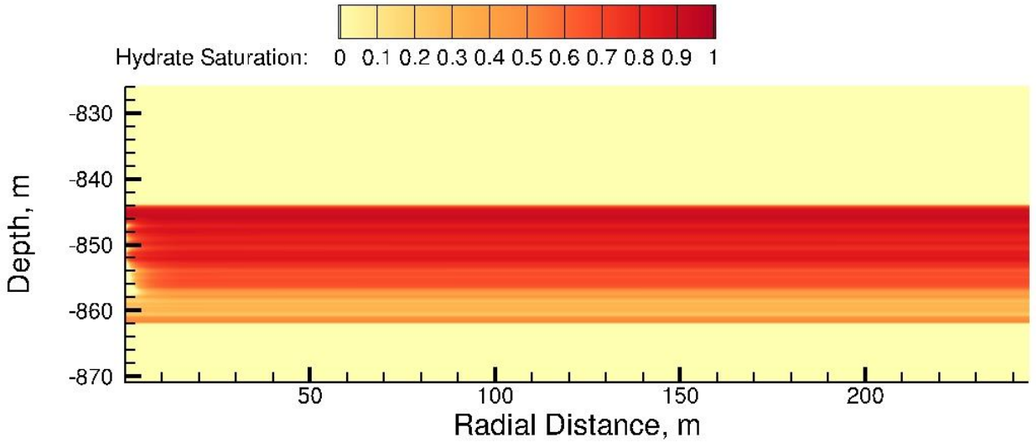


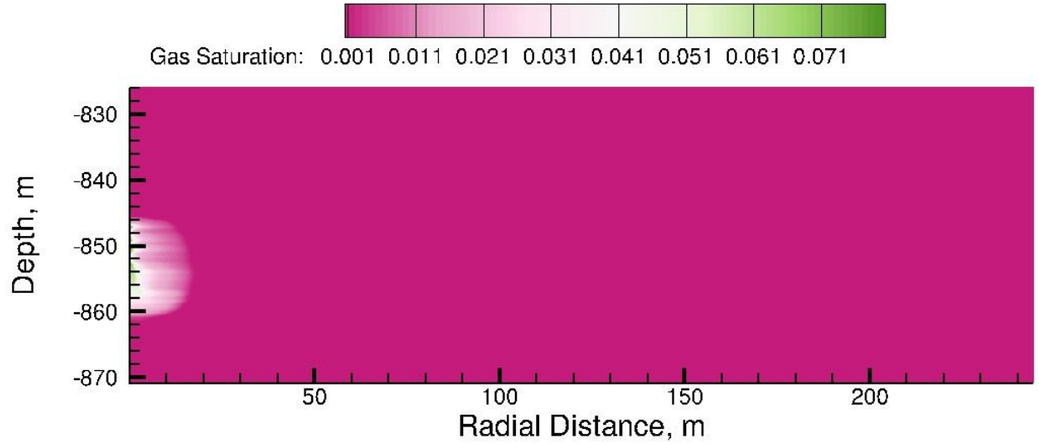


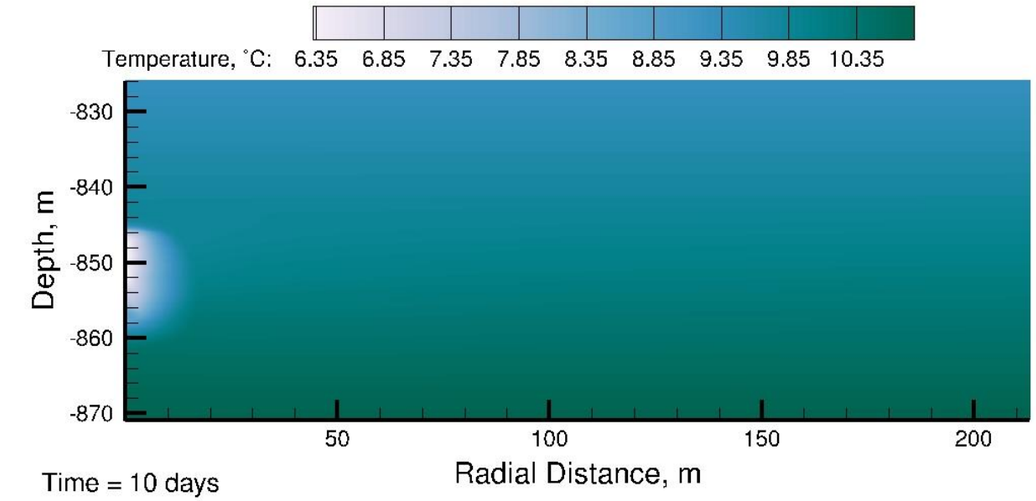


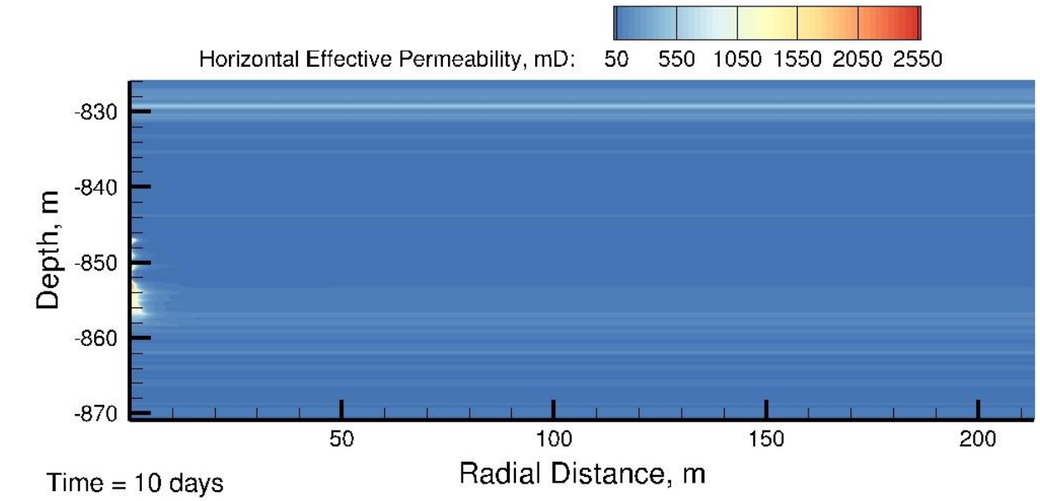

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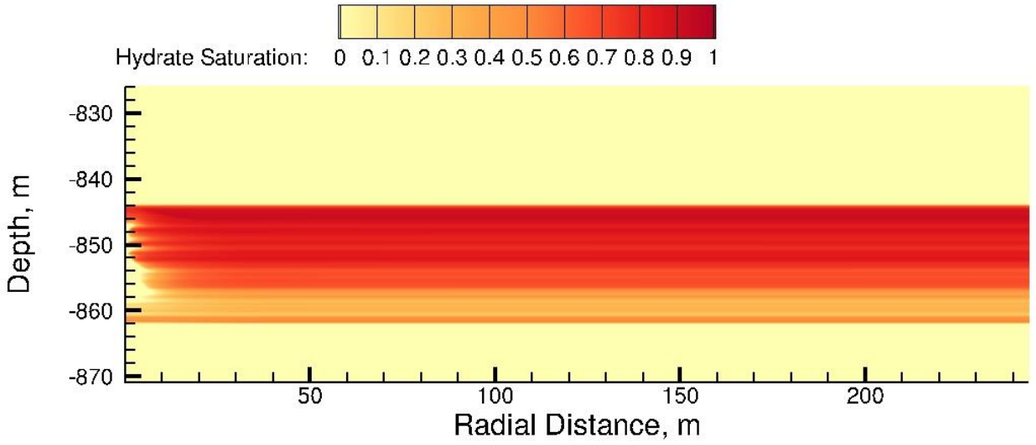


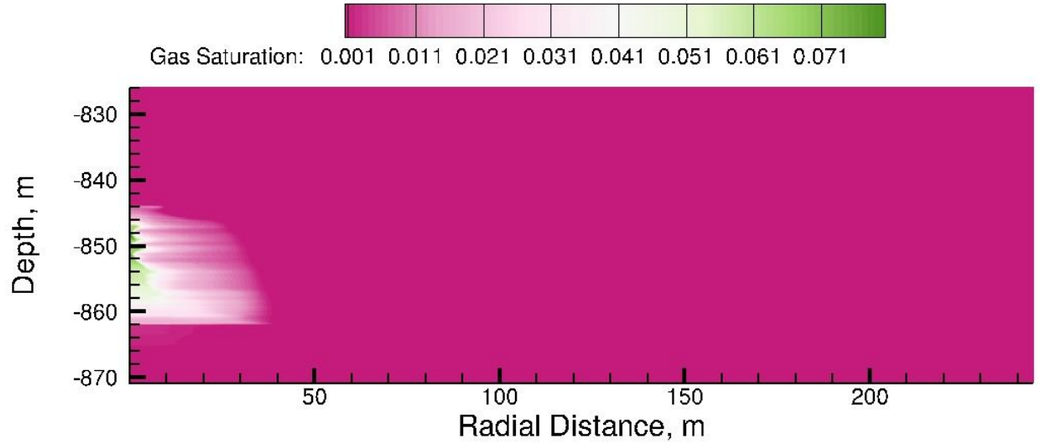


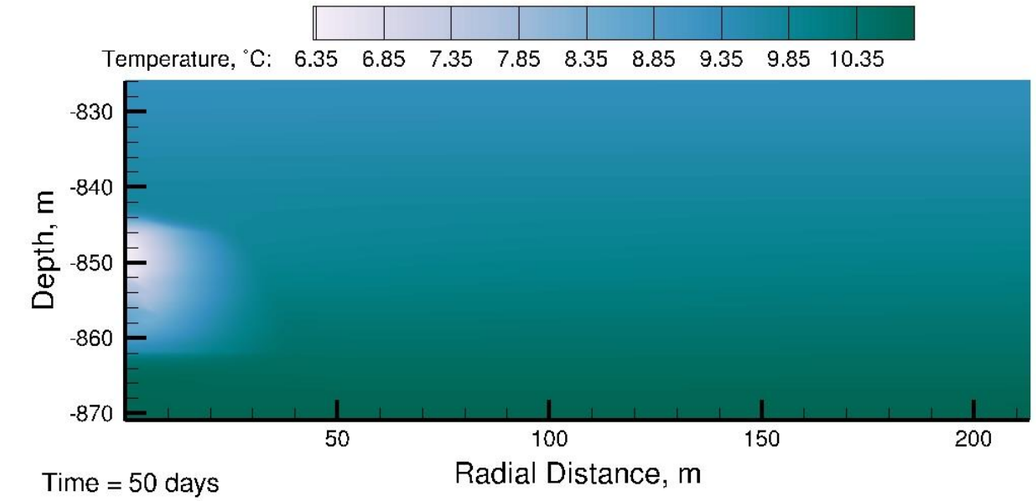


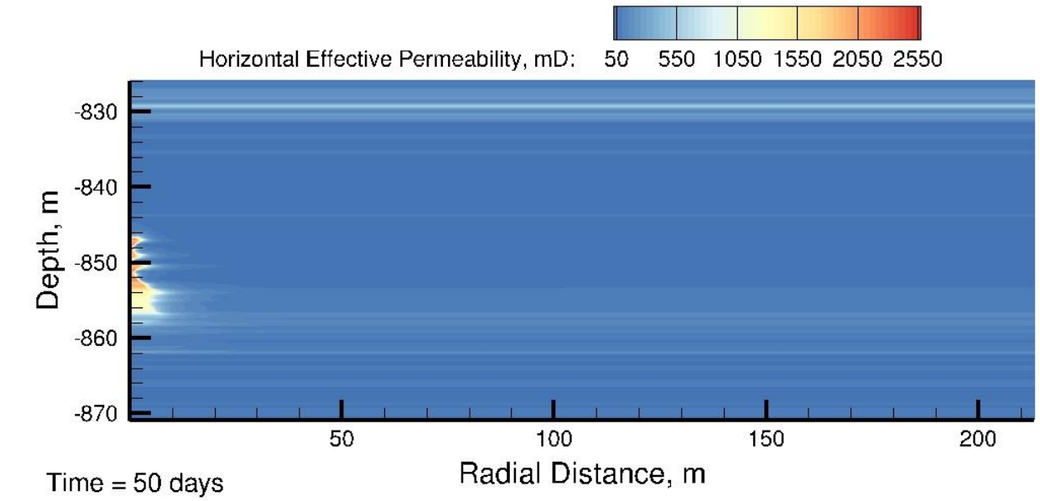

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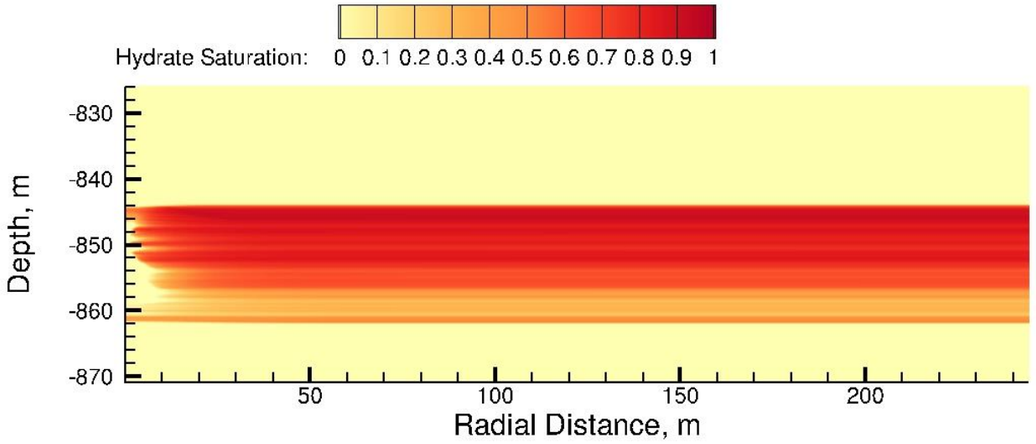


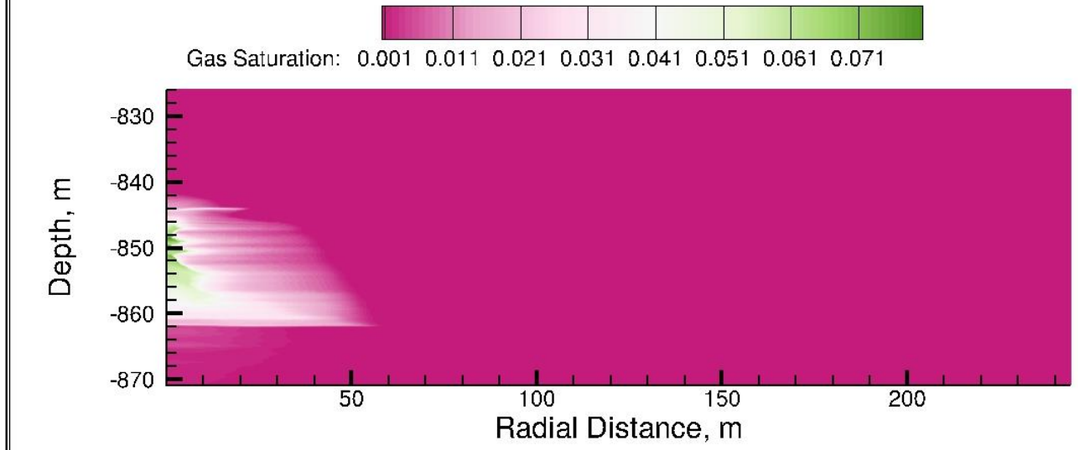


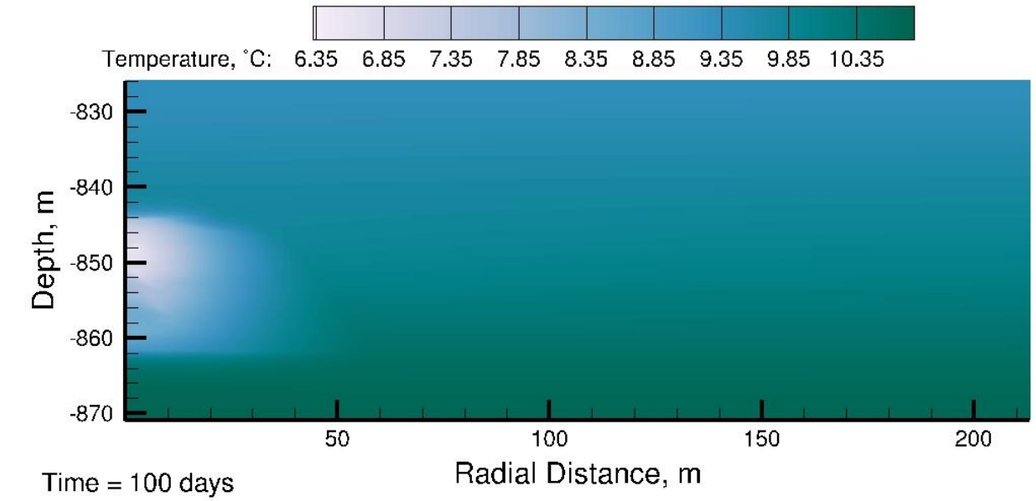


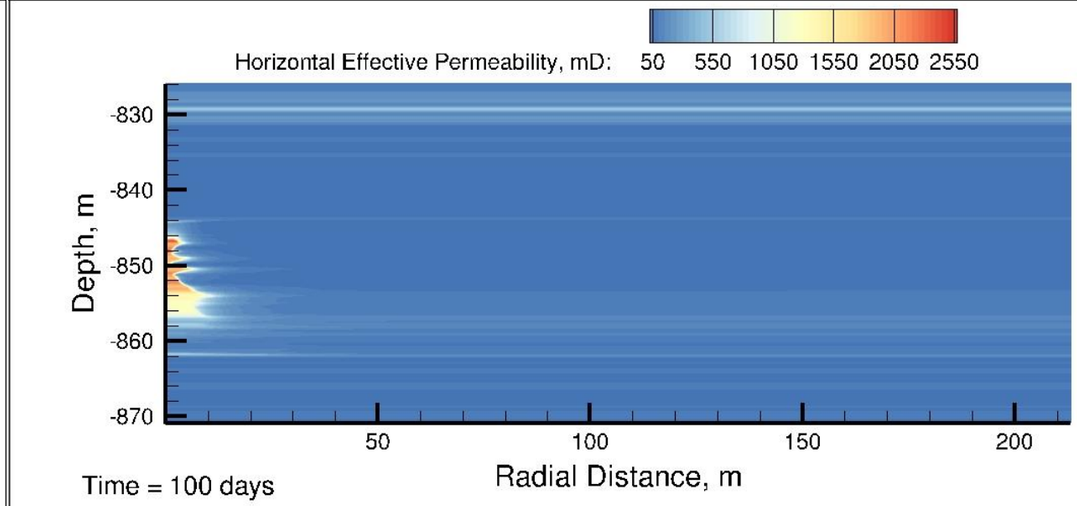

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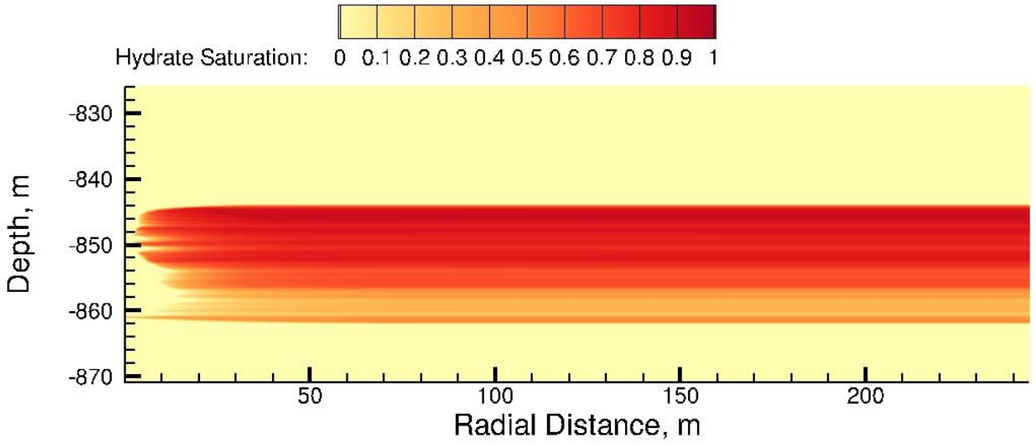


