Investigation of tribological properties of polysaccharides based green lubricants using non-equilibrium molecular dynamics simulations

Lakshmi Kumar Kunche, Fangxi Wang, and Sanket A Deshmukh
Department of Chemical Engineering
Virginia Tech, Blacksburg, Virginia

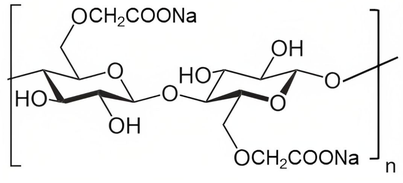
Introduction

Majority of the present day lubricants are derived from fossil fuels. These lubricants cause damage to the environment and moreover they are extracted from non-renewable resources. Thus, there is a need for the research on environmentally adaptable lubricants that are extracted from non-conventional sources of energy. Polysaccharides have characteristics of semi-flexible/rigid molecules and thereby exhibit shear thinning and elastic behavior even at high shear rates. Molecular-level understanding of lubrication mechanisms is still lacking, which is important to design efficient polysaccharide lubricants.

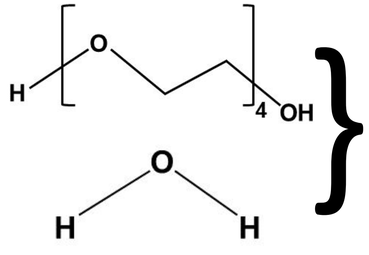
Research Question

Molecular Dynamics (MD) simulations can provide a detailed atomistic picture of polysaccharide structure and polysaccharide-metal interactions, which can aid us in the design of new polysaccharide based lubricants. The mechanism of lubrication is dependent on the structure and interactions of the lubricant with metal surface. It is also important to investigate the variation of frictional forces at different loads applied on the system and velocities of the surfaces.

Materials and Methods

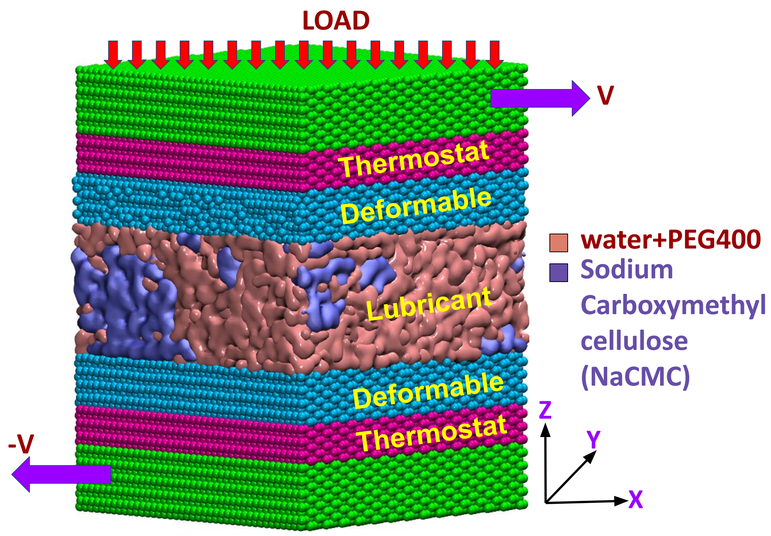


Lubricant
Sodium Carboxy methyl cellulose (NaCMC) anionic polyelectrolyte
30 ru polysaccharide

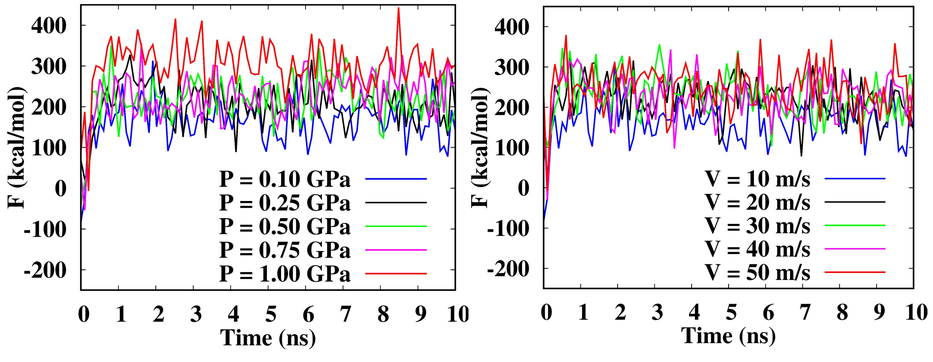


Base-fluid (50 - 50 wt%)
PEG-200 + water

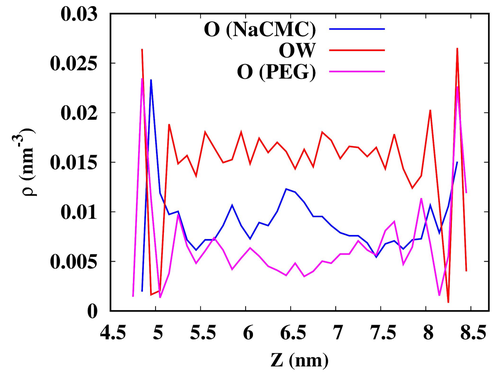
Simulation Setup



Results



- Frictional force was calculated as sum of forces on the atoms in top moving and top thermostat layers in x-direction
- Frictional force increase with the applied load and velocity. However this difference is not so obvious in the case of velocity behavior
- In experimental studies[1] also it was observed that frictional force was increasing with load



- Water, PEG and NaCMC oxygens, were mostly present close to the iron surface

Conclusions

- Non-equilibrium MD simulations provided deeper understanding of green lubricant structure under shear
- Frictional forces increase with load and velocity which is in agreement with experiments
- Water oxygens tend to stay near the iron surface and due to polar interactions between PEG and NaCMC oxygens with water, they also stay at surface increasing the efficiency of the lubricant

Acknowledgement

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References

1. Shetty, P., Mu, L., & Shi, Y. (2020). Polyelectrolyte cellulose gel with PEG/water: Toward fully green lubricating grease. *Carbohydrate polymers*, *230*, 115670.