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Multiscale Multiphysics Model of CRUD Transport and Deposition in Pressurized Water Reactors: Formulation and Preliminary Results Examining the Effect of Surface Potentials

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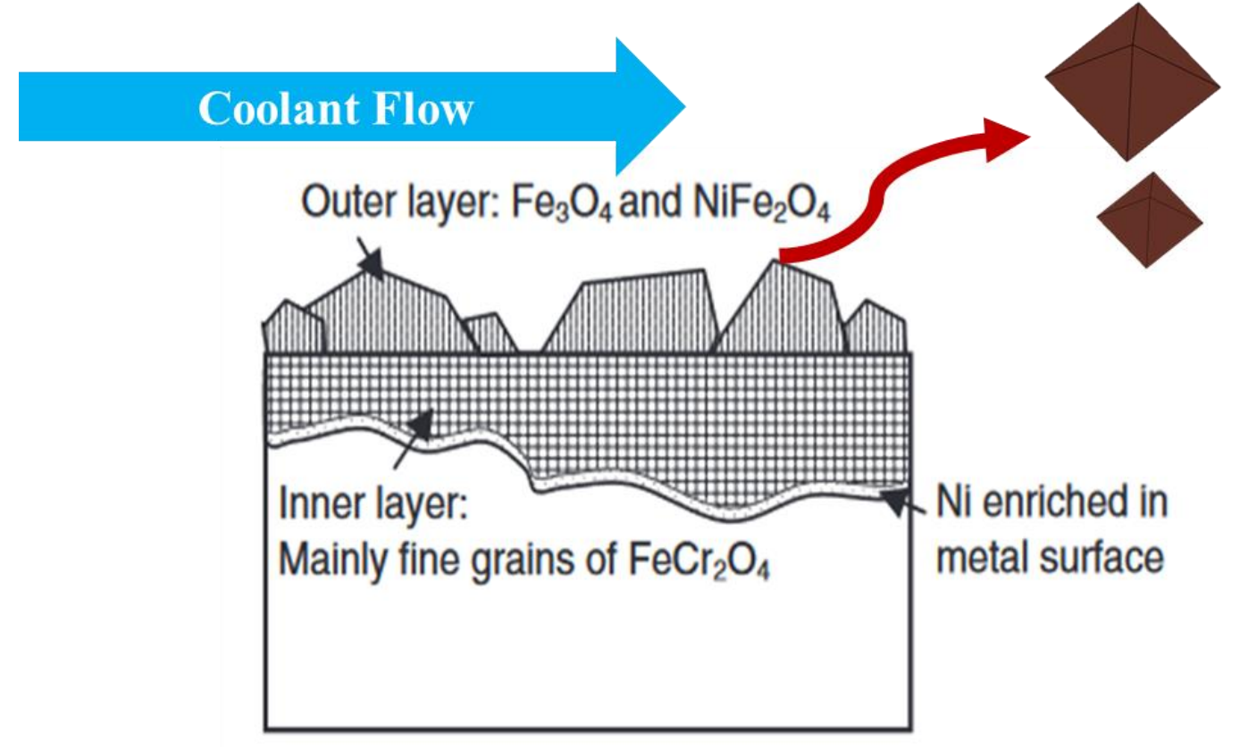
Naval Nuclear Laboratory

