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NEMD in Tribology
Methods and Applications

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UK FLUIDS NETWORK

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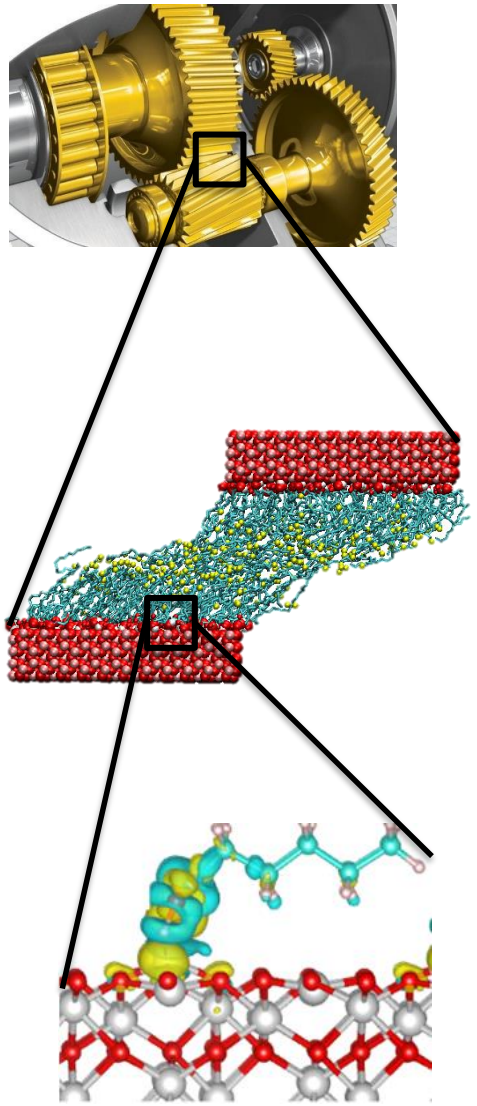
Topics

1. Modelling in tribology
2. NEMD of OFMs
3. NEMD of EHL
4. NEMD SIG – links to industry
5. Conclusions & next steps



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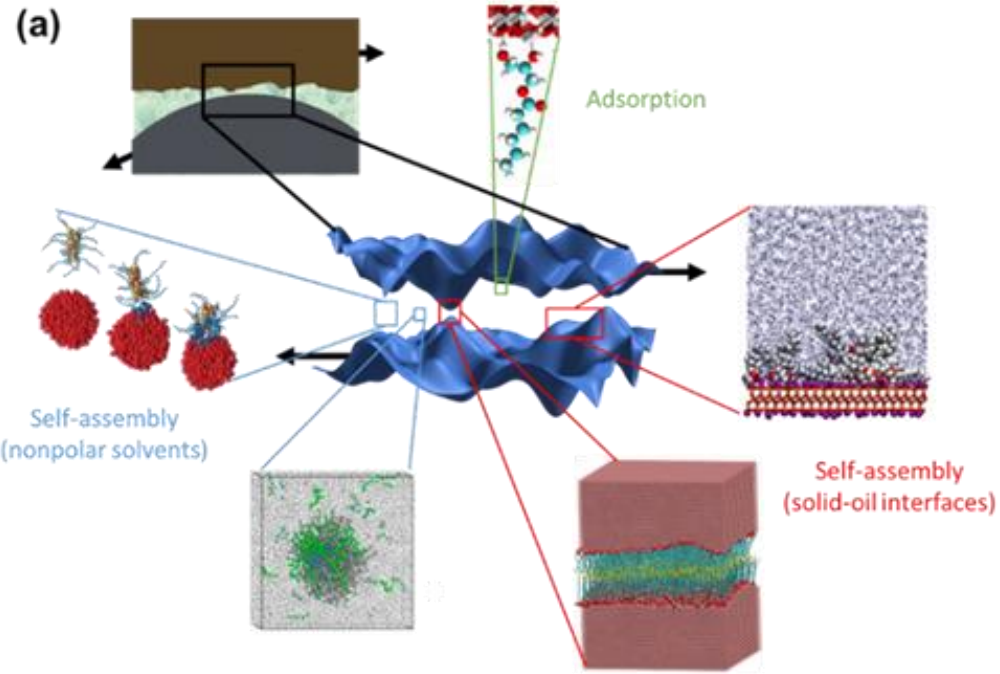
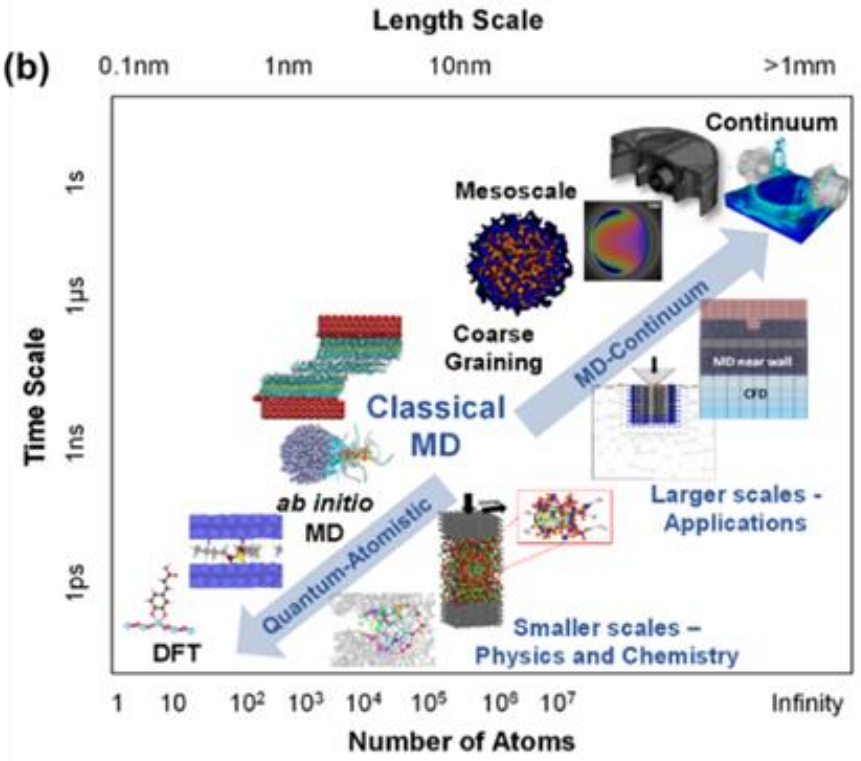
1. Modelling in Tribology





