lubricants

MDPI

A computational Study on the Role of Lubricants under Boundary Lubrication

Walter Holweger [1, 2, *], Luigi Bobbio [3, *], Zhuoqiong Mo [4], Joerg Fliege [3], Bernd Goerlach[5], Barbara Simon[1]

[1] Technology Consultant, Sailegärten 2, 72351 Erlaheim, Germany
[2] Operational Research Group, School of Mathematical Sciences, University of Southampton, Southampton SO17 1BJ, UK
[3] University of Southampton, Faculty of Social Sciences, School of Mathematics, Southampton SO17 1BJ, United Kingdom
[4] University of Southampton, Faculty of Social Sciences, Business School, Southampton SO17 1BJ, United Kingdom
[5] ASC Goerlach, Robert-Bosch-Straße 60/1, D-72810 Gomaringen, Germany
* Correspondence: walter.holweger@t-online.de; l.bobbio@soton.ac.uk;

1. Supplementary Material

In what follows, we explained more in deep the symbols used in the manuscript "A computational Study on the Role of Lubricants under Boundary Lubrication" and we provide some example and/ or figures that could help the reader in understanding the chemical status considered. All the figures were created with the aid of Hyperchem® software.

1.1 Symbols

With *Solvate BxAy, with x >> y*, we mean that plenty of baseoil molecules "x" cover the additive "y". As an example, take Figure S1: plenty of Baseoil Molecules (in red), surround (solvate) an Additive A (blue).

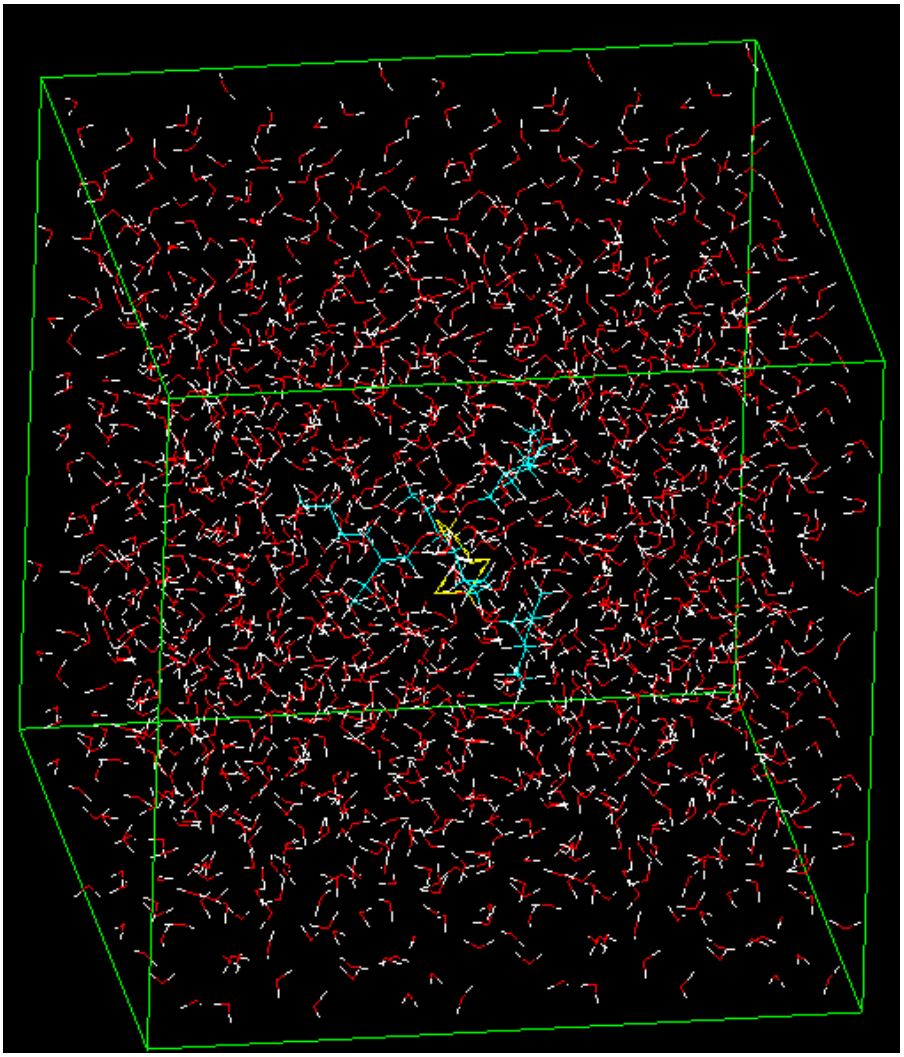

Figure S1: Meaning of BxAy: plenty (x>>y) of Baseoil Molecules B (red) solvate an Additive A (blue)

The notation *Clustering Bx [Ay]g, with x ~ y* means that B dissolves additives clustering together and a possible chemical status is represented in Figure S2. In extreme cases micelles are formed with a shell of baseoil encapsulating self-aggregates of additives, expressed as degenerated by a degree of $g \geq 2$.