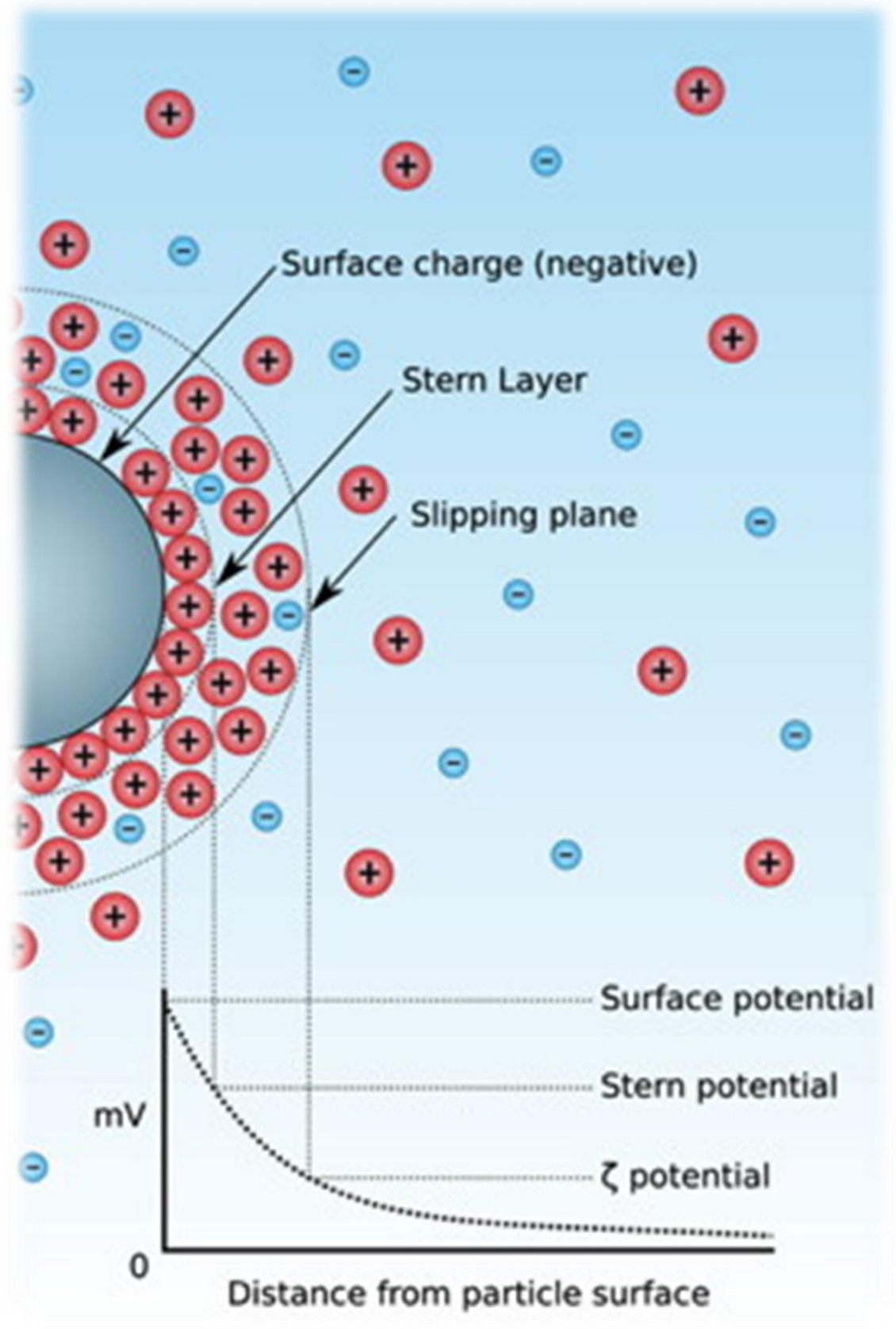
Motivation

Fouling caused by Corrosion products (CRUD) in PWR affect the operational performance of the Reactor (CRUD-induced power shifts, CRUD-induced localized corrosion, etc.,)

Goal: To develop a model in COMSOL™ that simulates the deposition of suspended particles inside a pipe representing a reactor environment



Transport and Deposition of CRUD



Thermodynamics

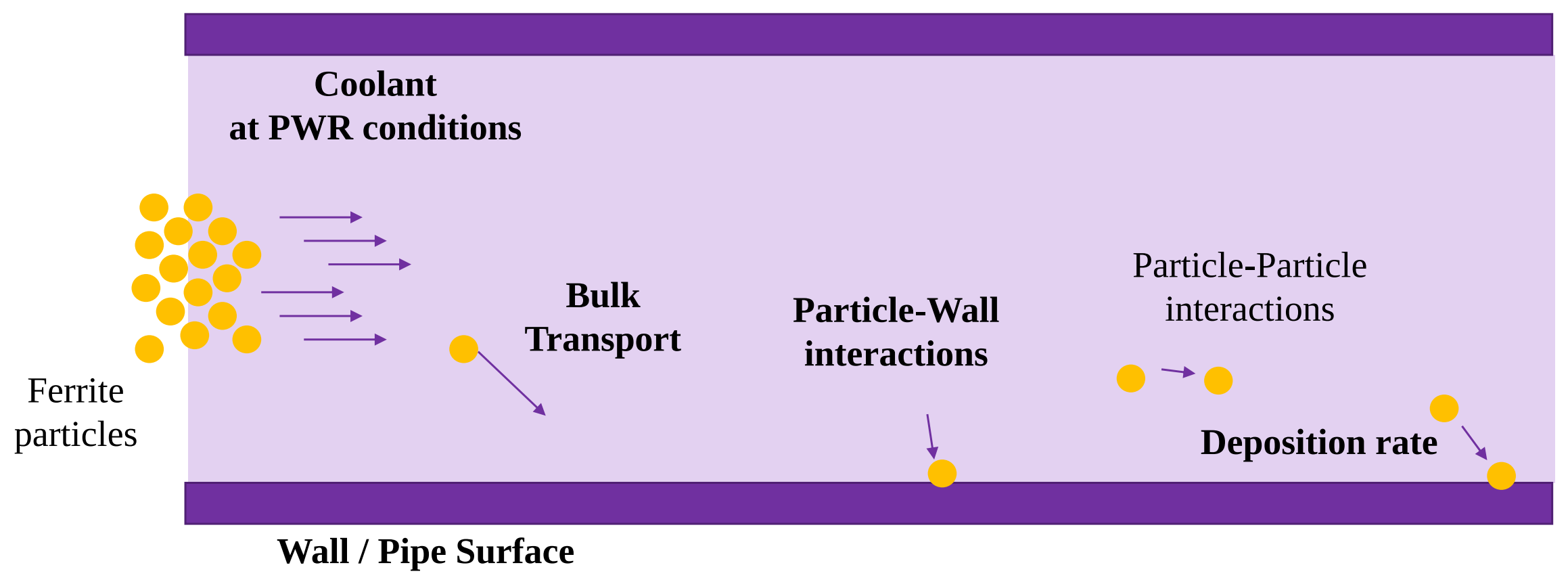
Will particles deposit on the wall?