Ewen et al. **Friction.** 6, 349-386, 2018

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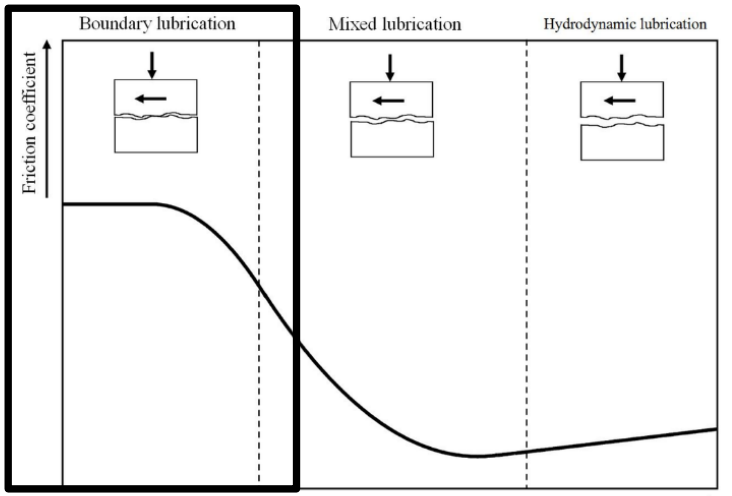
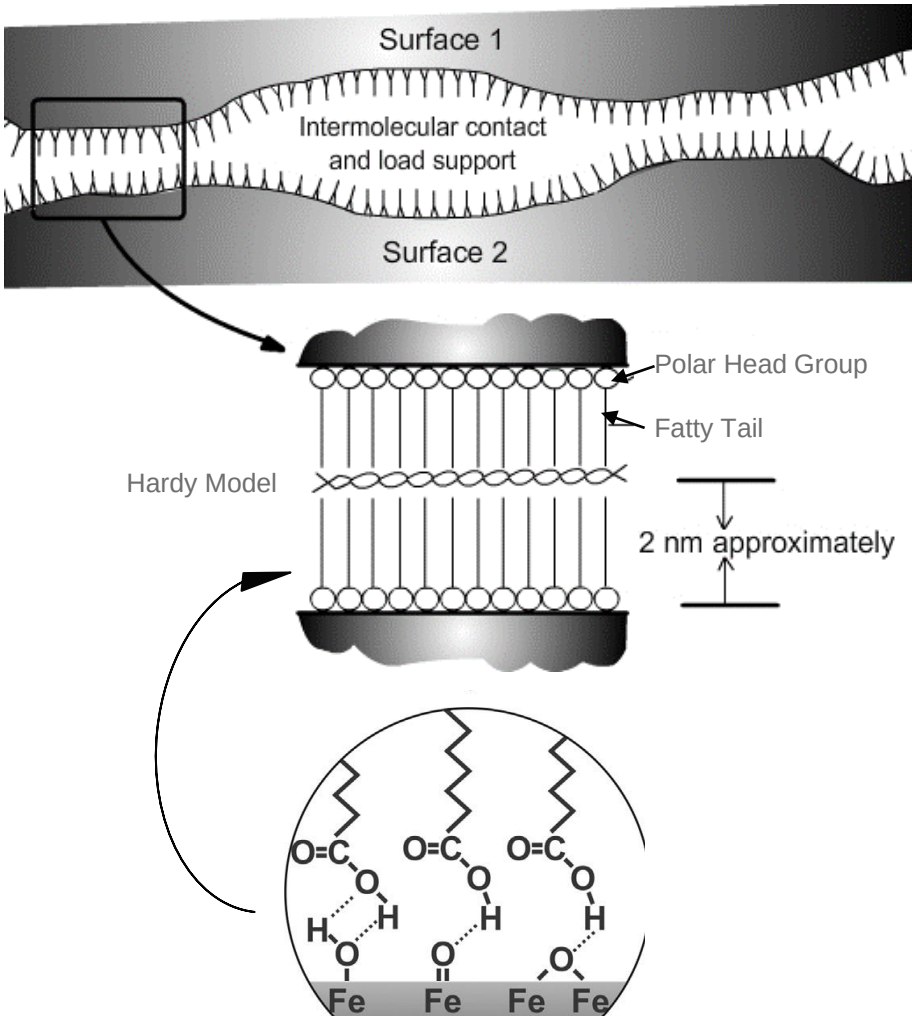
2. Organic Friction Modifiers (OFMs)



Generalised Stribeck Curve



- Boundary lubrication (low *v* / low η / high P) → **high friction and wear**
- OFM polar head groups adsorb onto surface
- Form monolayer – interchain Van Der Waals forces between tail groups
- Incompressible and prevents solid-solid contact → **reduces friction and wear**

Campen and Spikes, **Tribol. Lett.** 48, 237, 2012

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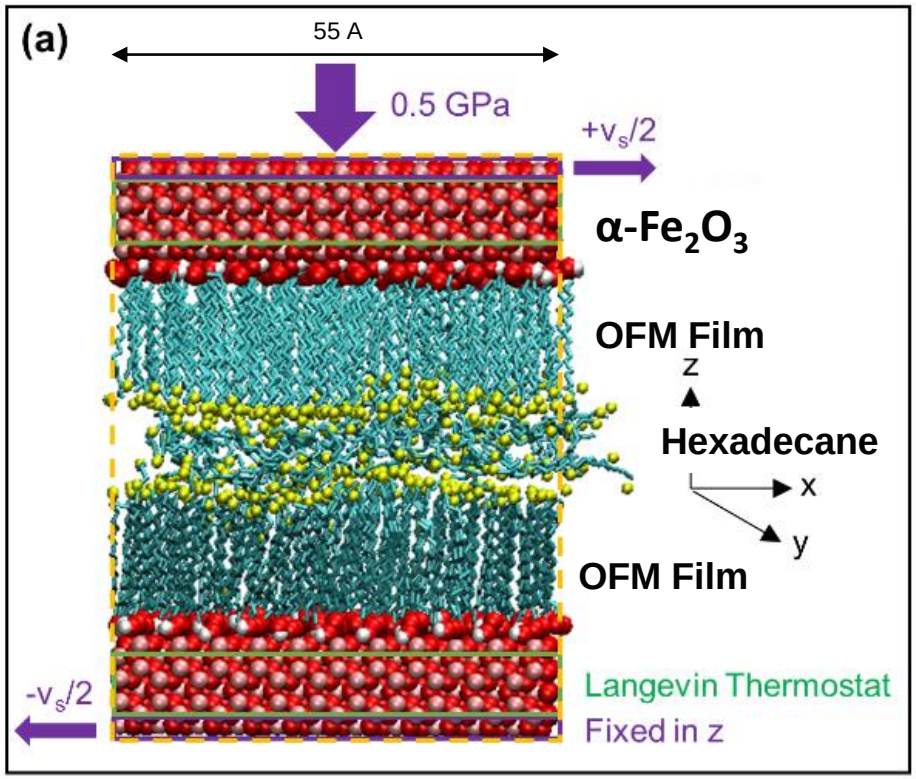
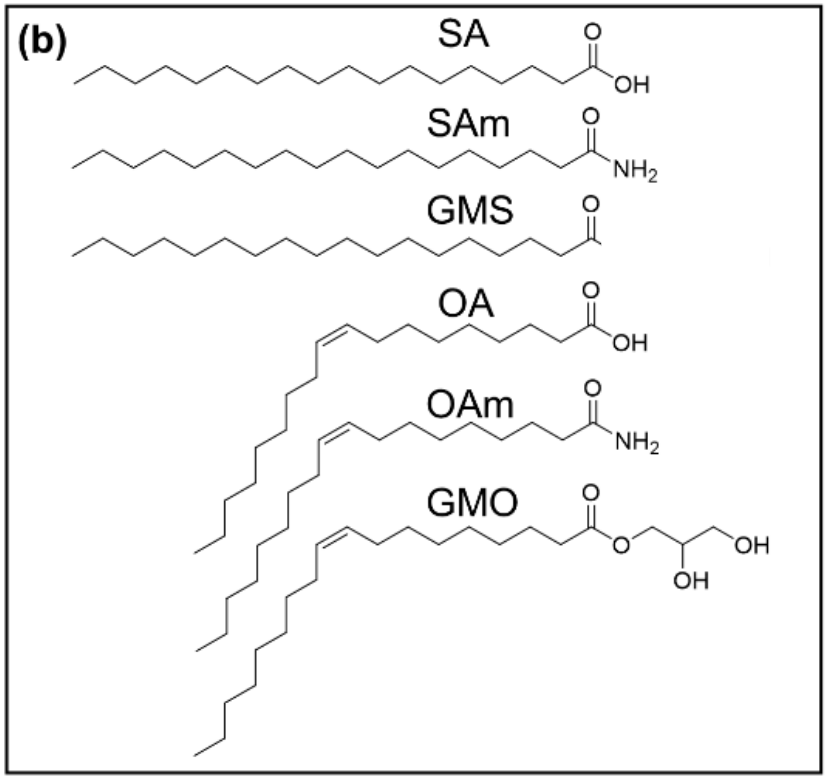
2. NEMD of OFMs





