

A CFD-based approach for thermochemical conversion of straw

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Abstract

In the framework of the development of an organic Rankine cycle (ORC), a straw fired small-scale furnace is analyzed and improved. It is intended to support this process with simulations in Computational Fluid Dynamics (CFD). In this study, the sub-model for the fire bed to be used for the CFD simulation is introduced. An existing model was improved and adapted for straw combustion. The model is designed as porous medium approach and covers evaporation of moisture, pyrolysis, gasification and combustion as well as heat and mass transfer. Simulations of a small biomass particle have been conducted to test the solver and its applicability to various types of biomass.

Introduction

Reduction of greenhouse gas emissions in power production is considered to be the main option in preventing or at least limiting global warming. While solar and wind power are fluctuating sources of renewable energy, biomass can be used in combined heat and power (CHP) systems on demand. For solid biomass, combustion is one of the main conversion technologies and is the base for water steam and organic Rankine cycles (ORC).

One of the main challenges in small-scale biomass combustion is emission reduction, especially when considering solid biomass fuels like straw or other agricultural residues. Emissions produced during biomass combustion are harmful for health and environment. One way to reduce pollution formation is to optimize the combustion chamber and process parameters using CFD.

Computational Fluid Dynamics (CFD) is an excellent supplement to practical experiments for the design and optimization of biomass combustion appliances. With the possibility to quickly and individually change parameters, it accelerates the development of stoves and boilers.

Biomass combustion is difficult to model, as various processes are involved and many details have to be considered. To account for this complexity, a CFD-based simulation is divided into bed model, gas phase reaction in the freeboard and additional models as it is shown in figure 1. For each step, there are several possibilities for realization.

Our research group develops a modular system containing various kinds of models for each section. These models can be combined to build a suitable CFD-simulation for the examined stove. Thus, it is possible to examine the parts of interest closely while simplifying other model components to save computational effort. A broad range of technology used in biomass combustion can be described and analyzed by this method.

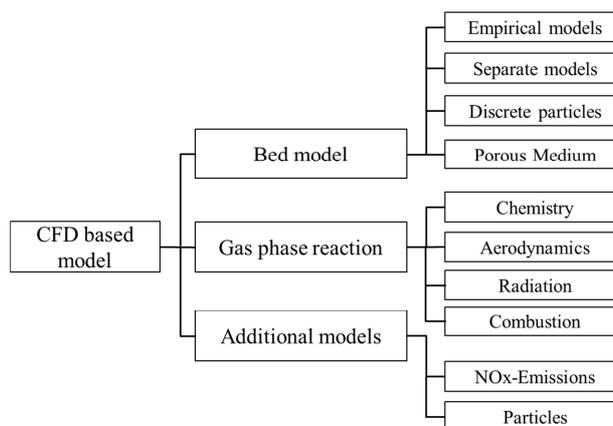


Fig. 1. Structure of a CFD-based model for biomass combustion in small-scale furnaces

Bed models

The bed model presented in this paper is part of the toolbox for CFD-based simulations. It can be easily adapted for various types of biomass, considering differences in shape as well as in physical and chemical properties. For this study, it is prepared to be used in the simulation of a straw fired furnace, which is part of an ORC system.

During thermochemical conversion in a fire bed, biomass passes through the phases drying, pyrolysis, gasification and combustion. The bed model contains all four phases and provides the results as input information for the gas phase simulation. In thermally thick fuel particles some of the steps may overlap or occur simultaneously.

A simple method to provide input data for gas phase reactions, is an empirical or semi-empirical model. For this purpose, fuel gas composition, mass flow and temperature are measured and used for the simulation. For a semi-empirical model, calculations based on measurements are made to provide input-data [1].

