Simulation of Reverse Osmosis Membrane Compaction using Material Point Method (MPM)

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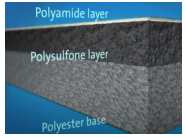
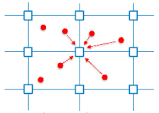
Motivation:



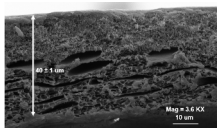
- 1.2 billion people across the world live in regions of water scarcity
- 2 million tons of sewage/industrial/organic waste discharged worldwide every day
- Replacing thermal desalination with high pressure reverse osmosis (HPRO) can reduce the energy consumption and cost of brine concentration
- High pressures (~ 100-200 bar) in HPRO leads to membrane compaction thus reducing its ability to filter efficiently.

Material point method:

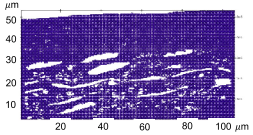


- Grid based finite element methods pose difficulties due to grid quality deterioration arising from severe material deformation
- Variant of the Particle-in-Cell method. Continuum simulated as a collection of material points embedded in a cartesian grid.
- Easy handling of large material deformations, complex geometry handling, easy incorporation of multiple constitutive models and amenability of large-scale computing

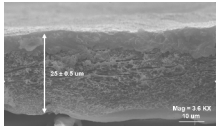
MPM Simulation of membrane compaction



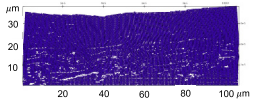
SEM image of uncompacted membrane



Uncompacted membrane in MPM

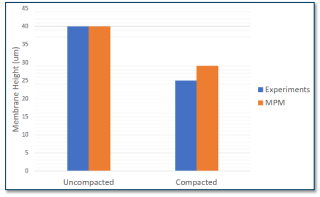


SEM image of compacted membrane



Compacted membrane in MPM

- Experimental compaction of Polysulfone membrane performed at UCLA. Initial material point distribution obtained from SEM image of uncompacted membrane
- Membrane simulated as a linear elastic material with Young's modulus (= 100 MPa) obtained from tensile test



Comparison of membrane heights from experiment and simulation

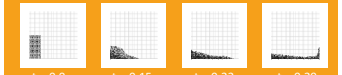
- Application of pressure on the membrane deforms it by 11μm as compared to 15 μm observed in experiments (accuracy ~16% with respect to experiments)
- Macro void deformations obtained in simulations are in close agreement with that observed in SEM images
- Further improvements in simulated results to be obtained by modifying Young's modulus to account for micro voids in membrane

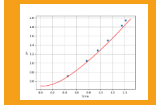
Exagoop MPM solver, features, validation and performance

EXAGOOP: KEY FEATURES

- Background cartesian mesh and particle generation and related operations handled using AMReX – a performance portable grid/particle software library.
- Linear hat, Quadratic B-Spline and Cubic B-Spline numerical schemes
- Embedded boundaries for modeling complex geometries
- CPU and GPU compatible

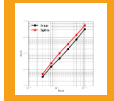
VALIDATION: DAM BREAK SIMULATION

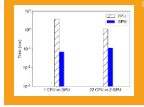




- Water simulated as barotropic fluid
- Excellent match with experimental measurements on water-front location

CONVERGENCE, PARALLEL PERFORMANCE





- Second-order convergence observed for 1D simulation of transverse string vibration problem (L2 norm of error used)
- GPU parallelization enables quicker simulation run times

NAWI CONNECTIONS

Period of Performance: Oct. 2021 – Till Date

Challenge Area/Topic Area:
- Materials and Manufacturing

NAWI Leverage

NAWI funding led to the development of Exascale capable MPM solver, capable of execution on both CPU and GPU architectures. NAWI funding enabled computations to be performed on National Lab supercomputers (Eagle, at NREL)

KEY FINDINGS AND CONCLUSIONS

- Development of a three-dimensional, block-structured, parallel MPM solver-*'Exagoop'* capable of execution on CPUs and GPUs
- Extensive validation of '*Exagoop*' solver for both solids and fluids show excellent match with exact solutions/available measurements
- MPM applied for the first time to study compaction of RO membranes. Membrane compaction predicted up to 16% accuracy with respect to experimental measurements.

REFERENCES

"Simulation of Reverse Osmosis Membrane Compaction using Material Point Method", Sreejith N. A., Hariswaran Sitaraman, Marc Day, Sina ShabazMohamadi, Jishan Wu, Eric Hoek, to be presented at SIAM International Conference on Computational Science and Engineering, 3rd March 2023

"**Exagoop Material Point Method Solver**", GitHub repository: *https://github.com/NREL/Exagoop*

ACKNOWLEDGEMENTS

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