DTU Mechanical Engineering
Department of Mechanical Engineering

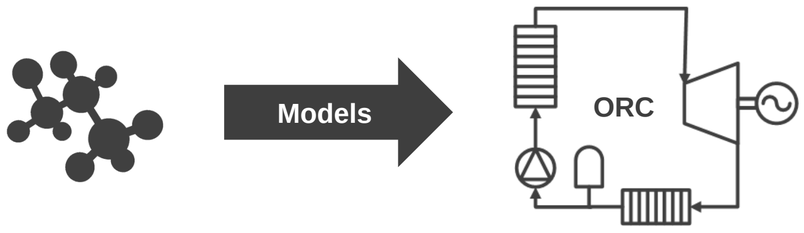
# Prediction of thermophysical properties of innovative fluids

**Maria E. Mondejar and Fredrik Haglind**
Department of Mechanical Engineering, Technical University of Denmark, Nils Koppels Allé, Building 403, 2800 Lyngby, Denmark
* Corresponding author, Tel. +45 4525 1409, e-mail: maemmo@mek.dtu.dk

## 1. Project NanoORC

The project NanoORC aims at evaluating the potential of innovative fluids as working fluids for organic Rankine cycles (ORCs) power systems.

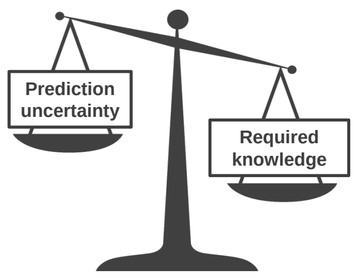
The project develops general models for the prediction of the thermophysical and transport properties of innovative fluids. The models will be used to evaluate the performance of new working fluids for the organic Rankine cycle technology.




## 2. Prediction of thermophysical properties

The thermophysical and transport properties of new working fluids can be predicted based on their molecular structure, and other core properties.

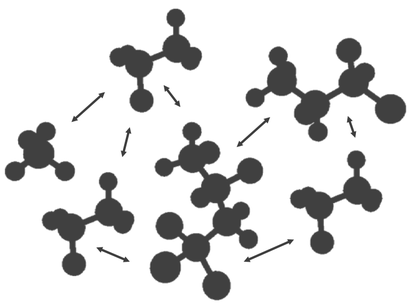
Predicting the properties of new working fluids imposes a compromise between the prediction accuracy and the amount of available information of the working fluid.




NanoORC investigates the combination of different predictive techniques for thermophysical properties to improve the overall accuracy of the predicted values.

## 4. Mixtures

The simplest approach to predict the behavior of mixtures of new working fluids consists of weighing the contribution of each component according to their mutual interaction.



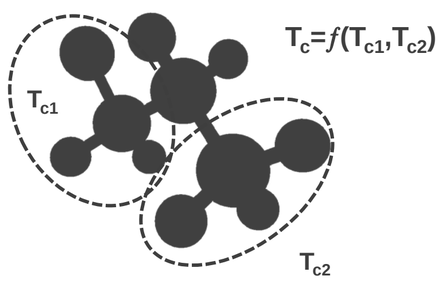
Mixing parameters

Equation of state for mixtures

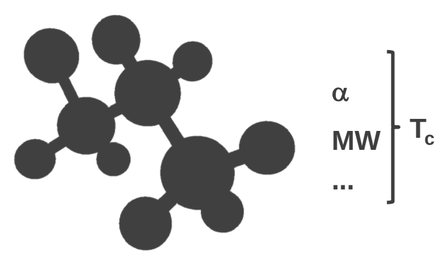
Mixing parameters in equations of state represent the mutual interaction (attractive and repulsive forces) of the mixture components' molecules. The mixing parameters for new fluid pairs can be estimated based on the molecular structure of the components.

## 3. Pure fluids

The most accepted approaches for property prediction are group contribution methods (GCMs) and quantitative structure–property relationship (QSPR) methods.




**GCMs** divide molecules in different functional groups for which the contribution to the total value of a specific property is known.




**QSPR** methods relate a property with molecular numerical features derived theoretically from the chemical structure.

### Partners

DTU

Turboden srl.

### Acknowledgements

The project is funded by the European Union's Horizon 2020 research and innovation programme under grant agreement No 704201 (project NanoORC). The financial support is gratefully acknowledged.

DTU Mechanical Engineering
Department of Mechanical Engineering
DTU Mechanical Engineering
Department of Mechanical Engineering
DTU Mechanical Engineering
Department of Mechanical Engineering