Reactive Transport in Porous Media: Multiscale Modeling and Experiments

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Outline

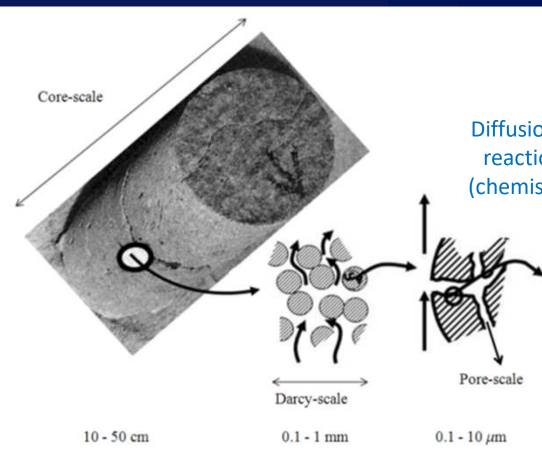
- Coupling of Physics at Multiple length Scales
- Upscaling Techniques
  - Bottom-up and top-down approach
  - Reduced Order Modeling
- State-of-art Measurement Techniques
  - Transport, Thermodynamic and Interfacial Properties
  - Kinetics and Adsorption Characteristics
- Coupling of Physics and Data Analytics
  - Blind ML vs Physics informed ML
- Petroleum Engineering Skills towards Energy Transition

Coupling of Physics at Multiple length Scales

Hierarchy of Length Scales (Continuum Regimes)

- Reactive transport (Diffusion, convection and reactions) are core phenomena in many chemical and petroleum processes
- Coupling of these processes at multiple length scales determine the macroscopic behavior of the system
  - Diffusion and reaction chemistry at micro- (or nano-) pores
  - Microscopic and macroscopic transport at meso- and macro-pores

— Ratnakar, RR. 2012. PhD Thesis



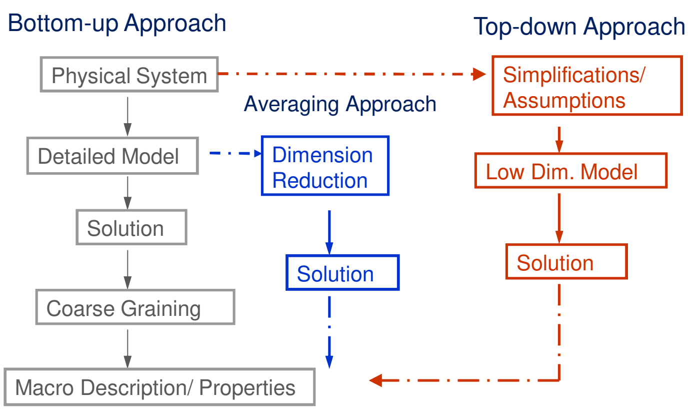
Diffusion + reaction (chemistry)

Macroscopic transport

Microscopic transport (Diffusion + convection + reaction)

Upscaling Techniques

Various Approaches of multiscale modeling



— *Ratnakar, RR. 2012. PhD Thesis*

— *Ratnakar, RR and Balakotaiah V., Multi-scale averaging of Diffusion-convection-reactions processes", McGraw-Hills, In preparation (2022)*

Averaging Approach

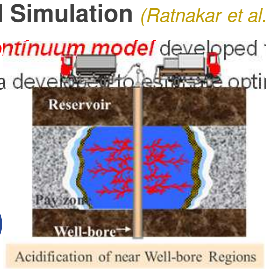
Lyapunov-Smidt Reduction; Center Manifold; Volume Averaging; Homogenization; Reynolds re-normalization

- ✓ Eliminate the local spatial degrees of freedom
- ✓ Enabling fast and inexpensive computation
- ✓ Real time optimization
- ✓ Design and performance evaluations
- ✓ Solving Inverse problems

