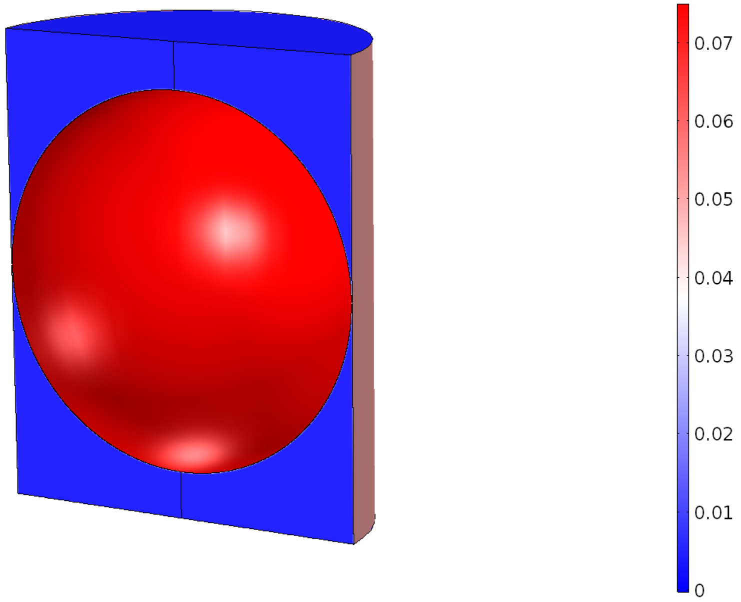
Electrostatic Interactions Between Charged Bubble Interface and Solid Wall



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BINGHAMTON UNIVERSITY
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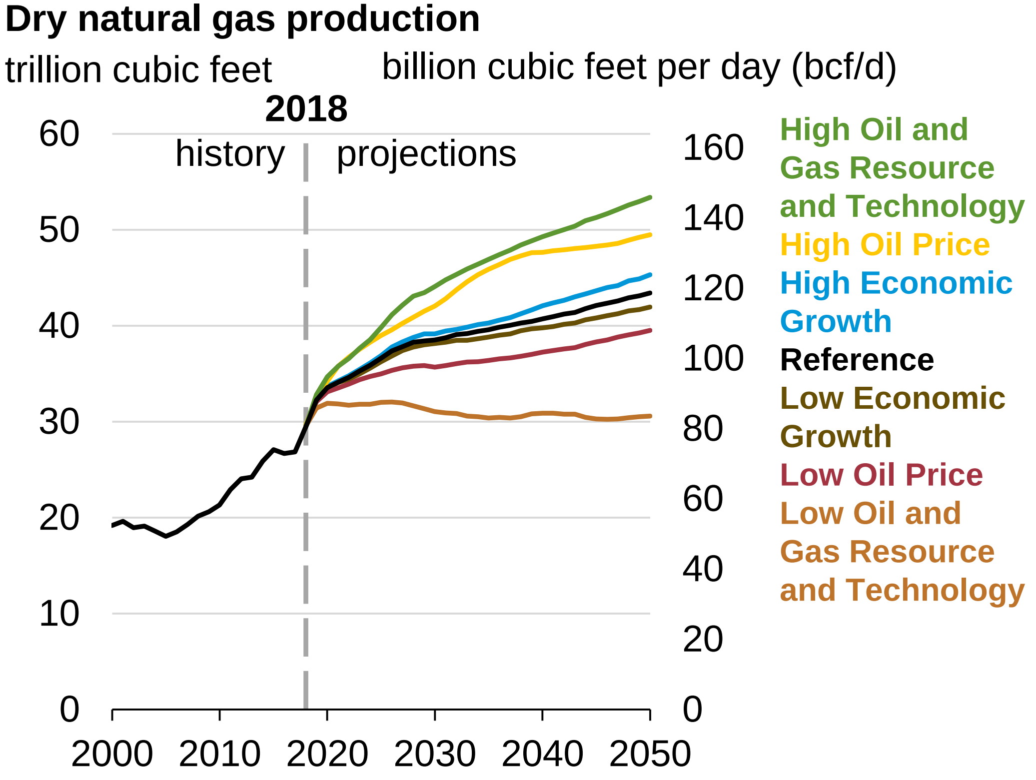
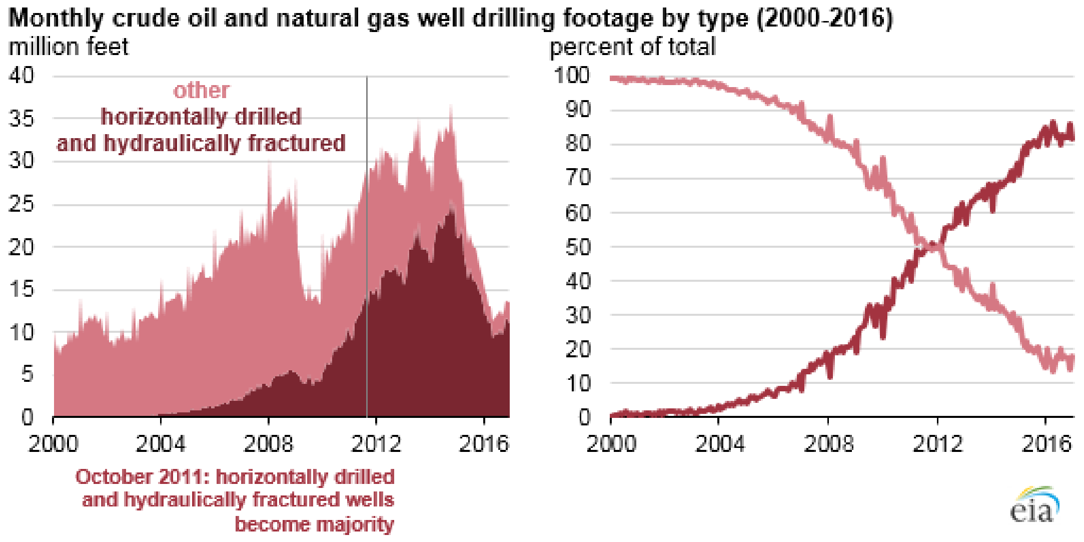
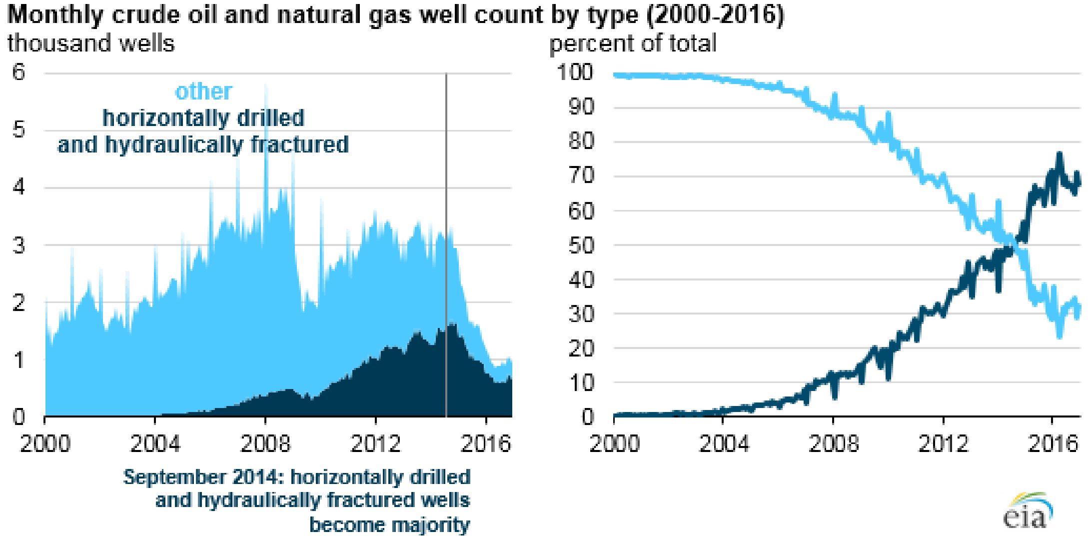
Mechanical Engineering

