LITHUANIAN ENERGY INSTITUTE

ADMISSION TO PHD STUDIES FOR THE YEAR 2023

DOCTORAL RESEARCH TOPIC:

Investigation of heat and mass processes by Molecular Dynamics methods

RESEARCH FIELD:

Energetics and Power Engineering (T 006)

BRIEF DESCRIPTION OF RESEARCH TOPIC:

For the evaluation of water evaporation/condensation processes, empirical regularities are used, which allow to estimate change of phases approximately in the macro-scale, but they are completely inconsistent with reality and may even be misleading in the micro- or nano- scales. In addition, creation of sufficiently accurate numerical models for drying various materials (eg biomass), requires to assess the water diffusion in the material in a sufficiently precise manner, which is very expensive or even mot always possible by experimental methods. Another important challenge is the heat and mass transfer processes in nano-channels, which experimental studies are also not always possible.
At present, the power of computers has already reached such a level that numerical studies are already available that would allow by the Molecular Dynamics methods to model heat and mass exchange processes with sufficient precision numerically. The aim of the research is to determine the regularities of heat and mass processes in nano-scales by methods of molecular dynamics.

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