(a) NEMD system set up, (b) OFM molecules simulated

- Three OFM coverages: 1.44, 2.88, 4.32 nm^{-2} (theoretical max = 4.55 nm^{-2})
- Stearic/oleic acid, stearamide/oleamide, glycerol mono-stearate/oleate
- T = 300 K, P = 0.5 GPa, v_s = 1-20 m s^{-1}

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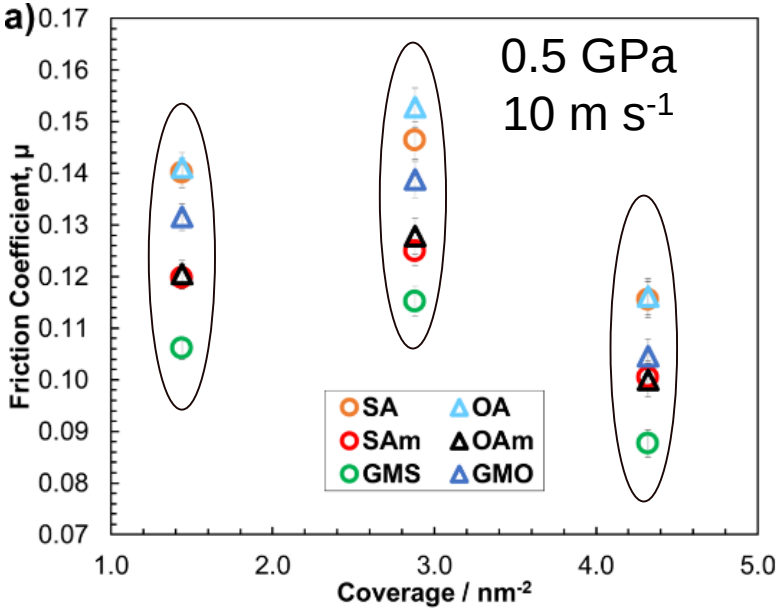
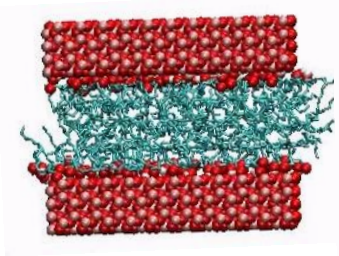
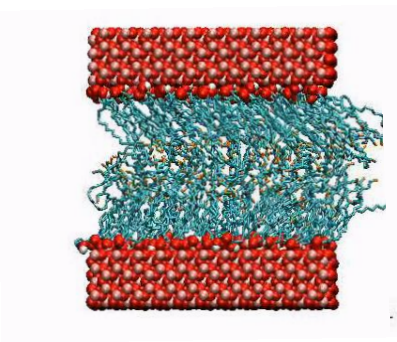
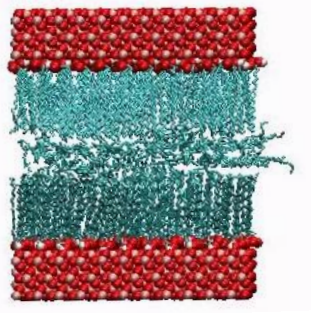
2. Effect of Surface Coverage



1.44 nm^{-2} 2.88 nm^{-2} 4.32 nm^{-2}







‘Liquid-like’ ‘Amorphous’ ‘Solid-like’

- Low coverage: **intermediate friction** → most interdigitation but molecular rearrangement relatively fast
- Medium coverage = **high friction** → interdigitation high, molecular rearrangement slow
- High coverage = **low friction** → very low interdigitation, slip between layers

Ewen et al. **Langmuir.** 32, 4450-4463, 2016

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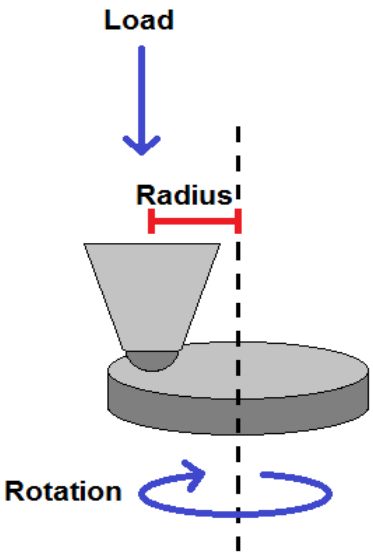
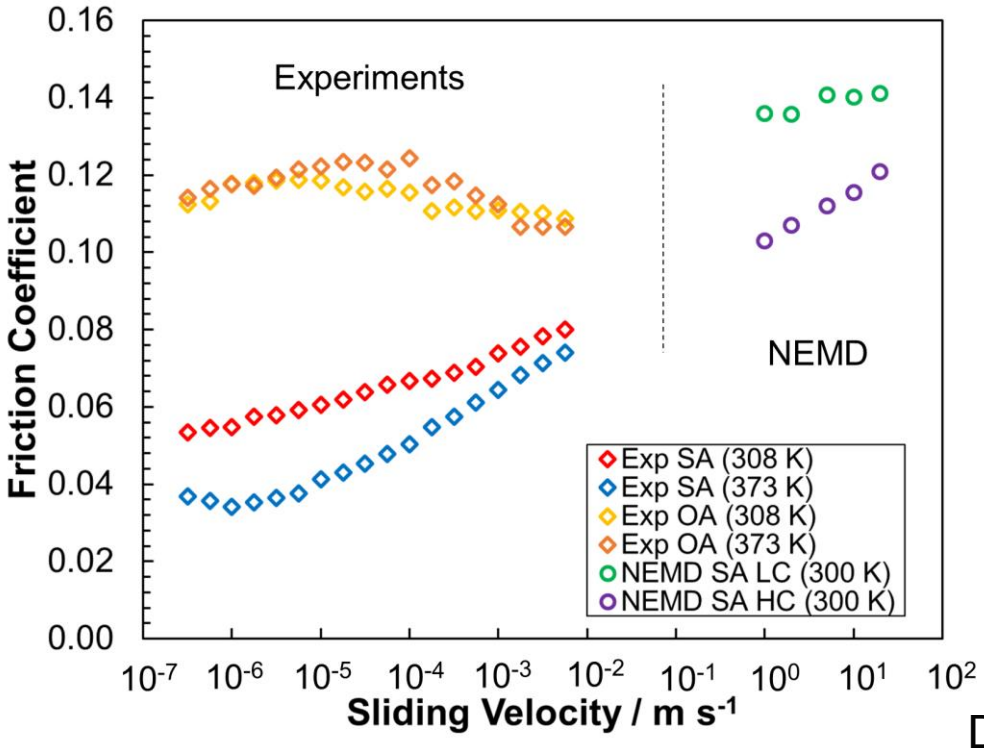
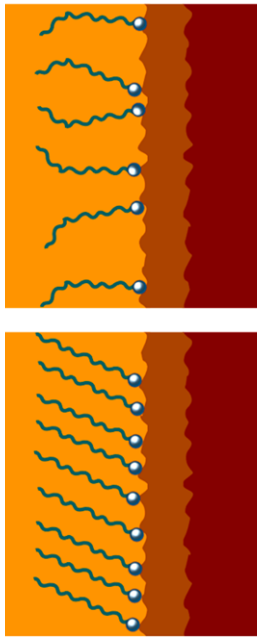
2. Links with Experiments