Upscaling Techniques

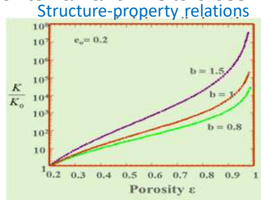
Example: Reactive Dissolution in Porous Media

- **Background**
  - Near well-bore damage during drilling and production phases: restrict the flow of hydrocarbon
  - Acid injection: dissolving carbonate near well-bore region to enhance permeability and hence oil production - success depends strongly on the temperature, mineralogy and heterogeneity
- **Modeling and Simulation** *(Ratnakar et al., 2012, 2013a,b)*
  - ***Two-scale continuum model*** developed for Newtonian and in-situ cross-linked acids.
  - Scaling criteria developed to estimate optimum ... rate etc.)

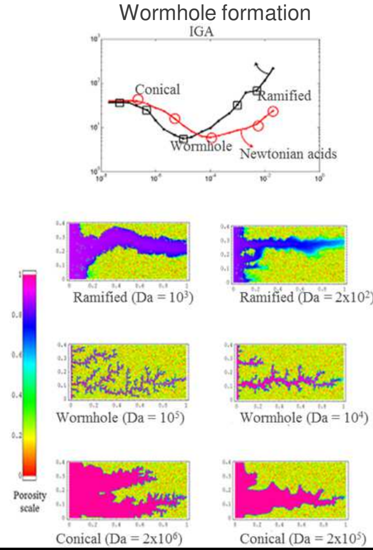


Acidification of near Well-bore Regions

Structure-property relations



Wormhole formation



— *Ratnakar et al., SPE-154936 (2012); CES, 90:179-199 (2013); CES, 90: 258-274 (2013)*

Upscaling Techniques

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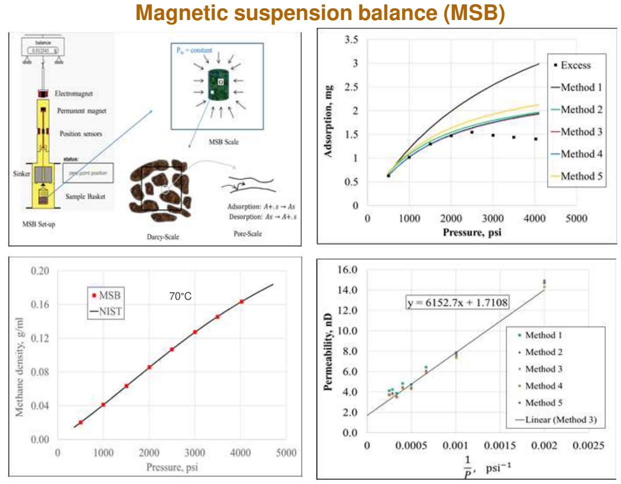
Example: Adsorption and Transport Characteristics in Tight Rocks

- **Background**
  - Characterization of adsorptive and transport behavior of unconventional reservoirs – accurate estimate of hydrocarbon reserves and proper design of recovery schemes
  - Dependency on various quantities such as organic material (maturity and type), pore structure, and mineralogy
- **Modeling and Experimental** *(Ratnakar and Dindoruk, 2018, 2019)*
  - Integrated workflow developed for simultaneous estimation of true adsorption isotherm and nano-Darcy range permeability from MSB experiments
  - Completed for three different unconventional recourses with methane and CO2

— *Ratnakar et al., SPE-191504 (2018, 2019)*

Magnetic suspension balance (MSB)



State-of-art Measurement Techniques

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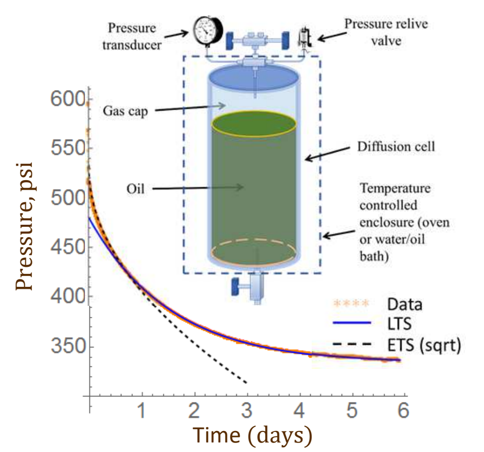
Example:
Thermodynamic (PVT) Properties – Fluid characterization (Vendor Labs)