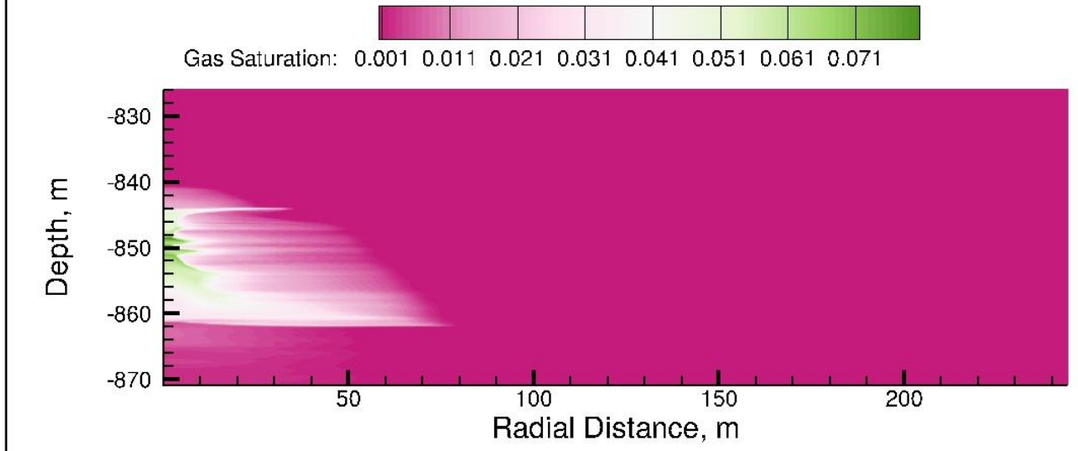


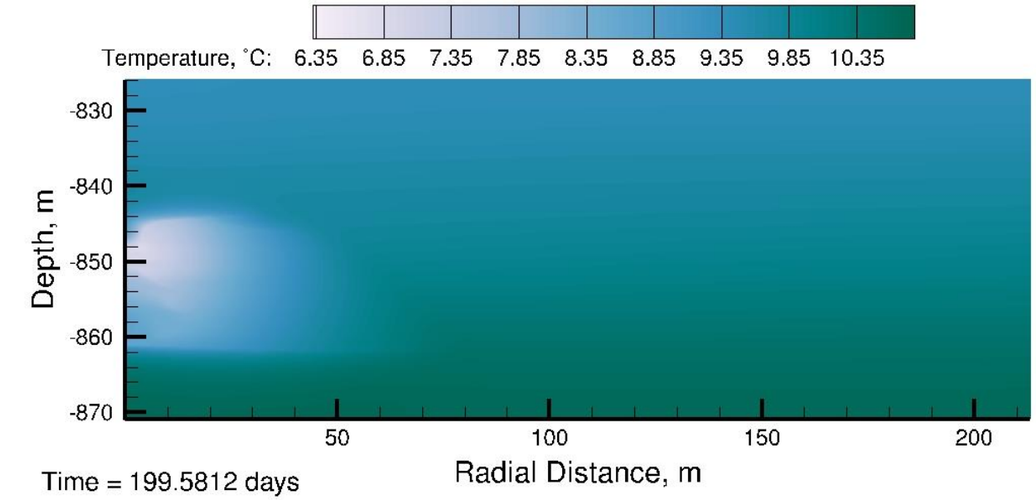


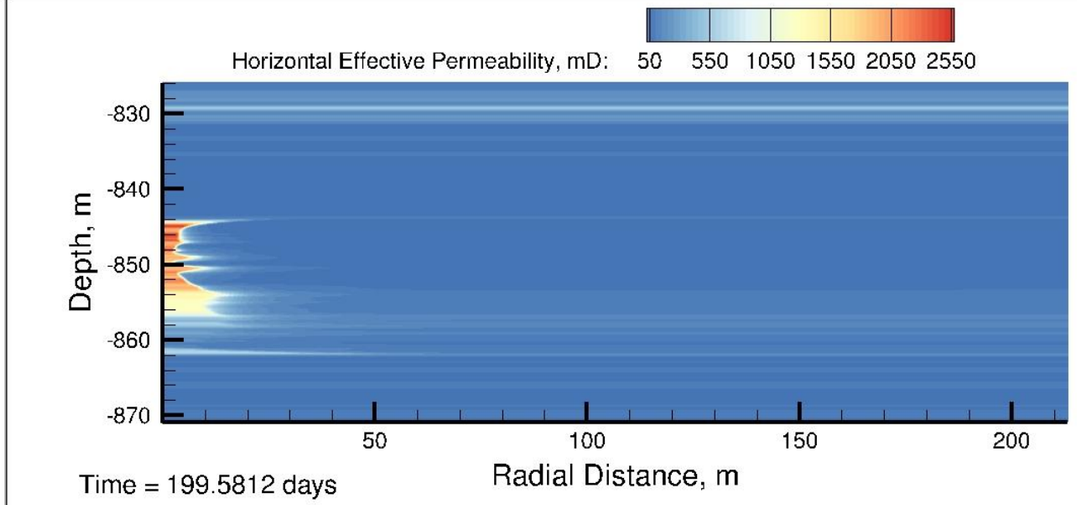

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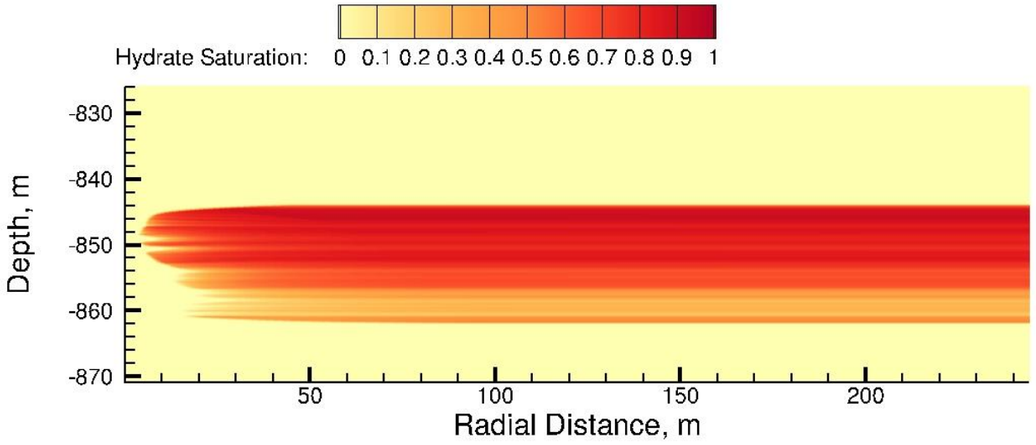


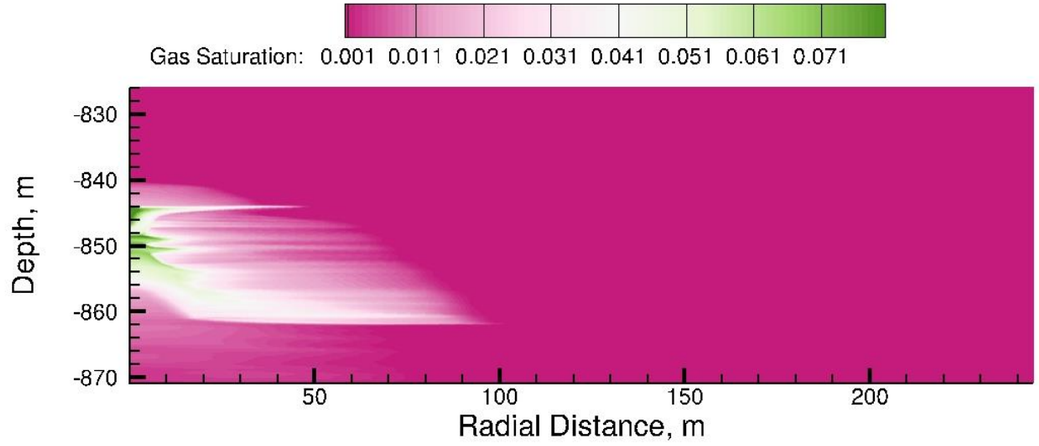


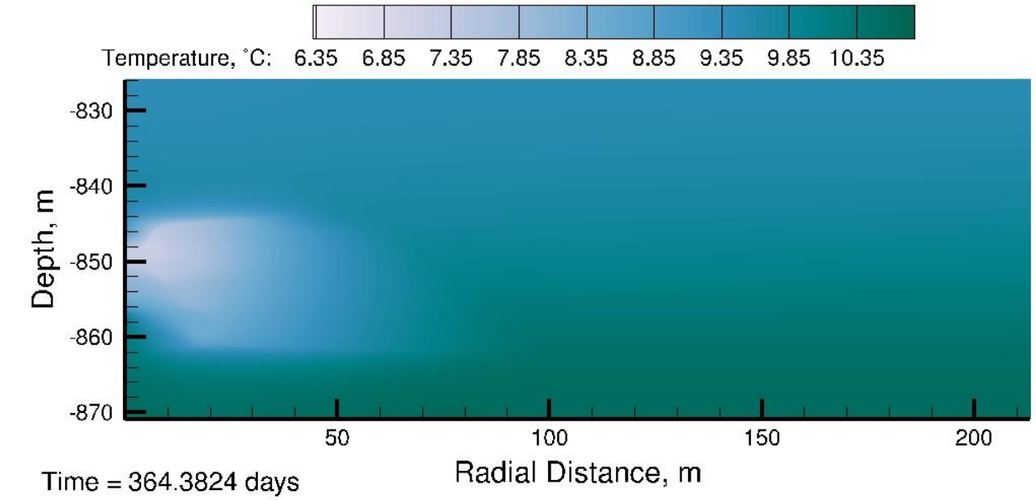


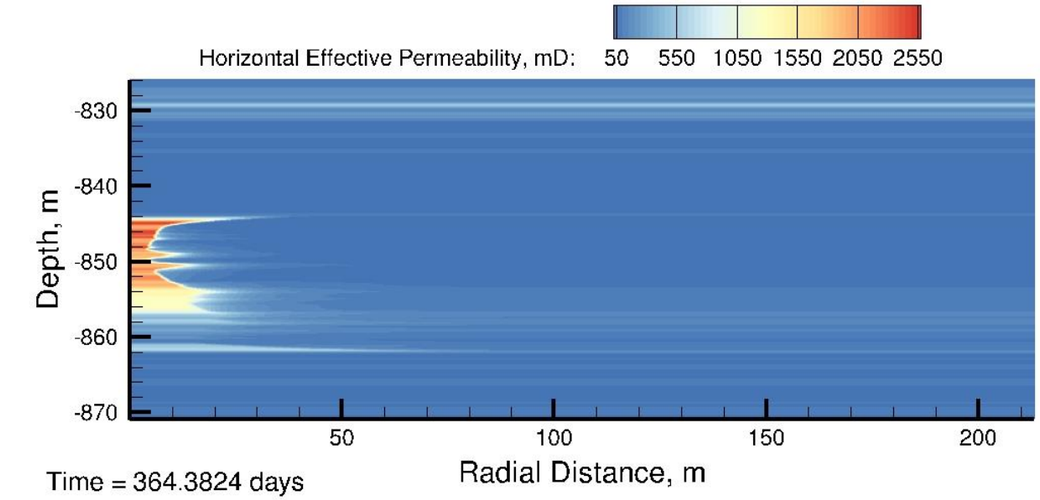

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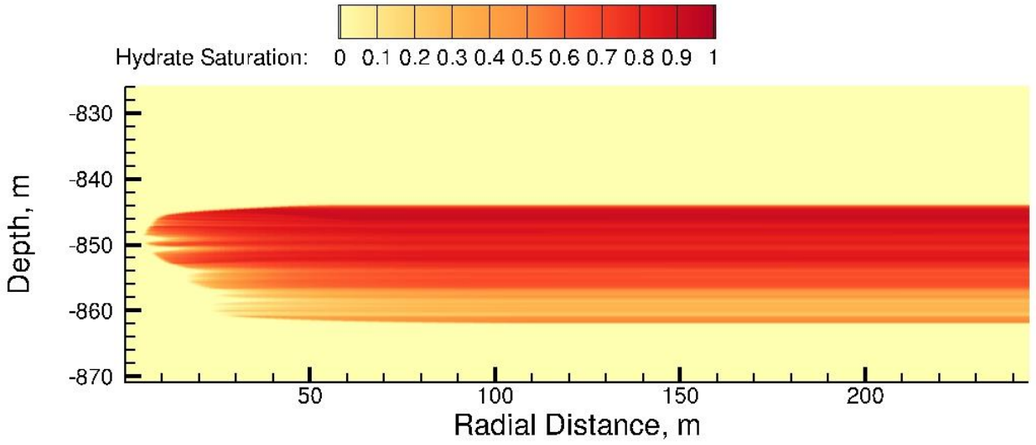