- Colloidal forces
  - Dipole interactions: van der Waal's (VDW) force
  - Electric double-layer (EDL) interactions
- Highly sensitive to surface properties such as Stern potential

Kinetics

At what rate do particles approach the wall?

- Bulk transport of particles due to turbulence and convective transport in the coolant
- Fluid flow solved with k-ω turbulence model taken for the Stokes' drag force calculations



COMSOL Modules

- Computational Fluid Dynamics
- Particle Tracing Module

Multiscale Multiphysics Model Formulation

Time scales of events

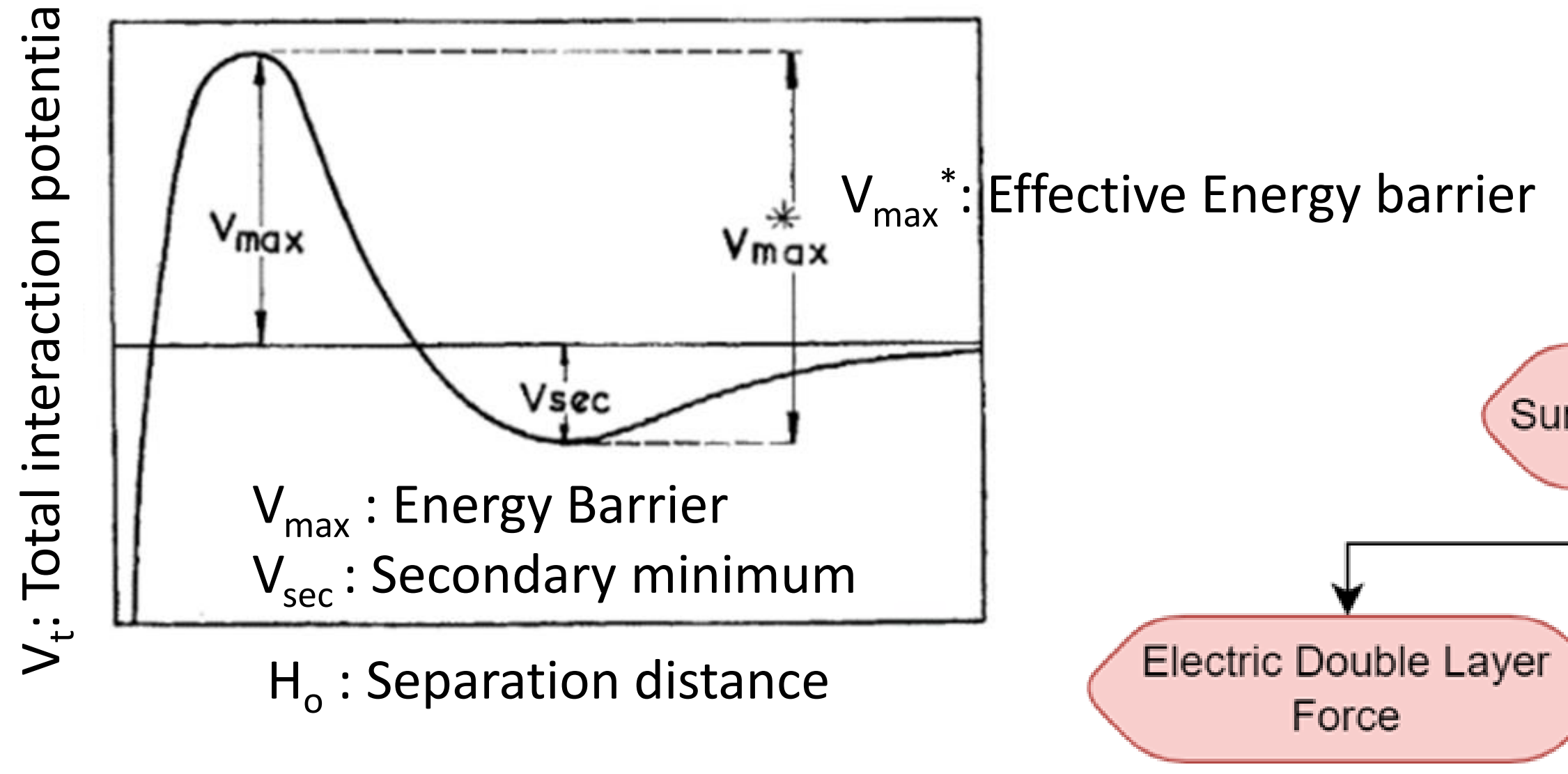
- Kolmogorov length and time scales for turbulence
- Range of EDL forces

