Juryreport
AkzoNobel Afstudeerprijs voor Chemie en Procestechnologie 2019

J.P. (Jonah) Poort MSc, Technische Universiteit Delft
Solving Vapor-Liquid Flash Problems Using Artificial Neural Networks

The jury was very much impressed by the quality of the work of all 11 candidates nominated by their MSc thesis supervisors. The jury took into their consideration the grades obtained by the nominees, their CV, and most importantly the MSc thesis submitted. The jury concluded that most of the nominees met all requirements to be awarded the AkzoNobel Afstudeerprijs.
The quality of the work nominated was very high. Nevertheless, the jury had no difficulty to select the winner: Jonah Poort MSc from the TU Delft. The title of his MSc thesis is: Solving Vapor-Liquid Flash Problems Using Artificial Neural Networks.
Vapor-liquid phase equilibrium (flash) calculations largely contribute to the total computation time of many process simulation models, absolutely crucial for the design and operation of processes in the chemical industry. As a result, process simulations are limited in the amount of detail that can be included due to computational time restrictions. Flash calculations can fail to provide acceptable results which can seriously hinder process modelling and design.

In the MSc thesis work of Jonah Poort, he presented for the first time, artificial neural networks (AI) that he developed to provide a much faster and robust alternative to traditional flash calculation methods. Although the potential importance of AI is well known, AI techniques have not been employed previously in thermodynamic calculations such as Vapor-Liquid Equilibrium (VLE) calculations. In addition to AI for conventional flash types, Jonah Poort developed neural networks for two new concept flash types: a constant entropy - constant volume (SV), and a constant enthalpy - constant volume (HV) flash, not only for classification but also for prediction of thermodynamic properties of the two phases. The results show that the developed neural networks are more than one order of magnitude faster than conventional methods at the same accuracy. The results and methods of Jonah are now used in process simulators in the chemical industry, with a first application at the company “Zero Emission Fuels (ZEF) BV”.

It is important to note this research was independently carried out by Jonah Poort, with very little supervision needed. The excellent quality of the thesis and its impact, combined with Jonah's independence, resulted in a graduation mark of 10/10, which is very rarely given. The work has led to a scientific publication in the journal Fluid Phase Equilibria, which is the leading journal in the field of thermodynamics and phase equilibria. The manuscript was written by Jonah Poort himself with virtually no corrections needed from his supervisors.

The jury established by the Koninklijke Hollandsche Maatschappij der Wetenschappen concluded that this work is the best among all submitted nominations and trusts it will have a big impact in the future.

Prof. dr. I.W.C.E. (Isabel) Arends, Lid decaan faculteit Bètawetenschappen Universiteit Utrecht, oud-hoogleraar biokatalyse en organische chemie, Technische Universiteit Delft
Prof. dr. A.W. (Aart) Kleijn, director Center of Interface Dynamics for Sustainability, CDCST, CAEP, Chengdu, hoogleraar sustainable energy and heterogeneous chemistry Universiteit van Amsterdam, bijzonder hoogleraar Universiteit Leiden, adviseur FOM-Instituut DIFFER

De jury vergaderde op 25 oktober 2019 onder leiding van Jhr. mr. Th.S. Röell, directeur KHMW. Daarnaast waren ter vergadering aanwezig Prof. dr. A.P. IJzerman, secretaris natuurwetenschappen, en Drs. S. van Manen, secretaris.