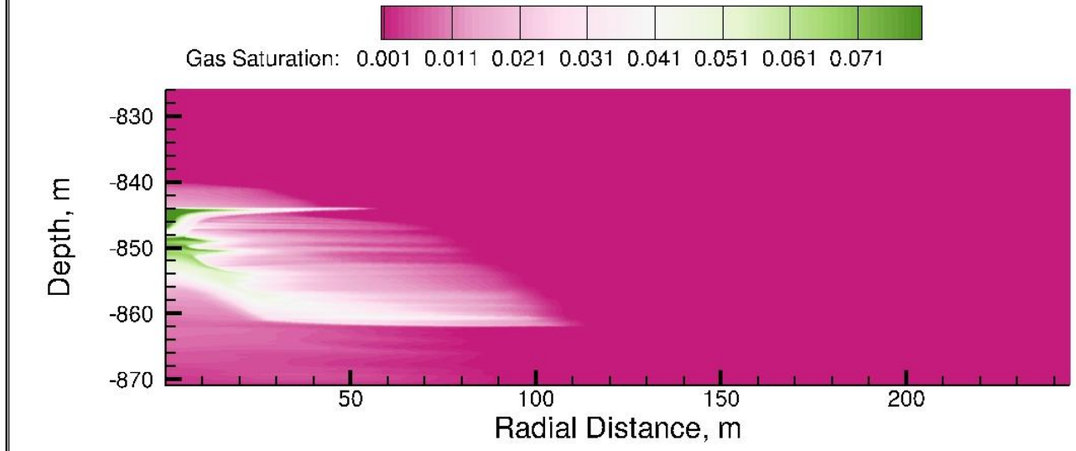


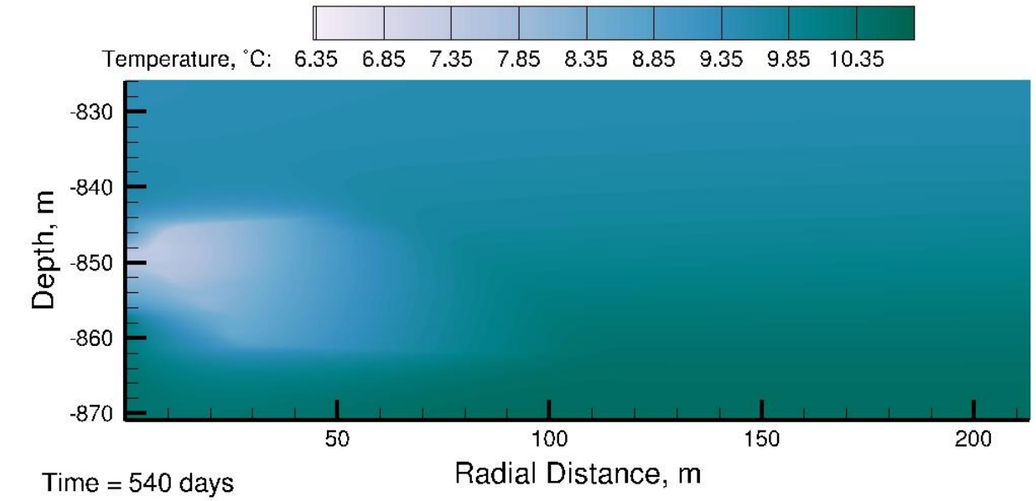


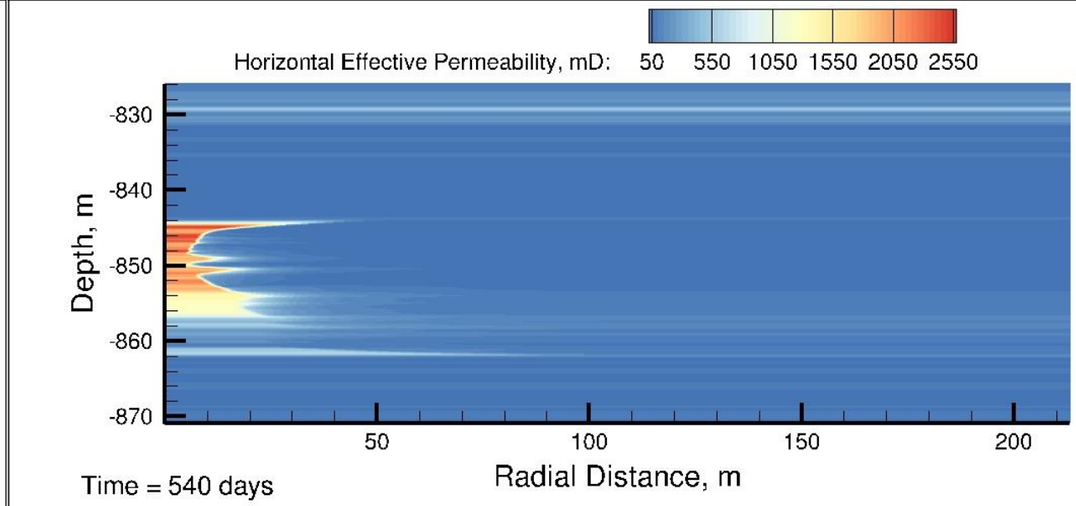

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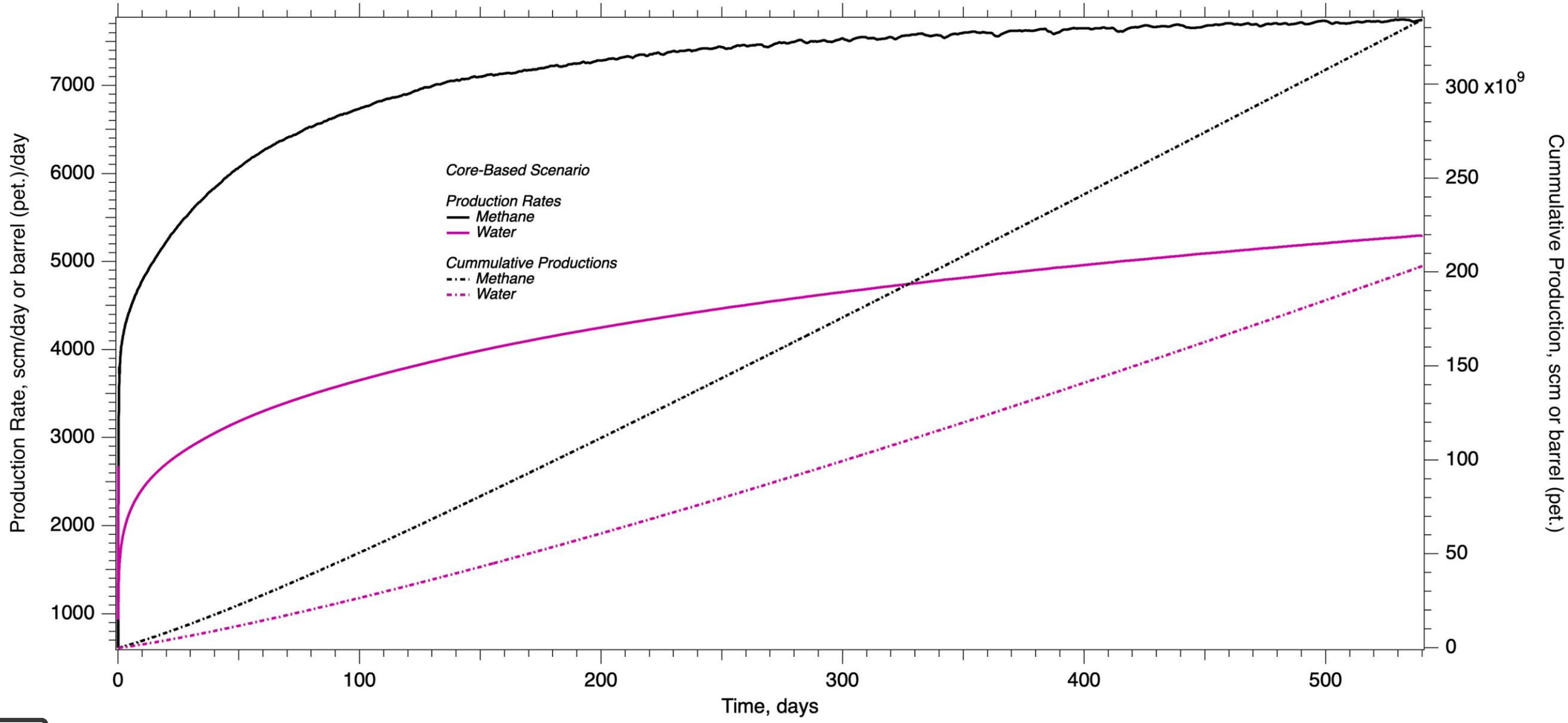
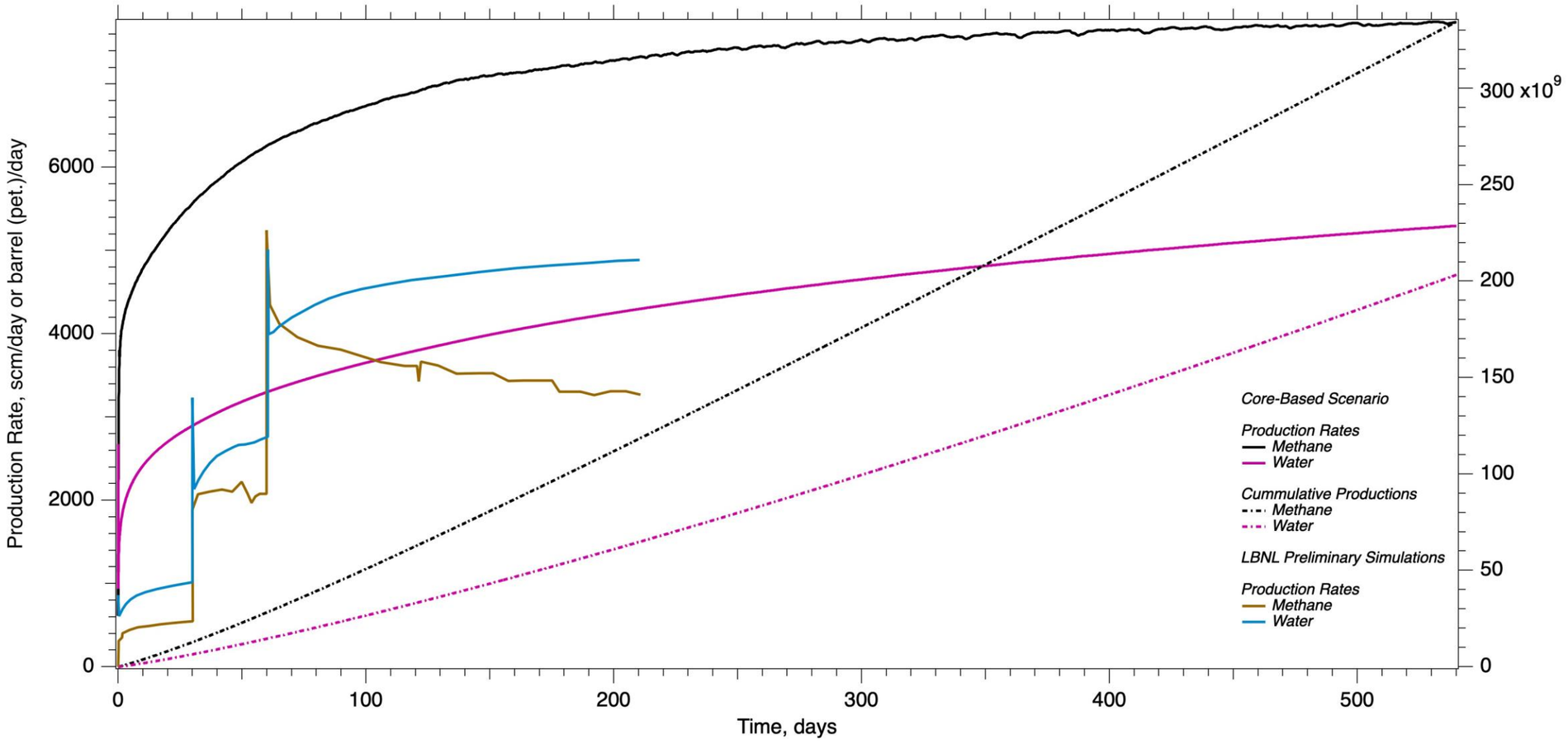
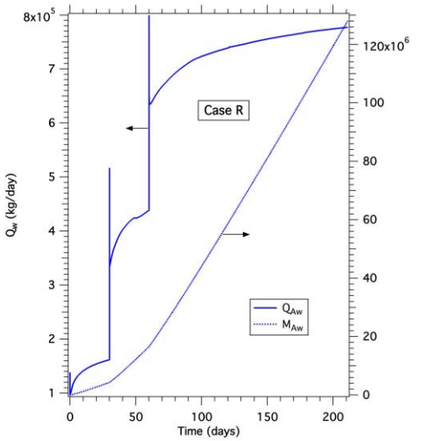
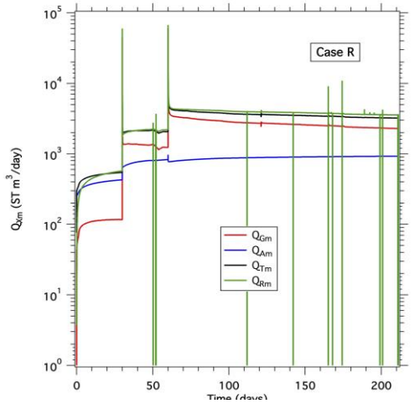


# Simulations in Support of the Alaska North Slope Project: Core-Based Scenario / Case R

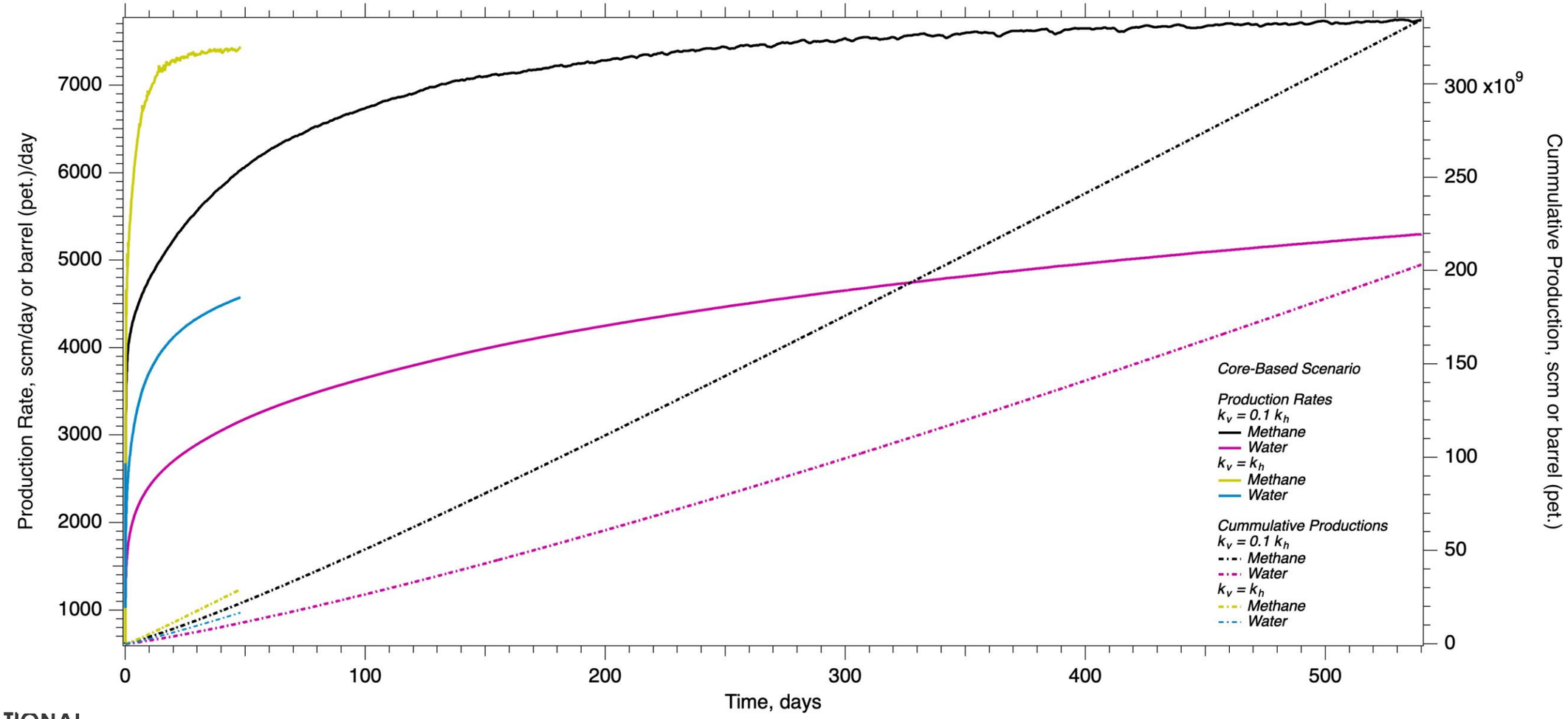


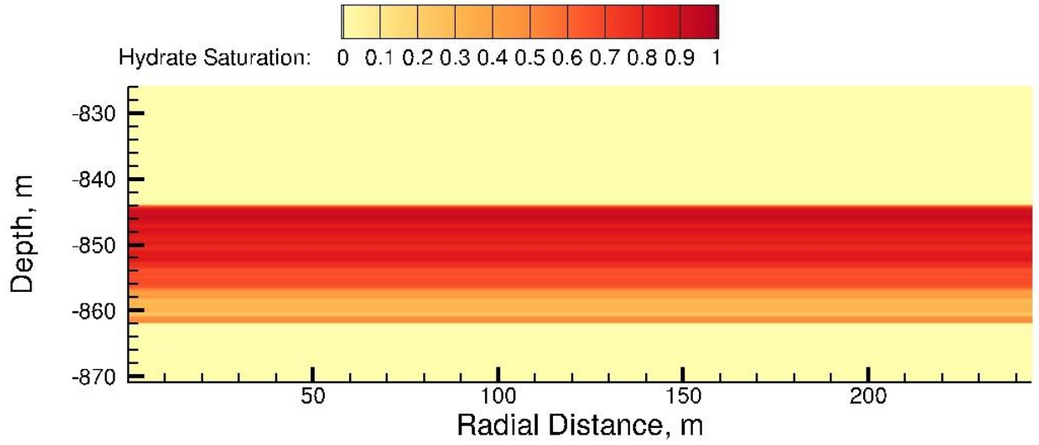

Reagan, M.T., G.J. Moridis, R. Boswell, T. S. Collett. 2020. “Preliminary Analysis of System Behavior During a Planned Long-Term Production Test at a Permafrost Hydrate Deposit in Alaska” Unpublished poster at the Gordon Research Conference on Natural Gas Hydrates, Galveston, Texas, February 23-28, 2020.

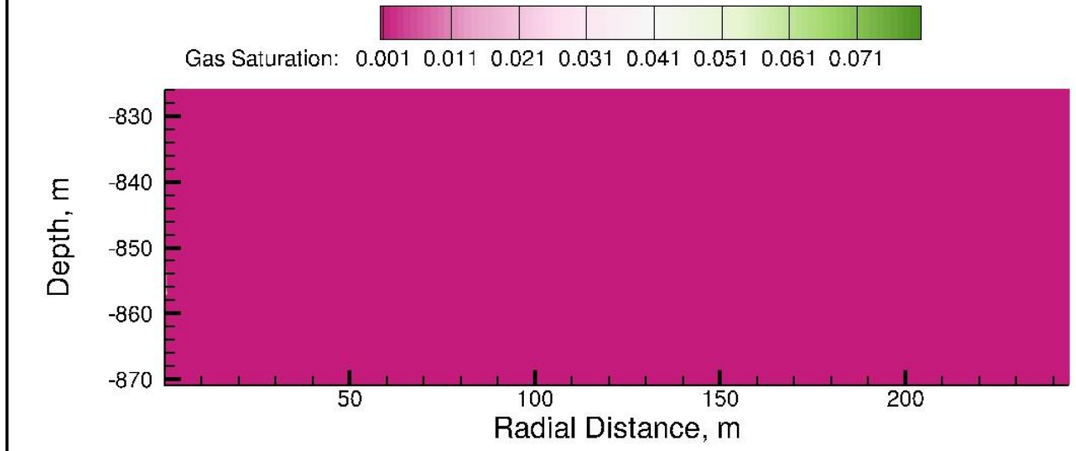
# Simulations in Support of the Alaska North Slope Project: Core-Based Scenario

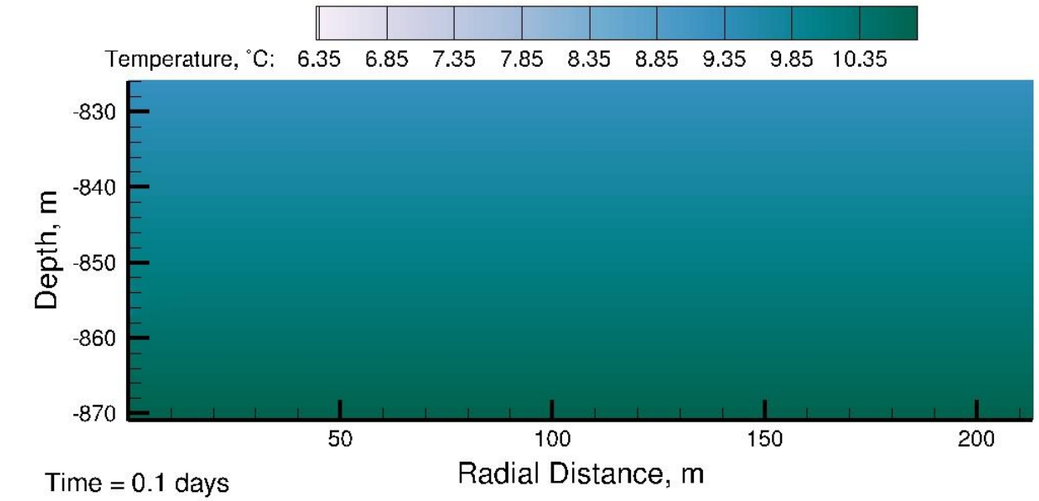


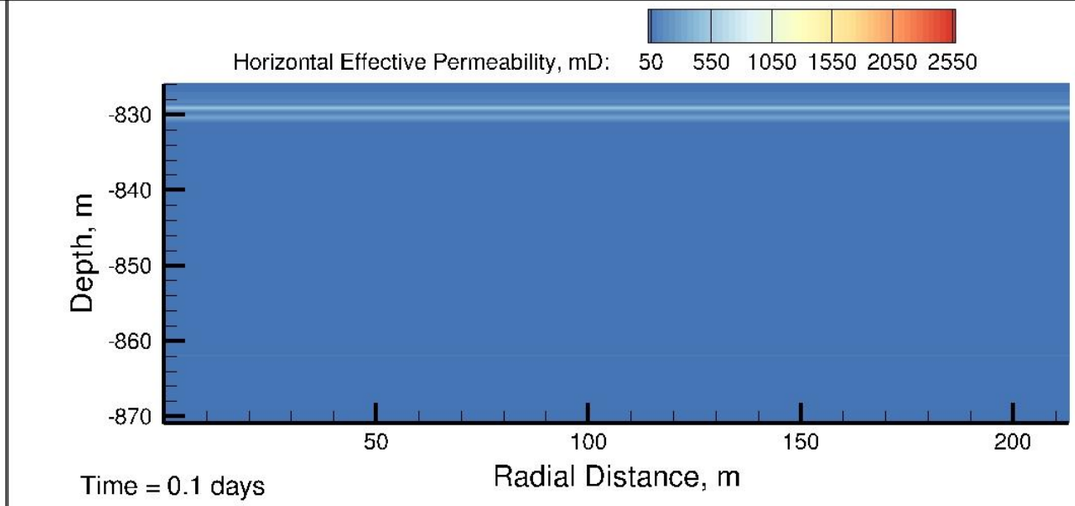
# Simulations in Support of the Alaska North Slope Project: NMR-Based Scenario

