



DGMK/ÖGEW – Frühjahrstagung 2018

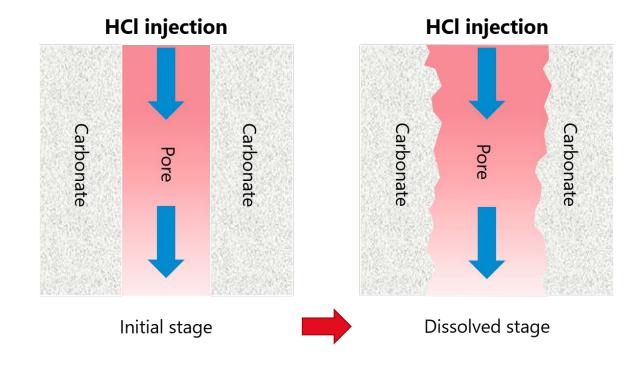
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MOTIVATION – REACTIVE FLOW



- Reactive Flow: HCl injection into carbonate
- Effect: Dissolution, enlargement of the pore space (permeability enhancement)
- Establish a higher permeability
- Keep mechanical stability
- Use numerical simulation to optimize the process parameters, e.g. acid concentration, injection velocity, ...

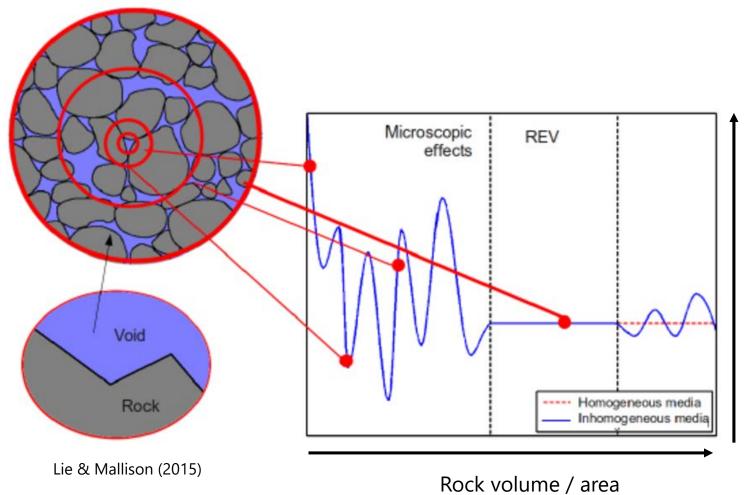


Rock property, e.g. permeability

WHY DO WE NEED A NEW NUMERICAL MODEL?

MATH 2 MARKET

- Lesson learned from digital rock physics: structure at the pore scale influences rock properties at the core scale
- Simulations at the pore scale require REV and, so, large computational domains
- Need for efficient solvers and simple rules for structure manipulation
- We developed a simple numerical model which can be applied to large computational domains (REV)





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Model Description and Implementation

Simulate HCI injection into a carbonate sample

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Model Workflow – Step 1



- Compute the flow field in the structure
- For a given fluid velocity or pressure drop
- Stokes or Navier-Stokes equations
- Export streamlines
- This step is implemented in the GeoDict software



MODEL WORKFLOW - STEP 2



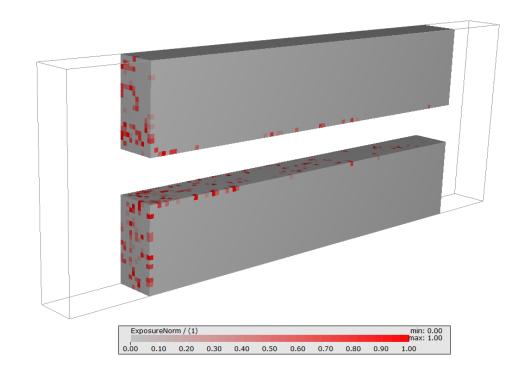
- Compute particle movement
- Particle transport is a combination of advective and diffusive motion (Streamlines + Brownian motion)
- A particle behaves like a single H⁺ Ion, while it represents a larger number of ions (we call this concept *Multiplicity*).
- We keep track of the collision points with the rock interface
- This step is implemented in the GeoDict software



