# **Master thesis**

Investigation of the influence of different wood polymers on their compaction behavior by using molecular dynamic simulation (MD-simulation)



# **BACKGROUND:**

The need to increase the use of renewable biomasses for energy supply, such as fuel pellets or briquettes is significant. In contrast, the automation of fuel production is not trivial. In order to produce high-quality pellets and briquettes, many years of experience in the operation of fuel production plants are necessary so that the requirements for the physical-mechanical fuel properties. can be fulfilled. However, to study the influence of individual wood polymers, they were separated in the laboratory and studied already individually during densification. The different wood polymers (lignin, cellulose, hemicellulose, etc.) react under high pressure different.

With this background, the theoretical principles for the compaction of woody biomasses are to be developed within the scope of a master's thesis and the densification of wood polymers is to be investigated with molecular dynamic simulation (MD-simulation). A software tool based on the MD is available for processing. Theoretically as well as practically, the following key areas of work result from this:

# **YOUR TASKS:**

- Determination of the state of the art in science and technology for the densification of woody biomass.
- Establishing a MD-Simulation of the previously created laboratory experiments from literature with the help of a MD simulation tool (LAMMPS)
- Understanding the influence of different types of wood polymers during densification and re-expansion (after pressure release) by parameter variation
- Validation of the simulation by laboratory experiments and verification of the setup used by sensitivity analysisEvaluation of results and derivation of raw material- and process-specific recommendations for further development

## **YOU HAVE:**

- Bachelor degree in natural or engineering sciences
- Results-oriented work and ability to analyze tasks and problems fast

## WE OFFER:

- A good introduction to the topic as well as competent and motivated support in the processing of the tasks
- A family-friendly, modern working environment in a collegial working atmosphere
- Good public transport connections

#### **BEGINNING:**

01.12.2024

## **DURATION:**

16 weeks

## LANGUAGE:

English

#### **PROCESSING LOCATION:**

Deutsches Biomasseforschungszentrum, Torgauer Straße 116, 04347 Leipzig

# **CONTACT:**

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## **APPLICATION DOCUMENTS:**

Please submit your compelling application (in a single attachement, preferably as pdf, max. 5 MB) e-Mail: bewerbung@dbfz.de

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