EMMC case study:

Atomistic simulations of properties of lubricants

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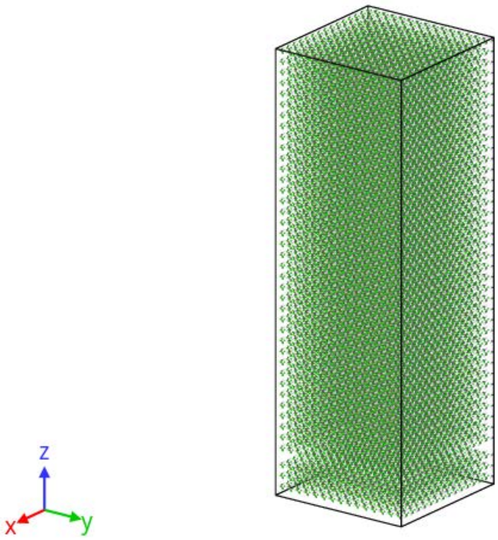


Figure 1 Initial configuration used for the calculation of the density and viscosity of a lubricant

About the Company

SKF group is a leading global supplier of products, solutions and services within rolling bearings, seals, mechatronics and lubrication systems. As a multinational company with headquarters in Gothenburg, Sweden, SKF employs more than 43000 people worldwide of which a few hundred contribute to R&D activities. Some of those activities are devoted to developments of advanced materials, where modelling is an important tool. The modelling specialists represent various backgrounds and expertise levels ranging from BSc to PhD with several years of professional experience. To strengthen its staff expertise, SKF provides both internal and external training for their employees.

About modelling – the nuts and bolts

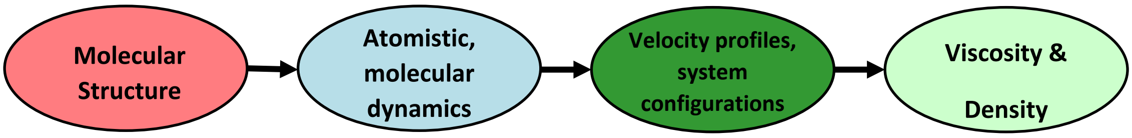
The modelling groups at SKF are familiar with various models including: electronic (DFT), atomistic (MD), mesoscopic (DPD, Discrete dislocations), continuum (CFD, continuum mechanics), and data-based. Multiscale modelling is also commonly used, linking different models. Some of the modelling activities are outsourced.

Modelling is used commonly in R&D projects and the different types of modelling are used according to the project's needs. Typical cases in which modelling is used include: assessment of information which cannot be obtained experimentally and when there is the need to improve the understanding of specific phenomena.

SKF modellers are experienced with commercial software, as well as free-ware and in-house developed software. External resources, typically academics and software vendors, are employed when there is a lack of specific capabilities or resources (including software and infrastructure) or there is the wish to explore new approaches to problems.

About the Case Study

The case study is based on the SKF's work on atomistic simulations of properties of lubricants.



For this particular case, what were your objectives as an industrial consumer of modelling?

We wanted to reduce the amount of property measurements of some simple lubricants since the measurements are complex and expensive.

How did materials modelling play a key role in problem solving?

We have developed and validated modelling strategies to determine key properties of lubricants, starting from the molecular structure.

Materials modelling played a key role in reducing costs and increasing the understanding at lower scales of the behaviour of the fluids.

What tools and methodologies have been applied?

All the initial systems were generated using a modified version of the open-source LAMMPS Builder software available at https://github.com/JE1314/LAMMPS_builder

The Molecular Dynamics simulation were run using the LAMMPS code (https://lammps.sandia.gov/).

The visualisation of the systems was done using the software Ovito (http://ovito.org/).

The postprocessing was done using LAMMPS itself, some python scripts and Gnuplot for the generation of the figures.

What were the expected improvements of the material behaviour simulation?

We expected to develop simple screen methods before going to detailed experimental measurements.

For this particular case, did modelling affect your value chain?

We improved the understanding of properties of known materials, we calculated viscosity and density of simple lubricants, and we reduced the number of needed experiments.

In the future we will extend the developed methodologies to predict new materials composition and see how this relates to the properties in order to identify better alternatives to the actual materials.

For this particular case, what was the quantitative value of materials modelling?

The use of modelling did not save person time initially, the development of the modelling workflow took quite some time (200-300h), so there was an important investment of time. However, once the methodology has been implemented, the number of experiments is expected to be reduced. We estimate that the cost of the simulations is 1/5 of the cost of the experiments. This will help to reduce the development cost for new lubricants.

In addition, the modelling speeds up the materials selection and the discovery process of new materials. These contributions are difficult to quantify, but in general fewer experiments leads to less time needed for materials selection and in-silico testing provides a larger design space.

What investments were made during the project?

For the development of the modelling strategy, about 200-300 person hours of time plus considerable computing time on our internal HPC cluster were necessary.

For this particular case, how did you measure the impact of Materials Modelling as a tool to assist in problem solving, process optimisation, product development?

We did not have a defined approach to measure the impact of Materials Modelling but would be interested in establishing one.

What technical and technological benefits resulted from the project?

We developed a new way (for the company) to pre-screen physical properties of simple lubricants.

What where the economic benefits/impacts when you did use modelling?

The number of experiments should be reduced in the future. The cost of experiments is estimated to be 5 times the cost of simulations.

What was the business impact versus previous approach?

The use of Materials Modelling should reduce the time and cost of development.