Separate bed models compute the thermochemical conversion of biomass independently from the CFD-domain and the result is used as boundary condition for

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Proceedings of the European Combustion Meeting 2015

the gas phase reaction. Depending on the application, the models can be 0- to 3-dimensional. Especially 1-dimensional bed models are widely used, because they deliver good results at reasonable effort. Bed model and CFD-domain are often coupled using radiative heat flux of the flame to set the temperature in the bed model and the volatile composition as fuel gas [2, 3].

For small-scale furnaces with bulk material like wood chips or pellets, a model that describes the conversion of each particle separately and considers the interaction between particles is suitable. This can be realized by using models based on Discrete Element Method (DEM) for the bed [4].

One possibility to approach the simulation of the fire bed is to describe the biomass as porous medium inside the CFD domain. This approach has become more popular since computational resources have advanced [5, 6]. The advantage of using a porous medium bed model is the presence of the bed as physical domain inside the CFD-simulation. In this way, the interaction between fluid flow and solid bed can be described. Not only the exchange of information about temperature and fuel gas composition, but also the influence of the bed on the flow field can be examined.

Straw combustion

Firing straw is challenging, because the high content of ash combined with low melting temperature leads to fouling and slagging inside the stove [7]. Inorganic salts cause formation of pollutants and the release of corrosive substances like hydrochlorid acid [8]. In addition, inorganic salts catalyze pyrolysis reactions [9]. To meet those challenges, simulations are used for stove design and improvement.

Straw is in many cases fired in furnaces with a moving grate. To simulate the decomposition of straw along the grate, a two-dimensional approach is commonly used. The models are developed as separate models, which are coupled with CFD code [10 – 12].

As deposition of ash inside the stove is often a reason to use CFD simulations for prediction and optimization several publications address this topic [7, 13]. The amount of deposited ash as well as its influence on fluid flow inside the stove and heat transfer to the outside is analyzed.

Aerosols consisting of fine ash particles are formed in the flue gas due to reactions of precursors released during biomass combustion. Nucleation, growth, motion, agglomeration, coagulation, precipitation and surface reactions of these particles can be described by the General Dynamic Equation (GDE) [8, 14]. Models to predict the formation and behavior of aerosols are developed to analyze the mechanisms and influences behind particle formation.

ORC technology

The organic Rankine cycle (ORC) uses an organic fluid as working medium. Usually, a second cycle with thermal oil is used for the transport of heat from the combustion chamber to the organic cycle to prevent the

organic working fluid from overheating. An example for a typical ORC cycle is given in figure 2.

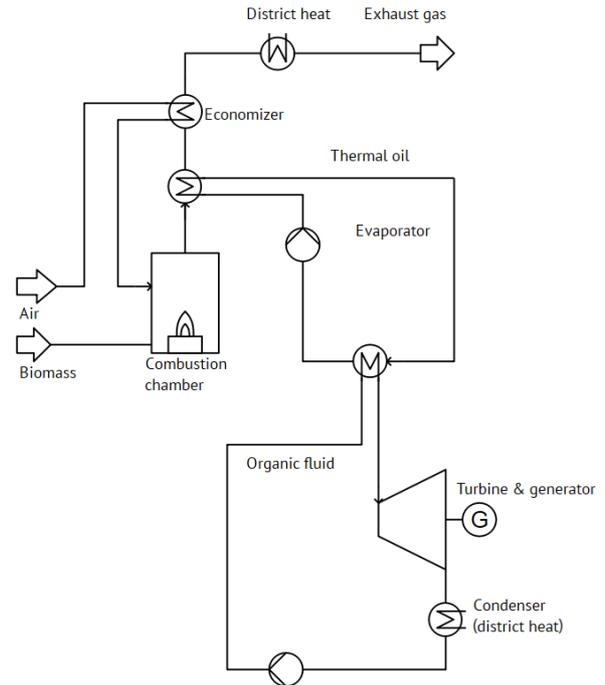


Fig. 2. Flow scheme for a typical organic Rankine cycle (ORC)

Methods

Calculations are conducted with the open source CFD software OpenFOAM 2.1.1 with the additional solver *biomassGasificationFoam* by Kamil Kwiatkowski [15]. The solver has been developed and validated for gasification of wood (*robinia pseudoacacia*). For this study it has been adapted to be used for combustion of straw. On that account, the property data of biomass were changed according to table 1. In addition to that, reactions for char gasification, char combustion and homogeneous gas phase combustion were added.