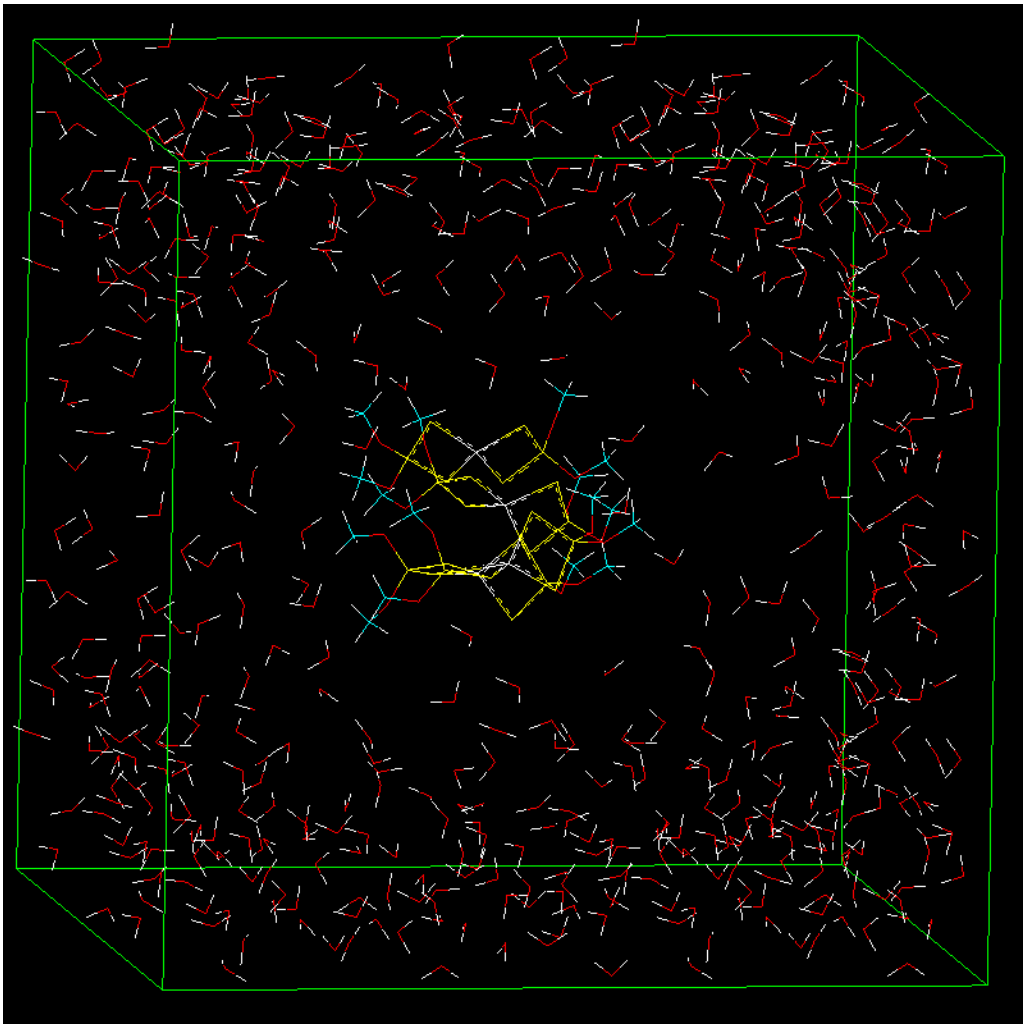

Figure S2: A Cluster of Additives A is surrounded by a shell of baseoil molecules (B), representing Bx-[Ay]g with g = 2

In Figure S3 we reported a situation where solely the baseoil is considered as an example of *Clusters of the baseoil [B]g* temporarily created random with a degree of g.