CETR UMT-2
P = 0.69 GPa





OA
≈1 nm^{-2}

SA
≈4 nm^{-2}

Depletion Isotherm

- Compared to saturated (SA), *Z*-unsaturated (OA) higher friction coefficient which is less sensitive to v_s
- OA forms films with lower surface coverage than SA

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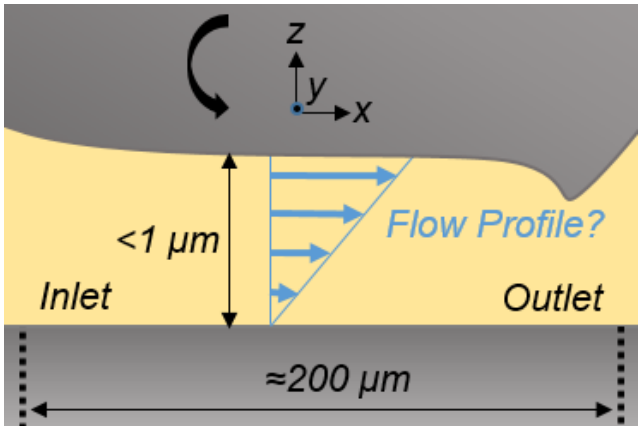
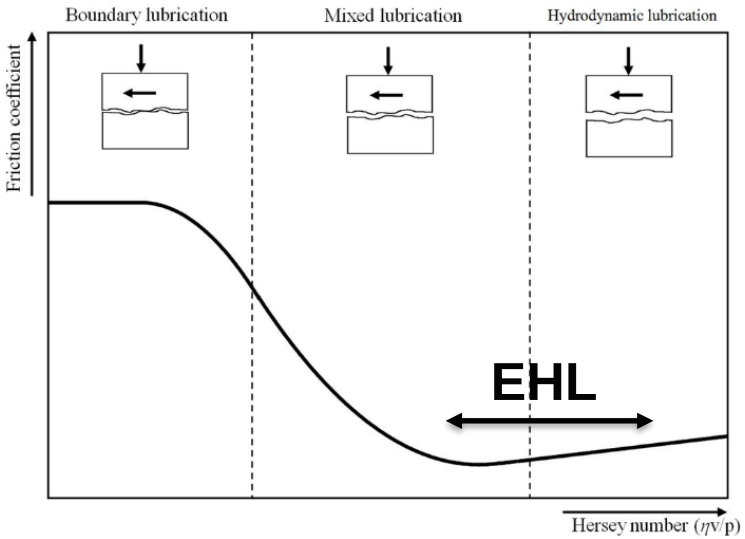
3. Elastohydrodynamic Lubrication (EHL)

- Many components roll and slide together e.g. rolling bearings, gears, CV joints and cam/followers
- Much of the friction loss is in the **elastohydrodynamic lubrication (EHL)** regime
- Thin lubricant film sheared at high strain rates and pressures





Spikes and Jie. **Tribol. Lett.** 56, 1-25, 2014

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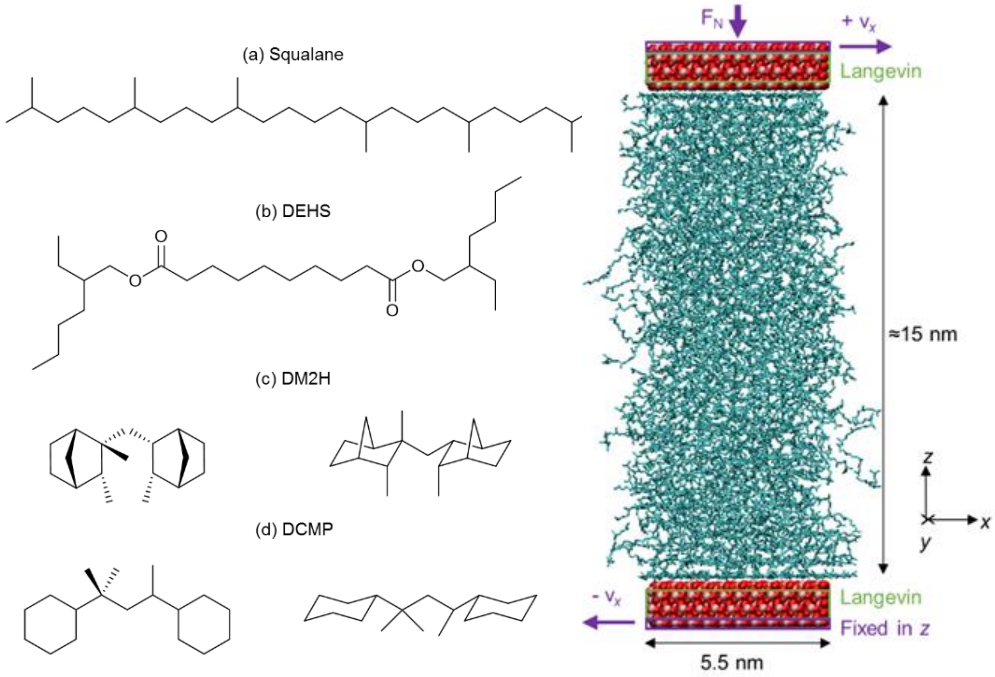
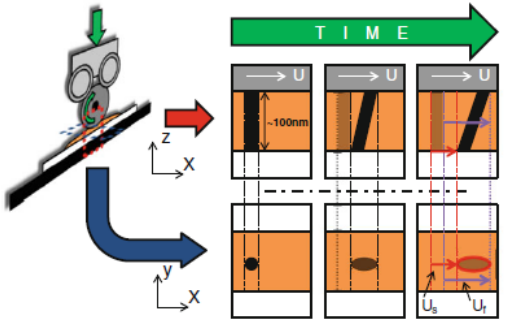
3. NEMD of EHL