$$\eta \equiv \left(\frac{\vartheta^3}{\varepsilon}\right)^{1/4}$$

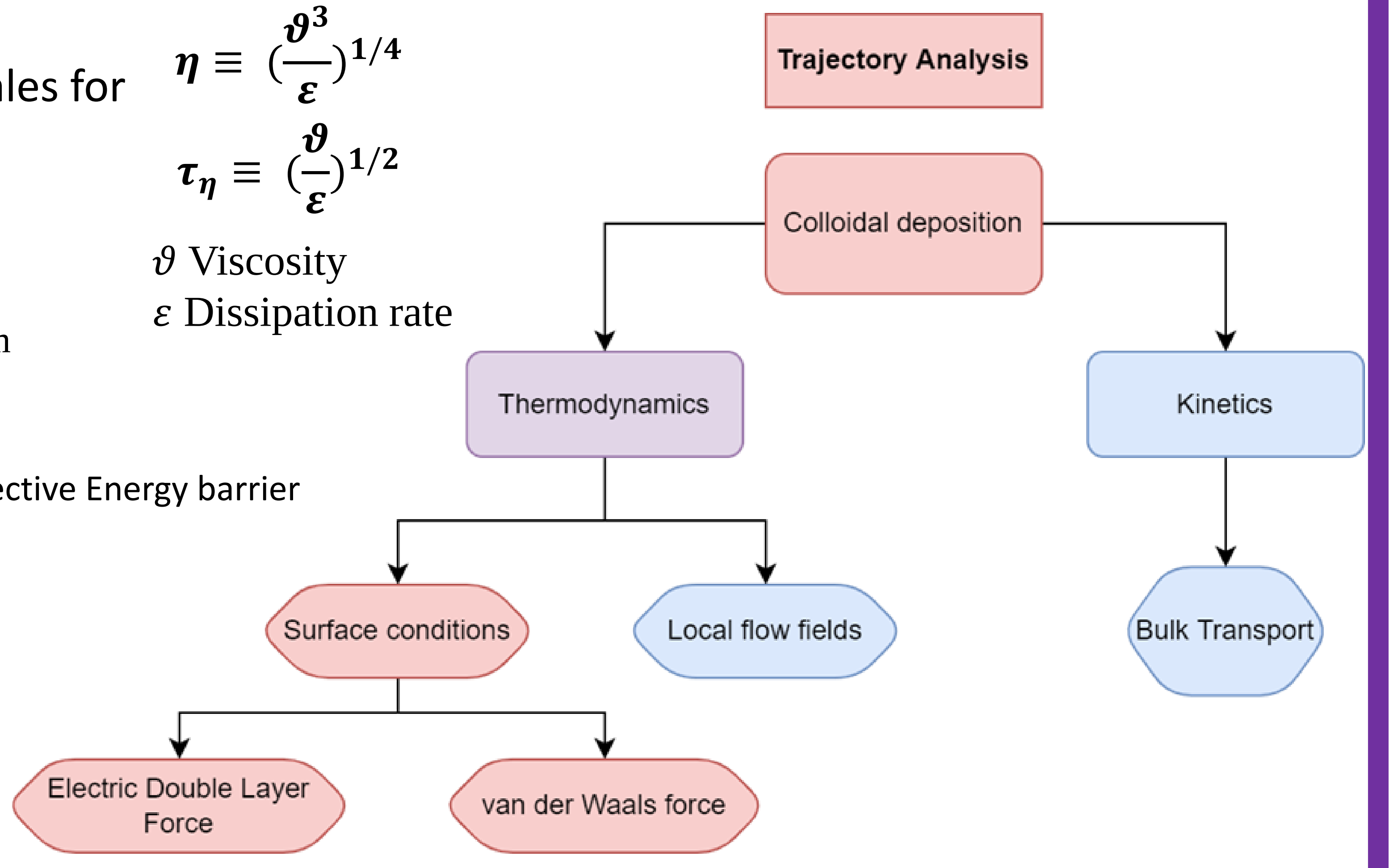
$$\tau_\eta \equiv \left(\frac{\vartheta}{\varepsilon}\right)^{1/2}$$