Example:
Adsorption and Transport Characteristics in Tight Rocks (MSB Previous slide)

Example: Diffusive Transport of Gas in Liquids (Oils/Bitumen)

- In reservoir simulation for design of recovery process, diffusion is one of the key properties and can be dominant in absence of convective mixing
- ***Pressure-decay test:*** Robust methodology integrating experiments and numerical inversion is developed and applied for various gas-oil systems from worldwide reservoirs
- Enable handling of intermittency and/or noise in data as well as speed up the experiments



— *Ratnakar et al, Transport in Porous Media (2019)*
— *Ratnakar and Dindoruk, SPE-170931 (2014, 2015); SPE-181514 (2016, 2019); SPE-191531 (2018, 2020)*

State-of-art Measurement Techniques

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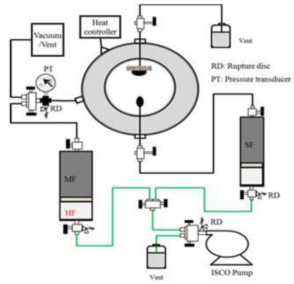
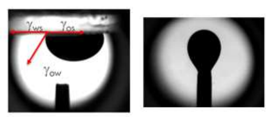
Example: Asphaltene Stability and Interfacial properties

- **Background**
  - Asphaltene precipitation is one of the commonly encountered issues in oil recovery operations and can add significant problems in petroleum production fields.
  - Wettability (interfacial properties) alteration due to asphaltene precipitation in a reservoir affects rock-fluid interactions that have potential impacts on oil production, recovery and flow in the production network
- **Measurement and Inversion** *(Ratnakar et al. 2017, 2018, 2019)*
  - Novel technique developed for measuring asphaltene onset pressures (AOP) based on sharp change in Interfacial tension (IFT)
  - Modeling for asphaltene precipitation and correlation with interfacial forces

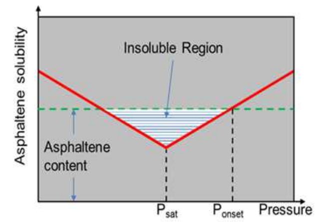
— *Ratnakar et al., SPE-183940 (2017, 2018); SPE-190385 (2018, 2020)*

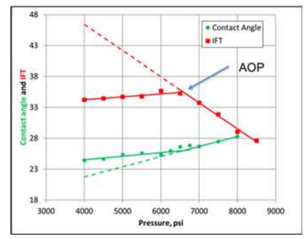
Pendant drop set-up





$\cos\theta = \frac{\gamma_{ws} - \gamma_{os}}{\gamma_{ow}}$





State-of-art Measurement Techniques

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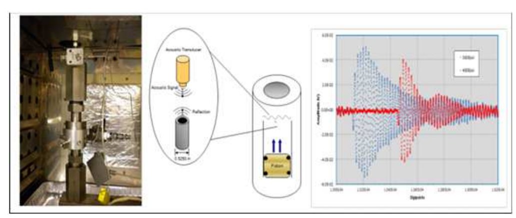
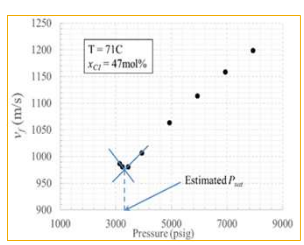
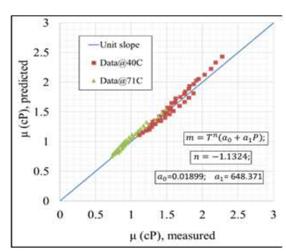
Example: Acoustic Velocity and Linkage to Other Fluid Properties