- Compare **friction** and **flow** behaviour of four **lubricant** and **traction fluid** molecules
- **Tribology experiments** used to investigate friction behaviour and
- **In-contact phosphorescence** used to investigate flow behaviour
- NEMD simulations can **simultaneously** probe friction and flow behaviour
- Wide range of conditions (pressure, strain rate) in both experiments and simulations (EHL)





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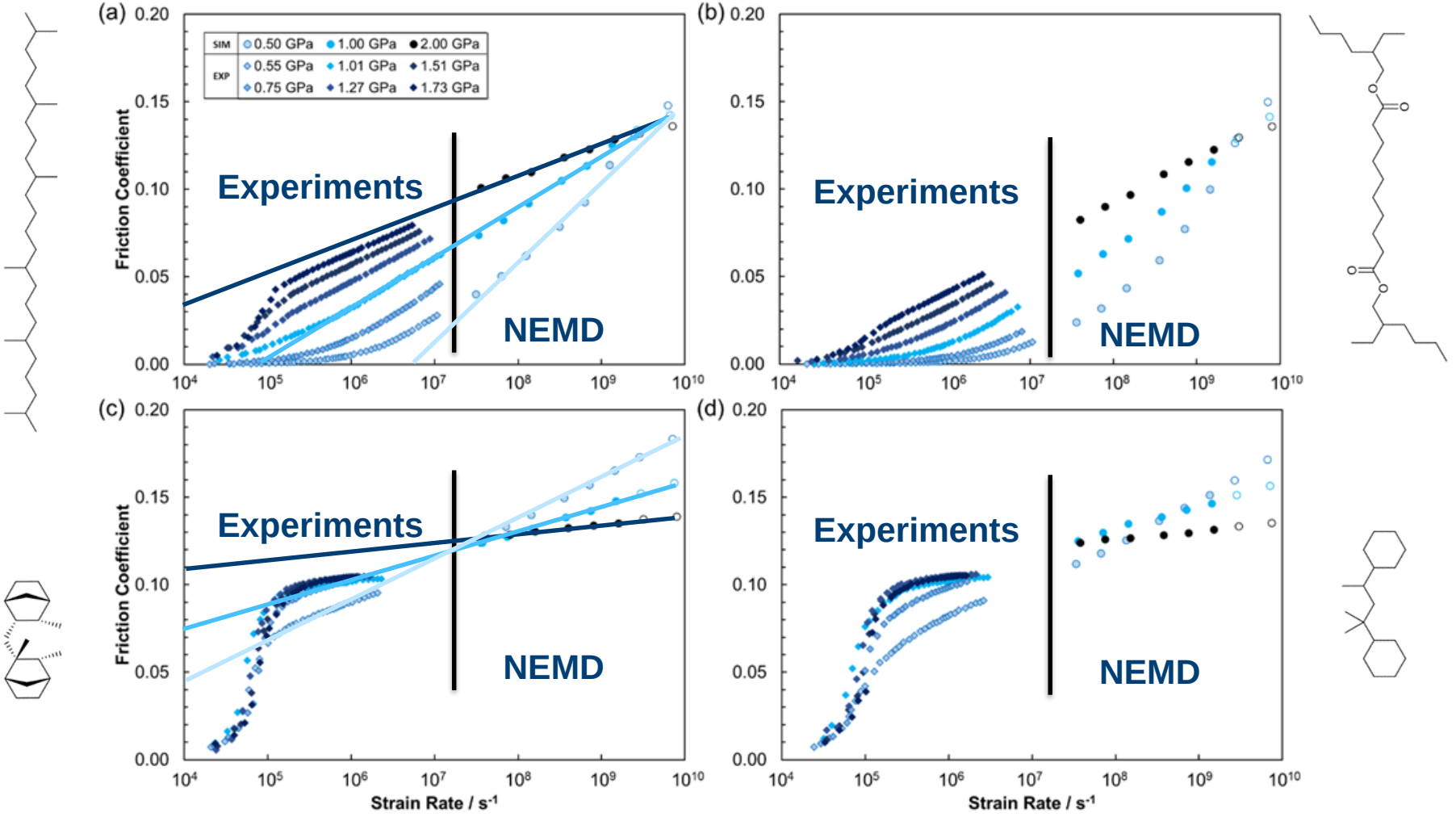
3. EHL Friction



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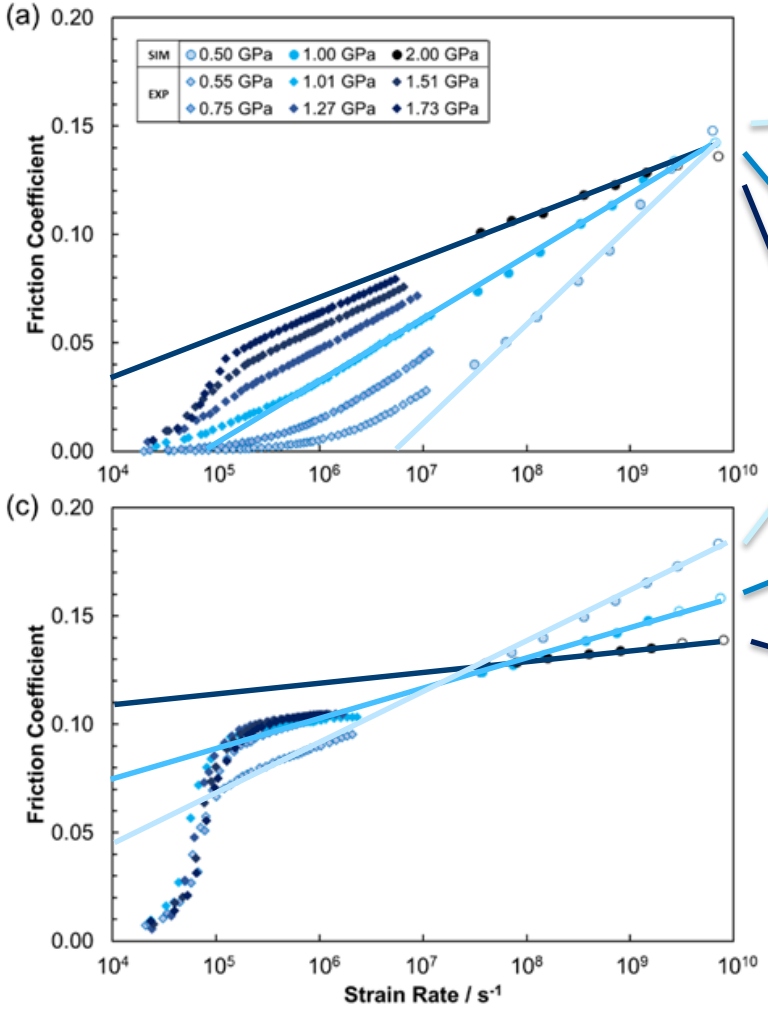
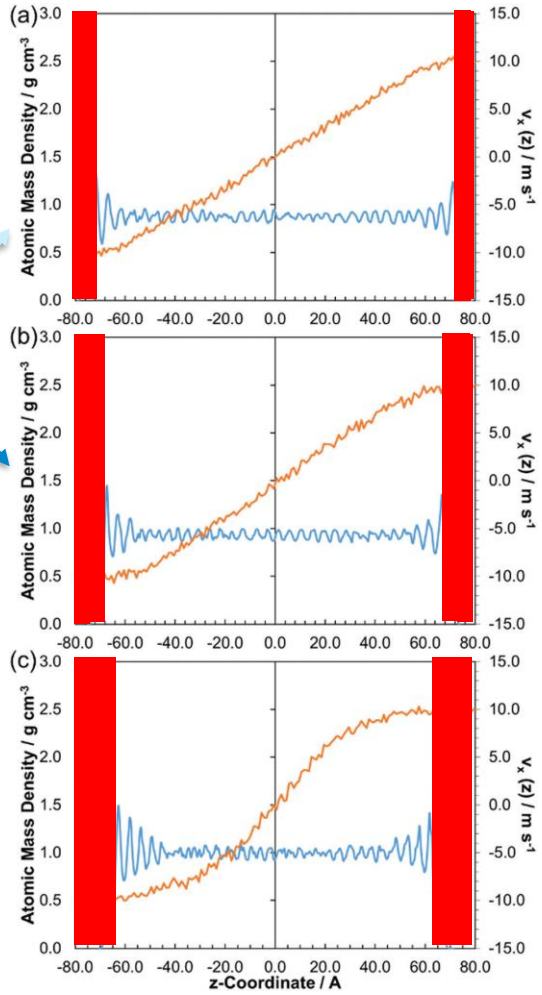
3. EHL Flow