Projected U.S. Natural Gas Consumption & Production



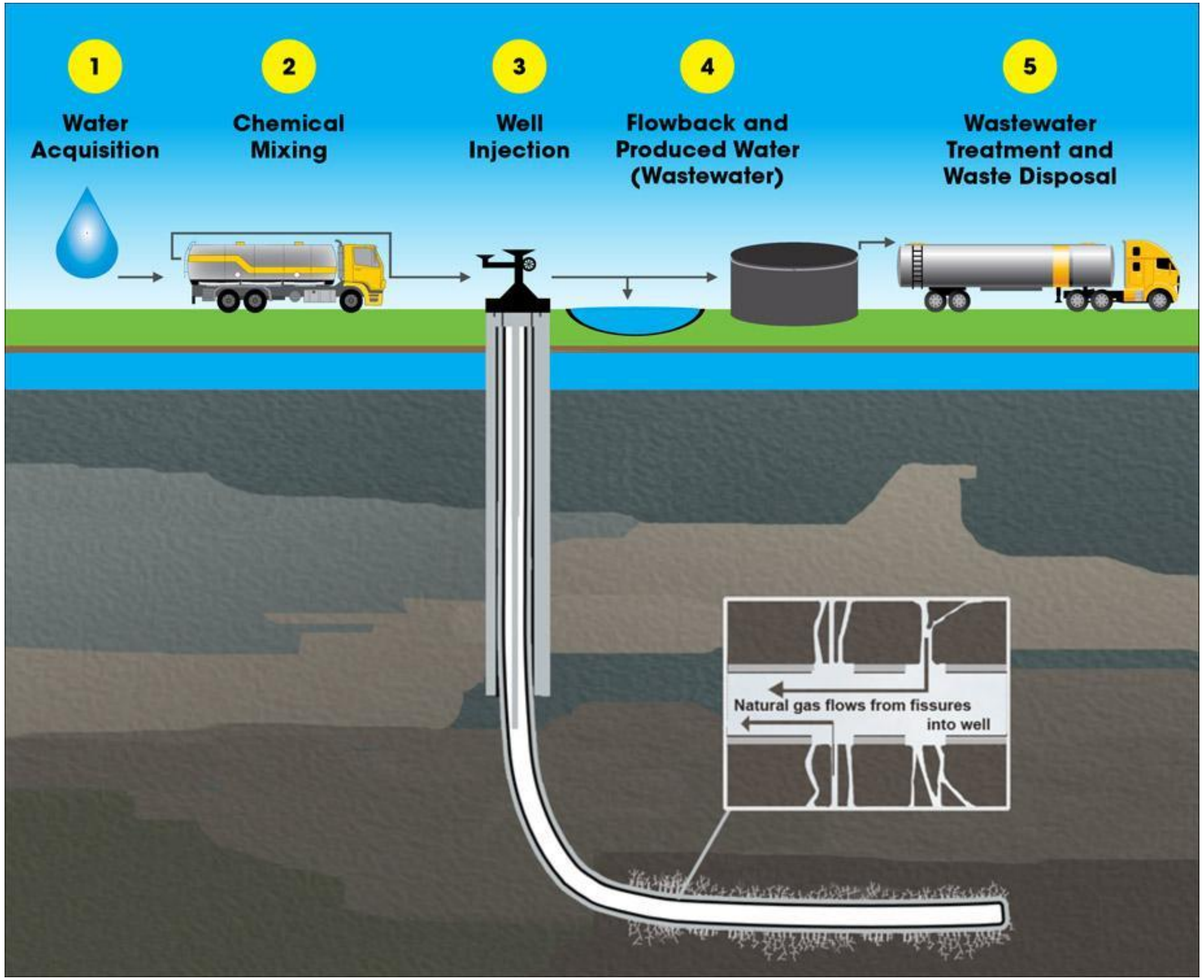
Source: U.S. Energy Information Administration Annual Energy Outlook 2019



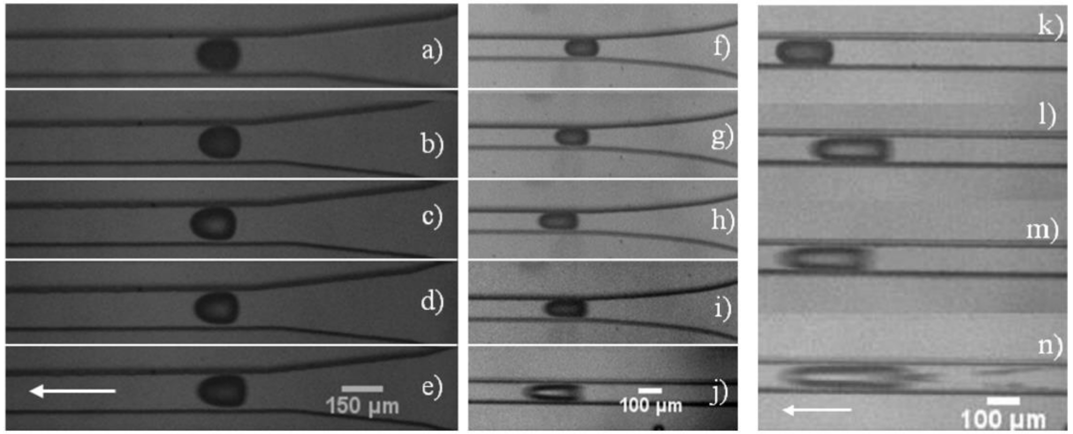


- Increase in production and consumption through next 30 yrs
- International Energy Agency: 2018 record high production of 139 tcf (4% increase from 2017)
- Hydraulic fracturing has become predominant method of extracting gas since 2011 and accounted for most of all new wells drilled since late 2014