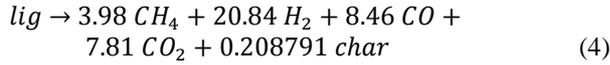
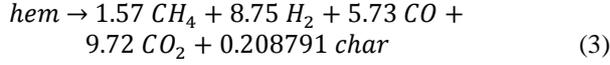
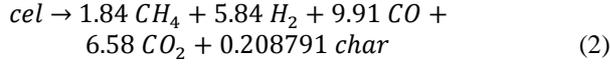
The straw particle is treated as porous medium inside the computational domain. Therefore, the flow of air is influenced by the presence of the particle. The porosity of the biomass particle changes during combustion due to the decomposition process. Governing equations of the code are described in detail in [3]. Solid components are represented by the species *hum* (*humidity*), *cel* (*cellulose*), *hem* (*hemicellulose*), *lig* (*lignin*), *char* and *ash*.

The model used in this study covers evaporation of moisture, pyrolysis, gasification and combustion for a fire bed of biomass. An Arrhenius expression is used to describe the kinetics of reaction (1) for evaporation.



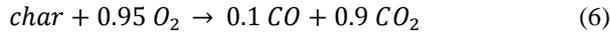
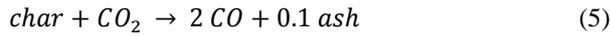
Pyrolysis is described by a mechanism based on the three components *cellulose*, *hemicellulose* and *lignin*. The decomposition of each component into gas and

char is described by an own reaction (equations (2-4)) with individual kinetic parameters [16].

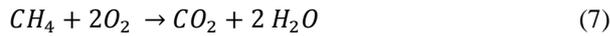


The advantage of this mechanism is the possibility to adapt it to other types of solid biomass fuels by changing the mass fraction of the solid pseudo-components. In addition, the composition of the fuel gas leaving the bed after pyrolysis depends on the content of *cellulose*, *hemicellulose* and *lignin* and changes with stage of combustion.

Gasification of *char* is represented by equation (5) [17], *char* combustion by equation (6). Reaction and kinetics of *char* combustion are based on [5].



Combustion is approximated by a global one step reaction for combustion of methane (eq. (7)). As this study focuses on the decomposition of straw during combustion, the gas phase reactions have been kept simple to save computational effort.



Heat transfer is implemented in the model according to [3]. Temperature of gas T and solid T_s are not equal and the heat transfer between phases is controlled by equation (8).

$$Q = \alpha \Sigma (T - T_s) \quad (8)$$

Q is the transferred quantity of heat, α is the heat transfer coefficient and Σ is the surface area of pores per solid state volume [3].

A single biomass particle during thermogravimetric analysis (TGA) is simulated. Geometry and mesh are the same as in [15]. A simple hexahedral mesh is used to represent the biomass particle and the cubic chamber around it, as it is shown in figure 3.

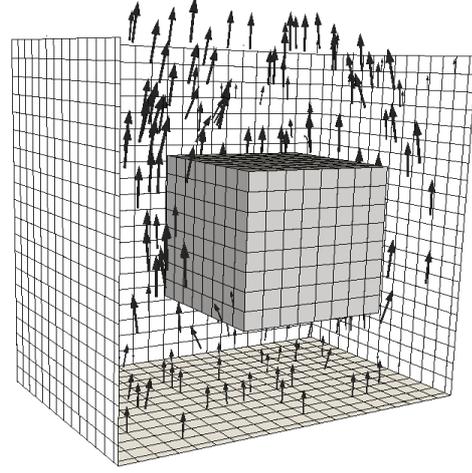


Fig. 3. Mesh used for the simulation of a single particle of wood and straw (based on [15])

A mixture of nitrogen (79 %) and oxygen (21 %) was introduced at the inlet on the bottom of the TGA chamber. Product gases left through the outlet at the top. Heat was applied by setting the temperature of bottom and walls according to a heating profile of 1 K/s. Heating started at 300 K and the temperature was kept constant after 1300 K were reached. Property data for wood and straw were chosen as stated in table 1. All other parameters were kept at constant values.