ϑ Viscosity
ε Dissipation rate

L ≡ 1/k(inverse Debye length) ~ 5-10 nm



$V_{max}{}^*$: Effective Energy barrier
V_{max} : Energy Barrier
V_{sec} : Secondary minimum
H_o : Separation distance



Critical velocity: minimum (radial) velocity for a particle to overcome barrier to deposit on the wall

Coolant (Water) Parameters	
Density	660 kg/m^3
Viscosity	1.01 x10^{-4} Pa.s
Temperature	598.15 K
Inlet velocity (average)	13.5 m/s
Outlet pressure	15.5 MPa
Length and radius of pipe geometry	10 m, 0.3685 m
Nickel ferrite particles	
Particle diameter	1 µm

- Critical velocity as a function of Stern potential

- Deposition rate
- Deposition velocity

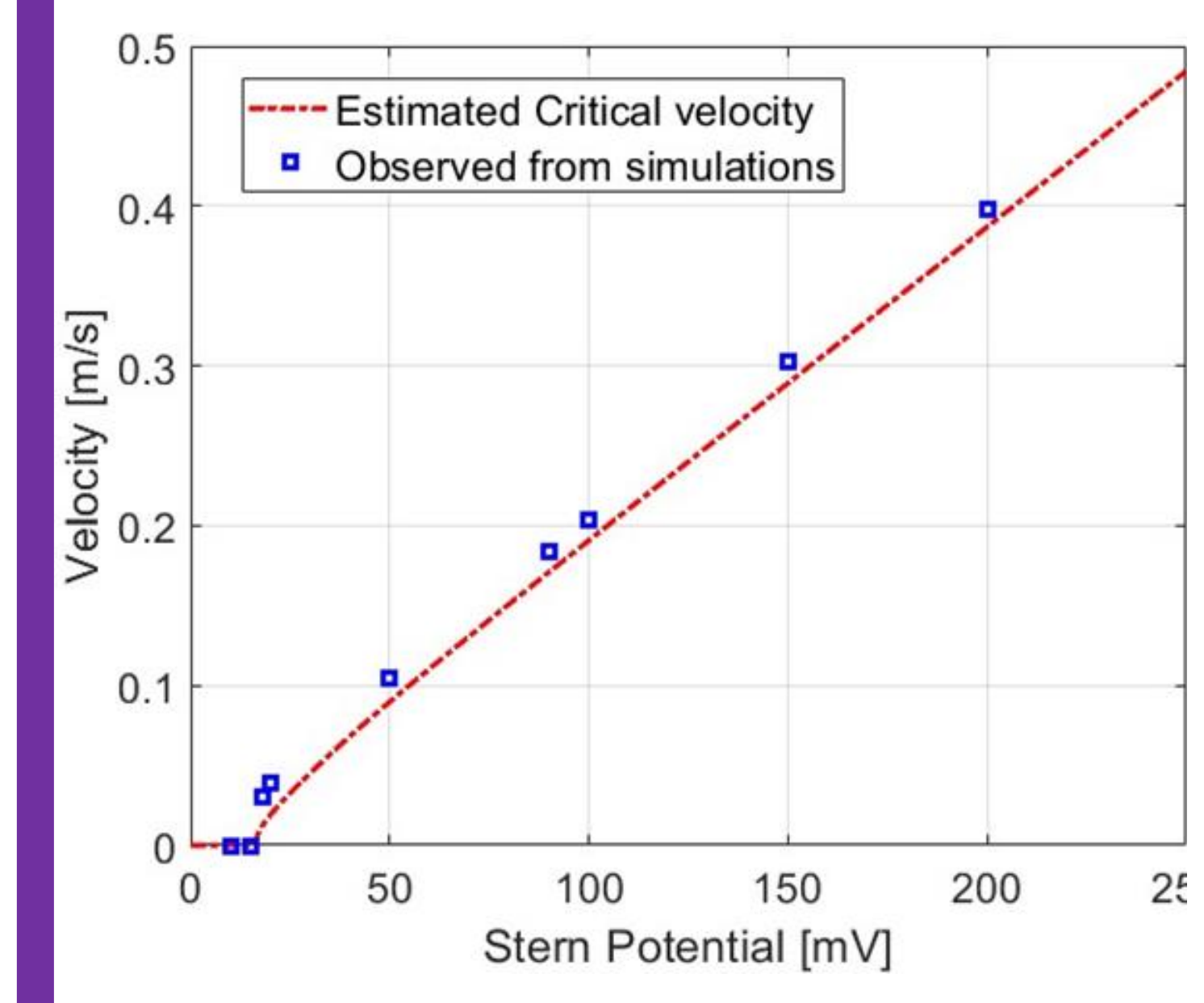
Sequential multiscale model

- Couples the thermodynamic details to the kinetic data
- Enables study of the influence of Stern potential on deposition probability

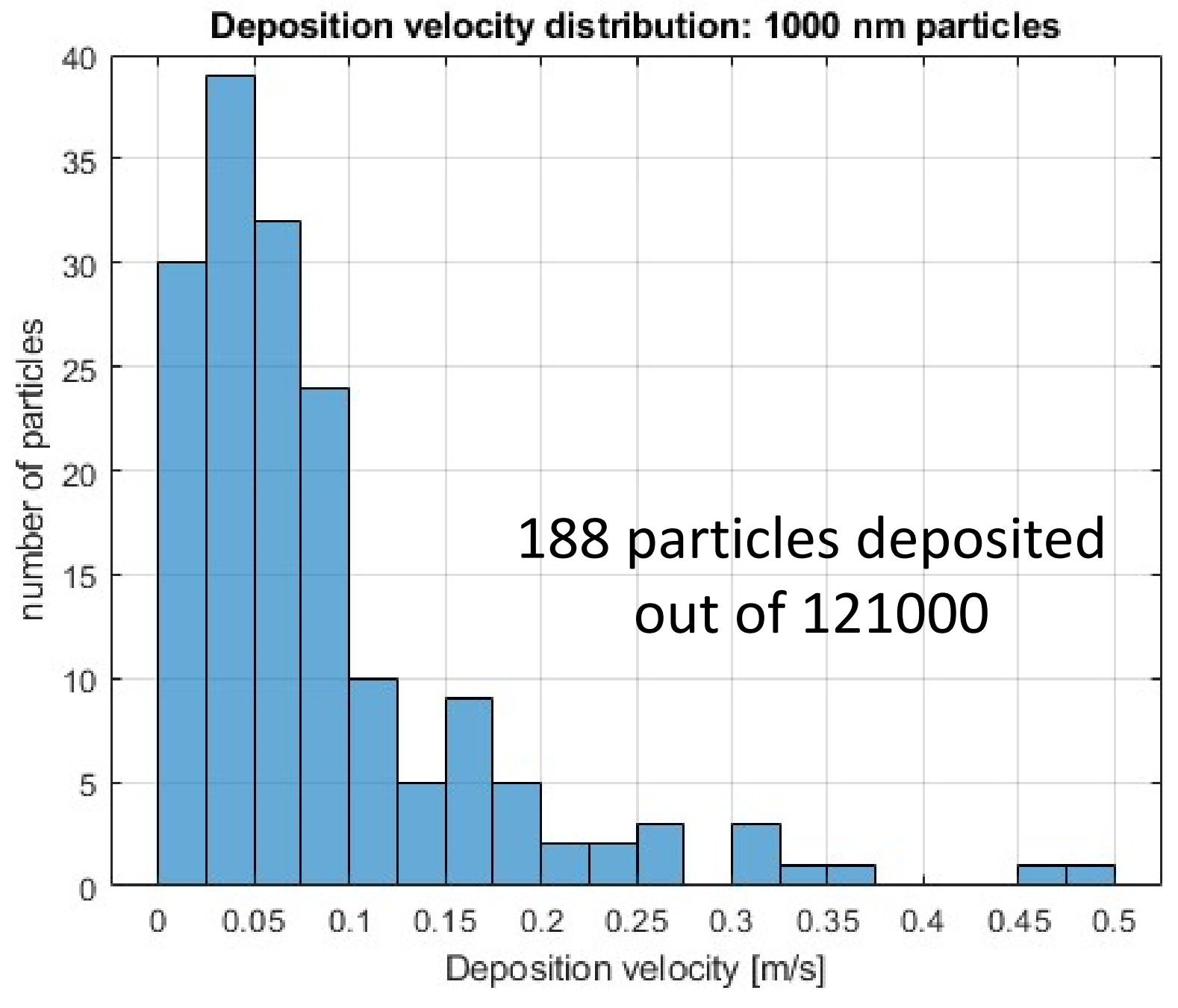
Preliminary Results: Sensitivity Analysis

