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Non-equilibrium molecular dynamics investigation of a model ionic liquid lubricant for heavy-duty applications

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In the current work, we present a modeling approach for simulating mesoscopic phenomena related to lubrication. Our geometry allows a variable confinement gap and a varying amount of lubricant in the gap. We have implemented and compared several coarse-grain molecular dynamics descriptions of an ionic liquid (spherical model and model with cation tail) as a lubricant that can expand into lateral reservoirs. The results have revealed two regimes of lubrication, and elastohydrodynamic one under low loads and one with low, velocity-independent specific friction, under high loads. The observed steep rise of normal forces at small plate-to-plate distances is an interesting behavior that could potentially be exploited for preventing solid-solid contact and wear.

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