Table 1. Property data for wood and straw used in the simulations. Reference is given for straw; all data for wood are taken from [15]

	Wood	Straw	Ref
Moisture (w-%)	0.07	0.075	[11]
Cellulose (w-%)	0.359	0.398	[18]
Hemicellulose (w-%)	0.276	0.305	[18]
Lignin (w-%)	0.285	0.157	[18]
Ash (w-%)	0.01	0.065	[18]
Porosity (-)	0.45	0.58	[10]
Density (kg/m ³)	1480	410	[10]
Pore size (m)	10 ⁻⁶	3.7·10 ⁻³	[10]
Heat capacity (J/kgK)	1380	2238	[10]

Results

In figure 4 the normalized masses of wood and straw particle during TGA are compared. The steps of evaporation, pyrolysis of the individual pseudo-components and *char* combustion can be identified clearly. Evaporation occurs first and almost simultaneously for both samples. During the pyrolysis of *hemicellulose* and *cellulose*, straw decomposes faster than wood. During *char* combustion the mass of the wood sample decreases more rapidly. The remaining mass is lower for wood, because its *ash* content is smaller. Because of the small size of the samples, differences in heat transfer do not affect the decomposition strongly.

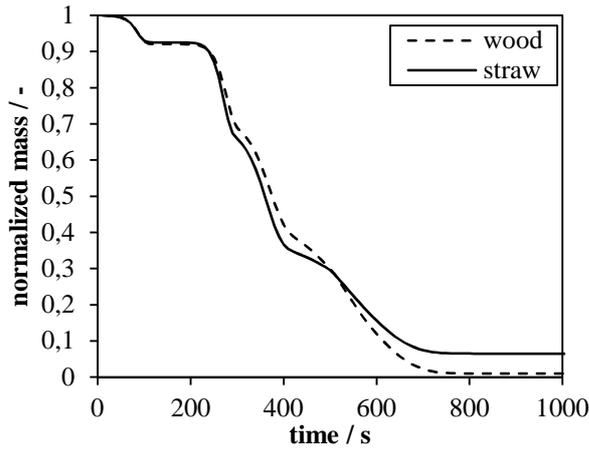


Fig. 4. Normalized mass of straw and wood particle during combustion

In figure 5 the decomposition of wood in the center of the modeled biomass particle is shown. The density of the individual components is presented in the illustration. First *humidity* evaporates, this process is completed after about 120 s when 420 K are reached. Pyrolysis of *hemicellulose* starts at 170 s and is almost completed, when decomposition of *cellulose* starts at about 300 s (600 K). *Lignin* is the last component to be decomposed, and the process takes the longest time to be completed. During the decomposition of the single components *char* is formed. Beginning at about 500 s (800 K) more *char* is consumed by *char* combustion and gasification than new *char* is formed. Therefore the density of *char* decreases from this point on. The amount of *ash* produced during gasification and combustion is too small to be observed in the presented figure. *Ash* is the only component remaining after evaporation, pyrolysis, gasification and combustion.

