Deep Learning Tool Enables the Identification of Alkanes For Lubricants With Superior Physical Properties

Deep learning tool Alchemite™ accurately predicts the physical properties of alkanes and will facilitate the development of new lubricants.

Cambridge UK | January 23, 2020. A recent study carried out by researchers from the Department of Physics at the University of Cambridge showed that a unique deep learning algorithm can accurately predict physical properties of alkanes and outperform several physico-chemical/thermodynamic methods. This cutting-edge technology is being commercialised by Intellegens as Alchemite™.

Lubricants are an essential component in industry and are widely used. They can protect surfaces from wear, reduce friction, transfer heat, and ensure the smooth functioning of mechanical devices. Given that lubricants are mixtures of predominantly alkanes, it is unclear whether contemporary lubricant formulations are the most optimal. Predicting the physical properties of alkanes and understanding the relationship between lubricant performance and alkane structure would facilitate the development of computationally-derived optimal base oils.

The study (Santak & Conduit, 2019), led by Dr Gareth Conduit (Research Fellow at the University of Cambridge and co-founder of Intellegens) and Pavao Santak (University of Cambridge) is published in *Fluid Phase Equilibria*. The authors implemented artificial neural networks that exploit property-property correlations to predict physical properties of alkanes. The deep learning algorithm (Alchemite™) inputs the molecular structure of alkanes to predict the boiling point, heat capacity, and vapor pressure as a function of temperature. The results reproduced by this algorithm are significantly more accurate and consistent than those reproduced by other methods. By combining sparse experimental data with molecular dynamics simulations to predict physical properties of alkanes, the algorithm can identify and speed up the identification of alkanes to be used for lubricant base oils with superior physical properties.

Dr Gareth Conduit (Research Fellow at the University of Cambridge and co-founder of Intellegens) said "We developed the deep learning tool Alchemite™ that is not only capable of predicting physical properties of alkanes, but has shown to accurately estimate intractable properties like density and shear viscosity. Alchemite™ could enable industries specialized in material formulations to substantially optimise their processes and yield better and faster results."

For more information on the Alchemite™ engine or Intellegens, go to: https://intellegens.ai or email ben@intellegens.ai.

About Intellegens

Intellegens is a spin-out from the University of Cambridge with a unique Artificial Intelligence (AI) toolset that can train deep neural networks from sparse or noisy data. The technique, created at the Cavendish Laboratory, is encapsulated in Intellegens first commercial product, Alchemite™ . The innovative deep learning algorithms that Alchemite™ is based on can see correlations between all available parameters, both inputs and outputs, in fragmented, unstructured, corrupt or even noisy datasets. The result is accurate models that can predict missing values, find errors and optimise target properties. Capable of working with data that is as little as 0.05% complete, Alchemite™ can unravel data problems that are not accessible to traditional deep learning approaches. Suitable for deployment across any kind of numeric dataset, Alchemite™ is delivering ground breaking solutions in drug discovery, advanced materials, patient analytics and predictive maintenance – enabling organisations to break through data analysis bottlenecks, reduce the amount of time and money spent on research, and support better, faster decision-making.