$$k_{vert} = 0.1\, k_{horz}$$



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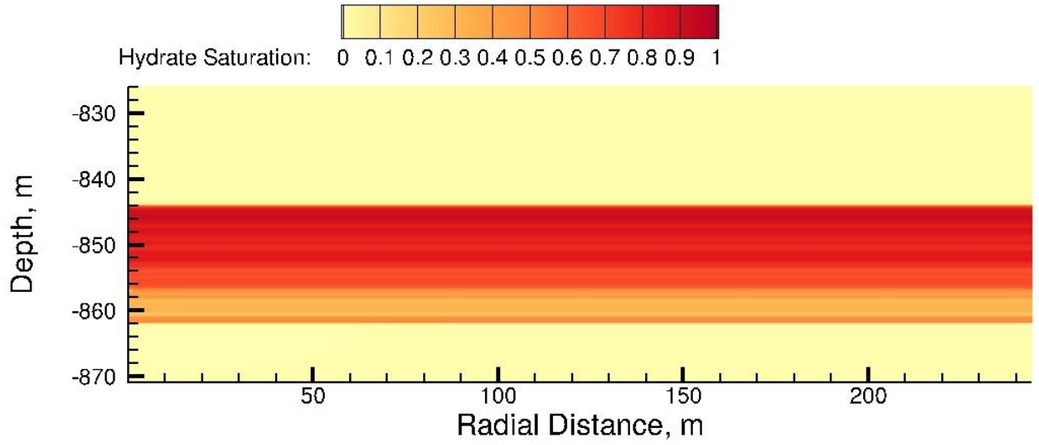
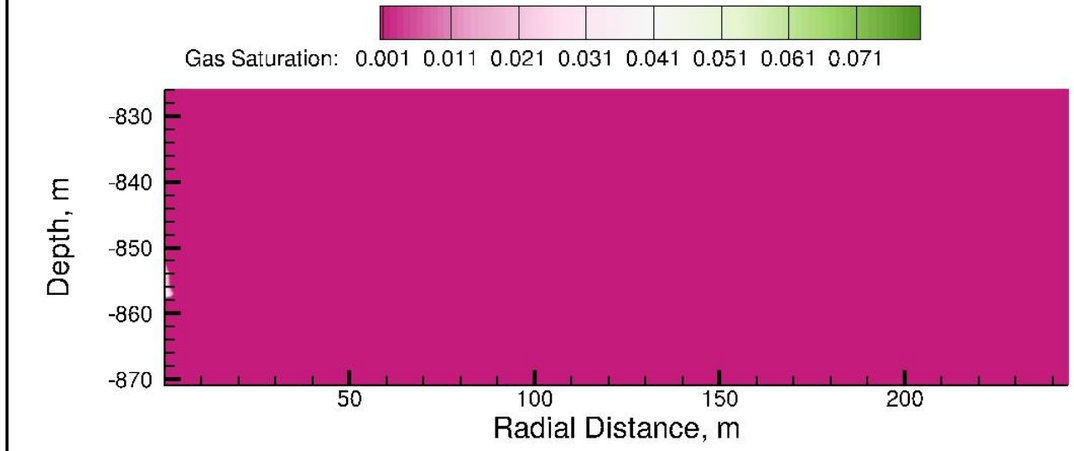
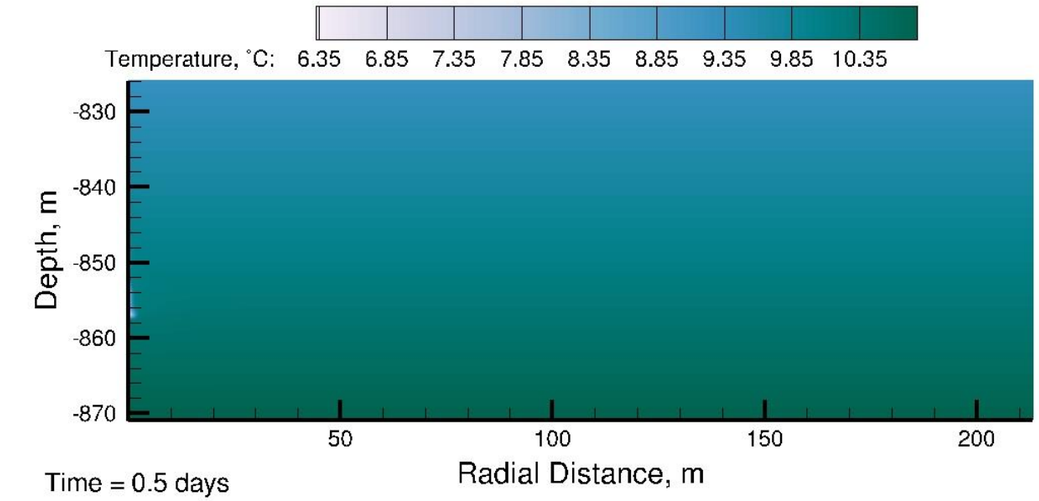
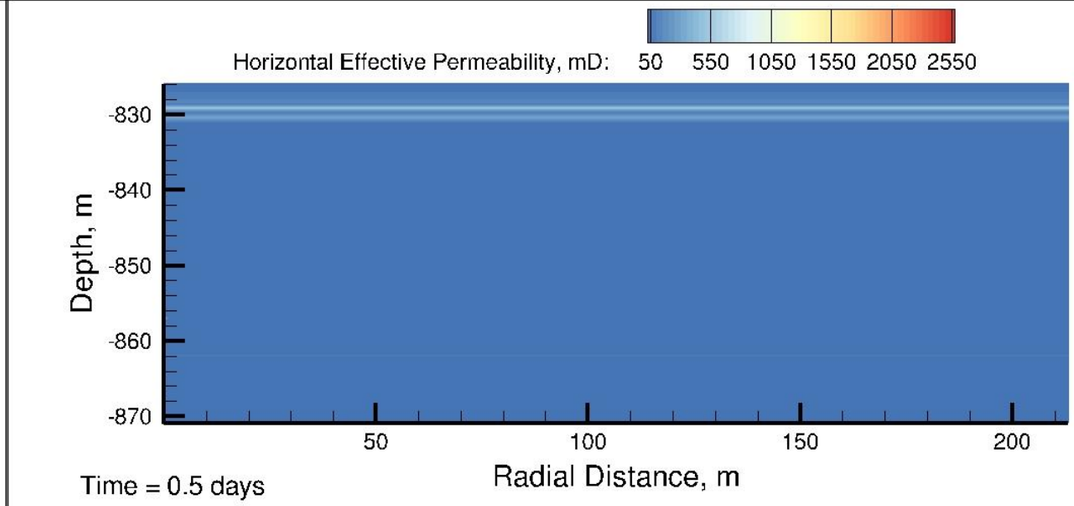


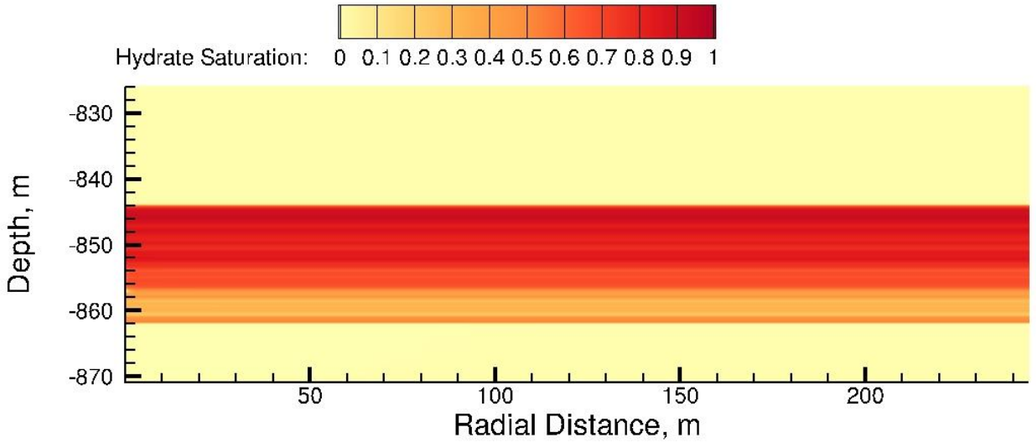



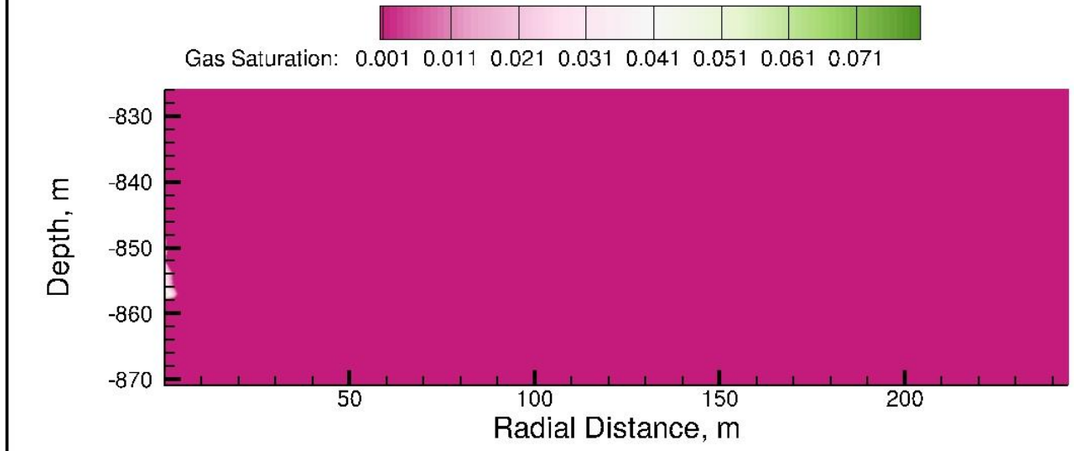



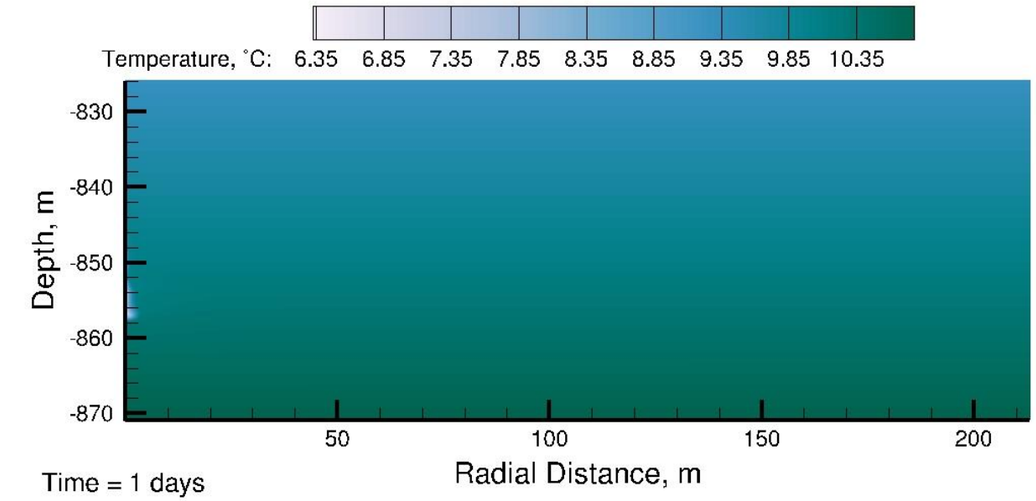



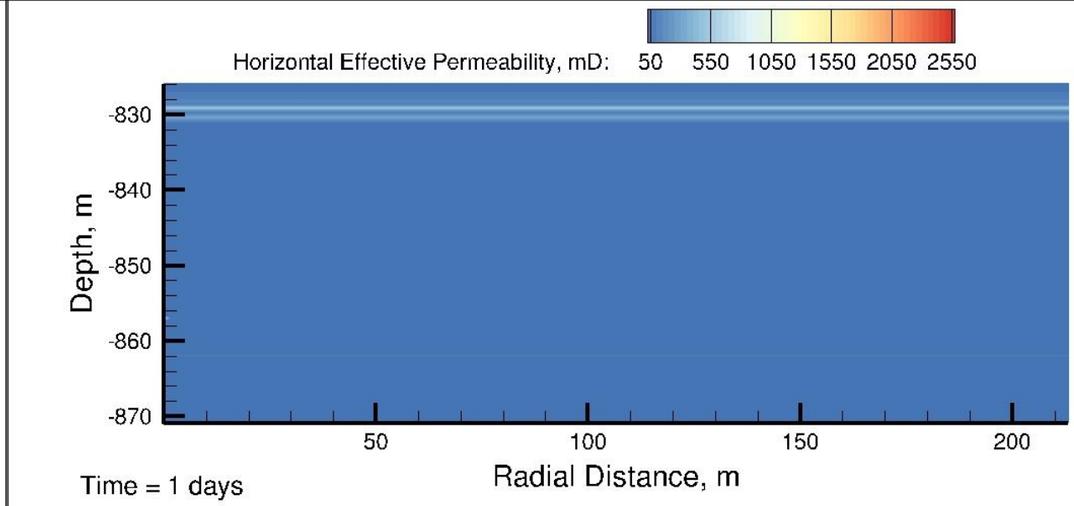
# Simulations in Support of the Alaska North Slope Project: NMR-Based Scenario

$$k_{vert} = 0.1\, k_{horz}$$



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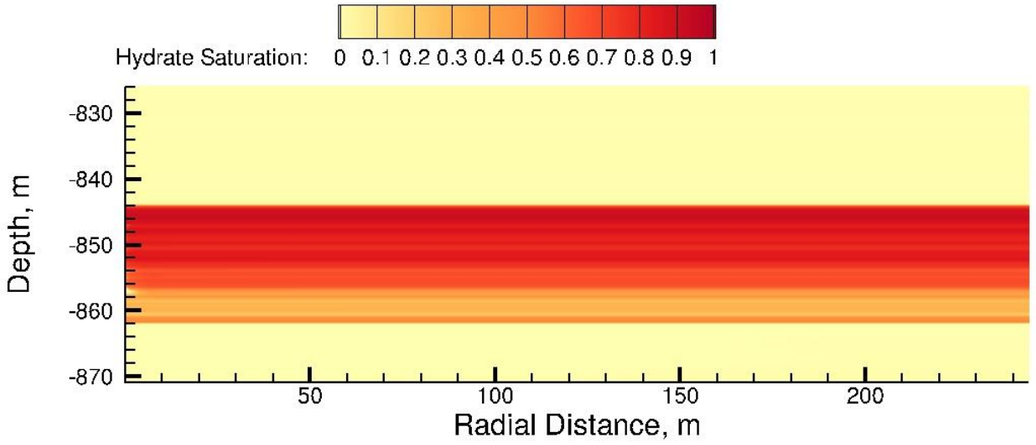


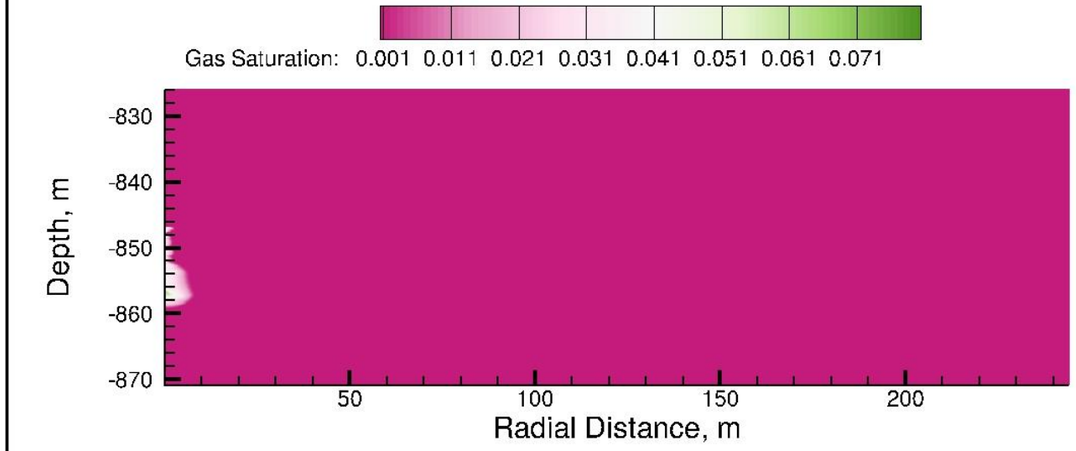


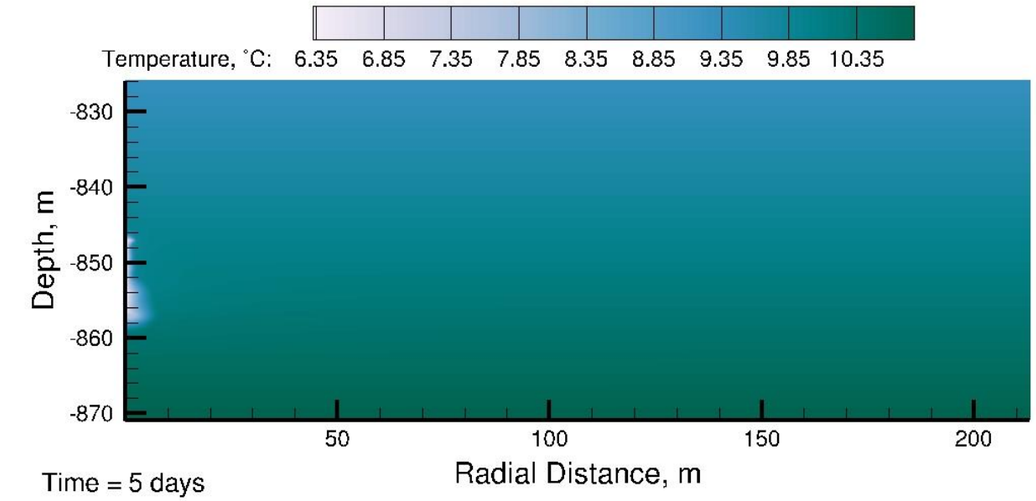


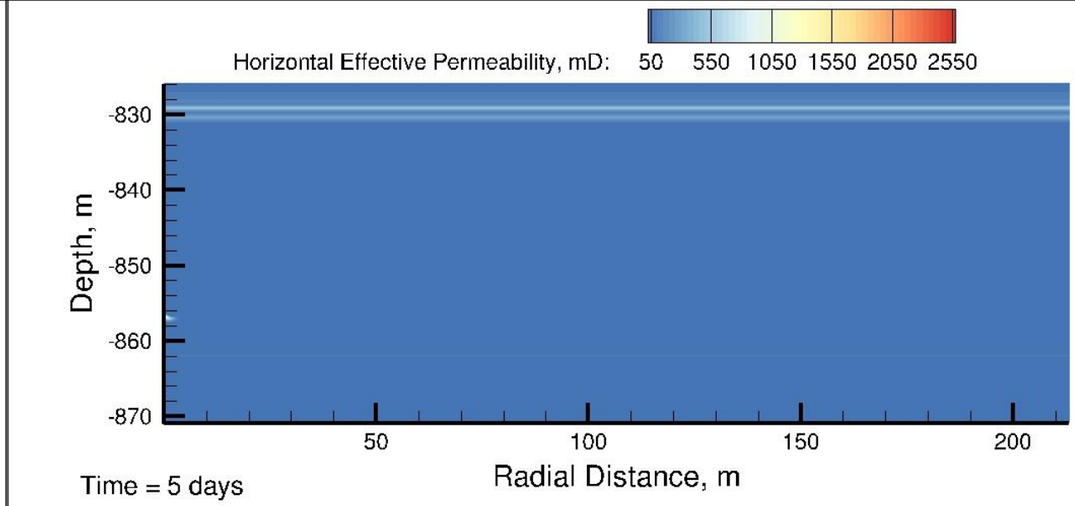

# Simulations in Support of the Alaska North Slope Project: NMR-Based Scenario

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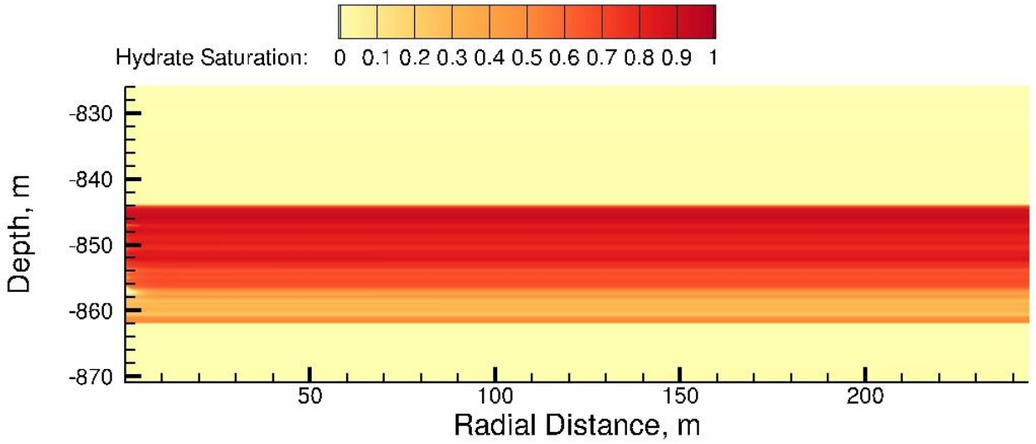