- **Background**
  - Fluid properties determination is one of core area of petroleum industries for accurate estimate of hydrocarbon reserves and recoverable volumes that translates directly to the revenue and profit of the industry
  - Some properties are very difficult to measure, e.g. viscosity of bitumen and very heavy oils, compressibility of any fluid etc.
- **Measurements and correlations** *(Ratnakar et al. 2018, 2020)*
  - Experimental capability developed for acoustic velocity measurements
  - linked to the estimation of viscosity and compressibility – correlation development and validation for three live crude oils from different fields

— *Ratnakar et al., SPE-190480 (2018, 2020)*







Coupling of Physics and Data Analytics

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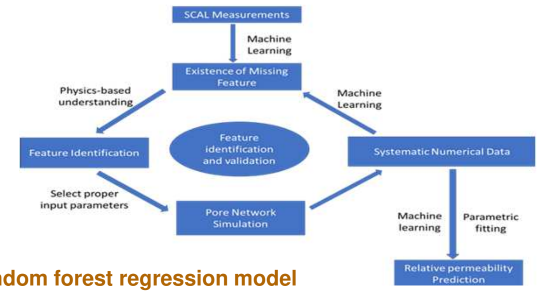
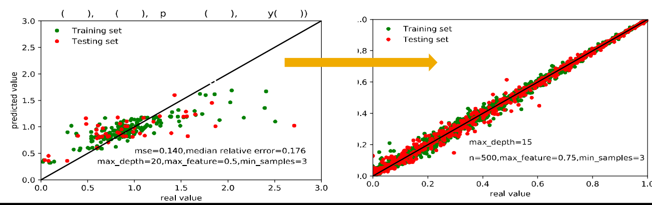
Example: Relative Permeability Predictions for Multiphase Flow in Porous Media/Reservoirs

- **Background**
  - Relative permeability is one of the most important quantities in multiphase flow in oil reservoirs – contains huge uncertainty in reservoir simulation due to lack of coherent experimental and modeling techniques
  - Can we use machine learning and extensive experimental data available in literature to develop a predictive tool
- **Coupling of data analytics and Physics** (*Bochao et al. 2018, 2020*)
  - Integrated workflow developed: determined the missing features using random forest algorithm and neural network
  - Developed empirical correlation that is fast and efficient to predict relative permeability for both drainage and imbibition processes.



Random forest regression model



— *Zhao, B., Ratnakar, R.R., Dindoruk, B. and Mohanty, K., SPE-196022 (2019, 2020)*

Petroleum Engineering Skills towards Energy Transition

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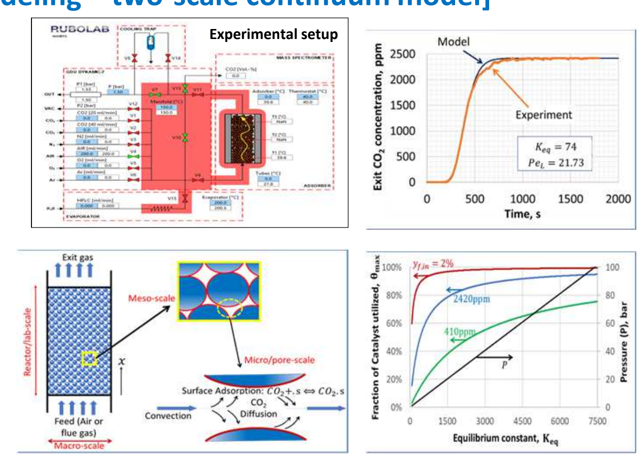
Example: Carbon Capture [Reduced order modeling – two-scale continuum model]