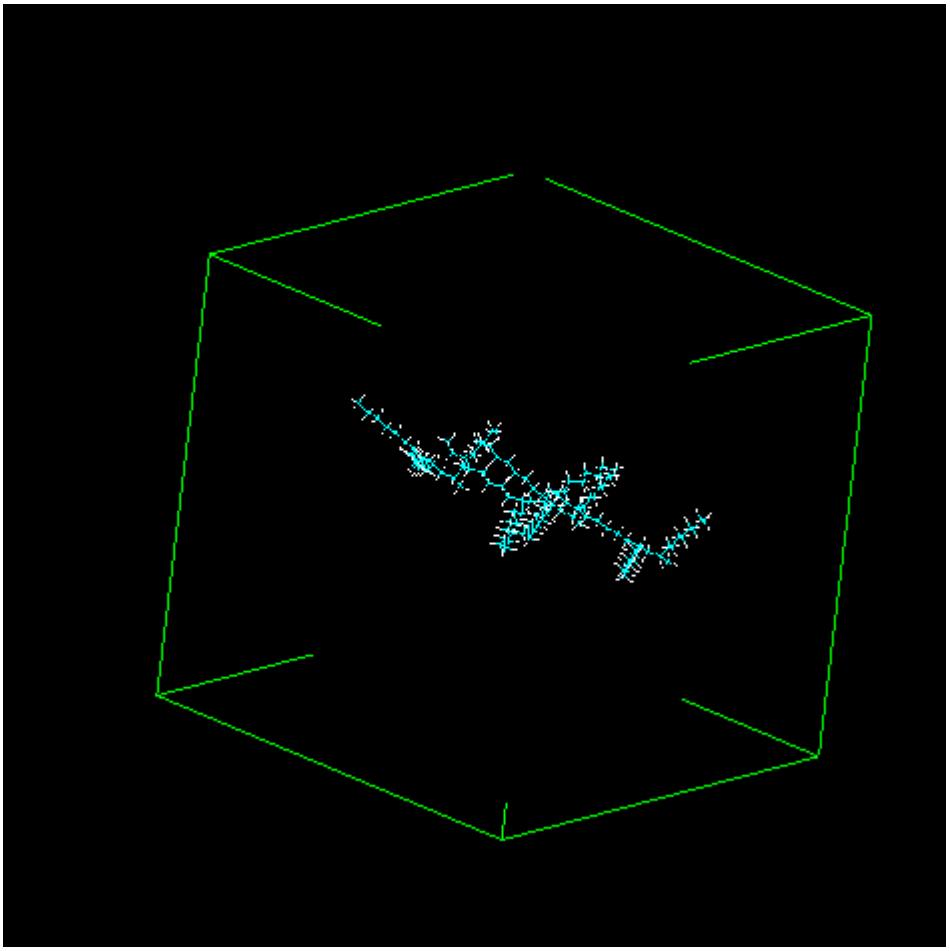

Figure S3: Clusters of baseoil molecules (g=4) in a box

On the other hand, Figure S4 exhibits a formation of *Clusters of the additive [A]g* temporarily created random with a degree of *g* (Example: g = 4). In this situation, only additives are shown.