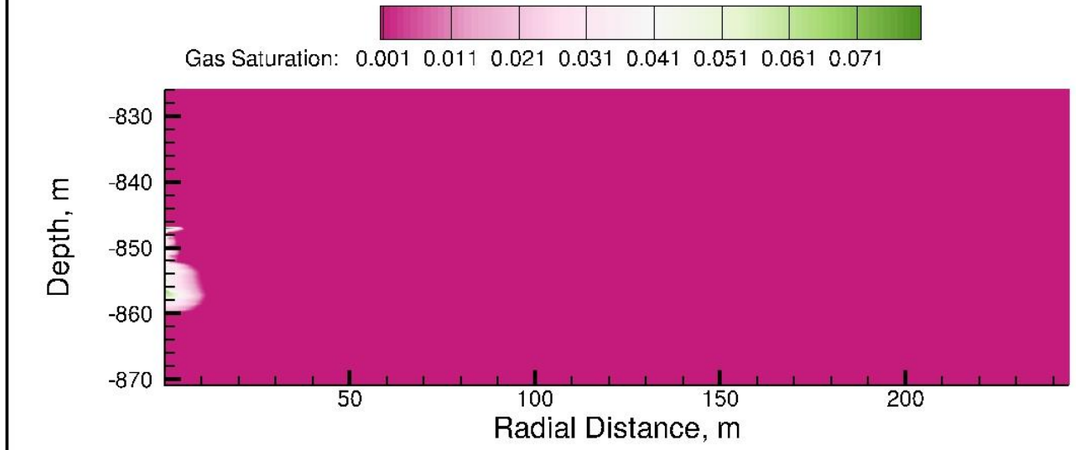


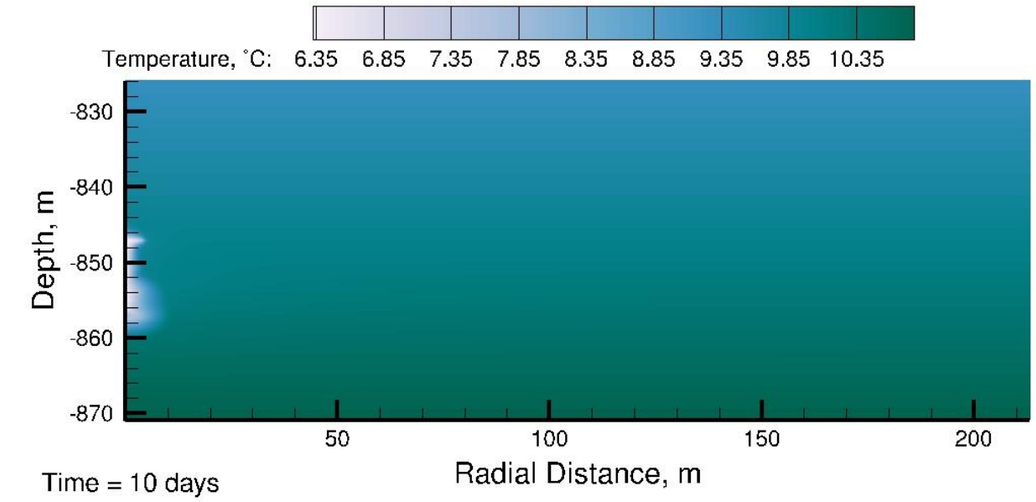


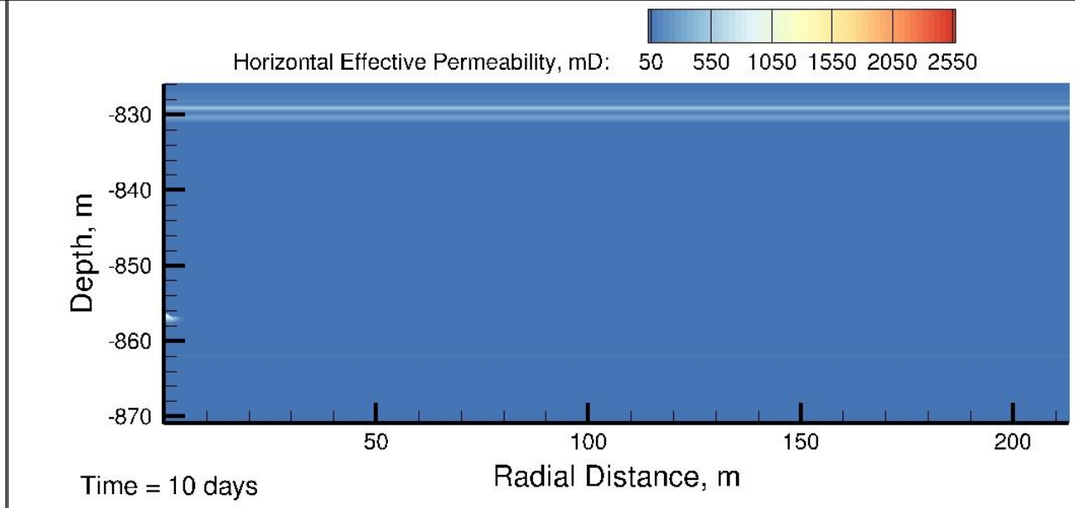

# Simulations in Support of the Alaska North Slope Project: NMR-Based Scenario

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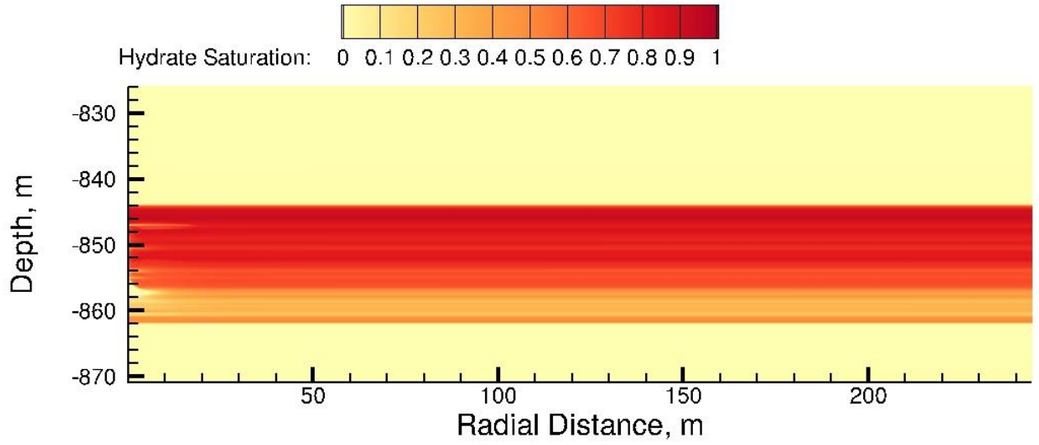


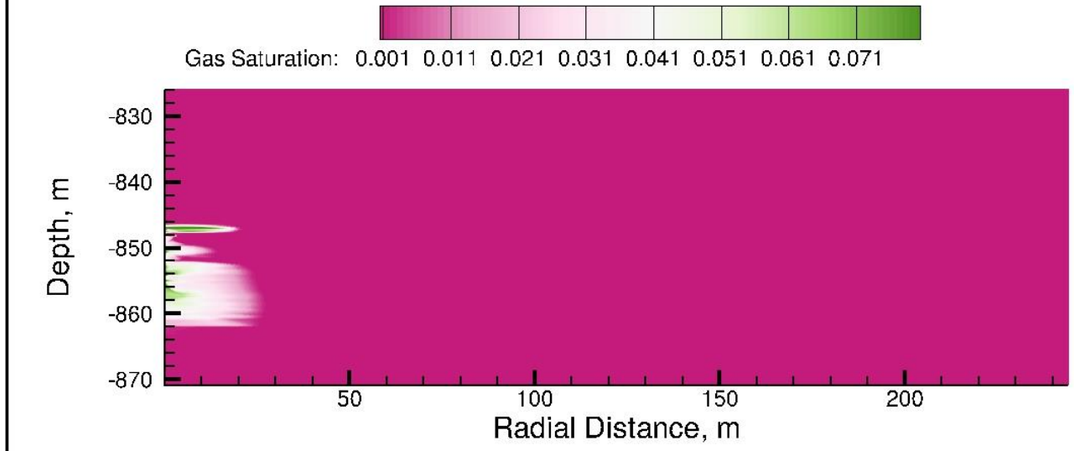


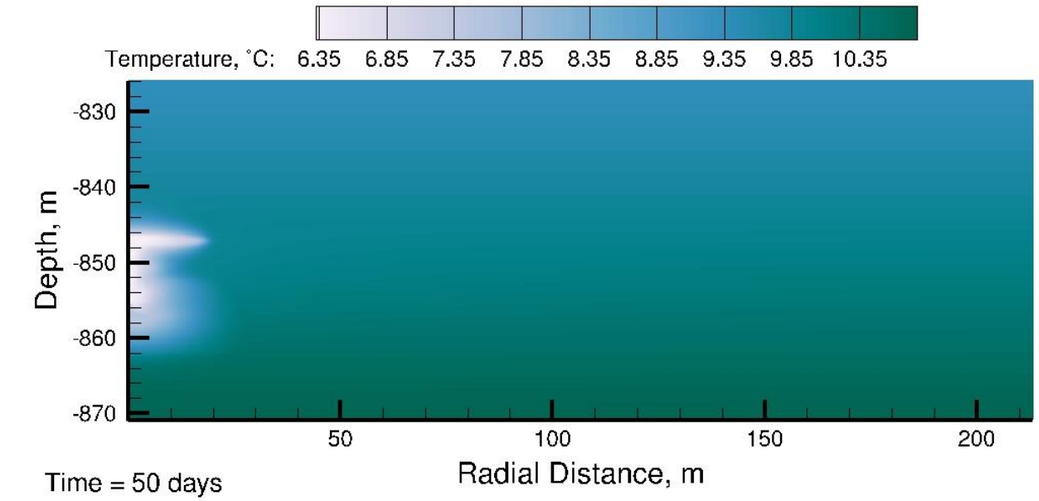


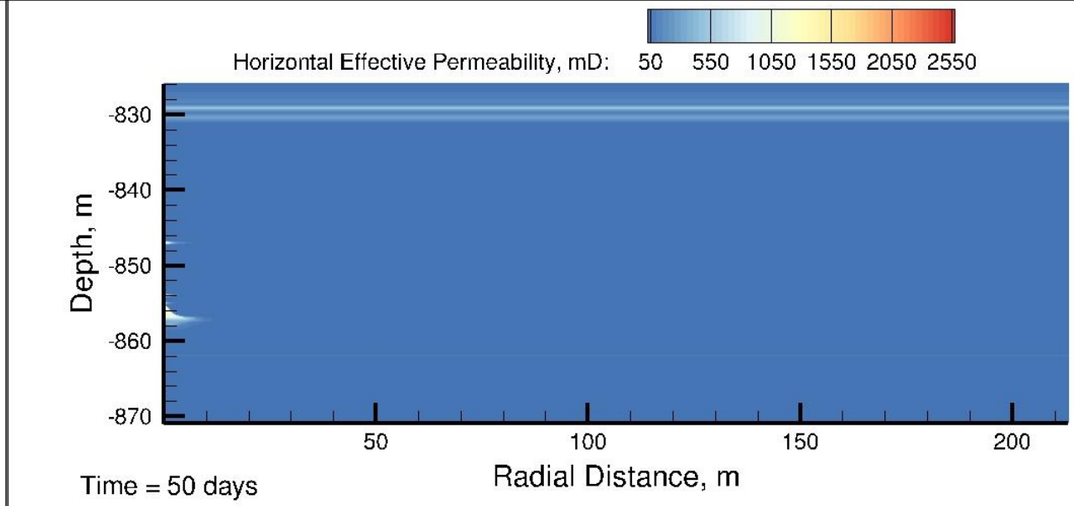

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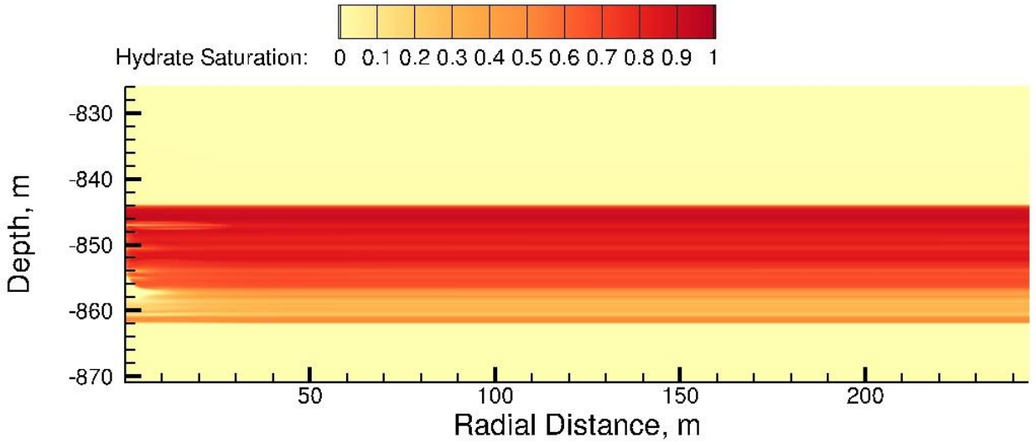