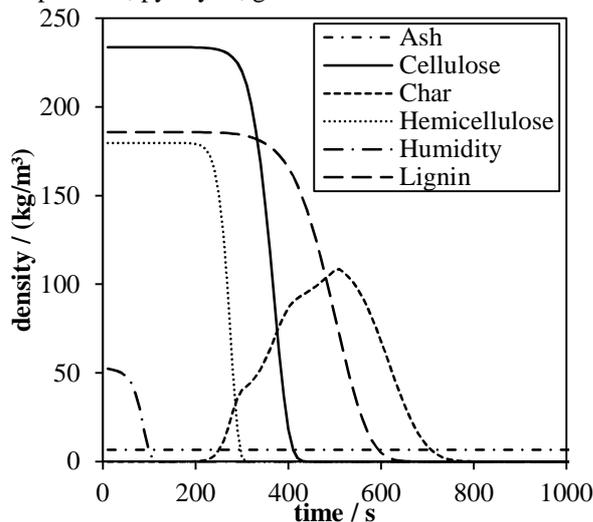


Fig. 5. Combustion of a wood particle in a TGA chamber with a heating rate of 1 K/s

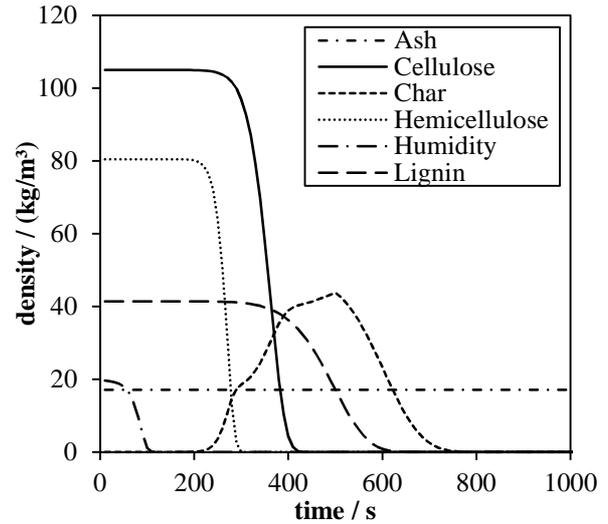


Fig. 6. Combustion of a straw particle in a TGA chamber with a heating rate of 1 K/s

In figure 6 the decomposition of straw is shown. In contrast to wood the *lignin* content is smaller, but significantly more *ash* is present. The densities of the components are lower for straw, because the initial density of straw is smaller and its porosity is higher.

The release of gases during combustion of the biomass particle is shown in the following figures (Fig 7 – Fig. 10). The individual decomposition of the pseudo-components *hemicellulose*, *cellulose* and *lignin* can be distinguished clearly in the peaks of the profiles. The first peak represents pyrolysis of *hemicellulose*, followed by *cellulose*. The slow decomposition of *lignin* can be found in the third peak.

Because of the smaller mass of the straw particle, the concentration of product gases emitted by straw is lower. The differences in composition can also be observed in the gas release profiles. Especially during *lignin* pyrolysis, the concentrations of methane and hydrogen deviate strongly between wood and straw. This is due to the lower *lignin* content of straw.

Methane combustion is considered in the code, but it appears only at high temperatures. When these temperatures are reached, most of the methane is already carried out.

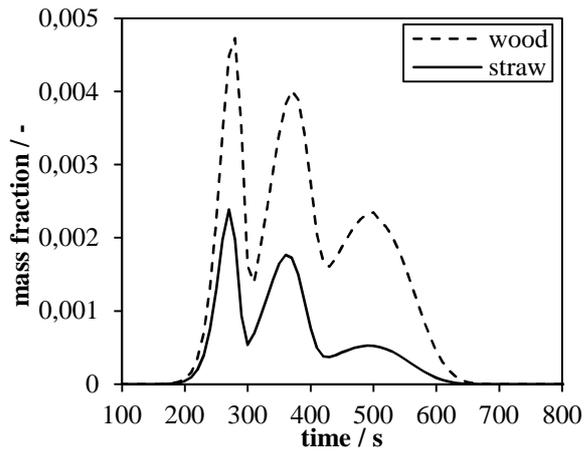


Fig. 7. Release of CH_4 during combustion of biomass particle; heating rate 1 K/s