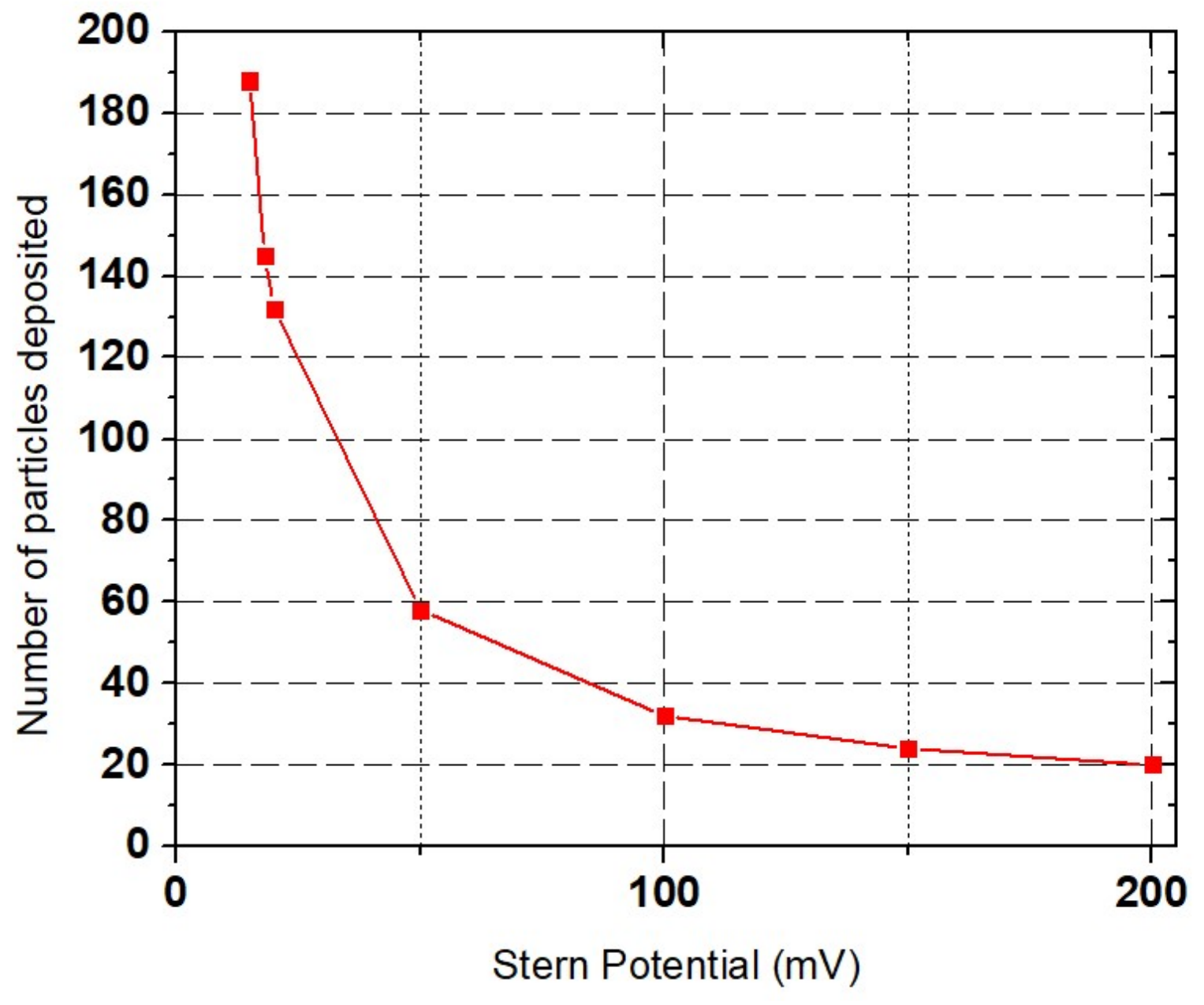
- Simulations were performed to understand the effect of the Stern potential on deposition
- Fine-scale simulations show a linear trend between critical velocity and the Stern potential, in agreement with the values estimated through DLVO alone (by extrapolating the potential barrier from DLVO to be kinetic energy required to deposit)
- Macroscale simulations provide the velocity distribution of deposited particles