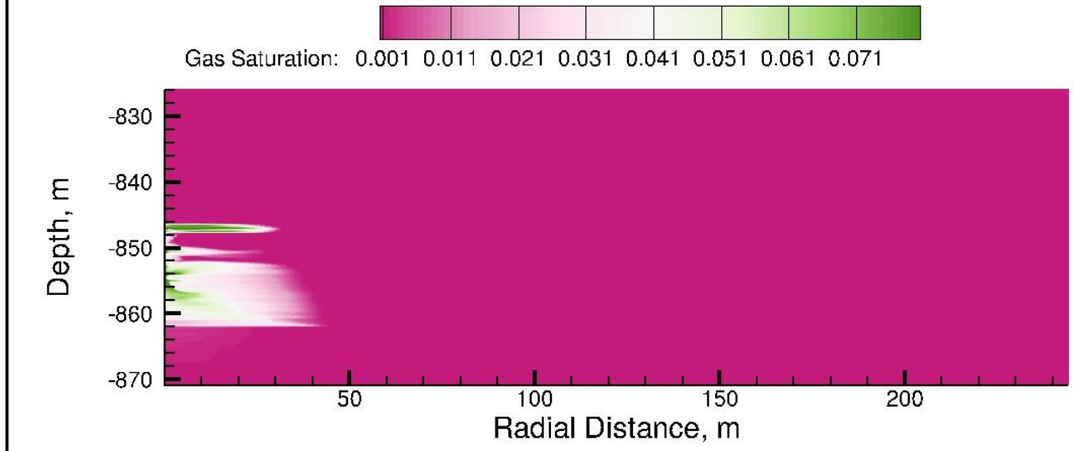


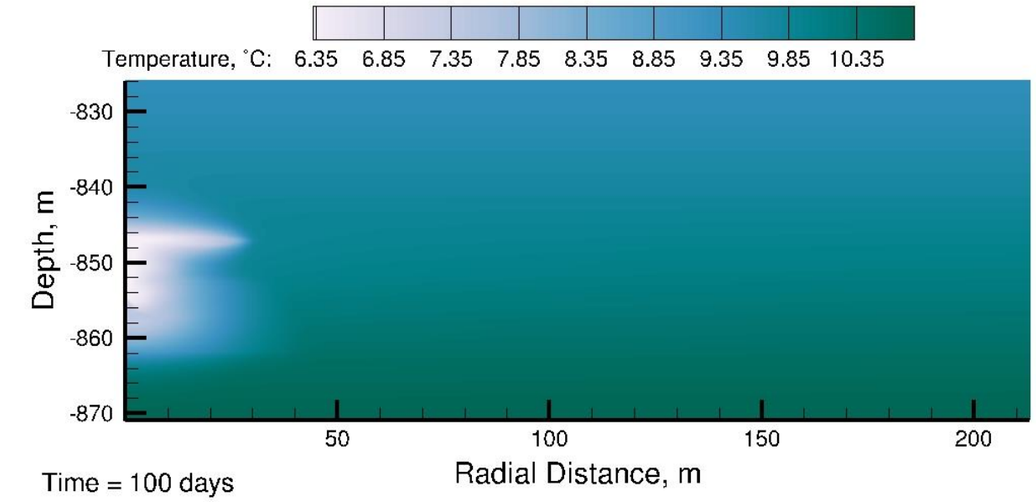


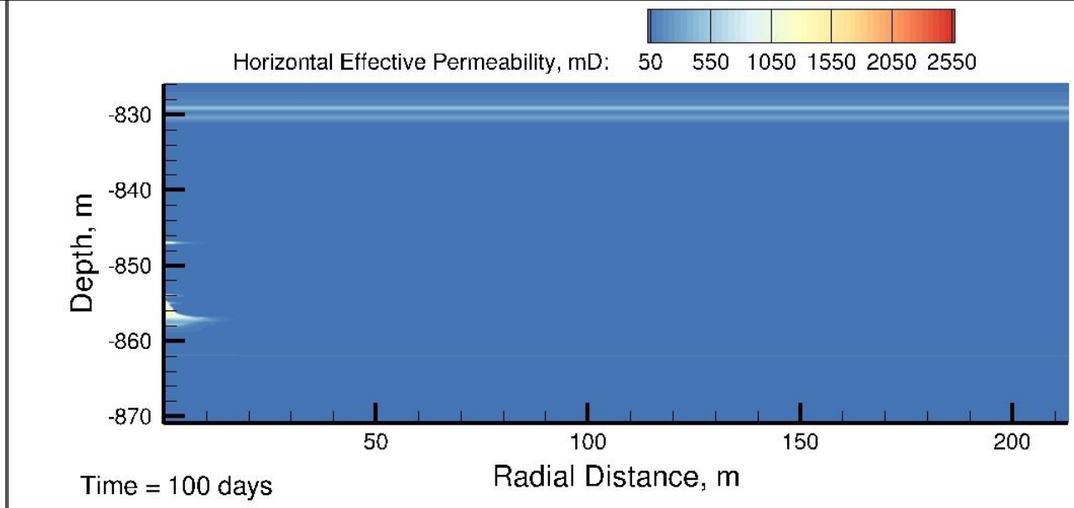

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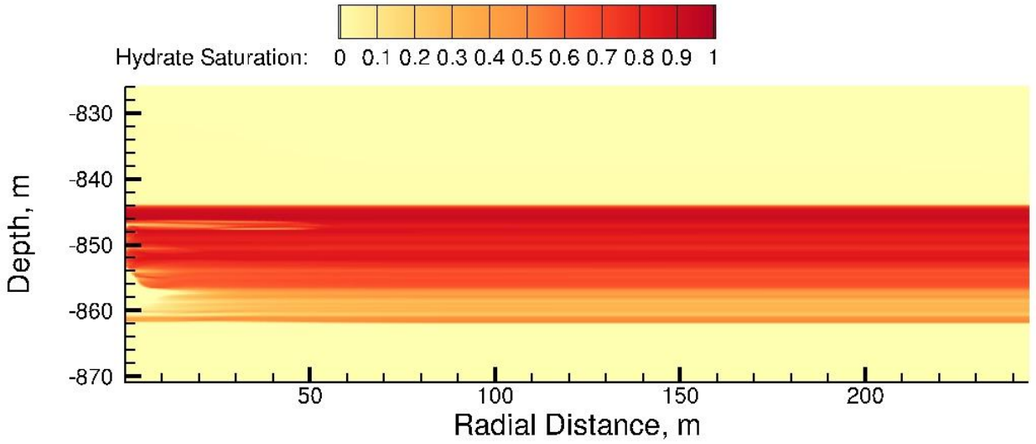
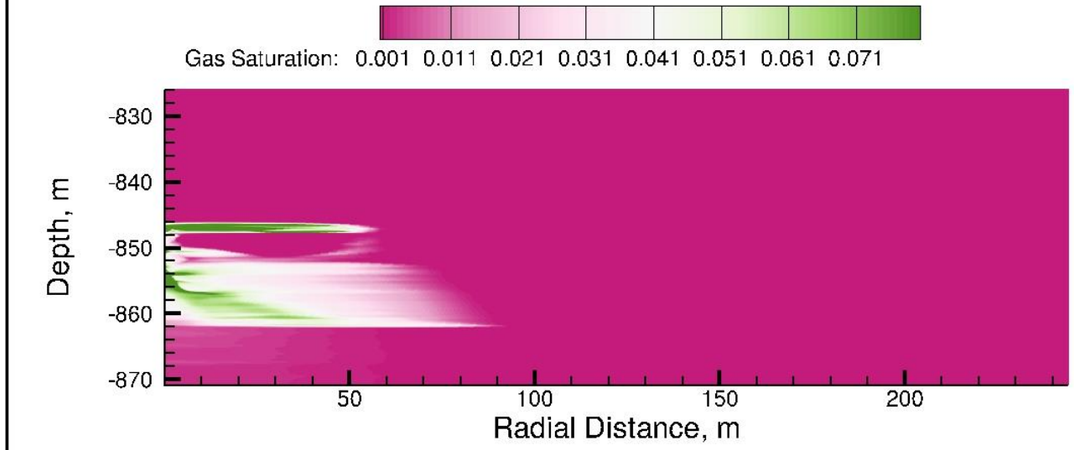
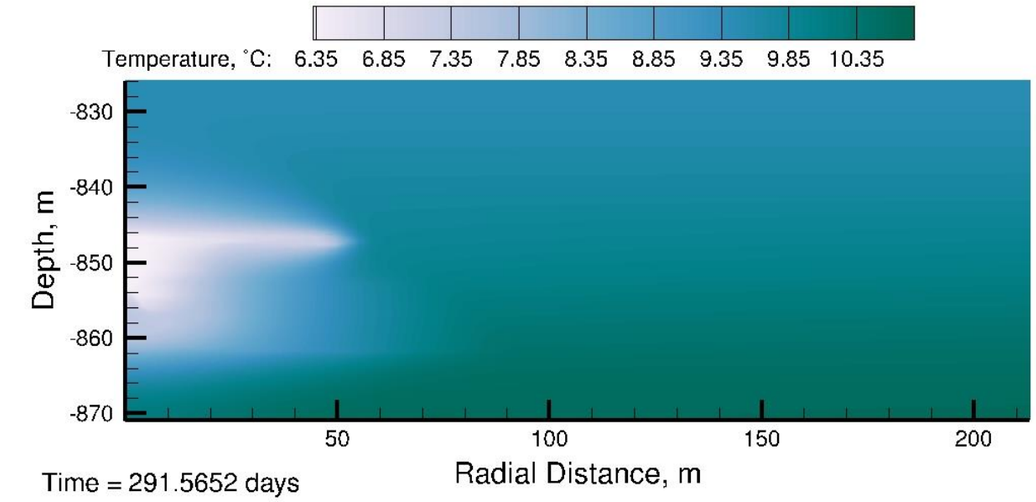
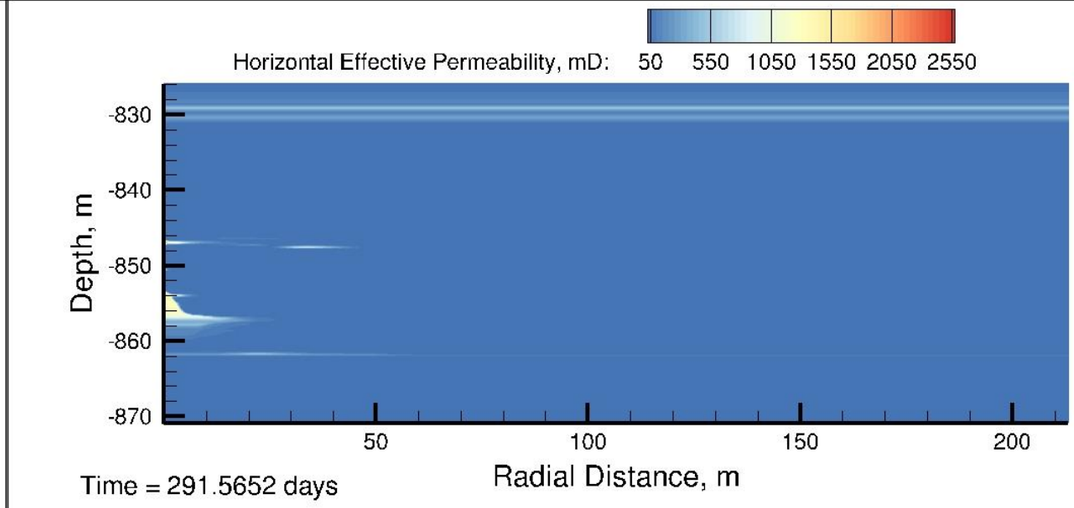


# Sequential and OpenMP Implementations of STOMP-HYDT-KE

## Solved Conservation Equations

energy
water mass
mobile mass of $CO_2$, $CH_4$, $N_2$
hydrate mass of $CO_2$, $CH_4$, $N_2$
inhibitor mass (e.g., salt)

## Active Phases

aqueous
gas
nonaqueous liquid
gas hydrate
ice
precipitated inhibitor
solid

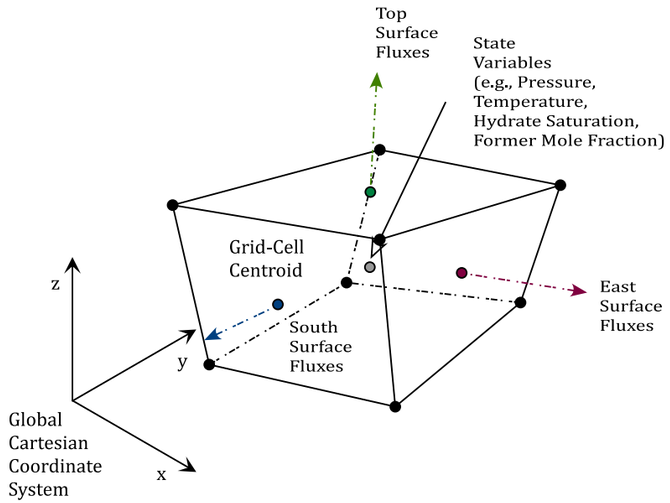
## Fully Coupled Solvers

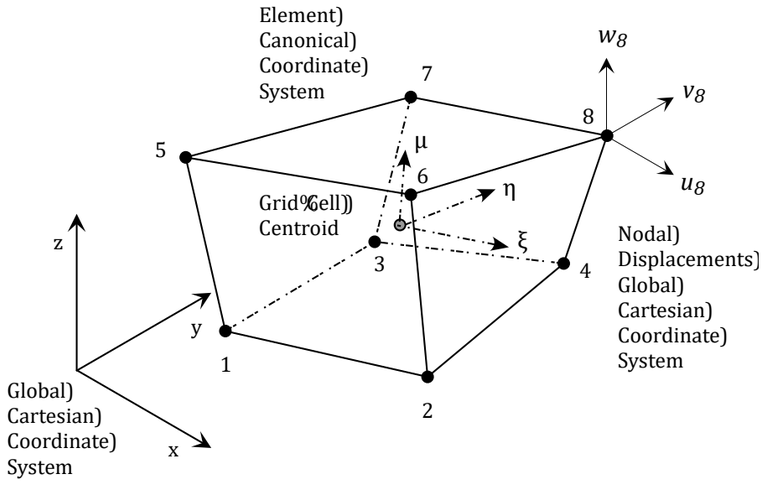
ECKEChem (geochemistry)

- finite volume
- operator split
- Courant number limiting

GeoMech (geomechanics)

- finite element
- hexahedron elements
- linear elastic
- static
- poroelasticity
- thermal expansion
- fixed-stress iterative sequential coupling



# Legacy Code Parallelization – Sequential and OpenMP Implementations

**ASCII (text) Input Files**

input (problem description)

tertiary mixture phase envelope ($CO_2$-$CH_4$-$N_2$)

tertiary mixture gas hydrate equilibria ($CO_2$-$CH_4$-$N_2$)

**Fortran 90 w/ or w/o OpenMP Source Code**

preprocessor to determine required memory

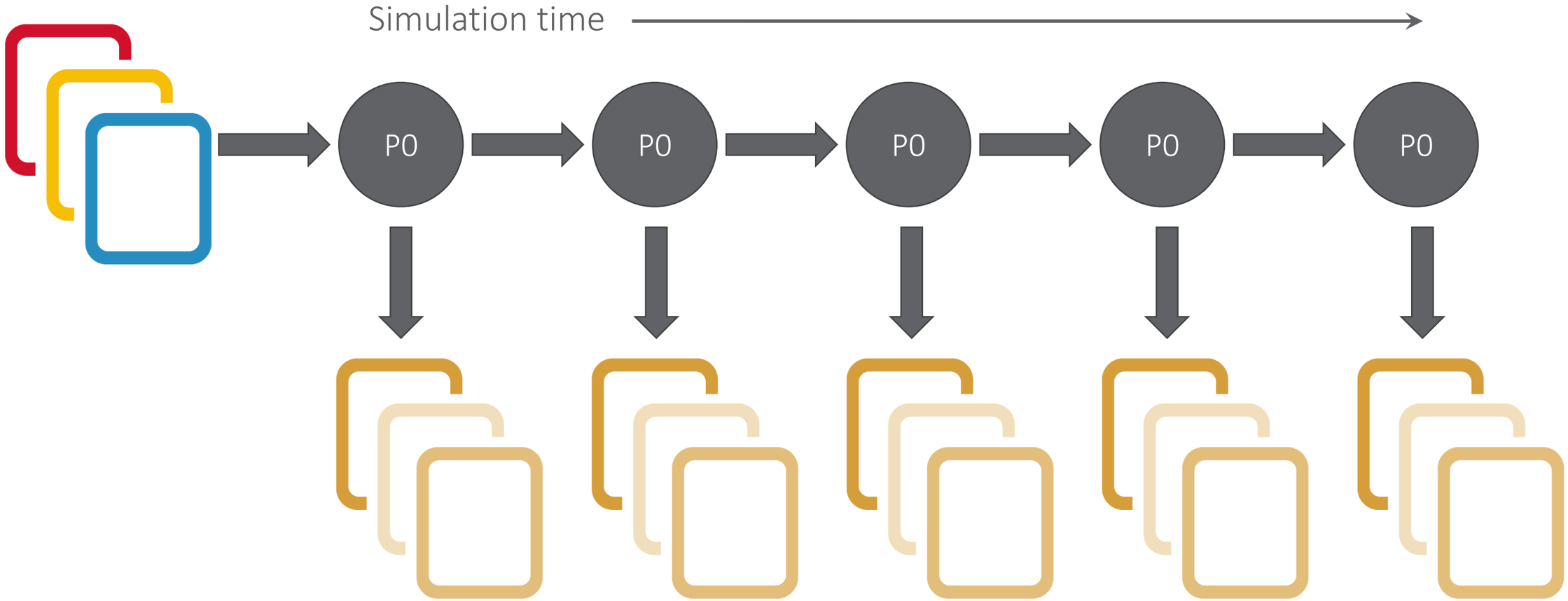
dynamic memory allocation

sequential looping over all field nodes (i.e., grid cells)

parallel looping over all field nodes (i.e., grid cells) via shared memory

coupled to a sequential or OpenMP external solver

# Legacy Code Parallelization – Sequential Implementation



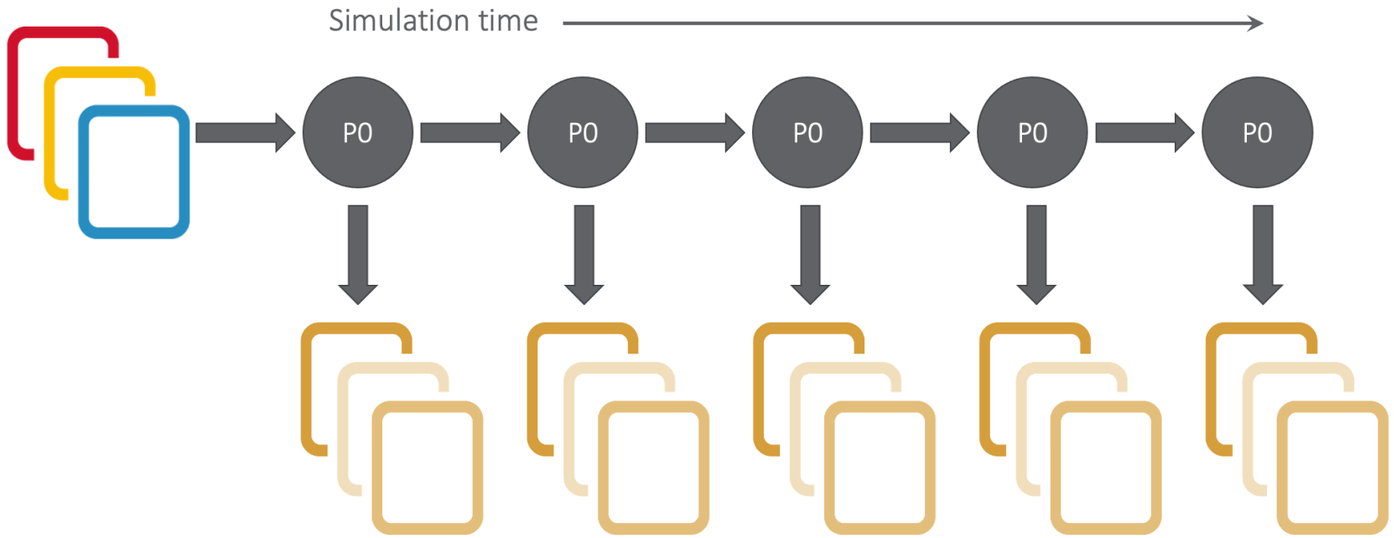
# Legacy Code Parallelization – Sequential Implementation

## Pros

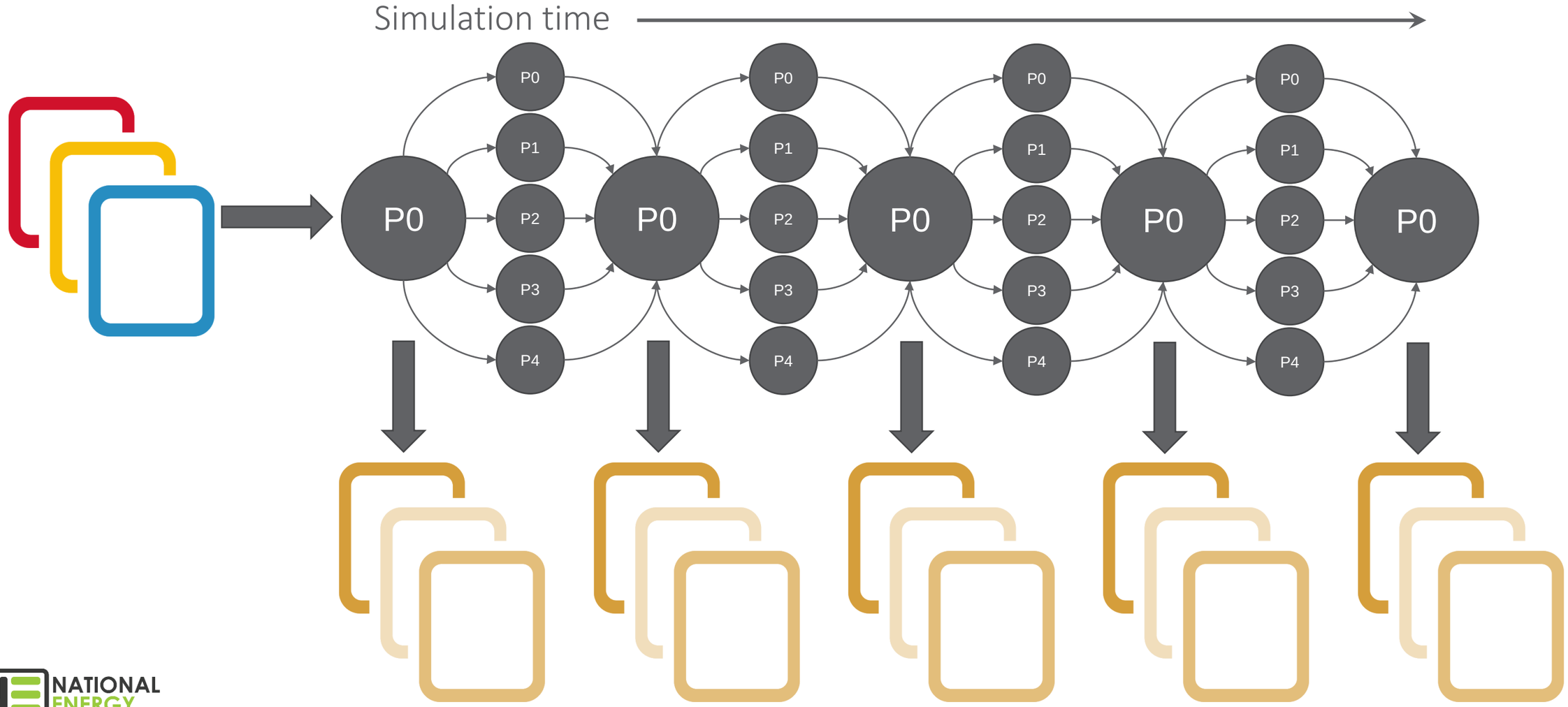
- Convenient screen output
- ASCII input and output files
- Multiple core computers not required

