



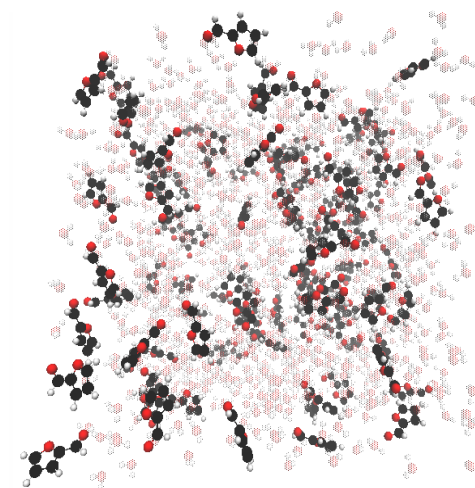
The European Materials Modelling Council

The presentation of an idea for the project

The presenter is: Inna Ermilova*,
inna.ermilova@mmk.su.se

A call topic number is: DT-NMBP-10-2019

The main contact is: Alexander Lyubartsev*,
alexander.lyubartsev@mmk.su.se



The project: **Finding out optimal conditions for hydrothermal carbonization processes and tailoring properties of new materials using molecular dynamics simulations**

* *Department of Materials and Environmental Chemistry,
Stockholm University, Sweden*



**Stockholm
University**

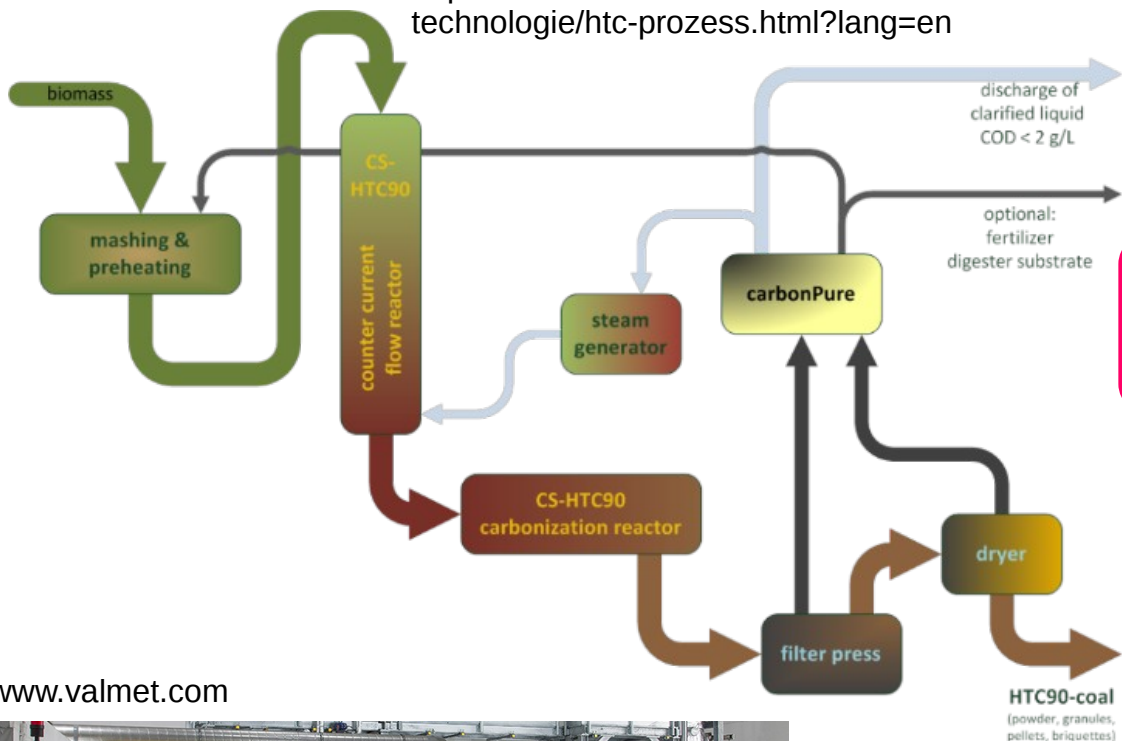


The European Materials Modelling Council

The main objectives and innovative aspects

Industrial process

<http://www.cs-carbonsolutions.de/cs-technologie/htc-prozess.html?lang=en>



www.valmet.com



Computational approach

Developing models for molecular dynamics simulations

Running MD simulations for different components and thermodynamic conditions; analyzing trajectories