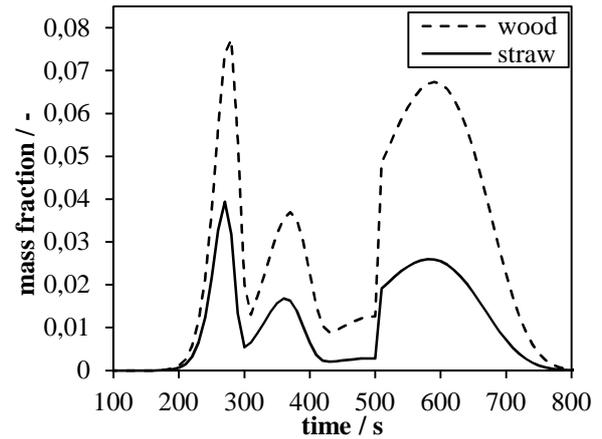


Fig. 10. Release of CO_2 during combustion of biomass particle; heating rate 1 K/s

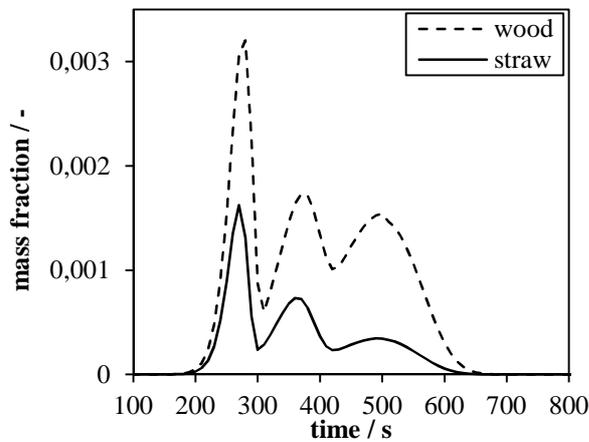


Fig. 8. Release of H_2 during combustion of biomass particle; heating rate 1 K/s

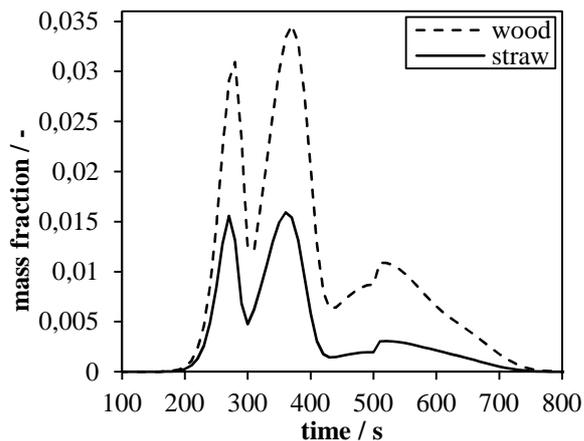


Fig. 9. Release of CO during combustion of biomass particle; heating rate 1 K/s

The profiles of CO and CO_2 (Fig. 9 and Fig. 10) show the same tendency as the other gaseous species during pyrolysis. The third peak is caused by *lignin* decomposition and *char* combustion which starts at 500 s, when the minimum temperature for *char* combustion (800 K) is reached. This behavior is more distinct for CO_2 than for CO .

Conclusions

The solver *biomassGasificationFoam* offers many features and has important mechanisms implemented. Therefore, it is an ideal basis for CFD simulations of biomass combustion in OpenFoam. As it is shown in this study, it is possible to simulate the combustion of various types of biomass by changing only property data. Still, enhancement regarding pyrolysis model and gasification and combustion mechanisms is needed. Further investigation of these issues is planned. In addition it is intended to use the solver for simulations of small-scale biomass combustion.

Acknowledgements

The work presented in this study has been supported by KIC InnoEnergy SE within the KIC Innovation Project “Construction of cogeneration system with small to medium size biomass boilers” (Reference: 13_2014_IP92_BioORC).

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