0.5 GPa

Increase P

2.0 GPa

Ewen et al. **Phys. Chem. Chem Phys.** 19, 17883, 2017

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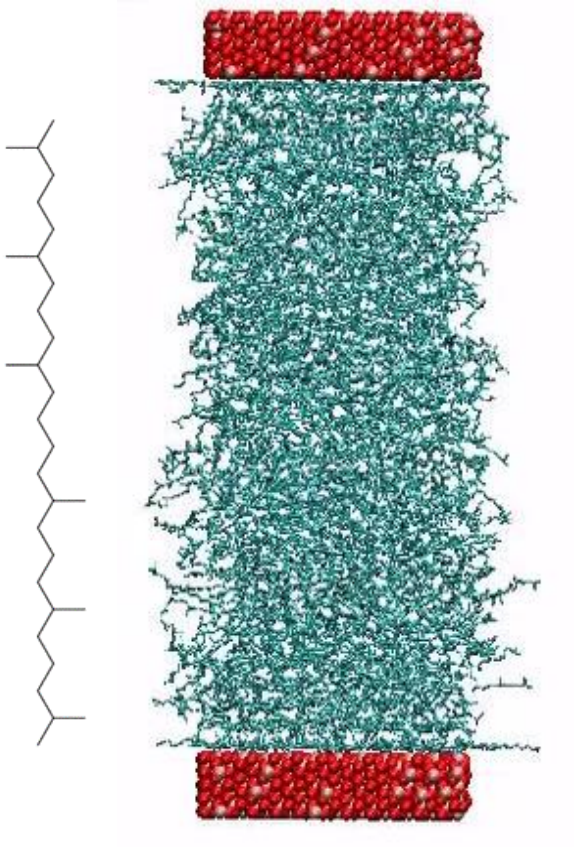
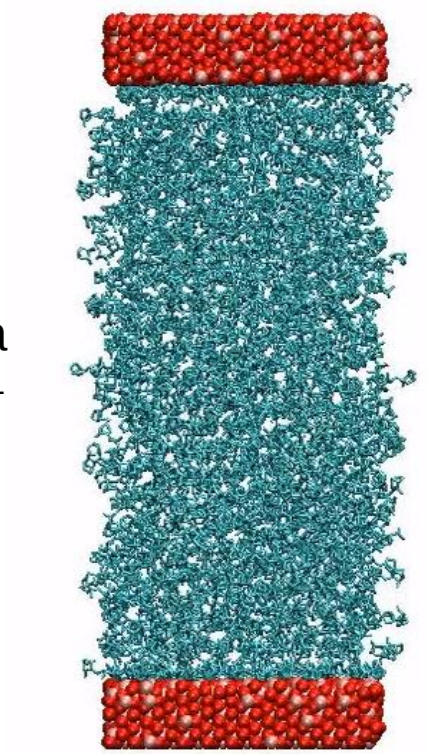
3. EHL Flow



Squalane
1.0 GPa
20 m s^{-1}

DM2H
2.0 GPa
20 m s^{-1}



- Lubricants Couette flow at low pressure, CL at high pressure
- Traction fluids CL at low pressure, PS at high pressure

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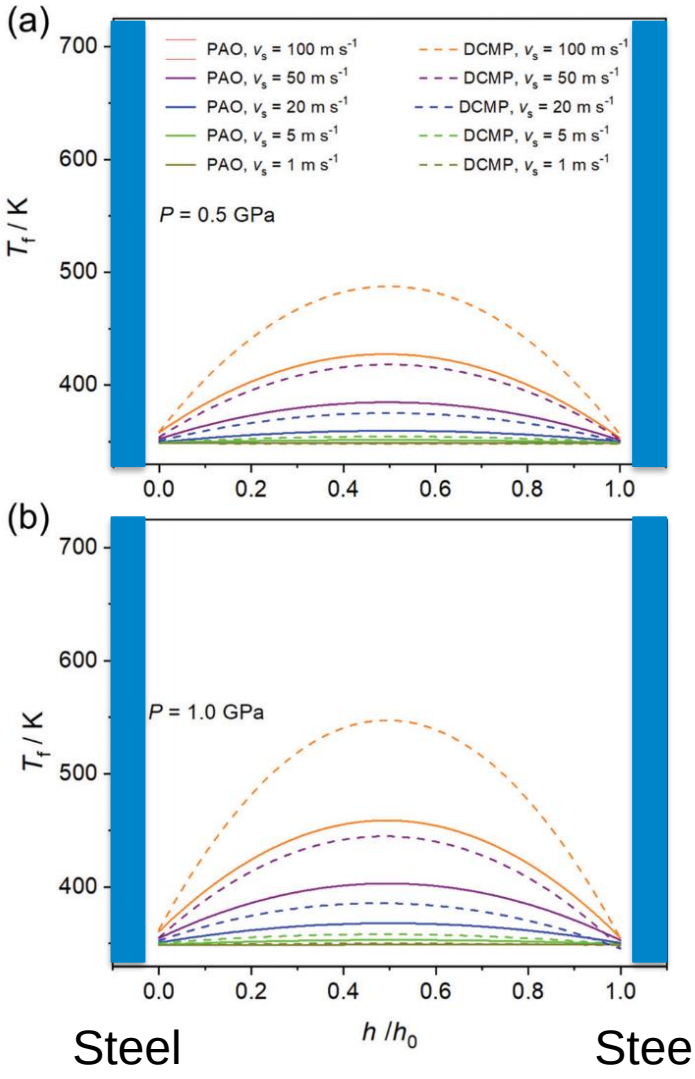
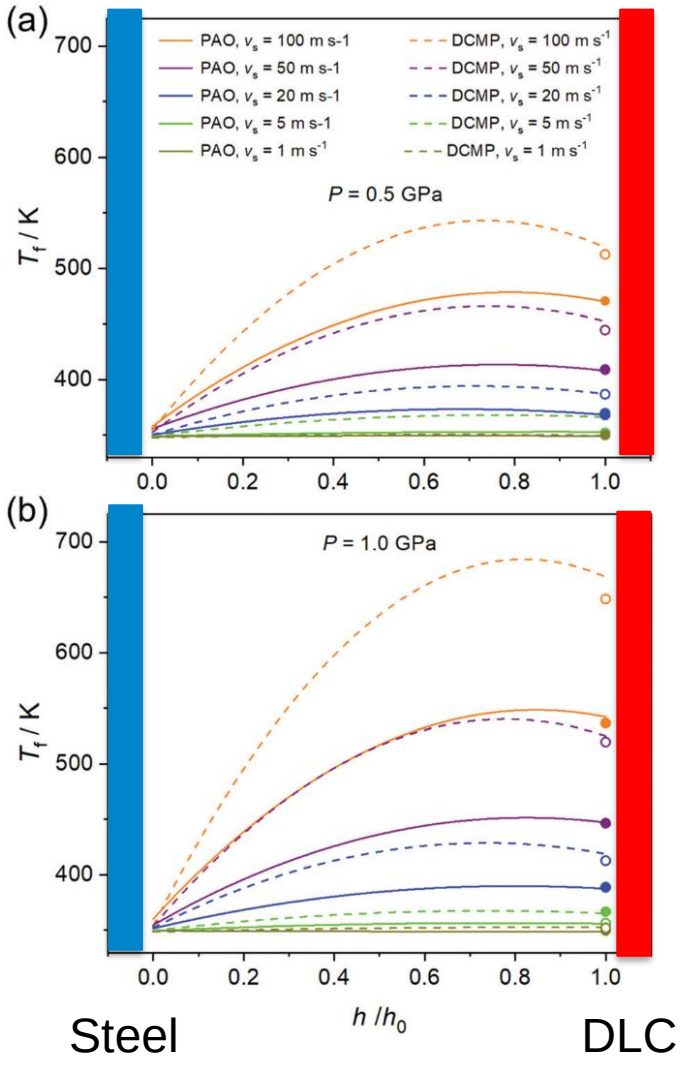
3. EHL Temperature