MODEL WORKFLOW - STEP 3



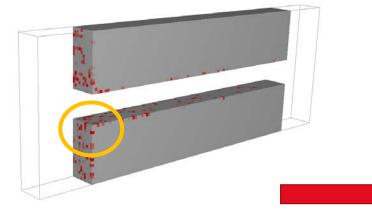
- Model the chemical reaction
- One particle represents a given number of H⁺ lons
- At every collision point a given number of H⁺ lons are transferred to the solid voxel
- We keep track of the consumed H⁺ ions in the particles and solid voxels
- This step is implemented as a Matlab function

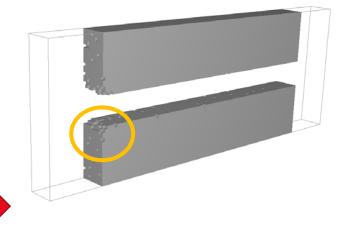


MODEL WORKFLOW - STEP 4

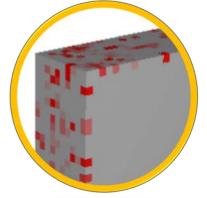


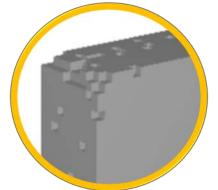
- Update rock structure
- Remove dissolved voxels
- The new structure is saved for the next iteration
- It can be used to analyze properties like: Mechanical stability (Bulk Modulus), Conductivity, Permeability
- This step is implemented as Matlab function





Remove voxels which have "collected" enough H+ lons for a complete dissolution





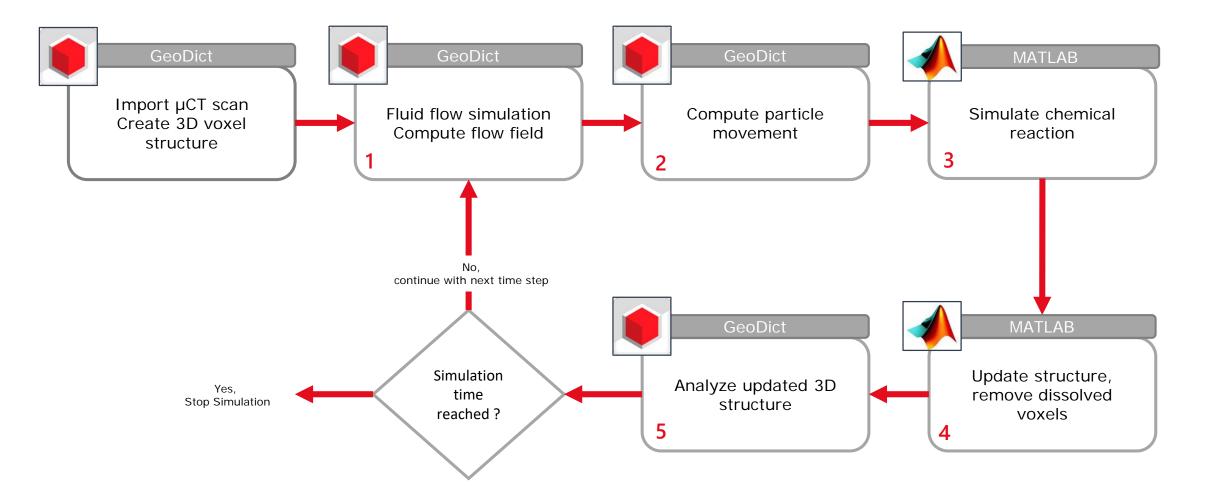


- Particle/Continuum approach
- Fluid flow as continuum (Stokes/ Navier-Stokes)
- Reactants (e.g. H+ lons) as particles
- One particle behaves like a single H+ ion, but represents a larger number
- Upon collision, H^+ ions dissolve the rock (CaCO₃): $CaCO_3 + H^+ -> Ca^{2+} + HCO_3$
- Keep track of consumed H⁺ and dissolved volume