Coupled results shows that deposition is sensitive to the Stern potential



Deposition velocity distribution: 1000 nm particles





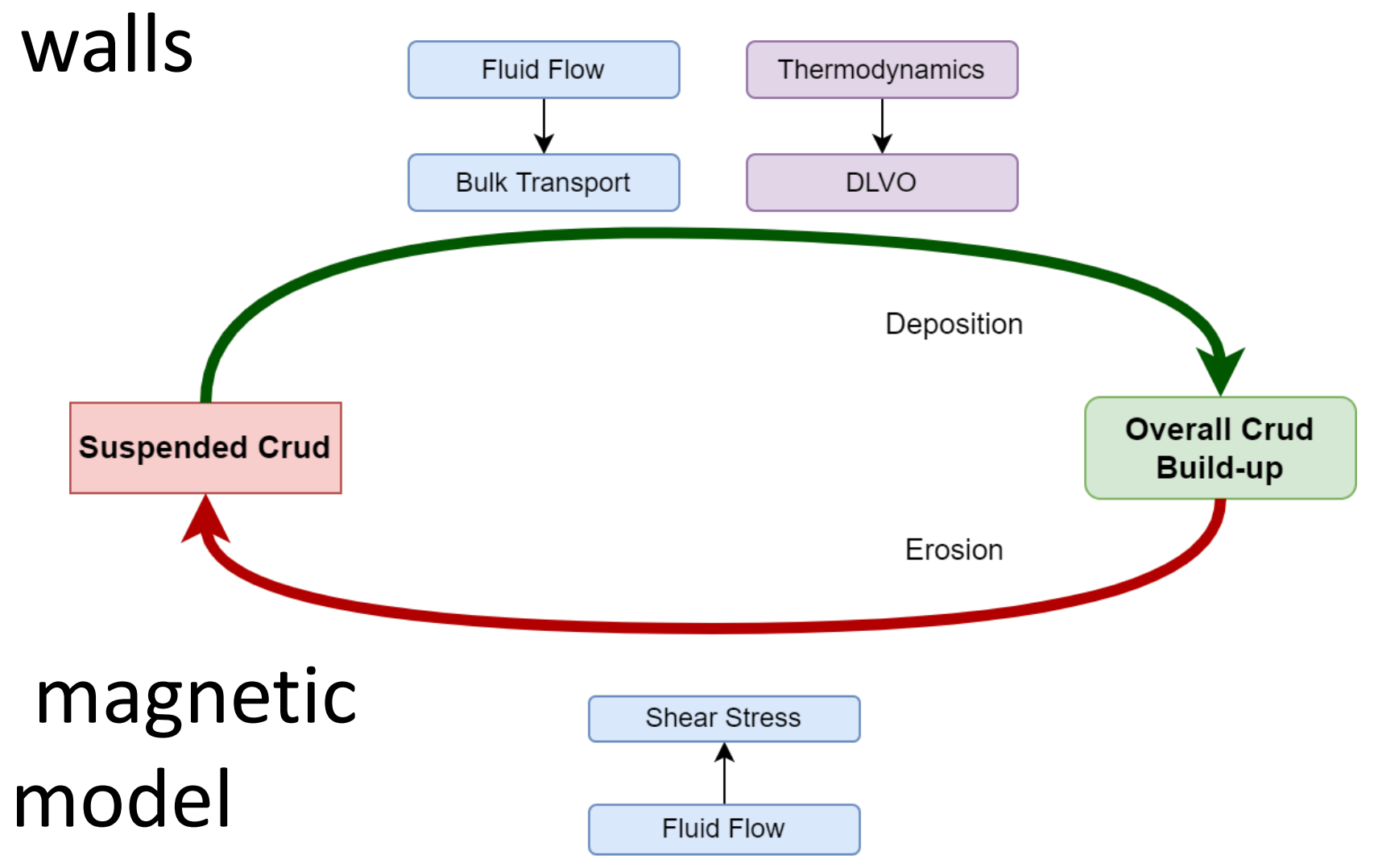
The coolant pH which would determine the Stern potential and affect the deposition significantly.

Summary

- Formulated a Multiscale Model for the deposition of CRUD in primary coolant circuit.
- Quantitative and qualitative verification for fine-scale model: obtained values and trends match with DLVO theory predictions
- Preliminary investigations confirmed deposition is highly sensitive to Stern potential of particle, which is pH-dependent

Future Work

- Investigate the effect of particle size on the deposition (drag forces, surface charge)
- Incorporate possible re-entrainment of particles from the walls
- Include magnetic forces in model



Acknowledgments

This material is based upon work supported by the U.S. Nuclear Regulatory Commission, Office of Nuclear Regulatory Research under Award Number 31310020M0006, with additional support from the New York State Center of Excellence in Nanoelectronics and Nanotechnology (NYS CENN).

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