HPC Multi-physics Biomass Furnace simulations as a Service

Xavier Besseron¹
Henrik Rusche², Bernhard Peters¹, Alban Rousset¹
Ralfas Lukoševičius³, Linas Paukštaitis³, Laimonas Narbutas³

1: University of Luxembourg
2: Wikki GmbH, Germany
3: Enerstena UAB, Lithuania

11th International SuperComputing Camp 2020
→ Virtual

Nov. 30th to Dec. 11th 2020
http://www.sc-camp.org/
Challenges in the simulation of biomass combustion
Introduction

Biomass combustion (e.g. wood chips)
- widely used for generating electric and thermal energy
- renewable and potentially carbon-neutral energy source

Combustion process
- very complex
- requires advanced techniques to minimize harmful gas emissions

Alternative biomass
- wood waste, straw, bark, olive pits, nut shells, grain husks, bagasse, etc.
- can cause problems due to their chemical composition, ash melting temperature, humidity, ash content, calorific value and others.
Combustion process in a biomass furnace

Combustion chamber of a biomass furnace
- forward acting grate
- transports the fuel through the furnace

The fuel undergoes a number of steps
- drying, pyrolysis, char burning, cooling in which it releases hydrocarbons.
- hydrocarbons are burned in the gas phase

Use numerical simulations
- to study efficiency and performance
- and reduce the costs of experiments
Numerical Approach: Multi-Physics Simulation

Two-way coupling between Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD)

**XDEM** (Lagrangian) for:
- Motion and collisions of biomass particles
- Conversion of biomass particles

**OpenFOAM** (Eulerian) for:
- Flow of gas phase
- Reactions in the gas phase

CFD-DEM coupling is required to capture the physics of biomass furnaces and offers unprecedented insight.
Complexity of biomass furnace simulations

The setup, execution and post-processing of biomass furnace simulations is challenging.

The necessary steps include:
- Generation of furnace and grate geometry
- CFD mesh generation and CFD case setup
- Calculation of the initial particle bed
- DEM case setup
- Calculation of fuel properties from ultimate analysis

This complexity is a serious obstacle, in particular for SMEs
- The adoption of such technologies requires substantial investment in computer hardware, software licenses and training of engineering staff.
HPC Multi-physics Biomass Furnace simulations as a Service

a simplified workflow for end user
CloudiFacturing Overview

- The CloudiFacturing solution is designed to support manufacturing SMEs and their needs for advanced cloud- or HPC-based ICT solutions.
- The CloudiFacturing solution will be open, empowering different stakeholders to become members of the community.
- All the services offered in the CloudiFacturing Solution will be based on a pay-per-use or subscription business model with a unified billing process.
Objective: a simple user workflow

From the spreadsheet to the report

Prepare Input File
- define the geometry and the settings of the furnace
- based on a Spreadsheet

Submit Input File
- via the CloudiFacturing web portal

Run the Simulation
- on the HPC platform
- no interaction needed from the user

Visualize the results
- download archive from the web portal
- pre-generated report
Spreadsheet Input File

Automatic generation of the CFD+DEM case

Furnace Geometry

Fuel composition

Air inlet settings
Job submission

Biomass Furnace Simulation Workflow

Welcome! This workflow takes an Excel file that contains the input parameters of a bio mass furnace simulation. The simulation uses XDEM (discrete particles) and foam-extend (computational fluid dynamics). It automatically generates all necessary inputs (geometry, mesh, input files) and returns a report for download.

Workflow steps
1. Select input Excel file
2. Perform simulation
3. Download results

Step 1: Excel-file selection
Select the Excel file that contains the inputs for the furnace simulation.

Choose selected file
Reset tree

HPC Simulation

HPC job running
The job is running but didn’t set its own status yet. Please wait ...

DPM Input File: biomass_furnace_3D.h5
DPM Output Directory: /output_biomass_furnace_3D/

Progress Report

HPC Multi-physics Biomass Furnace simulations as a Service
Simulation Results

Download link

Average bed surface temperature over time

Average particle composition over the bed length

Report
Under the hood
How to much input is required?

Furnace and grate design
• parametrised with a few numbers
• geometry is generated automatically

Fuel / Wood chip
• characterised by ultimate analysis
• thermo-physical values obtained from standard experiments

Air inlets
• can be placed at any position
• require the full composition when recirculation is used

→ A few hundred degrees of freedom!
• Designing and implementing a web interface was out of scope
Internal workflow

Particle bed generation
Mesh generation
DEM case setup
CFD case setup
HPC Furnace Simulation
Post-processing
Report

HPC Multi-physics Biomass Furnace simulations as a Service
SC V-Camp 2020
HPC Biomass Furnace Simulation

Two-way Direct Coupling
- DEM → CFD and CFD → DEM
- XDEM and OpenFOAM linked into one executable
- All coupling data exchange via shared memory

Hybrid Parallelization Scheme
- OpenFOAM running in parallel using MPI
- XDEM parallelized using OpenMP

HPC Execution
- Portable execution using Singularity
- HPC Job submission using SemWES
- Execution on IT4Innovations HPC platform
Biomass Furnace simulation using XDEM+OpenFOAM
Summary and Future Work

Multi-Physics Biomass Furnace Simulation
• Cloud-based interface and submission portal
• HPC execution back-end
  → Application as a Service (AaaS)

Simplified Workflow for end user
• All input settings provided in a spreadsheet
• Automatic generation of the case
• Automatic execution on HPC platform
• Generation of a report with the results

Part of the CloudiFacturing project
• Experiment 15 BioOpt
• To be integrated in the Digital Marketplace
• Target audience: SMEs
Thank you for your attention!


Acknowledgement

The project CloudiFacturing receives funding from the European Union’s Horizon2020 research and innovation programme (Grant No. 768892).