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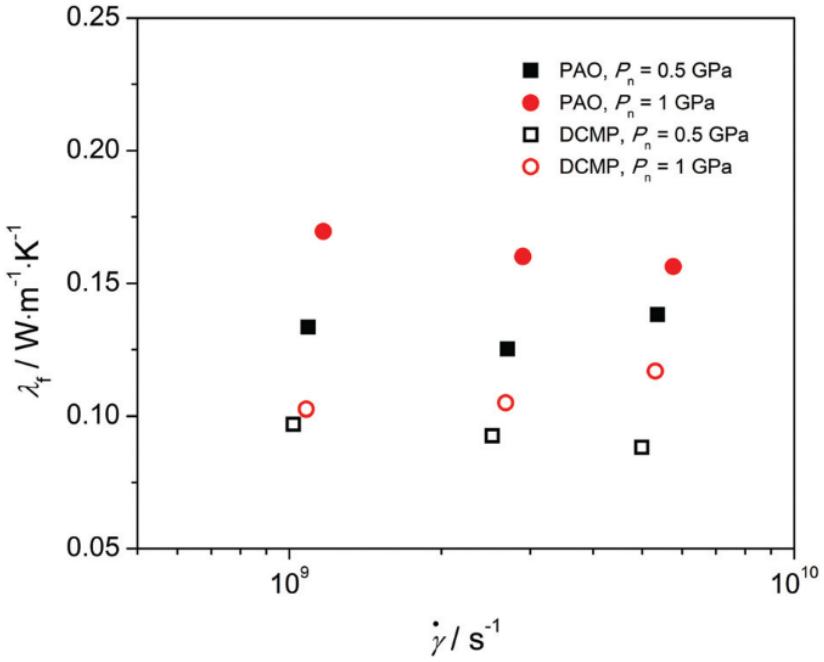
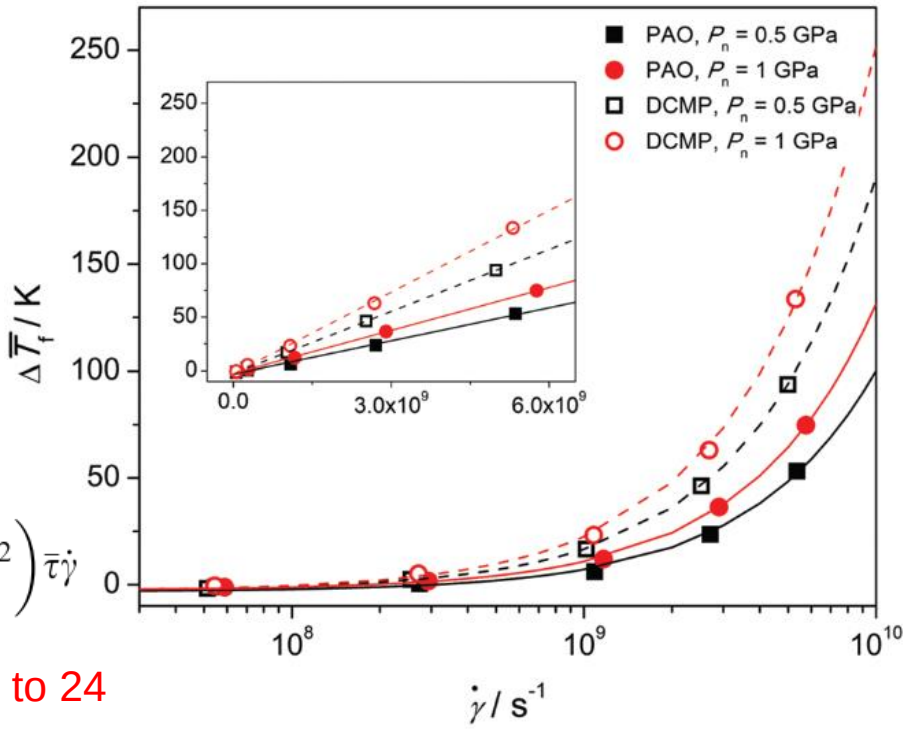
3. EHL Temperature



Fourier

$$T_f = -\frac{\bar{\tau}\dot{\gamma}z^2}{2\lambda_f} + T_{s-f}, \quad 0 \le z \le z_1$$



Archard

$$\Delta\bar{T}_{total} = \Delta\bar{T}_s + \Delta\bar{T}_f = \left(\frac{1}{(2\pi\lambda_s\rho_s c_s)^{0.5}} t_i^{0.5} h + \frac{1}{(b\lambda_f)} h^2\right)\bar{\tau}\dot{\gamma}$$