Developing materials using parameters for the process from simulations and characterizing them

Obtaining the material with desired properties

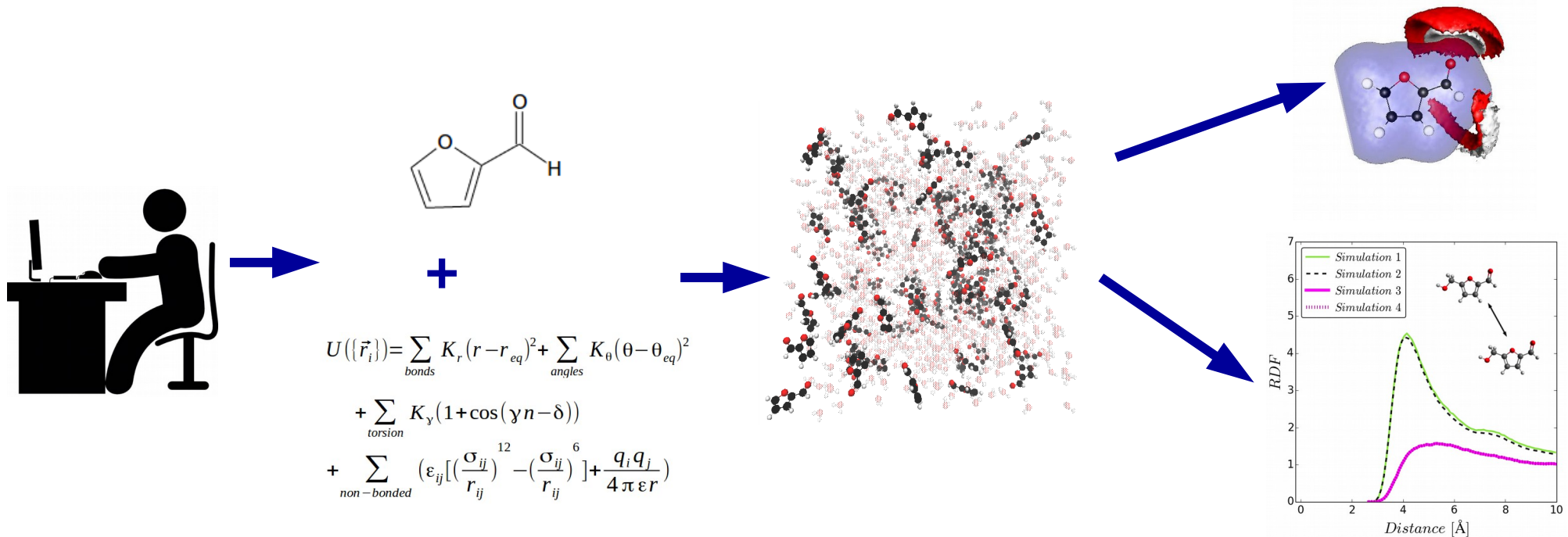
INNOVATION: Molecular modelling of these processes in hydrothermal conditions hasn't been done before so as behaviour of the compounds wasn't studied not only by modelling but even by experimental techniques.



The European Materials Modelling Council

The main objectives and innovative aspects

- Obtaining models which will help to control and “tailor” properties of future materials
- Optimal parameters for industrial processes
- Environmentally friendly production of new materials
- * Have already done preliminary simulations for hydrothermal carbonization (HTC) conditions for furfural and 5-hydroxymethylfurfural





The European Materials Modelling Council

The expected impact, available buildings, partners?..

Expected impact:

- Reduced costs of the development of materials by preliminary computer modelling of the synthesis process
- Development of environmentally friendly materials from naturally abundant sources

Available buildings and partners:

- Computational work can be done at Stockholm's University
- Collaboration is desired:
 - * lab on experimental characterization of HTC process (IR, NMR, X-ray etc.)
 - * industrial partners for demonstration



The European Materials Modelling Council

Acknowledgements

Alexander Lyubartsev for bringing up the idea and supervision

Fredrik Grote for doing the bachelor thesis entitled “Molecular Dynamics Simulations of Furfural Derivatives at Conditions of Hydrothermal Carbonization”



HPC2N - High Performance Computing Center North



PDC CENTER FOR
HIGH PERFORMANCE COMPUTING