## Cons

- Sequential performance
- Idle cores



# Legacy Code Parallelization – OpenMP Implementation




(Shared-Memory Computers/Nodes Only)

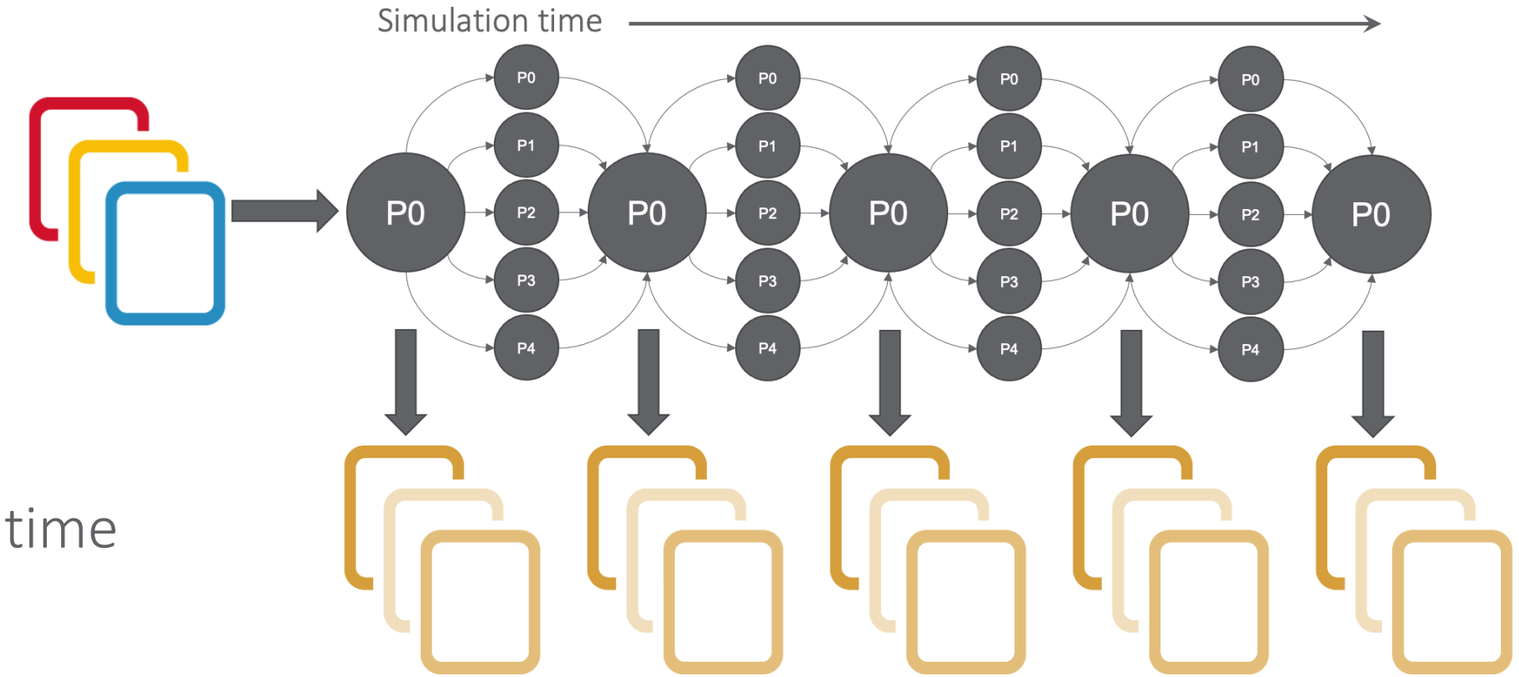
# Legacy Code Parallelization – OpenMP Implementation

## Pros

- Convenient screen output
- ASCII input and output files
- Parallel sections of code

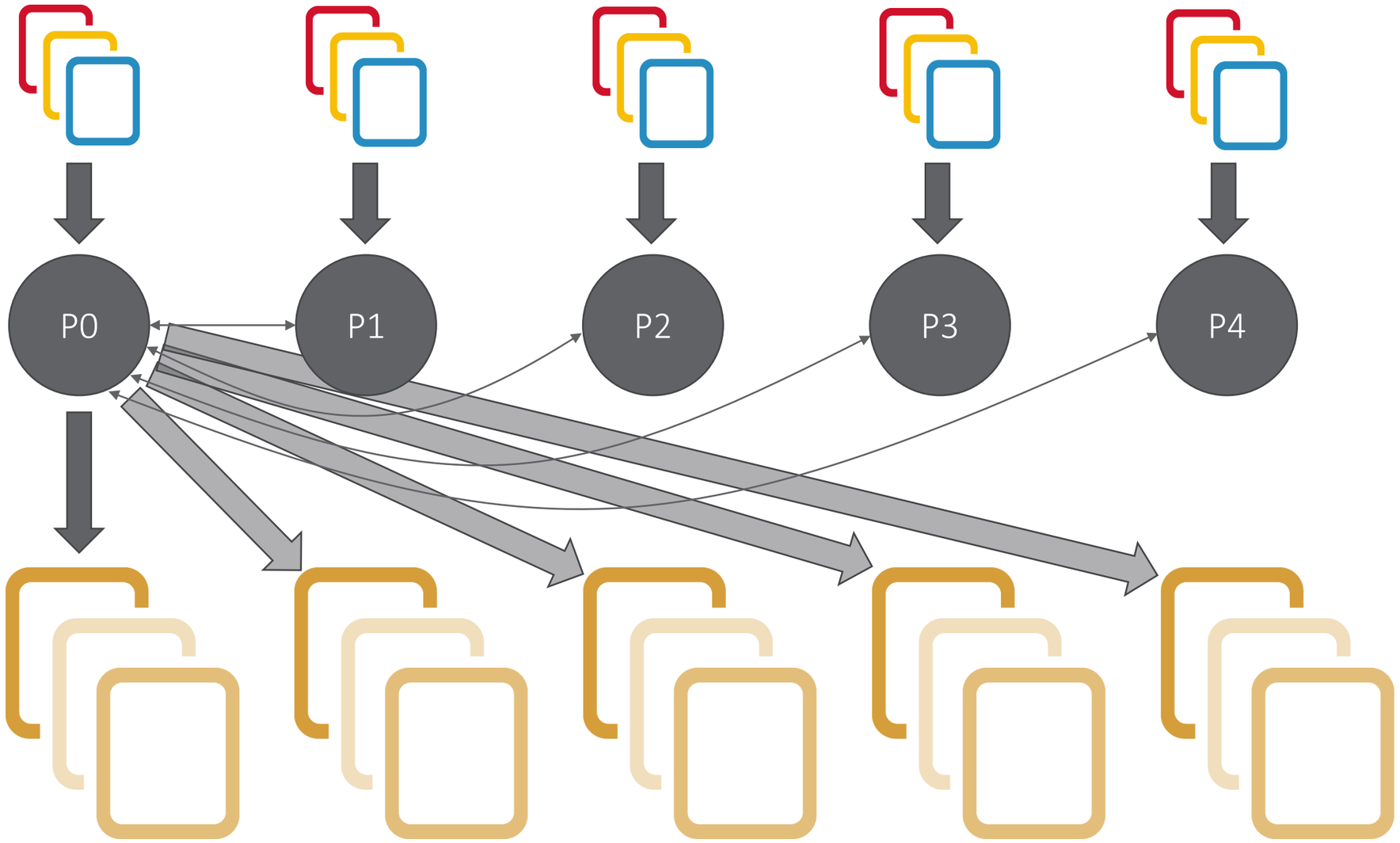
## Cons

- Looping setup can consume time saved in parallel processing
- Limited scaling
- Worse than sequential performance possible




(Shared-Memory Computers/Nodes Only)

# Non-parallel Input/Output




https://wgropp.cs.illinois.edu/courses/cs598-s16/lectures/lecture32.pdf

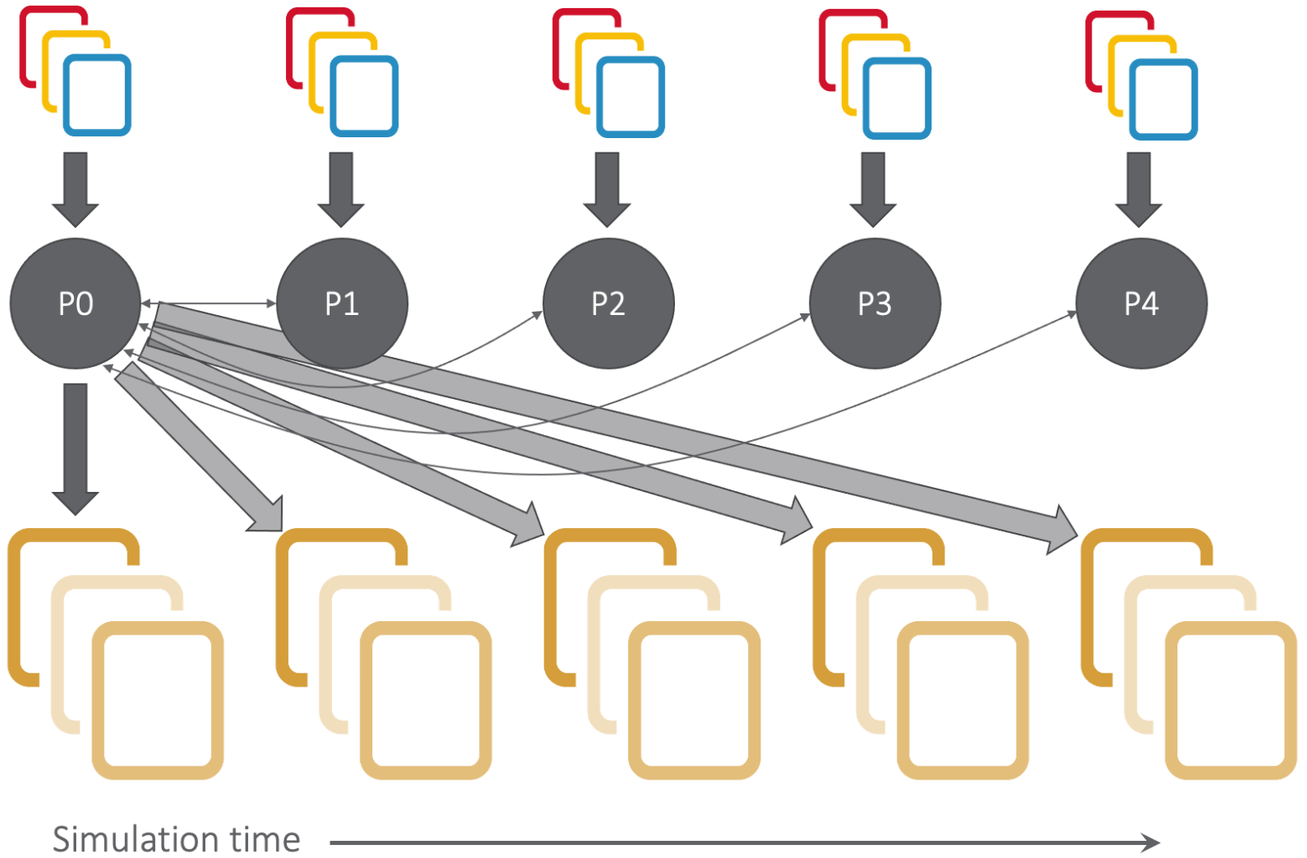
# Non-parallel Input/Output

## Pros

- Convenient screen output
- ASCII input and output files
- Parallel sections of code

## Cons

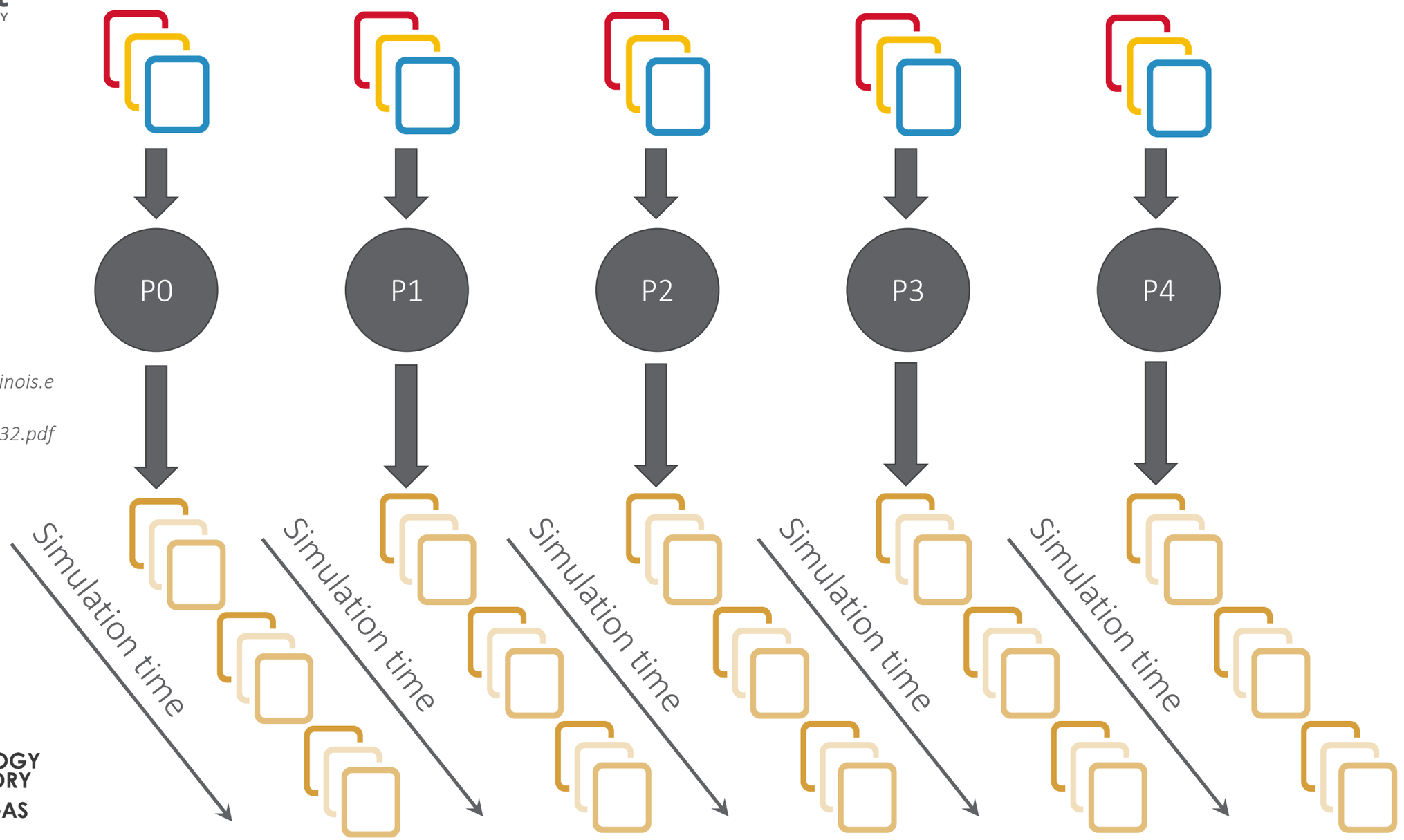
- Distribution of inputs across processors required
- Limited scaling
- Worse than sequential performance possible




(Shared- or Distributed-Memory Computers)

*https://wgropp.cs.illinois.edu/courses/cs598-s16/lectures/lecture32.pdf*

# Independent Parallel Input/Output




*https://wgropp.cs.illinois.edu/courses/cs598-s16/lectures/lecture32.pdf*

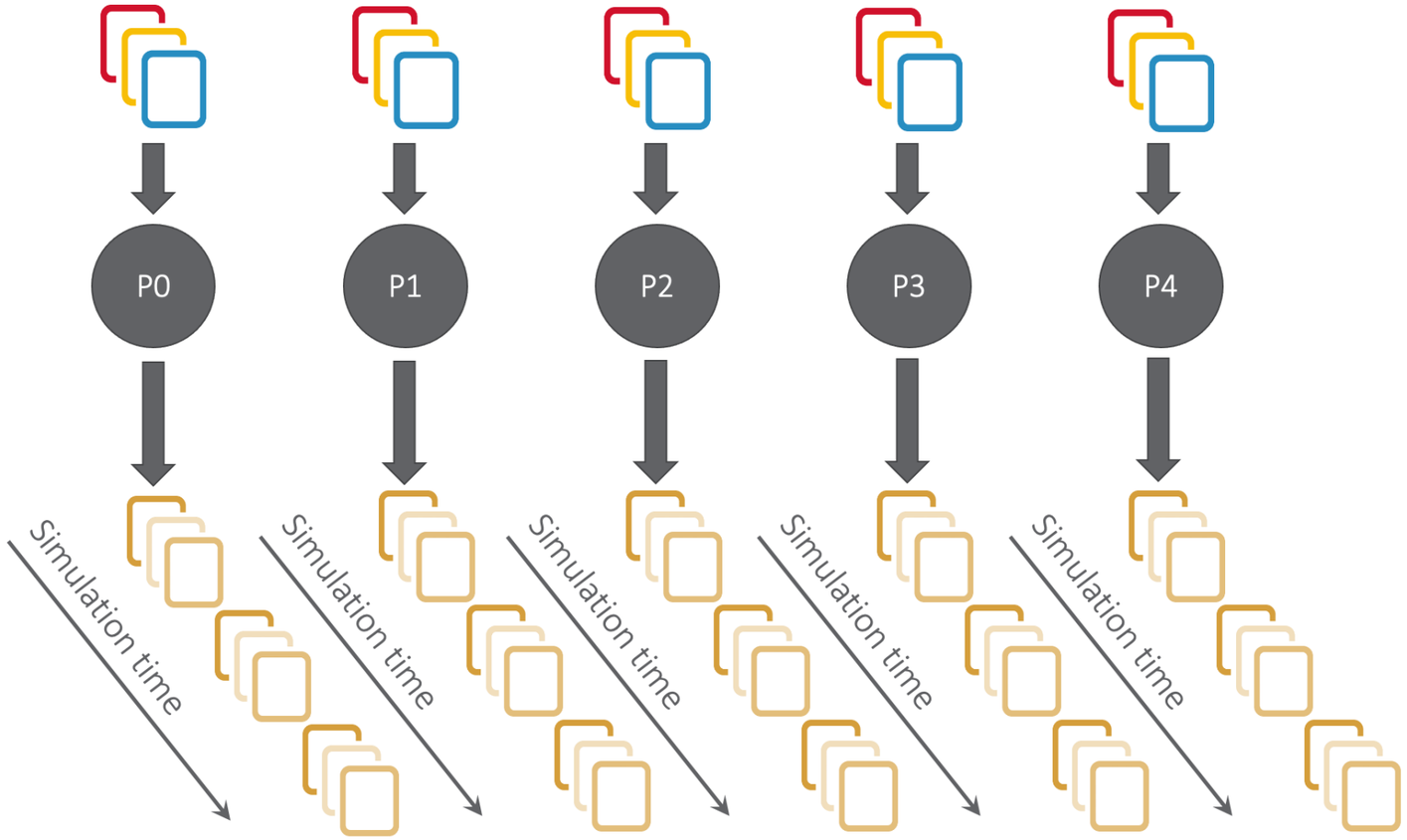
# Independent Parallel Input/Output

## Pros

- Parallelism
- Favorable strong scaling

## Cons

- Distribution of inputs across processors required
- Recombination of output files