Hydraulic Fracturing Overview

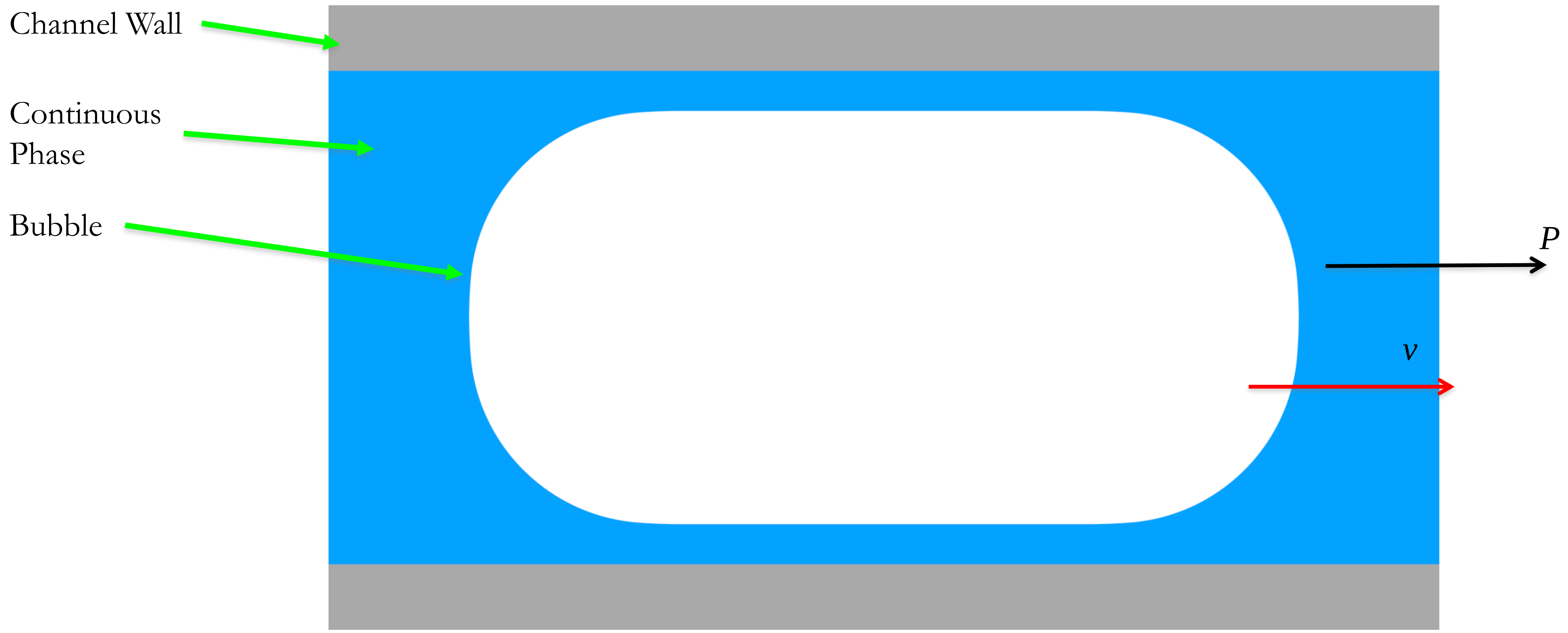


Source: U.S. Environmental Protection Agency

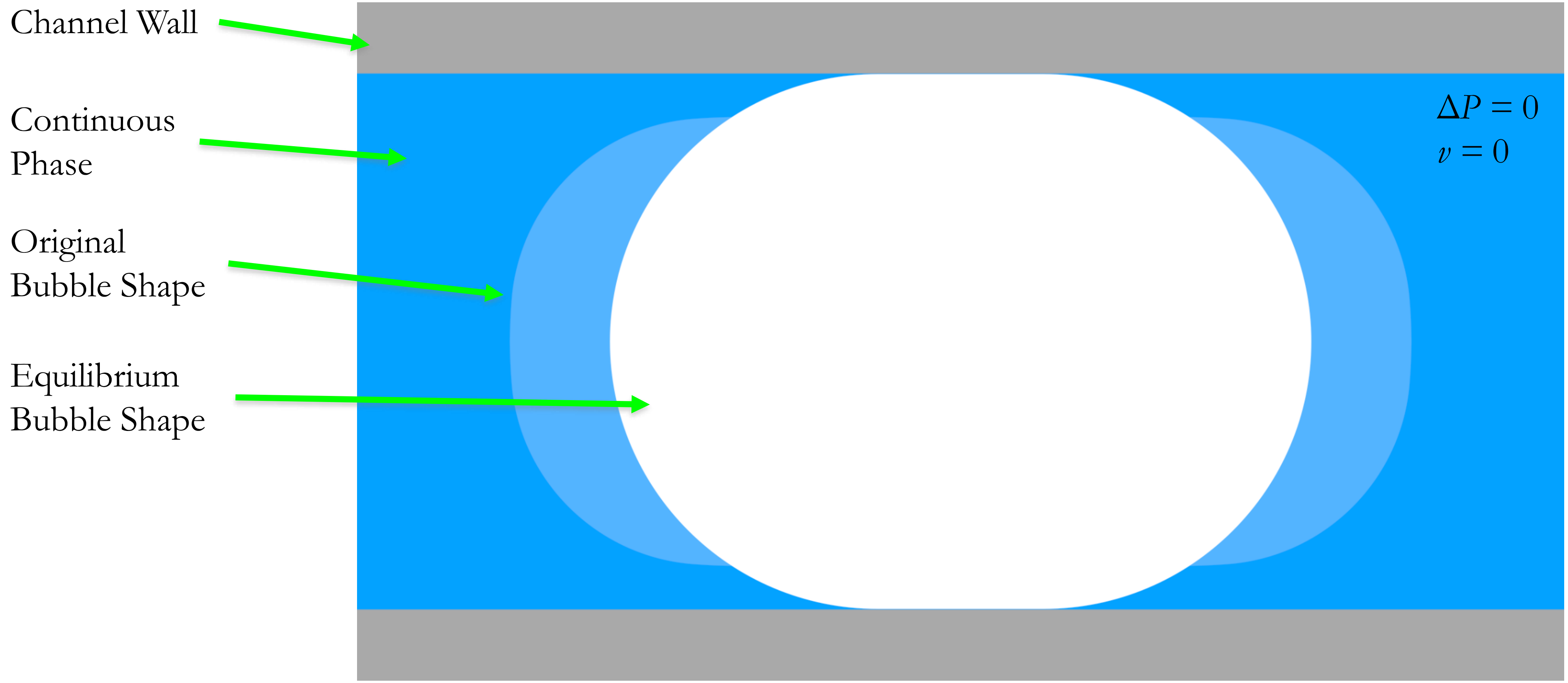


Source: M. K. Mulligan and J. P. Rothstein. Deformation and Breakup of Micro- and Nanoparticle Stabilized Droplets in Microfluidics Extensional Flows. Langmuir, 27(16):9760–9768, July 2011