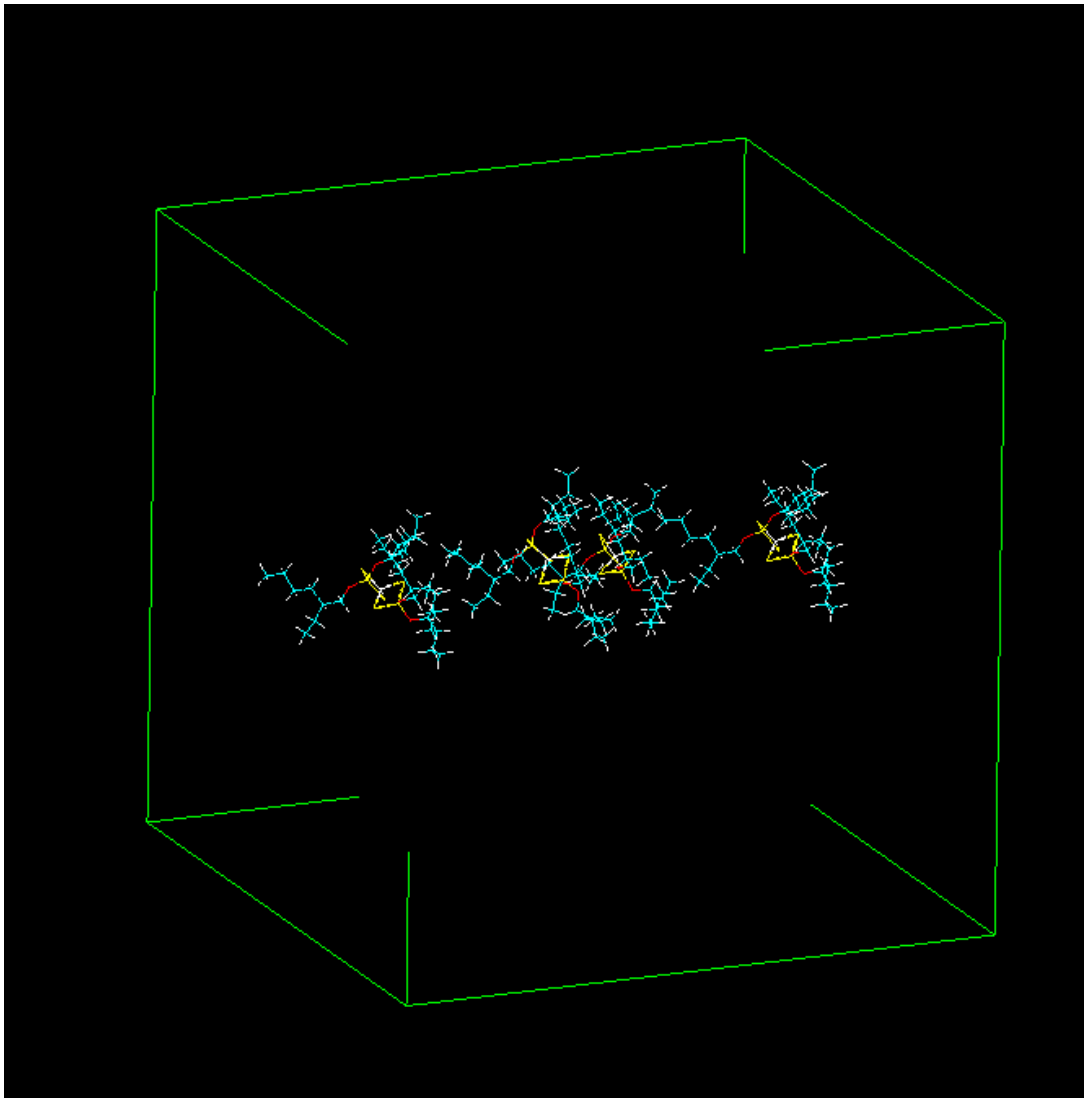

Figure S4: Assemblation of Additives (g = 4) in a box

Finally, in Figure S5 we show a situation where additives, single solvated ($g = 1$) or clustered ($g > 1$, in green) in a solvent (red, randomized), are competing with a surface S (red and white block). The surface is assumed as metal (white dots) and oxides (red dots). The additive surface interaction (grey arrow) competes with interaction of the additives with the solvent (blue arrow).

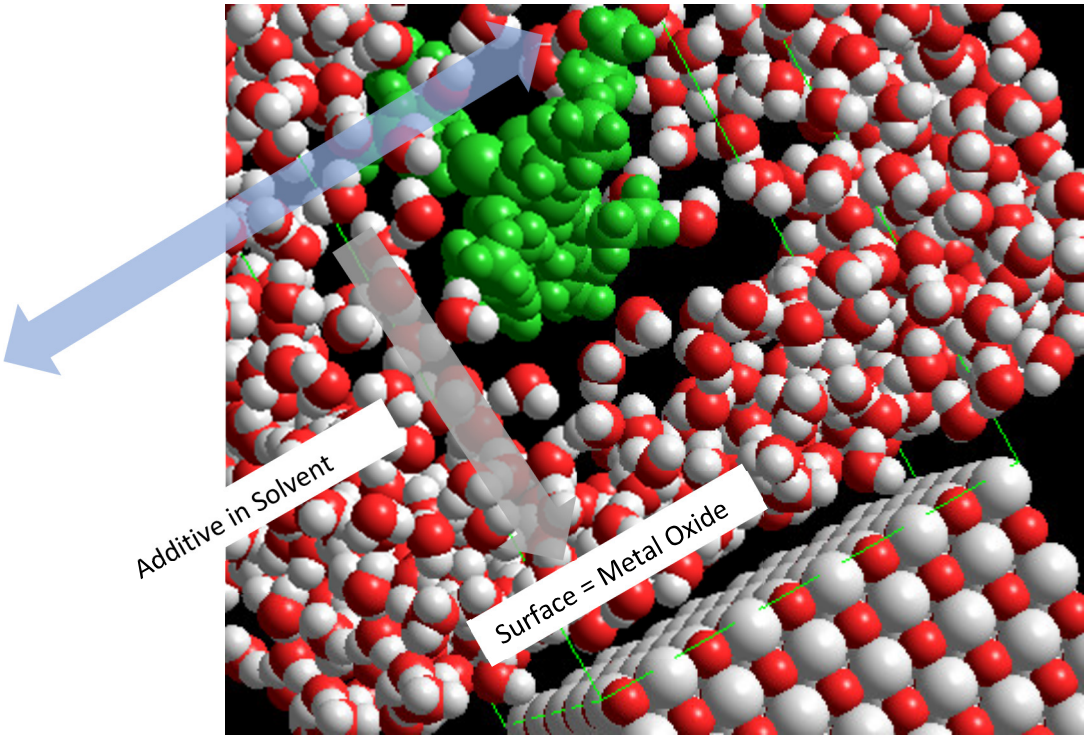

Figure S5: Additives, single solvated (g =1) or clustered (g>1)(as green dummy) in a solvent (red dummies, randomized), compete with a surface (red and white ordered dummies). The surface is assumed as metal (white dots) and oxides (red dots)

In a similar fashion, it is possible to create example for all the other cases mentioned as variances.