Ranges from 4 to 24

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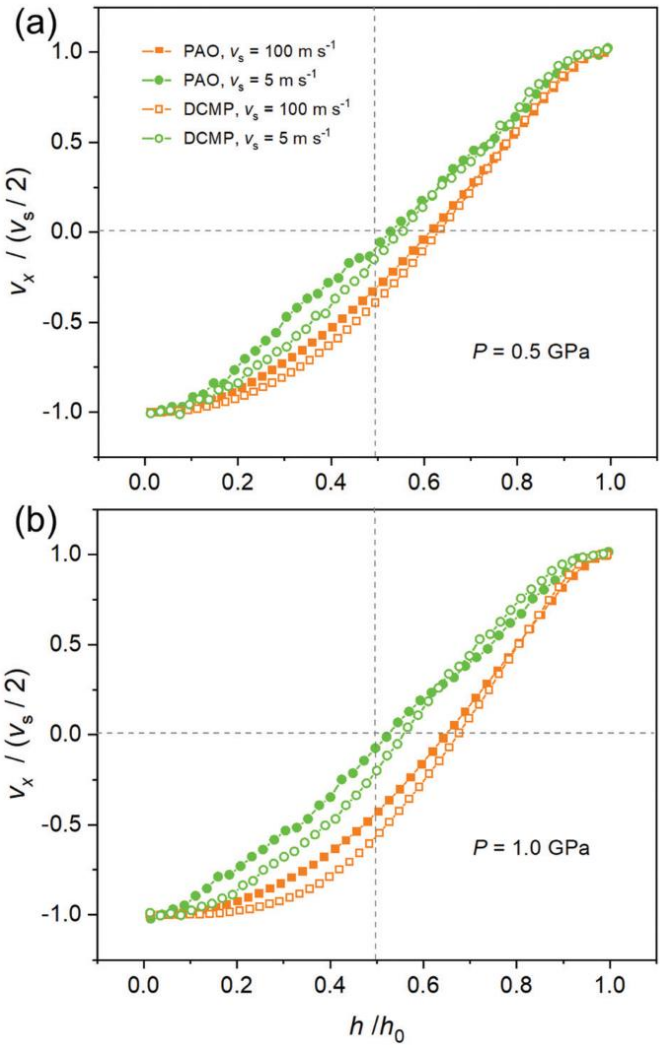
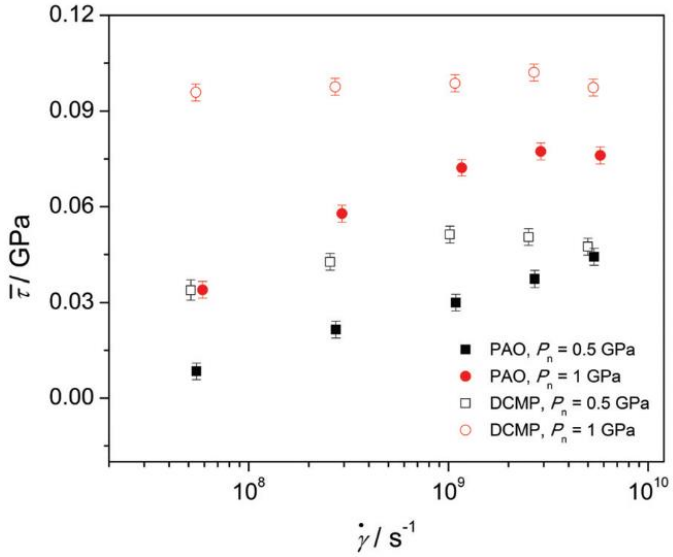
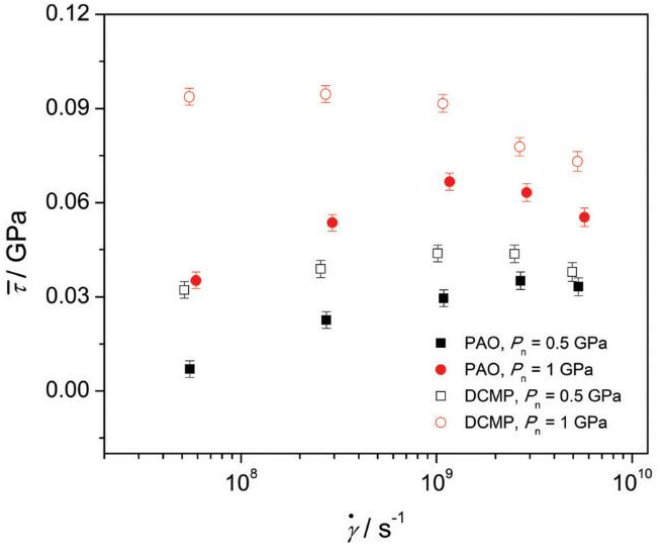
3. EHL Effect of DLC Surfaces





steel-steel



steel-DLC

Ewen et al. **Phys. Chem. Chem Phys.** 21, 5813, 2019

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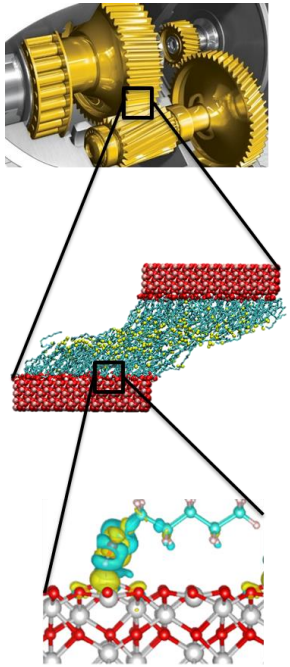
5. Conclusions & Next Steps

- NEMD has yielded unique insights into structure and friction of OFM films
- Accuracy has reached a level to discriminate between experimentally-relevant molecules
- Results show good agreement with experiments (conducted at several orders of magnitude lower shear rates)
- Industry increasingly interested in applied NEMD



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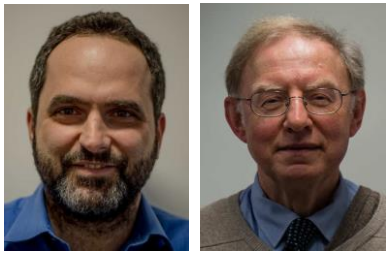
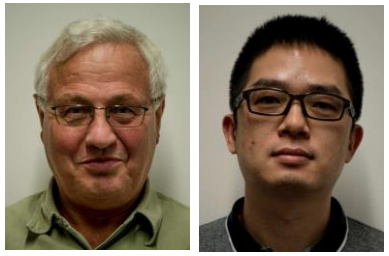
Acknowledgements

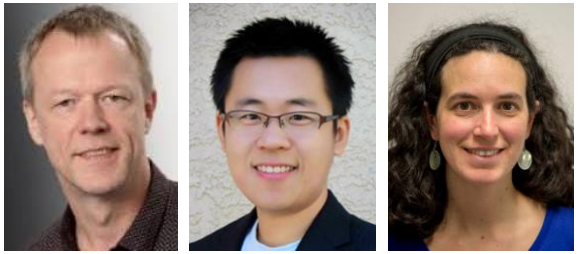
Simulations



Experiments



Collaborators



Funding

EPSRC
Engineering and Physical Sciences Research Council

Software

https://github.com/JE1314/LAMMPS_builder

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LAMMPS

VMD
Visual Molecular Dynamics

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VASP
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