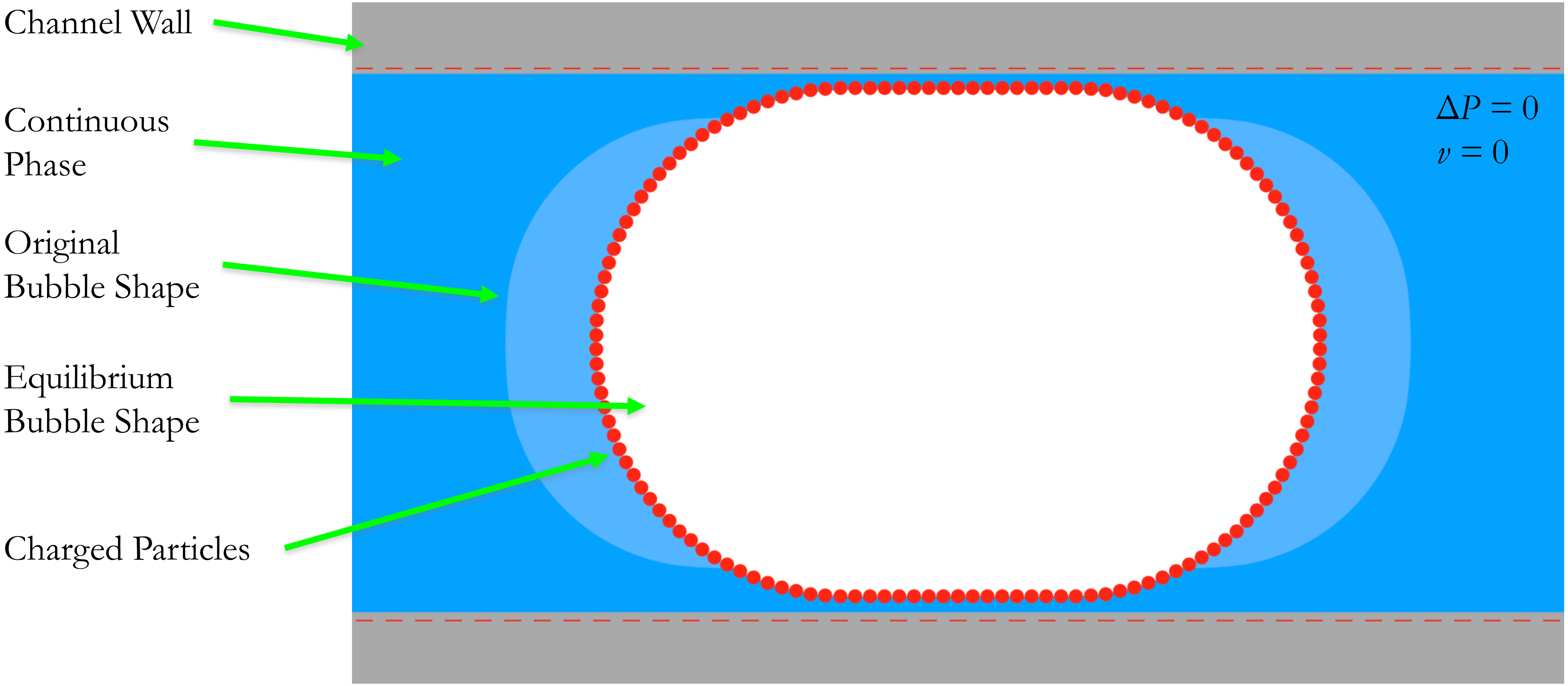
Problem



Problem


Channel Wall
Continuous Phase
Original Bubble Shape
Equilibrium Bubble Shape
$\Delta P = 0$
$v = 0$

Problem



Deformation and Contact Considerations:

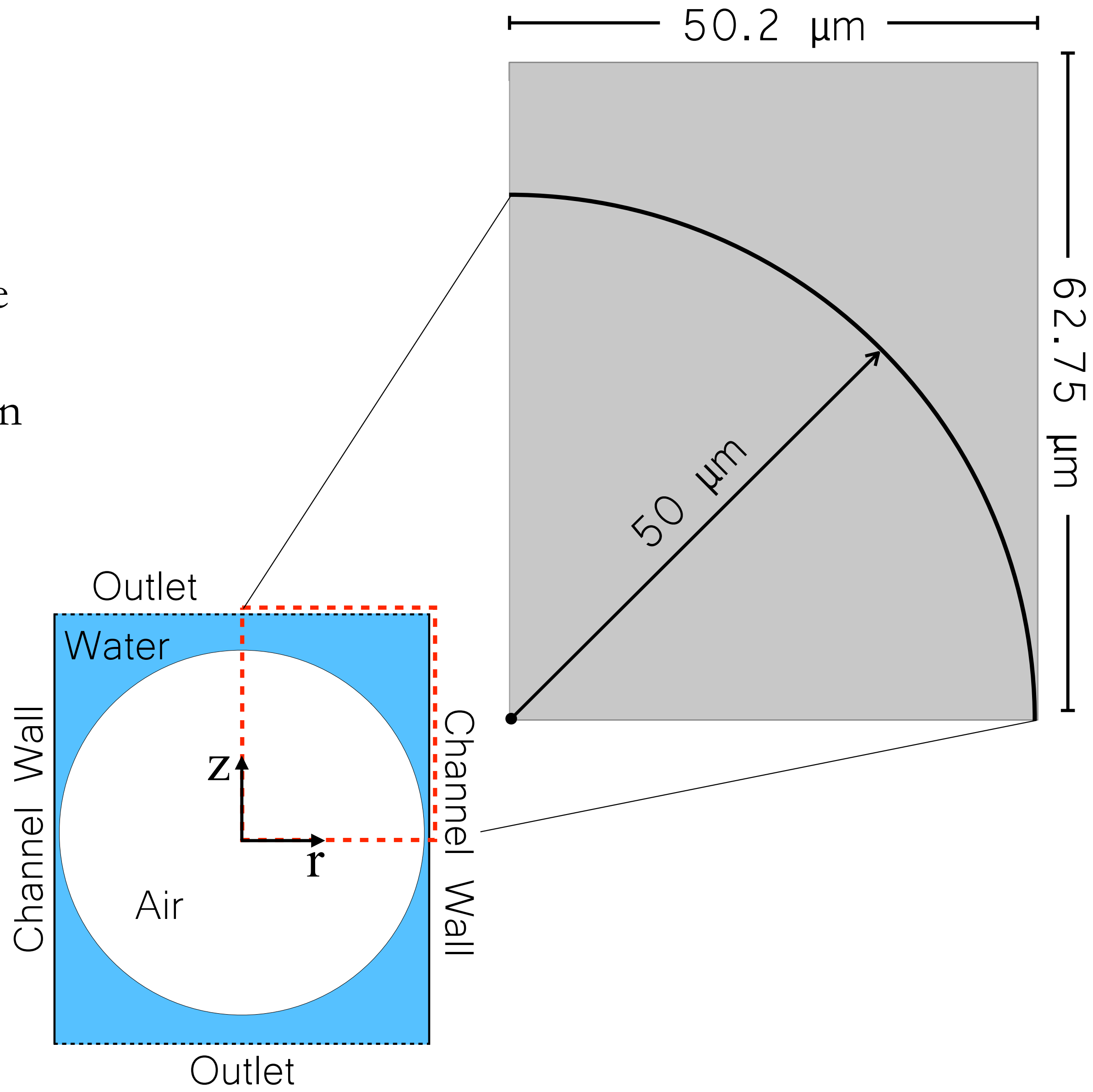
- Surface Tension
- Disjoining Pressure
- Electrostatic Forces