- **Background**
  - Increased energy demands, society challenges and stricter emission regulations/restrictions – Necessitates the development of net-zero emission fuels
  - Possible future scenario suggests that oil/natural gas remains major source of energy – Necessitates Carbon capture
- **Modeling and experiment** (*Ratnakar et al. 2019, 2021*)
  - Developed a two-scale continuum (TSC) model for carbon capture from air or flue gases using fixed-bed reactors
  - The model is robust and validated against in-house experimental observations
  - The model enables the understanding of commercialization and techno-economical challenges – and can simulating various scenarios for evaluating efficient reactor design & performance



— *Ratnakar, et al., AIChE (2019); JNGSE (2021)*

Petroleum Engineering Skills towards Energy Transition

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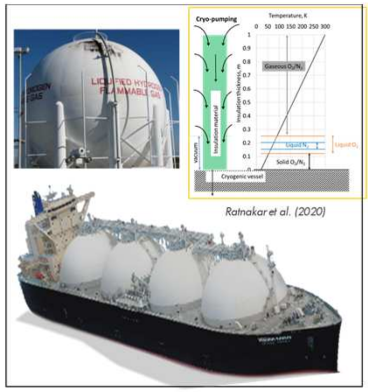
Example: Large-scale Liquid hydrogen storage [Thermodynamics; Upscaling of effective transport properties of insulations (porous media); Heat transfer and Natural convections]

- **Background**
  - Hydrogen - key future energy carrier that links with existing natural gas-based production enabling long distance carbon free energy transport – no intermittency issues
  - Hydrogen storage I skey element of global hydrogen supply chain
  - Because of the ultra-low boiling point (20 K) and low heat of vaporization, the liquid storage tank needs to be well insulated to minimize the boil-off loss
  - Challenges: cryopumping; hydrogen embrittlement during thermal cycling; Insulation property model in low T-ranges; Mechanical stability; Safety & Scalability



Ratnakar et al. (2020)

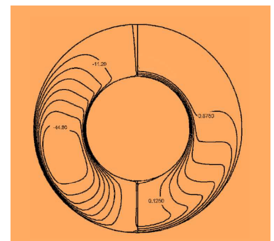


Figure 5 Streamlines (left) and isotherms (right) for $Ra = 1000, A = 1.0$

Natural convection

— *Sangita et al. (2014)*

— *Ratnakar, et al., 2021., Hydrogen supply chain and challenges in large-scale LH2 storage and transportation. Int. J. of Hydrogen Energy*
— *Ratnakar, et al., 2022., Effective Thermal Conductivity of Insulation Materials for Cryogenic LH2 Storage Tanks: A Review. Int. J. of Hydrogen Energy*

Petroleum Engineering Skills towards Energy Transition

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Other Examples:

- ❑ Gaseous storage of hydrogen for mobility applications [*Ratnakar et al. JNGSE, 81 (2020):103463*]
  - ✓ Thermodynamics; Separation; electrochemical compression
  - ✓ Infra-structure and fuel distribution, transportation/pipeline
- ❑ Subsurface hydrogen storage and CO2 sequestration [*Ratnakar et al., JNGSE, 81 (2020) 103450*]
  - ✓ Thermodynamics/solubility/storage capacity; subsurface engineering,
  - ✓ Separation, carbon capture
- ❑ Enhanced Geothermal System *[Ratnakar et al., SPE-209362 (2022)]*
  - ✓ Drilling and Well construction; Heat transfer and carrier fluids; thermodynamics;
  - ✓ Thermal technology; Subsurface engineering

Summary

- Flow in Porous Media is well established area for various disciplines especially for Petroleum Engineers
- Need to focus on advancement towards
  - state-of-art measurements of transport/thermodynamic properties from nano/micro scales to large/macro scales
  - Reduced order model development for enabling the solution of stiff problems, performance evaluation of large-scale systems, control and optimization, design and scaleup
  - Handling large datasets and apply data analytic methods (integrated with physics-based understanding) for enhanced computation
- Petroleum Engineering skills are diverse and applicable in various other disciplines including key elements of energy transition (Hydrogen, CCUS, Geothermal etc.)

Thank you

Questions?