(Shared- or Distributed-Memory Computers)

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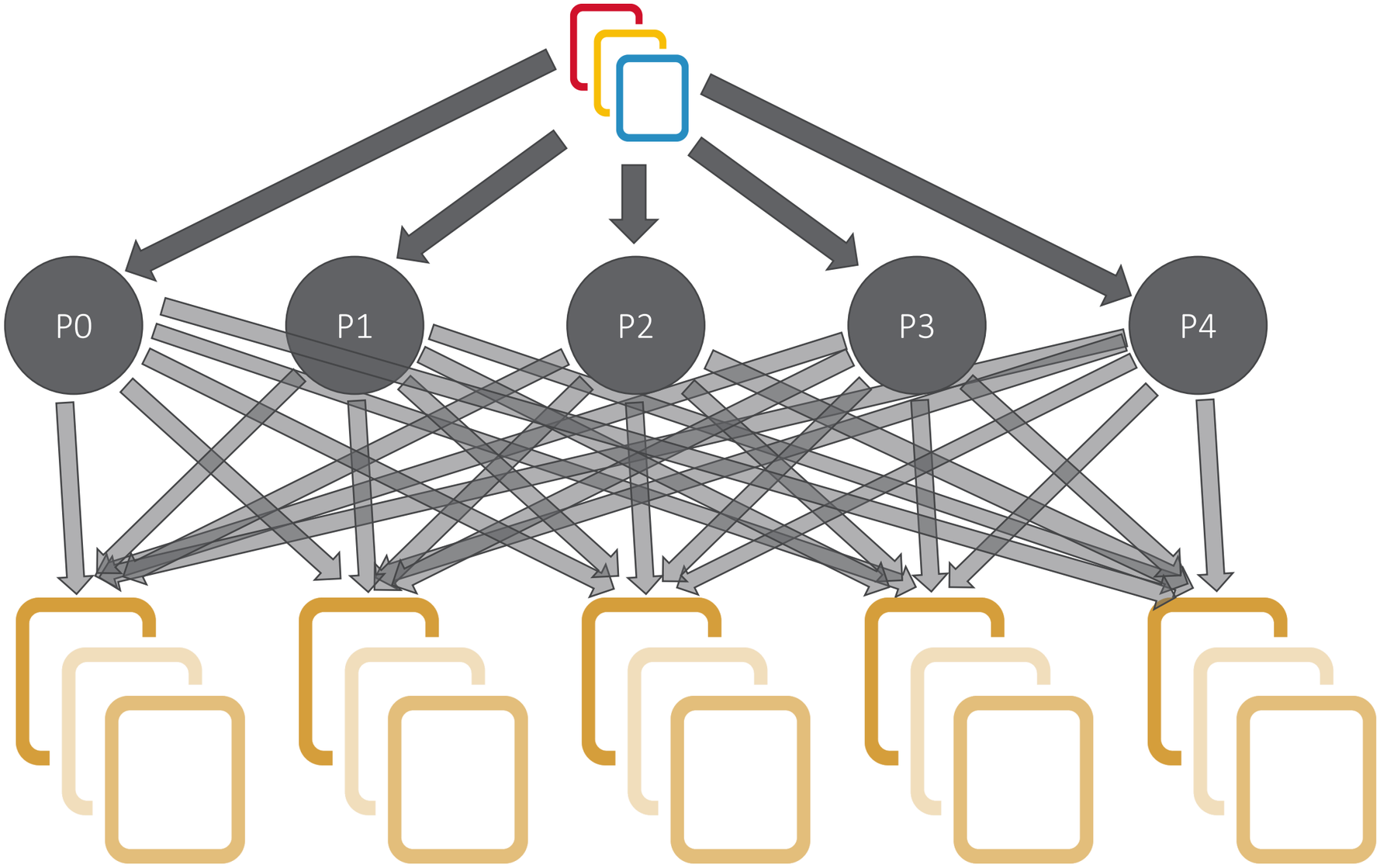
# Cooperative Parallel Input/Output

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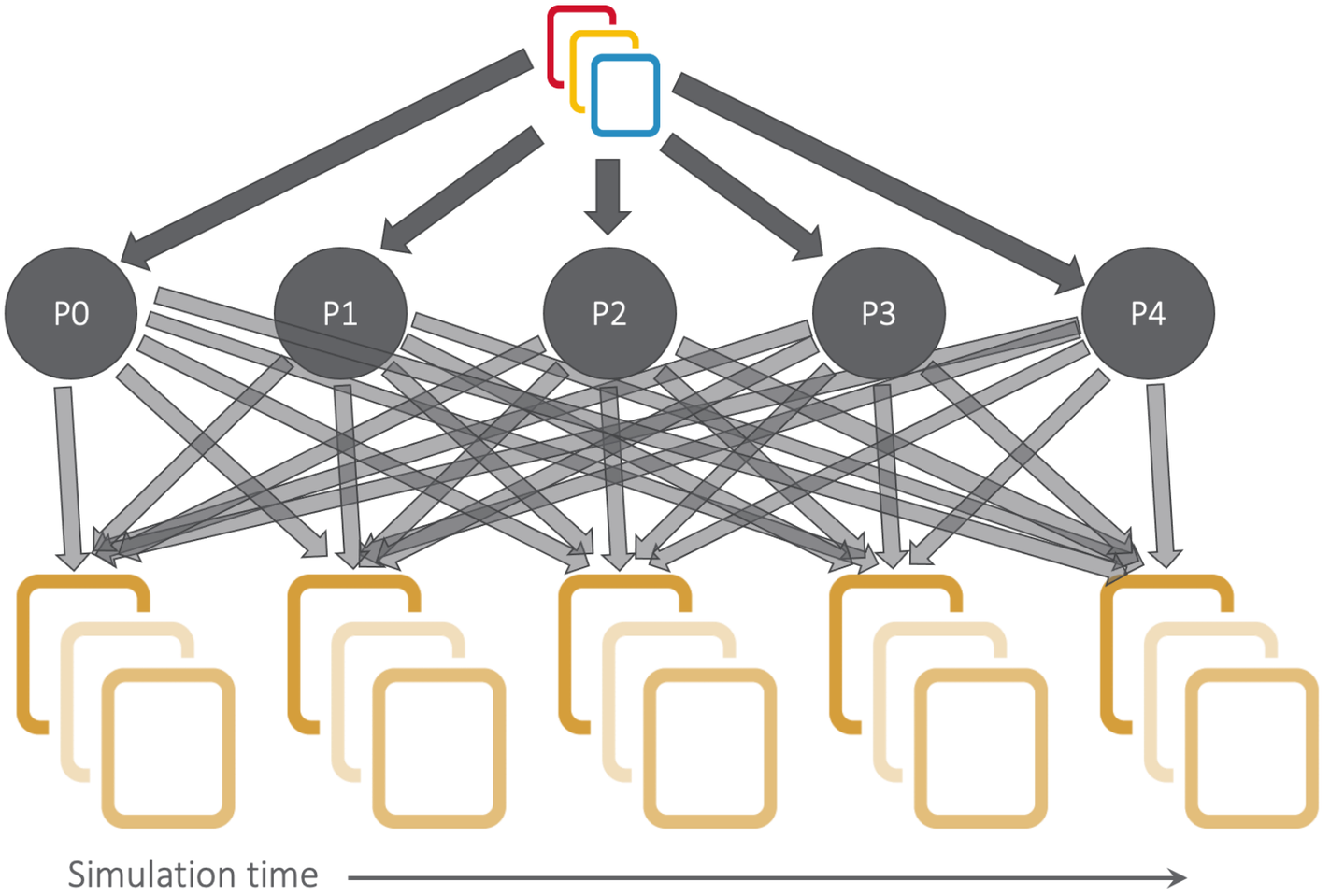
NATIONAL ENERGY TECHNOLOGY LABORATORY
OIL & GAS

# Cooperative Parallel Input/Output

Pros
- Parallelism
- Favorable strong scaling

Cons
- Can only be expressed in MPI
  - MPI_File_open
  - MPI_File_read
  - MPI_File_write
  - MPI_File_close
- Binary input and output files

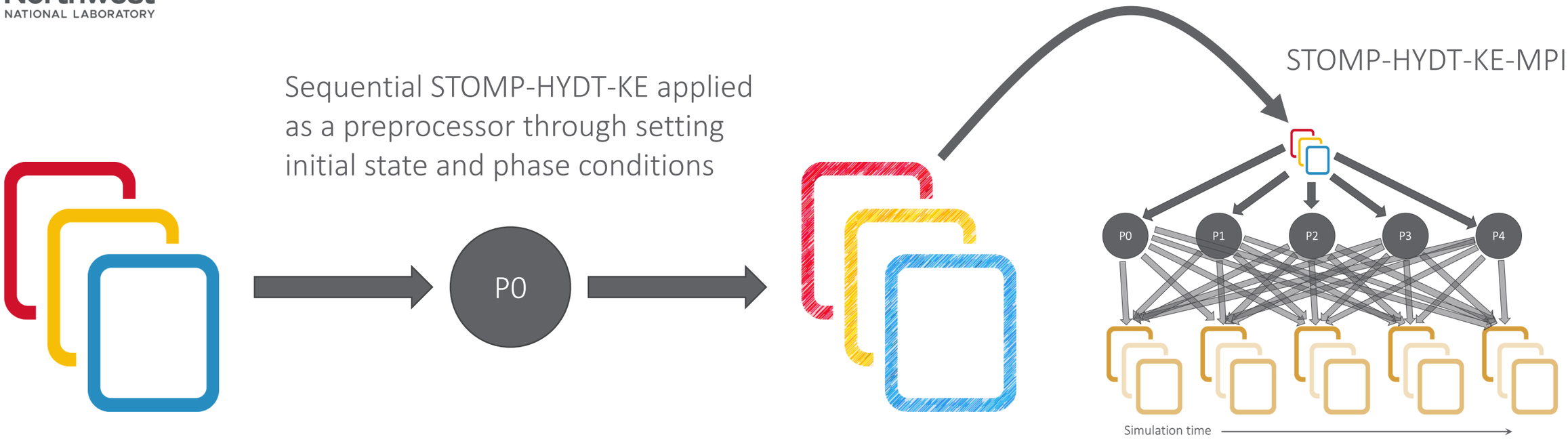



(Shared- or Distributed-Memory Computers)

*https://wgropp.cs.illinois.edu/courses/cs598-s16/lectures/lecture32.pdf*

# Development Concept for Legacy to MPI Conversion

Sequential STOMP-HYDT-KE applied as a preprocessor through setting initial state and phase conditions



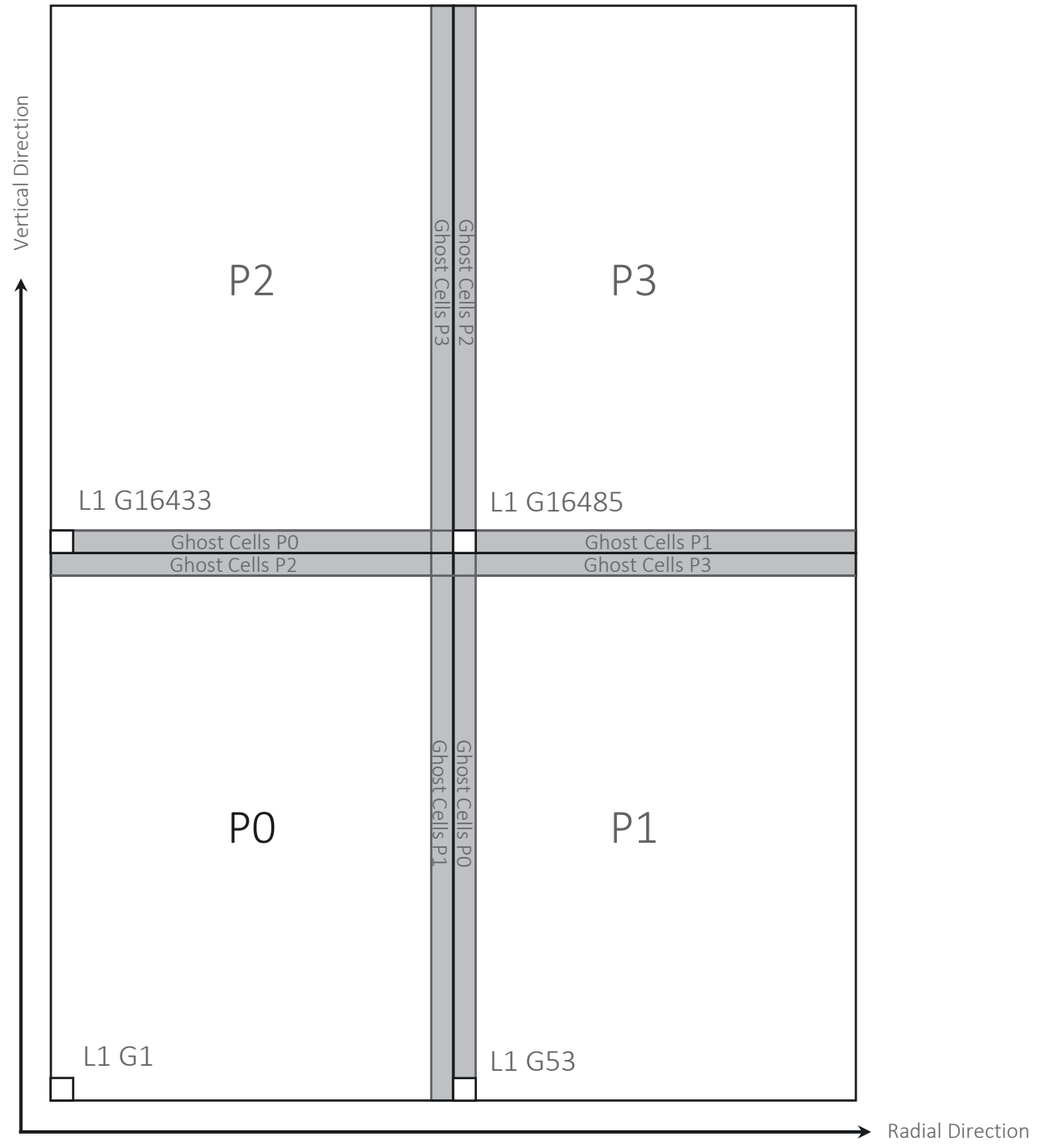

## ASCII (text) Input Files

input (problem description)
tertiary mixture phase envelope ($CO_2$-$CH_4$-$N_2$)
tertiary mixture gas hydrate equilibria ($CO_2$-$CH_4$-$N_2$)

## Binary Input Files

boco.bin
grid.bin
solu.bin
state.bin
inhibitor.bin
sorc.bin
prop.bin
co2_ch4_n2_pe.bin
hyd_co2_ch4_n2_eq.bin

# Verification Example 2D Cylindrical Domain of the Alaska North Slope Problem



# Verification Example 2D Cylindrical Domain of the Alaska North Slope Problem

## Sequential Execution Output

```
ROS =   0.000000000000000  N =   1
ROP(  1 ) =  -2.122732312030147E-013
ROP(  2 ) =   1.150409577254115E-015
ROP(  3 ) =  -2.006866894888049E-013
ROP(  4 ) =   3.188162625213245E-006
ROS =   0.000000000000000  N =   53
ROP(  1 ) =  -8.236512094708164E-010
ROP(  2 ) =   4.463768505649288E-012
ROP(  3 ) =  -7.786944422605302E-010
ROP(  4 ) =   1.237056801220587E-002
ROS =   0.000000000000000  N =   16433
ROP(  1 ) =  -9.108418610106376E-009
ROP(  2 ) =   9.525194614181432E-009
ROP(  3 ) =  -5.017687654262915E-016
ROP(  4 ) =  -5.565692837956595E-006
ROS =   0.000000000000000  N =   16485
ROP(  1 ) =  -3.534208418655472E-005
ROP(  2 ) =   3.695924005644069E-005
ROP(  3 ) =  -1.946887095982675E-012
ROP(  4 ) =  -2.159575588851399E-002
```

## Parallel 4-Processor Execution Output

```
ROS =    0.000000000000000       N =          1  ID  =           0
ROP(           1 ) =   -2.1227323120301472E-013  ID  =           0
ROP(           2 ) =    1.1504095772541154E-015  ID  =           0
ROP(           3 ) =   -2.0068668948880486E-013  ID  =           0
ROP(           4 ) =    3.1881626252132453E-006  ID  =           0
LIS_FINALIZE: IERR =           0 ID =           0
FINI: ID =           0
ROS =    0.000000000000000       N =      16485  ID  =           3
ROP(           1 ) =   -3.5342084186554715E-005  ID  =           3
ROP(           2 ) =    3.6959240056440685E-005  ID  =           3
ROP(           3 ) =   -1.9468870959826745E-012  ID  =           3
ROP(           4 ) =   -2.1595755888513989E-002  ID  =           3
LIS_FINALIZE: IERR =           0 ID =           3
FINI: ID =           3
ROS =    0.000000000000000       N =         53  ID  =           1
ROP(           1 ) =   -8.2365120947081643E-010  ID  =           1
ROP(           2 ) =    4.4637685056492882E-012  ID  =           1
ROP(           3 ) =   -7.7869444226053020E-010  ID  =           1
ROP(           4 ) =    1.2370568012205872E-002  ID  =           1
LIS_FINALIZE: IERR =           0 ID =           1
FINI: ID =           1
ROS =    0.000000000000000       N =      16433  ID  =           2
ROP(           1 ) =   -9.1084186101063759E-009  ID  =           2
ROP(           2 ) =    9.5251946141814327E-009  ID  =           2
ROP(           3 ) =   -5.0176876542629145E-016  ID  =           2
ROP(           4 ) =   -5.5656928379565951E-006  ID  =           2
LIS_FINALIZE: IERR =           0 ID =           2
FINI: ID =           2
```

Radial Direction

Pacific Northwest
NATIONAL LABORATORY

# Questions?

NATIONAL ENERGY TECHNOLOGY LABORATORY
OIL & GAS

# Summary

BP1-Task 1.0 Project Management and Collaborative Research
Collaborative project with KIGAM via the Joint Korea-U.S. Gas Hydrate Project, investigation of nitrogen injection for the Ulleung Basin of the Korean East Sea

BP1-Task 2.0 IGHCCS2
Study paper published in Journal of Marine and Petroleum Geology

BP2-Task 1.0 Project Management and Collaborative Research
Collaborative project with KIGAM via the Joint Korea-U.S. Gas Hydrate Project, investigation of air injection for the Ulleung Basin of the Korean East Sea

BP2-Task 2.0 Simulations in Support of the Alaska North Slope Project
Completed simulations of core- and NMR-based scenarios, continued investigations of kSP models, and modeling scenarios.

BP2-Task 3.0 Well Model Implementation in STOMP-HYDT-KE
Start pending.

BP3-Task 1.0 Project Management and Collaborative Research
Collaborative project with KIGAM via the Joint Korea-U.S. Gas Hydrate Project, pending new contract with KIGAM

BP3-Task 3.0 STOMP-HYDT-KE Parallelization
Currently ongoing