Model – Geometry

Objectives:

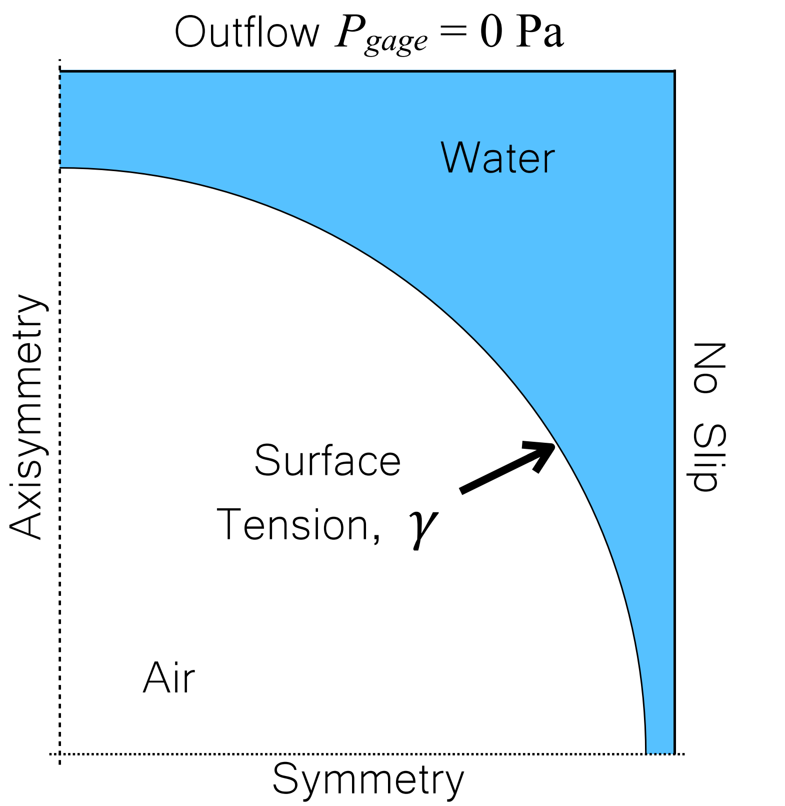
- Find conditions of maximal electrostatic repulsion between bubble interface and channel wall
- Simulate bubble morphology due to electric charge effects from channel wall on spherical bubble interface using the customized weak contribution in COMSOL

- Spherical bubble in microchannel
- 2D axisymmetry & planar symmetry
- Initial bubble radius = 50μm
- Channel radius = 50.2μm
- Half channel height = 62.75μm



Model – Boundary Conditions

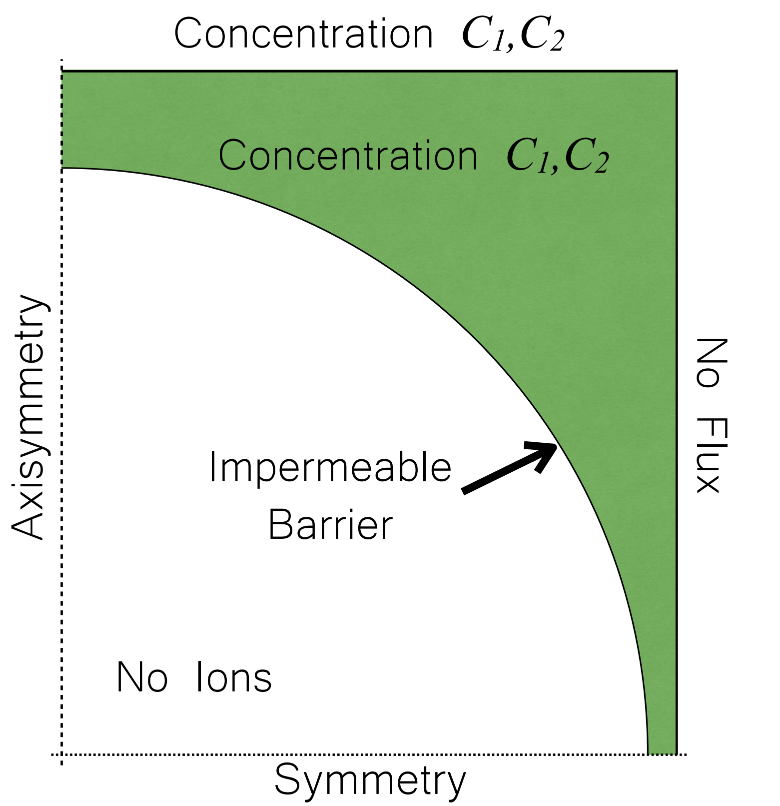
Fluid



$$\rho\nabla \cdot \vec{u} = 0$$

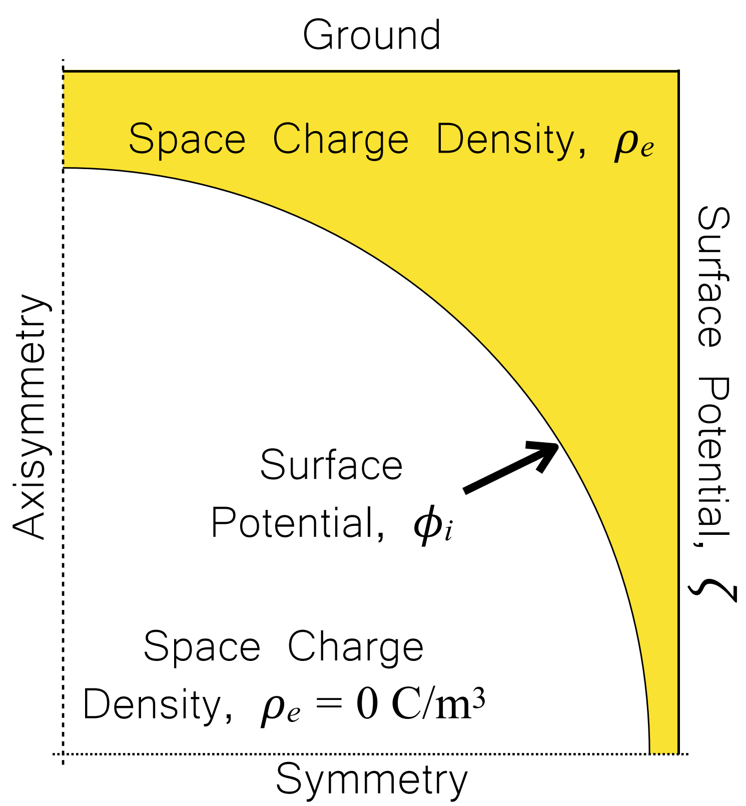
$$\rho\frac{\partial \vec{u}}{\partial t} + \rho(\vec{u}\cdot\nabla)\vec{u} = \nabla\cdot\left[-p\vec{I} + \mu\left(\nabla\vec{u} + (\nabla\vec{u})^T\right)\right] + \vec{F}$$