WORKFLOW - OVERVIEW







Simulation on a real rock structure

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CARBONATE SAMPLE



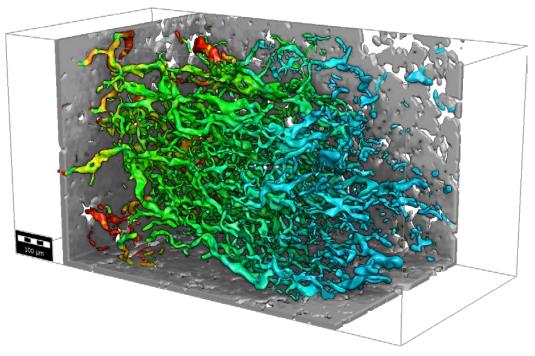
- Grosmont formation, Alberta, Canada
- Dimensions: 1024x1024x1024 voxel
- Resolution: 2.02µm
- Porosity: 21%, permeability range: 150 mD 470 mD -> heterogenous pore space
- Data set is published in DRP benchmark paper (Andrae et al. 2013)

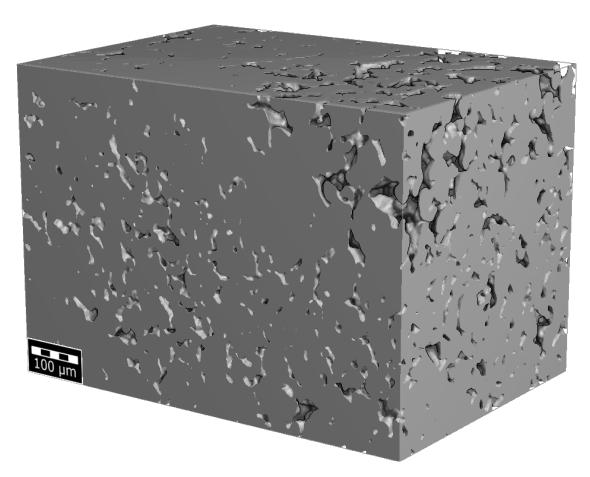


CARBONATE SAMPLE - SUBVOLUME



- Computational domain 256x256x362 voxel
- Porosity of subdomain: 21.9 %
- Homogeneous pore distribution



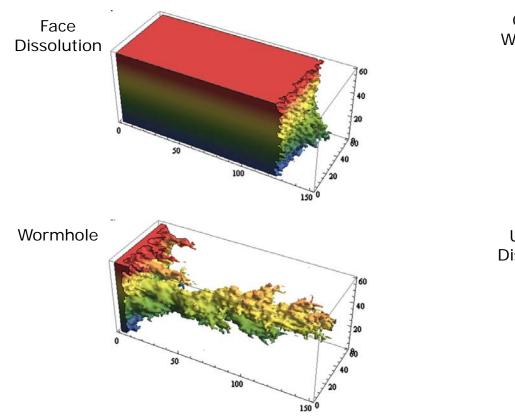


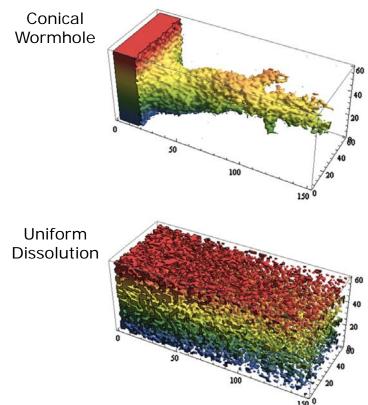
Flow simulation, red: high pressure, blue: low pressure

MODEL EVALUATION



Goal: Replicate characteristic dissolution patterns





Images from Maheshwari et al. 2013

DISSOLUTION PATTERN - FACE DISSOLUTION



Simulation settings:

Domain: 256x256x512 voxel

Runtime: 50 h

Average velocity: 0.001 m/s

pH value: 3.2

Simulation time: 700s

Number of particles: ~2000

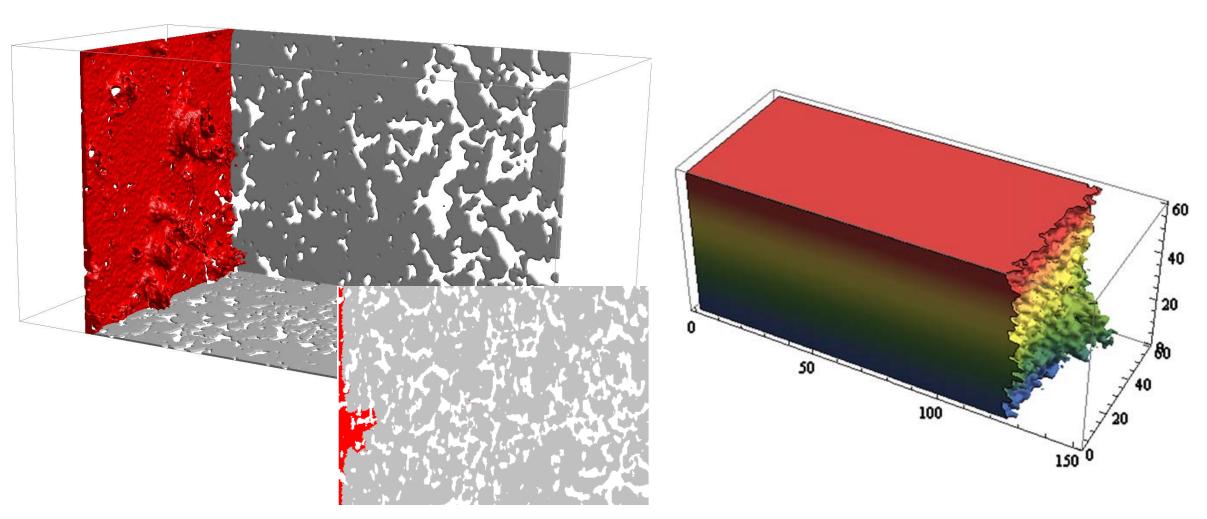
Material Information:

ID 00: Porespace [invis.]
ID 01: Dissolved Structure
ID 02: Original Structure



COMPARISON FACE DISSOLUTION PATTERN





GeoDict simulation

Maheshwari et al. 2013

DISSOLUTION PATTERN - CONICAL WORMHOLE



Simulation settings:

Domain: 256x256x362 voxel

Runtime: 36 h

Average velocity: 0.01 m/s

pH value: 3.2

Simulation time: 100s

Number of particles: ~2000

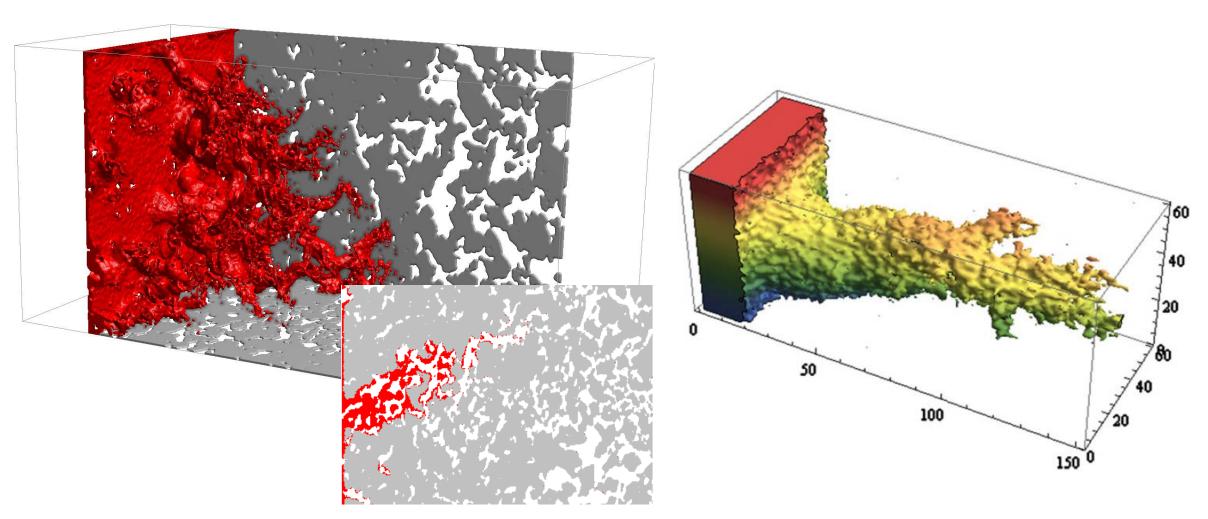
Material Information:

ID 00: Porespace [invis.]
ID 01: Dissolved Structure
ID 02: Original Structure



COMPARISON CONICAL WORMHOLE PATTERN





GeoDict simulation

Maheshwari et al. 2013

DISSOLUTION PATTERN - WORMHOLE



Simulation settings:

Domain: 256x256x362 voxel

Runtime: 28 h

Average velocity: 0.1 m/s

pH value: 3.2

Simulation time: 20s

Number of particles: ~2000

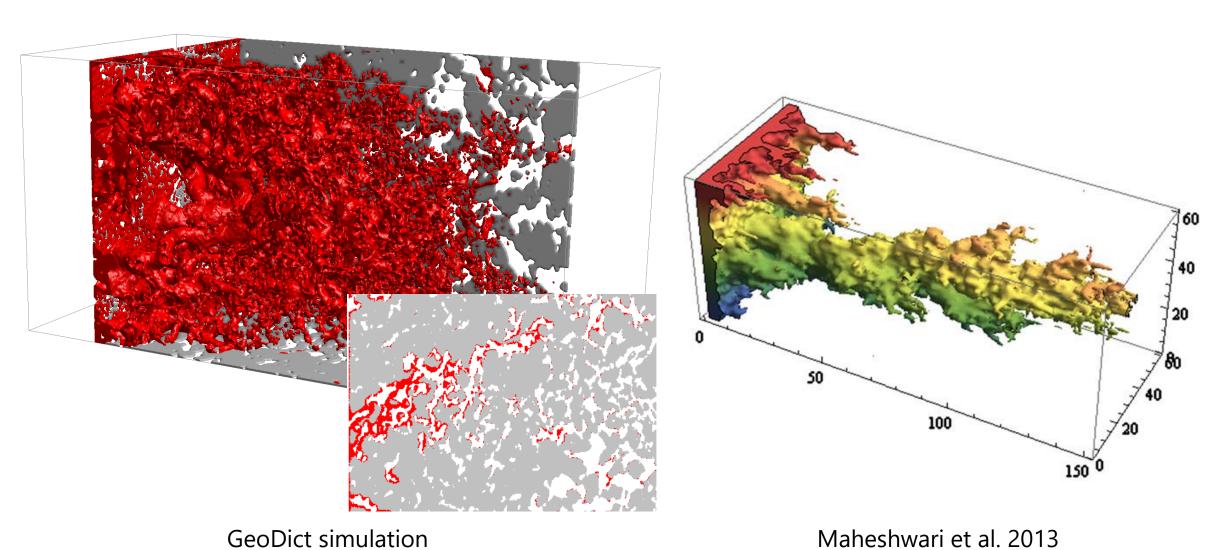
Material Information:

ID 00: Porespace [invis.]
ID 01: Dissolved Structure
ID 02: Original Structure



COMPARISON WORMHOLE PATTERN





DISSOLUTION PATTERN - UNIFORM DISSOLUTION



Simulation settings:

Domain: 256x256x362 voxel

Runtime: 29 h

Average velocity: 0.1 m/s

pH value: 2.8

Simulation time: 20 s

Number of particles: ~2000

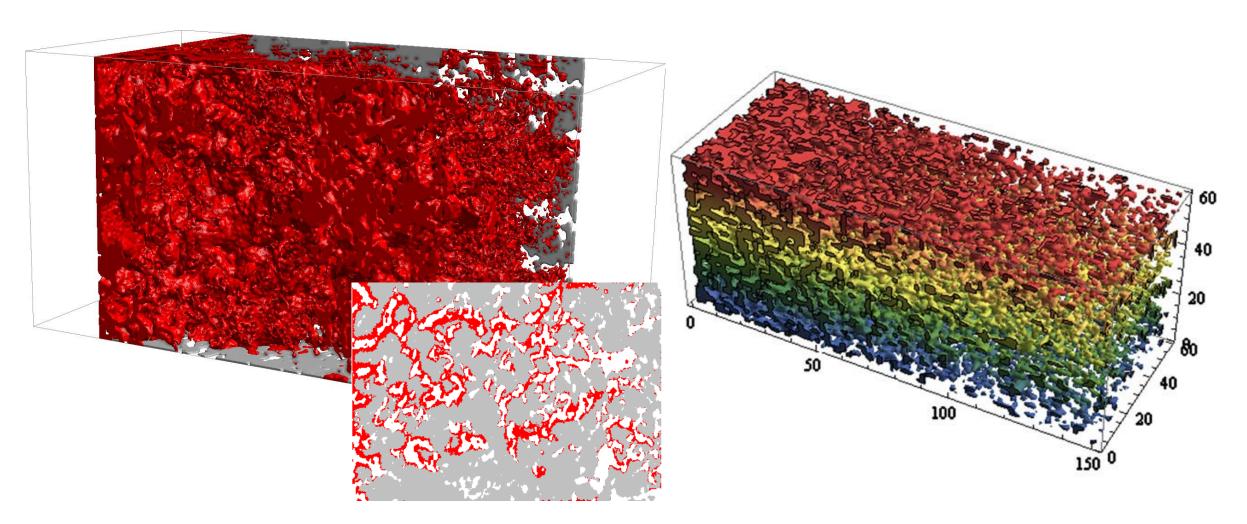
Material Information:

ID 00: Porespace [invis.]
ID 01: Dissolved Structure
ID 02: Original Structure



COMPARISON UNIFORM DISSOLUTION PATTERN



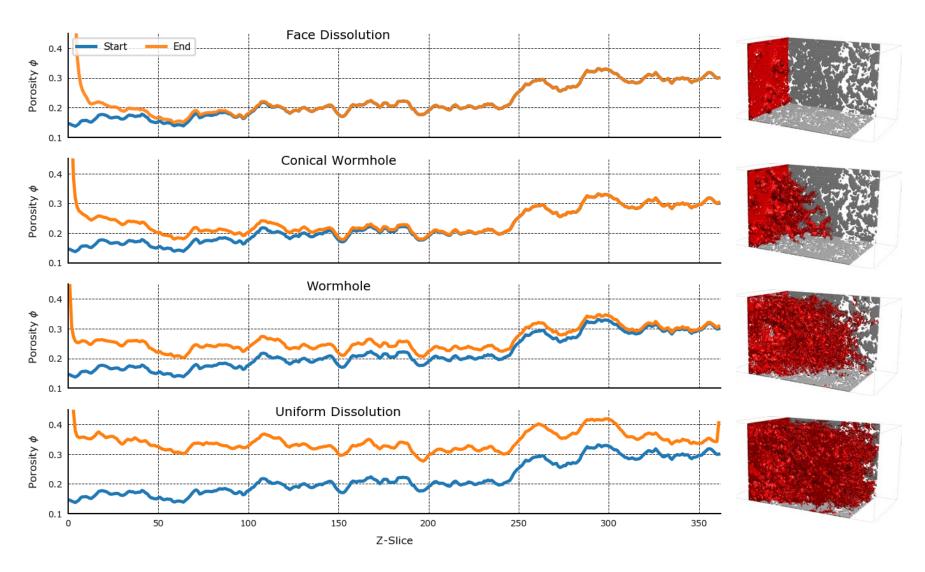


GeoDict simulation

Maheshwari et al. 2013

POROSITY ANALYSIS

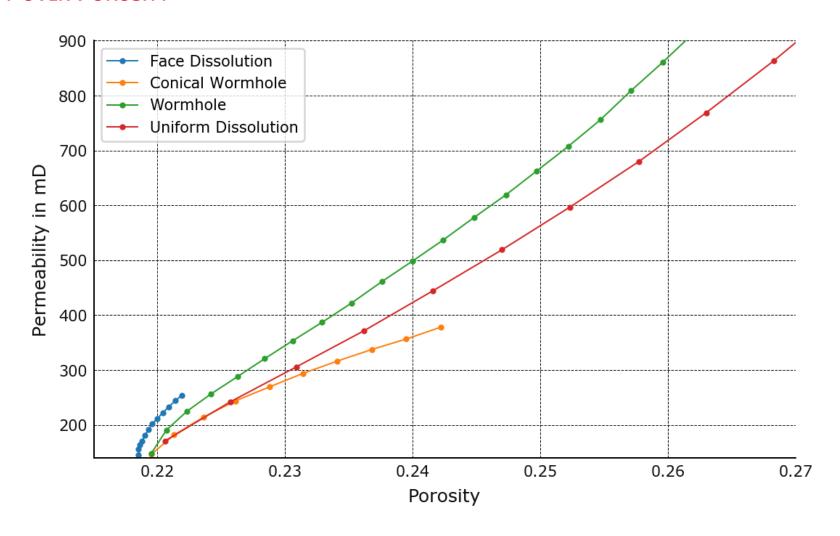




PERMEABILITY ANALYSIS

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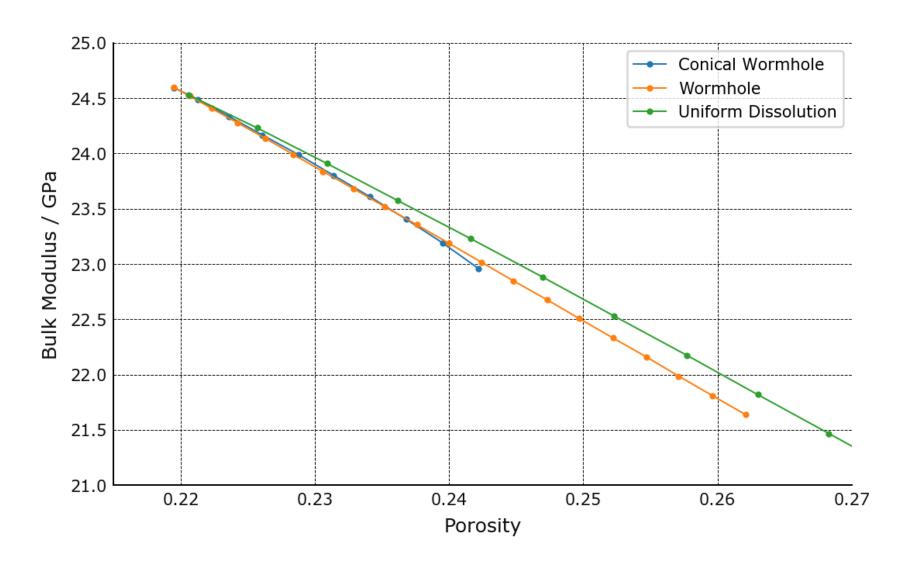
PERMEABILITY OVER POROSITY



MECHANICAL ANALYSIS

BULK MODULUS OVER POROSITY





"LARGE" SIMILIATION



Simulation settings

Domain: 512x512x51 Average velocity: 0.1

pH value: 3.2

Simulation time: 20 s Number of particles: Runtime: 120 h (16 cor

Material Information:
ID 00: Porespace [invis
ID 01: Dissolved Struct
ID 02: Original Structu



CONCLUSION & OUTLOOK



- Numerical model to simulate reactive flow presented
- Model evaluated by reproducing characteristic dissolution patterns
- All included in the commercially available DRP software GeoDict
- GeoDict simulations can be run on a state-of-the-art desktop workstation, using very efficient and reliable numerical solvers
- Current work to incorporate the Matlab functions into GeoDict to reach computational domains of > 2000^3 voxels

THANK YOU FOR YOUR ATTENTION



Please come to our booth for more information about GeoDict®



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REFERENCES

Andrae, H., Combaret, N., Dvorkin, J., Glatt, E., Junehee, H., Kabel, M., Keehm, Y., Krzikalla, F., Lee, M., Madonna, C., Marsh, M., Mukerji, T., Saenger, E., Sain, R., Saxena, N., Ricker, S., Wiegmann, A., Zhan, A., "Digital rock physics benchmarks Part I: Imaging and segmentation", Computers & Geosciences, 43, 25-32, 2013.

Lie, K. A. and Mallison, B. T., Mathematical models for oil reservoir simulation. In *Encyclopedia of Applied and Computational Mathematics*, Springer-Verlag Berlin Heidelberg, 2015.

Maheshwari, P., Ratnakar, R.R., Kalia, N. and Balakotaiah, V., 3-D simulation and analysis of reactive dissolution and wormhole formation in carbonate rocks. Chemical Engineering Science, 90, 258-274, 2013.