SORPTIVE BEHAVIOUR OF NANOPOROUS MATERIAL AS MOLECULAR SIEVE FOR COMPRESSOR APPLICATIONS: A COMPUTATIONAL STUDY

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Although esters are used as base oil for lubricants in applications as hydraulic and chainsaw oils and metalworking fluids, no biolubricants are known for compressor applications except for food industry. One of the main concerns of biolubricants is their performance which is improved using additives. The use of additives allows to increase the performance and physical properties of an oil but they also increase the cost of lubricants an may even be harmful to health or environment[1].

Our research aims to avoid the use of antioxidant additives in biolubricants for compressor applications by replacing them with a nanoporous material able to trap the oxidation products. In this way the development a nanoporous material based filter may lead to obtain a cost effective and environmentally friendly alternative to antioxidant additives.

Computational methods have become a tool to study absortive systems[2][3]. In this work Monte Carlo (MC) and Molecular Dynamics (MD) simulations have been carried out to study the absorption of oxidation products of an ester based biolubricant.

The ability of the material to absorb the oxidation products was obtained from the absortion isotherms and absortion isobars calculated by means of a configurational bias grand canonical monte carlo (CB-GCMC) method used to simulate the absortion of oxidation molecules at temperatures and pressures ranging from room conditions to the working conditions of a real compressor. Both surface and bulk sorption were studied. Isosteric heats, preferred absortion sites and minimum energy configurations have also been obtained. The configurations obtained from CB-GCMC were used as input for MD calculations in the NPT ensemble in order to study the dynamical behaviour of the system under compressor working conditions. Berendsen methods[4] were used to control temperature an pressure during simulations. The results obtained from MD simulations were used to calculate the diffusion coefficients of the molecules.

References:

[1] F.L. A. Lee; J.W. Harris. Lubricant additives. (2003) 575-577.
[2] S. Chempath, J. F. M. Denayer, K. M. A. De Meyer,G. V. Baron, R. Q. Snurr. Langmuir **20 (**2004), 150-156
[3] I. Daems, G. V. Baron, S. Punnathanam, R. Q. Snurr, and J.F. M. Denayer. J. Phys. Chem. C **111** (2007), 2191-2197
[4] Berendsen, H. J. C.; Postma, J. P. M.; van Gunsteren, W. F.; DiNola, A.; Haak, J. R., J. Chem. Phys., **81** (1984), 3684-3690.

Figures:

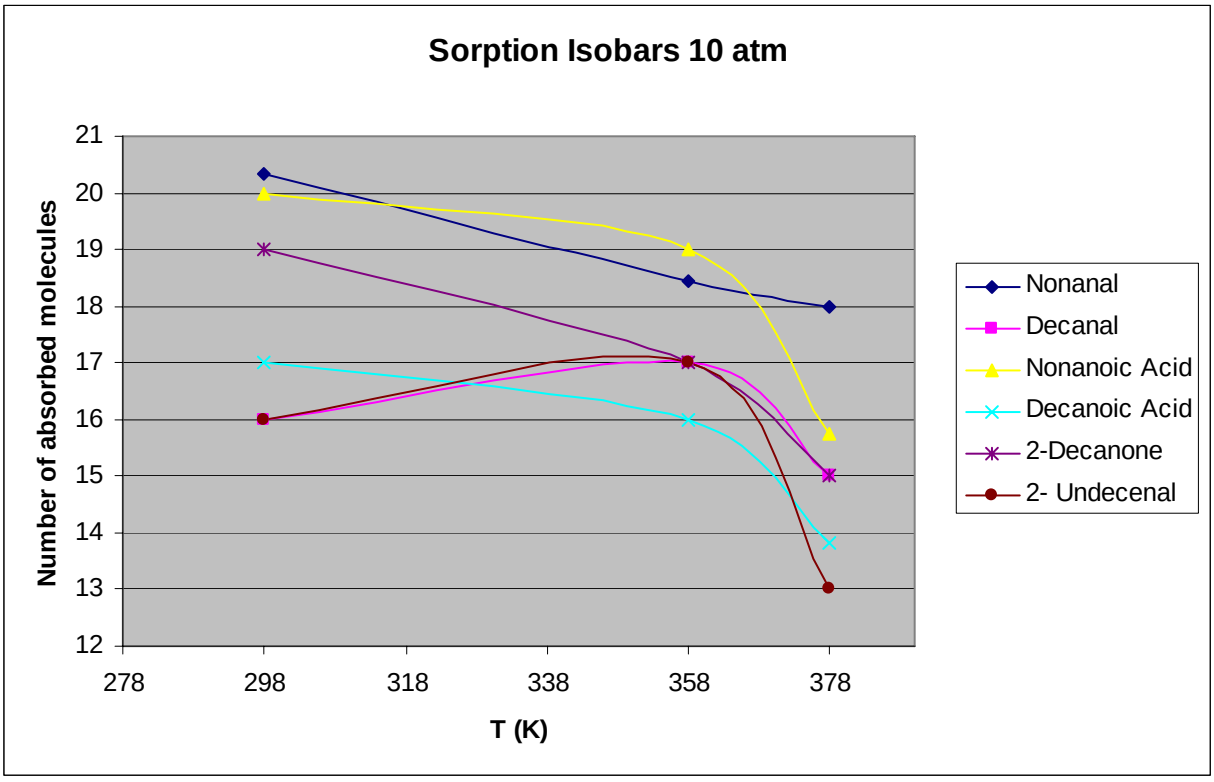

Figure 1. Sorption isobars for different oxidation products

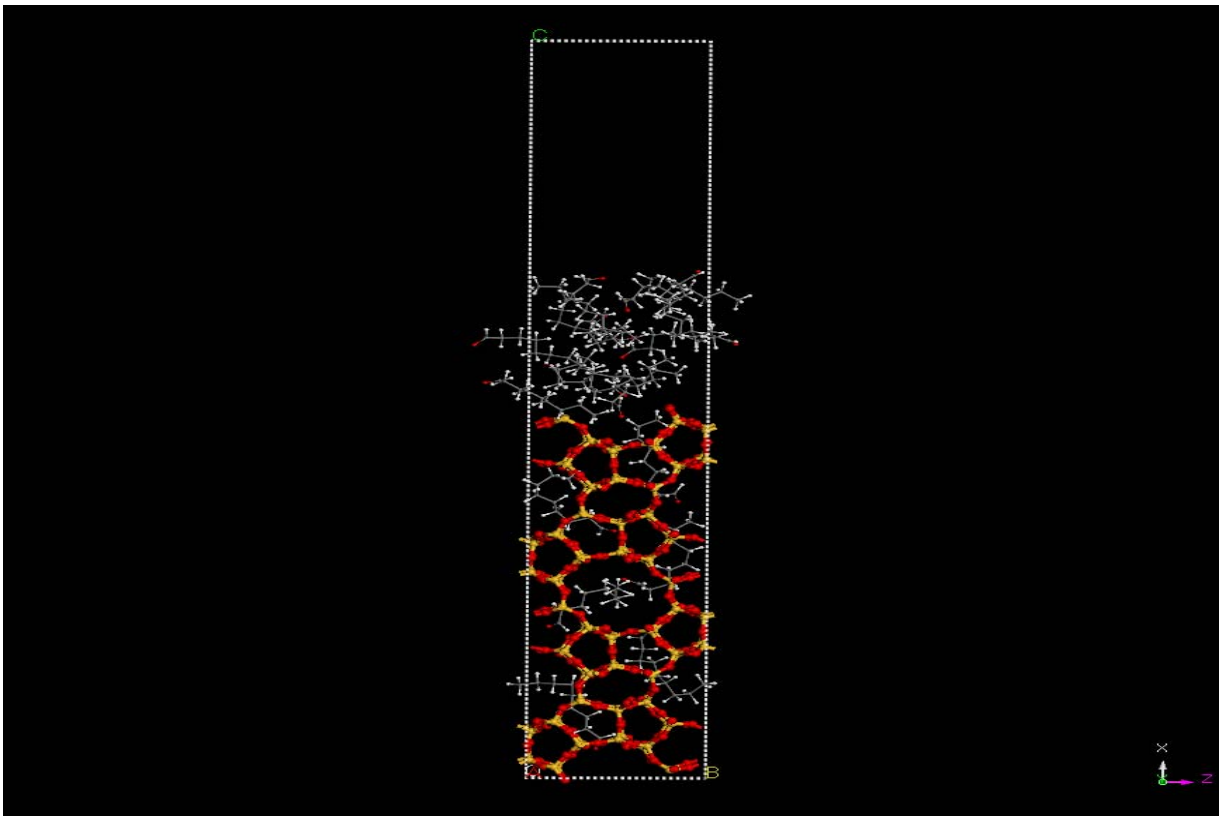

Figure 2. Minimun energy configuration from CB- GCMC calculations