Transport of Dilute Species



$$\frac{\partial c}{\partial t} + \nabla\cdot(-D\nabla c_j) + \vec{u}\cdot\nabla c_j = R_j$$

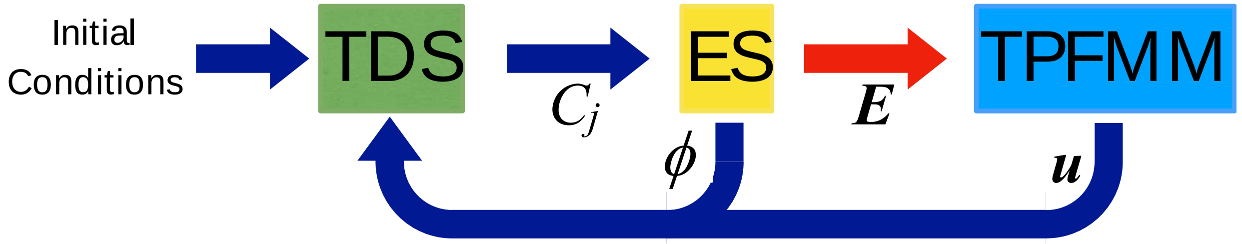
Electrostatic



$$\nabla\cdot\vec{D} = \rho_e$$

Model – Module Implementation & Weak Formulation

- Two Phase Flow Moving Mesh Method (TPFMM) – Multiphase, interfacial tracking
- Transport of Dilute Species module (TDS) – Ion concentration
- Electrostatics module (ES) – Electric field



$$\rho\left[\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\,\vec{u}\right] = \nabla\cdot\bar{\bar{\sigma}}$$

Navier-Stokes Eqn

$$\hat{n}\cdot\left(\bar{\bar{\sigma}}_A - \bar{\bar{\sigma}}_B\right) = \Gamma\gamma\hat{n} - \nabla_s\gamma - \rho_s\nabla\phi$$

Boundary Condition at Fluid-Fluid Interface

Total Stress
With unit normal from gas B to liquid A

Surface Tension

Electrostatics

Weak Form

$$\int_\Omega \rho\left[\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\,\vec{u}\right]\cdot\vec{v}\,d\Omega = -\int_\Omega \nabla\vec{v} : \bar{\bar{\sigma}}\,d\Omega + \int_S \gamma\left(\nabla_s\cdot\vec{v}\right)\,dS - \int_S \vec{v}\cdot\rho_s\nabla\phi\,dS.$$

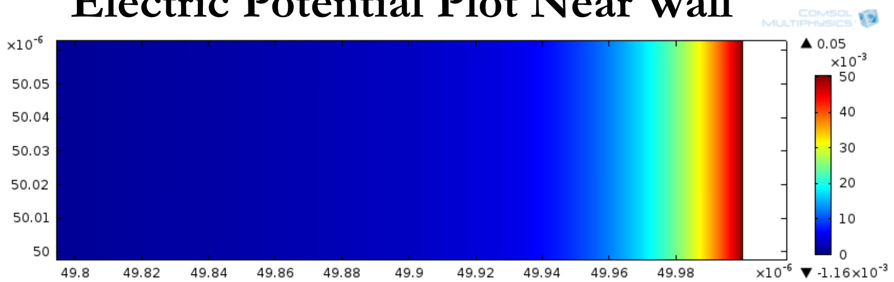
Time Deriv | Advection | Diffusion | Surface Tension BC | Electrostatic BC

Implemented as
Weak Contribution for **E**

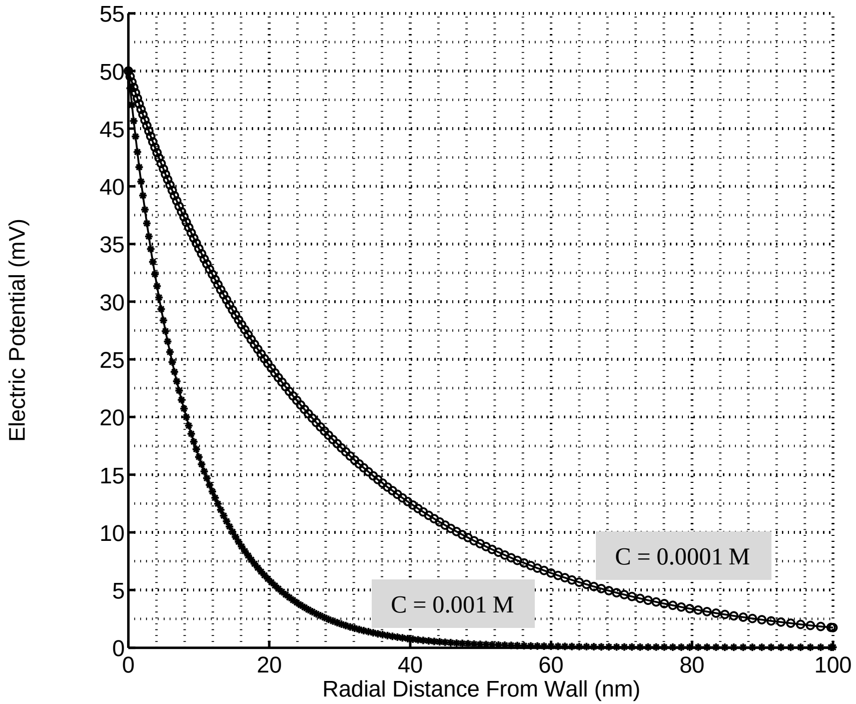
Results – Electric Double Layer

Verify COMSOL Capability for Steady State EDL Profile

Electric Potential Plot Near Wall



Electric Potential Profile Away from Wall



Numerical Debye Length

$$\psi(x) = \zeta e^{-x/\lambda}$$ (Boltzmann distribution)

$$\ln\psi = -\frac{1}{\lambda}x + \ln\zeta$$

Theoretical Debye Length

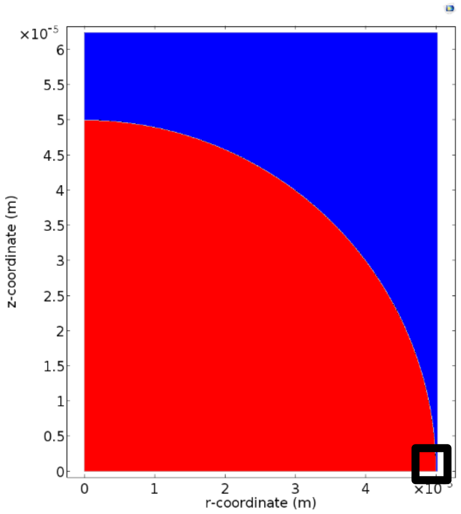
$$\lambda = \left(\frac{F^2}{\epsilon\epsilon_0 RT}\sum_i z_i^2 C_{i,b}\right)^{-1/2}$$ (Debye-Huckel approximation)

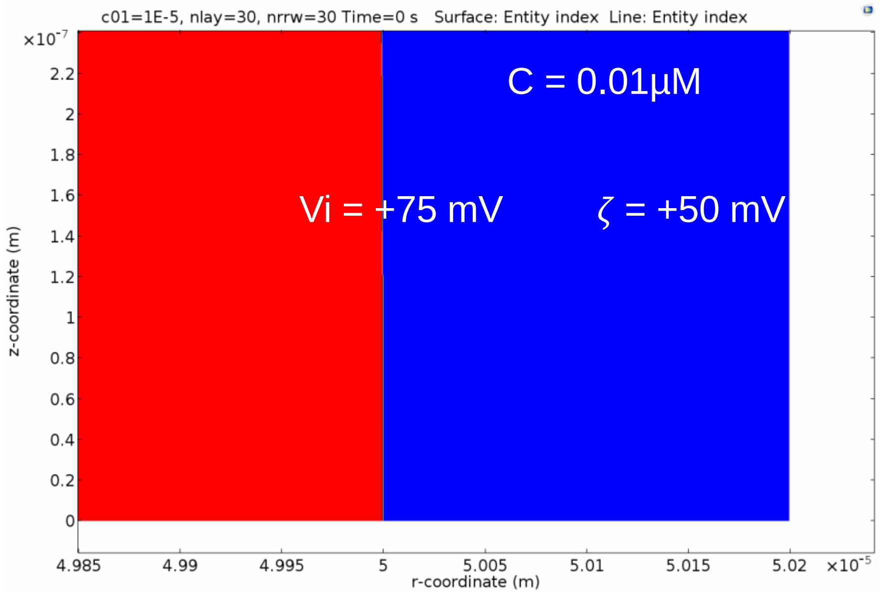
$$\lambda = \left(\frac{2C_b F^2}{\epsilon\epsilon_0 RT}\right)^{-1/2}$$ (Univalent-Univalent, Symmetric Electrolyte)

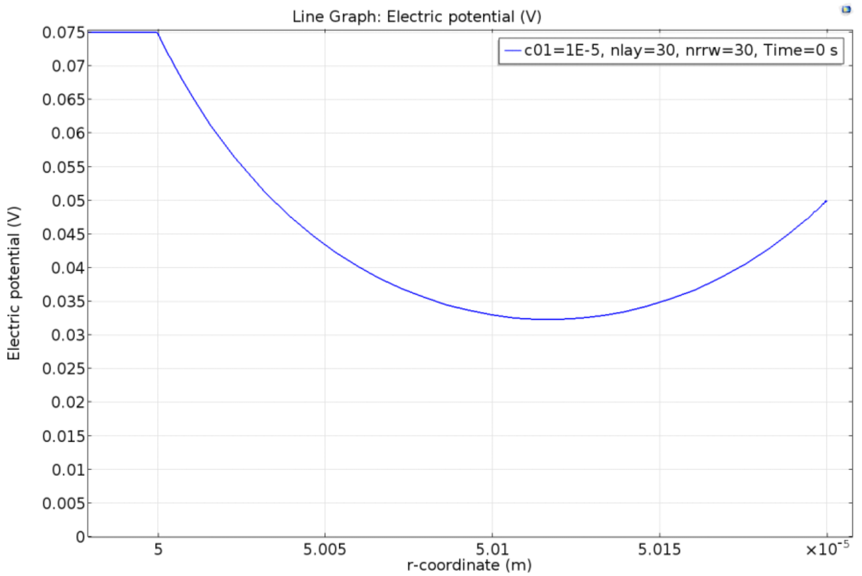
C (M)	λ_{nm} (nm)	λ_{th} (nm)	$\frac{\lambda_{th}-\lambda_{nm}}{\lambda_{th}} \cdot 100$
0.001	9.60	9.63	0.3
0.0001	29.9	30.4	1.6

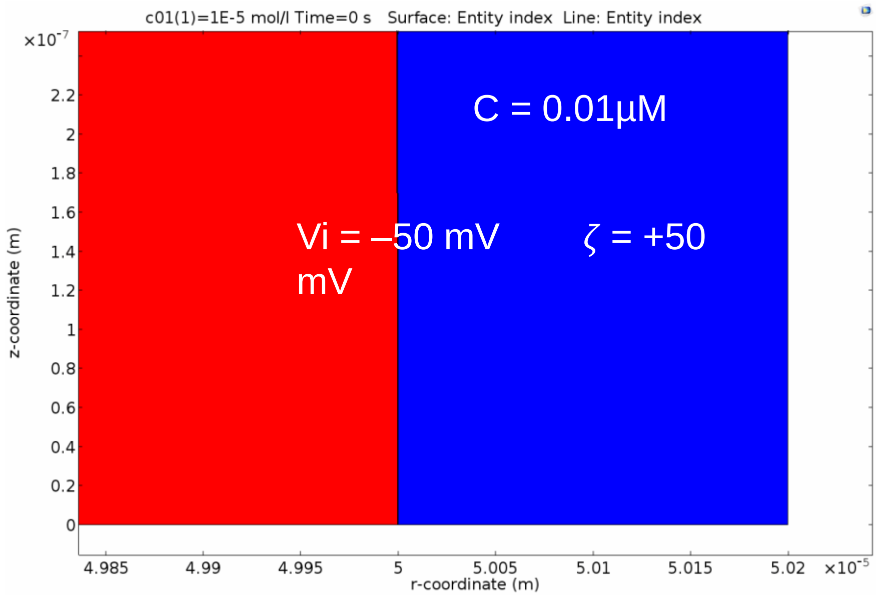
Strong Theoretical & Numerical Agreement

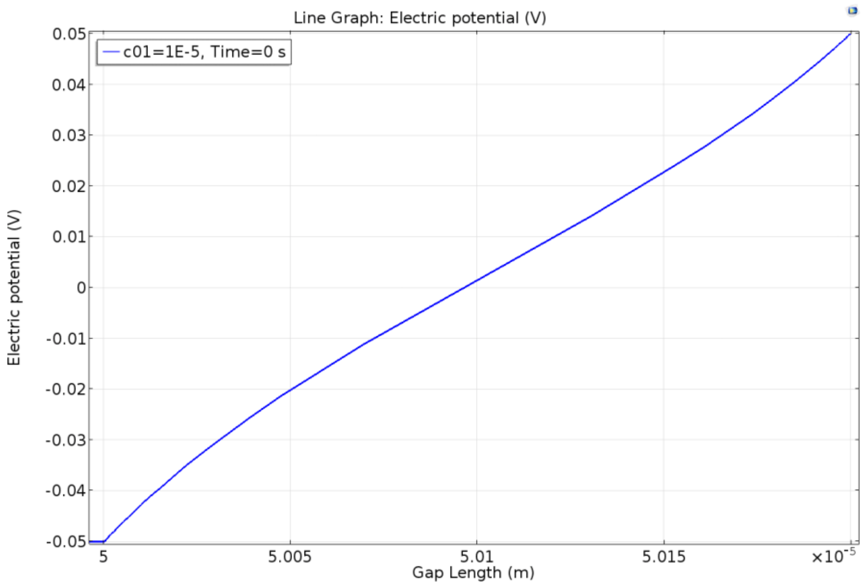
Results – Repulsion/Attraction







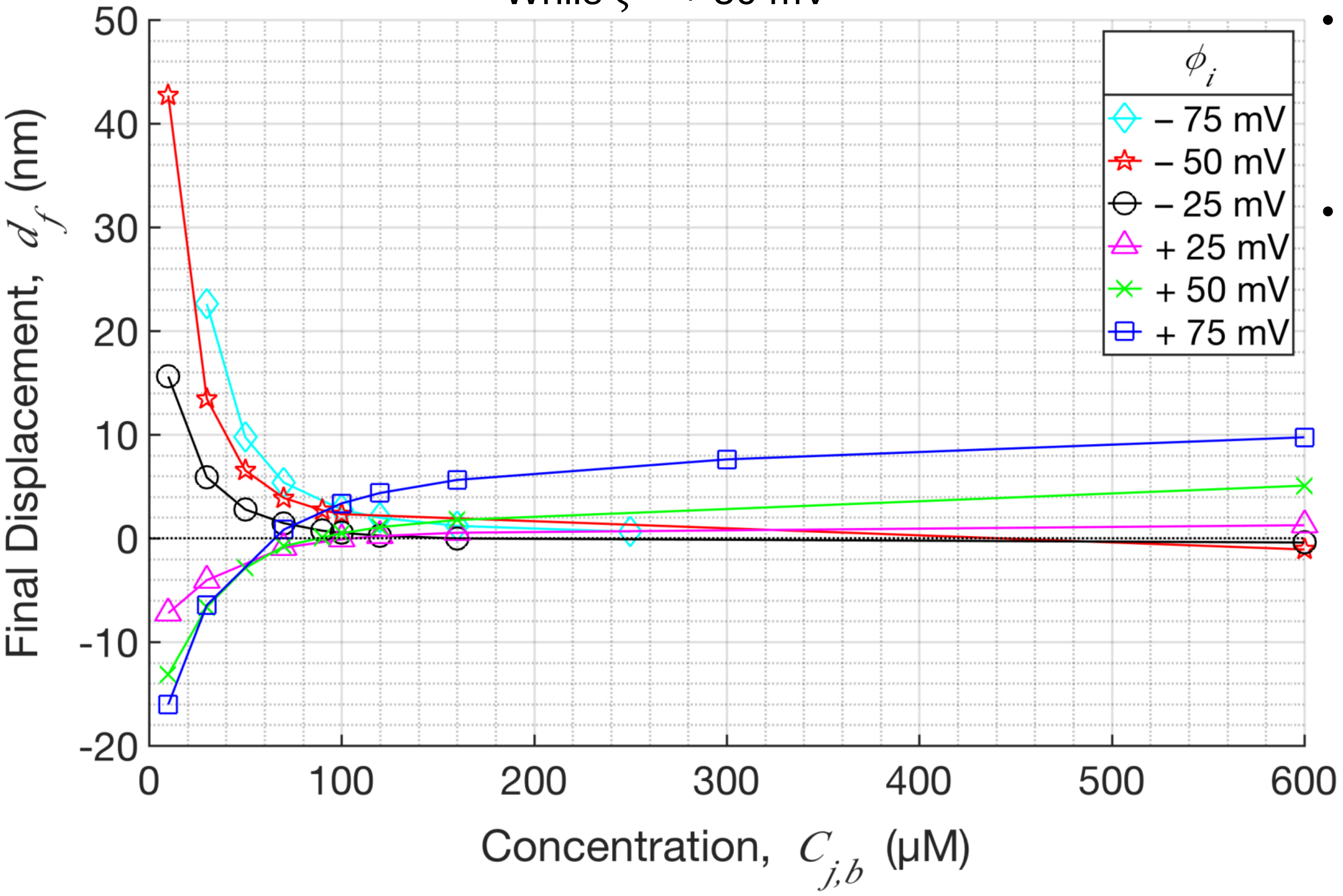




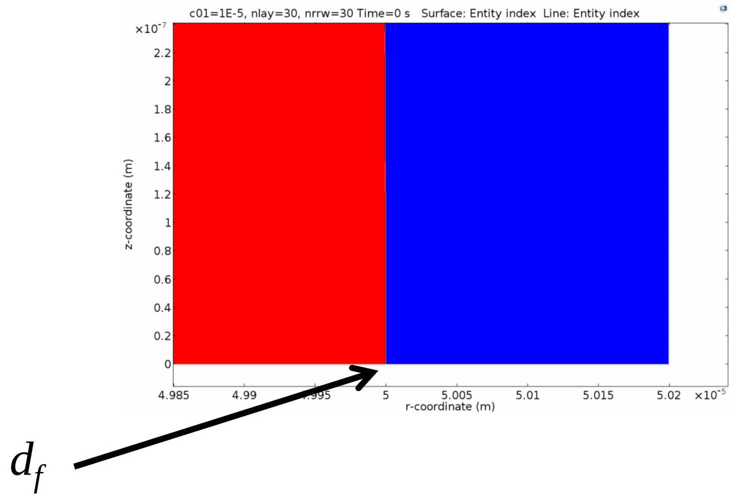
- Repulsive behavior with like electric potential
- Attractive behavior with unlike electric potential
- Double layer overlapped and updated through time

Results –Attraction/Repulsion

Final Displacement vs. Concentration at Various Interfacial Potential
While ζ = + 50 mV

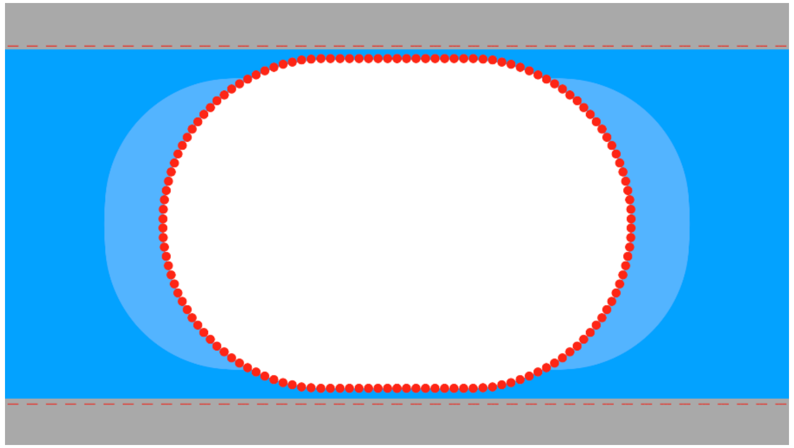


- Unlike Potential
  - Attractive behavior for low concentration
  - Neutral behavior for high concentration
- **Like Potential**
  - **Repulsive behavior for low concentration**
  - Attractive behavior for high concentration



Conclusion

- Developed a customized model to couple electrostatic influence on bubble interfacial morphology
- Quantify repulsive and attractive interactions between charged bubble interface and charged channel wall
- Key parameters: Electric potential and ion concentration for a given geometry
- Below certain ionic concentration threshold, larger electric potentials of like polarity maintain thicker lubrication layers
- Ability to create repulsive environments indicates strong possibilities for precluding bubble contact



Acknowledgements:

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