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Computational fluid dynamics modeling of biomass fast pyrolysis in a fluidized bed reactor, using a comprehensive chemistry scheme

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HIGHLIGHTS

- We have used an advanced kinetic model for pyrolysis coupled with CFD in 3D.
- The yields are compared to experimental results and shows a not too far-off prediction.
- The simulations are very time consuming but makes it possible to explore secondary reactions.
- For example, a number of thermal cracking reactions are applied to the tar components to see the effect.

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ABSTRACT

The CFD modeling for fast pyrolysis has previously focused on the major pyrolysis products; liquid, char and gas. This paper introduces a new approach to biomass pyrolysis; integrating a complex scheme of reactions including formation of such components as levoglucosan. The 3-D simulation takes into account the complex breakdown of each biomass subcomponent, the fluid dynamics of the process as well as the heat and momentum transfer of three Eulerian phases.

The pyrolysis products include reference species that reflects the composition of the bio oil, gas fraction and char fraction. A number of reactions are in addition applied to account for the thermal cracking of tar compounds and the final compositions are compared to experimental yields. The results show that the predicted pyrolysis products reflect the experimental yields satisfactorily, apart from the water content which is under predicted. Most importantly though, the approach is computationally feasible and it should be useful for future work.

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1. Introduction

Pyrolysis of biomass is considered as a potential source of fuel for various applications such as transportation, combined heat and power production as well as reduction agents. From a practical standpoint, *fast pyrolysis* means processing with optimized conditions for liquid production which implies fast heating rate and a temperature not exceeding 500 °C.

Modeling such processes is challenging in many ways and even more so in fluidized bed reactors. Those challenges are linked to the complex thermo-physical environment of fluidized bed reactors and the complex structure of biomass and the decomposition with an immense number species as products.

Much of the earlier CFD simulation work assumed three superficial components as representatives for the liquid, gaseous and solid components. Some studies elaborated on the non-uniformity of a reacting biomass particle and some studies focused more on the kinetics and the composition of the samples related to pyrolysis products [1]. No one has yet been able to device a complete model which takes into account all phenomena of fast pyrolysis in fluidized beds but both approaches improved the outcome and lead to increased understanding.

From the CFD direction, Papadikis [2] argues that: “The most crucial of the assumptions is that the particle is assumed to maintain uniform temperature along its radius”. In contrast, Dupont et al. [1] claims that “the accurate knowledge of the reaction kinetics appears to be a crucial parameter for a reliable modeling of the pyrolysis process”. This work can be seen as a unifying effort, where the in-depth chemistry is included in a comprehensive CFD model which accounts for heat and mass transfer as well as entrainment of particles.

Previously, a CFD model was developed (described in Mellin et al. [3]) with a two phase framework for time-effectively studying the behavior of the gas. Now this model has been extended in order to report the specific components of pyrolysis and thus obtain a composition of the liquid, gas and char. Therefore a new kinetic model has been implemented as well as a third

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Nomenclature

Alphabetic letters

A	pre-exponential factor (s^{-1})
a	interfacial area concentration ($m^2\ m^{-3}$)
C	heat capacity ($J\ kg^{-1}\ K^{-1}$)
c	coefficient (–)
d	diameter (m)
E	activation energy ($J\ mol^{-1}$)
e	coefficient of restitution (–)
g	gravitational acceleration ($m\ s^{-2}$)
h	heat transfer coefficient ($W\ m^{-2}\ K^{-1}$)
K	momentum exchange ($kg\ m^{-3}\ s^{-1}$)
k	heat conductivity ($W\ m^{-1}\ K^{-1}$)
m	mass (kg)
Q	heat transfer (W)
q	heat transfer per surface area ($W\ m^{-2}$)
R	universal gas constant ($J\ mol^{-1}\ K^{-1}$)
S	source term, due to e.g. reactions ($[kg, J\ldots]\cdot m^{-3}\ s^{-1}$)
T	temperature (K)
t	time (s)
u	intrinsic velocity ($m\ s^{-1}$)
v	velocity ($m\ s^{-1}$)
Y	mass fraction (–)

Greek letters

α	volume fraction (–)
ρ	density ($kg\ m^{-3}$)
μ	viscosity (Pa s)
π	pi (–)
τ	stress (Pa)
φ	sphericity (–)

Dimensionless numbers

Re	Reynolds number (-)
Pr	Prandtl number (-)
Nu	Nusselt number (-)

Common subscripts

g	gas
s	sand
b	biomass
i	any specie
mf	minimum fluidization
D	drag

Eulerian phase which in greater detail renders the biomass flow. Experiments are in addition made alongside the simulation to compare with the results. More information on the basis of the numerical model can be found in the previous publication [3], as well as more details on tuning of the drag law. The far-reaching purpose of the work is up-scaling of the technology.

In this paper, the pilot reactor is firstly described with analysis results of the pyrolysis products. Then the numerical model is described with focus on the additions to the previous work; finally the results, comparison with experiment, discussion and conclusion is presented. Throughout the work we made extensive use of User Defined Functions (UDF) and solution methods included in the commercial software package ANSYS Fluent 14.5.

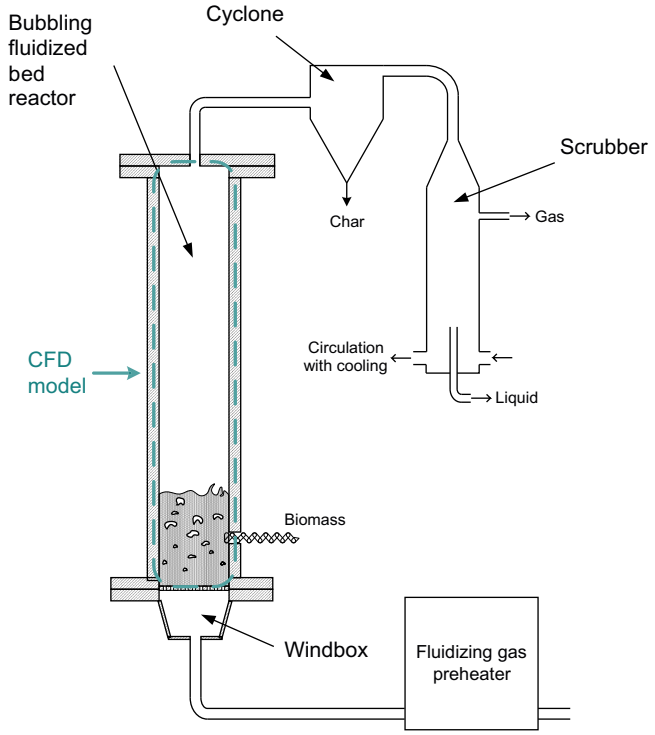

Fig. 1. Cross section of the bubbling fluidized bed reactor system with boundaries indicated for the CFD model.

2. Pilot reactor

A pilot fast pyrolysis setup with has been assembled at KTH, Sweden. The setup includes a preheater for the fluidizing-gas, the fluidized bed reactor, a cyclone and a scrubber. A schematic overview of the plant is shown in Fig. 1, with the domain of the CFD model indicated.

The biomass is introduced by a screw feeder directly into the fluidized bed at height of 5.75 cm above the distributor plate. The biomass is fed at rate of 2 kg/h, which is the designed capacity of the rig. The biomass is a mix of pine and spruce, see proximate and ultimate analysis in Table 1.

The gas species and the main groups of bio oil components are given in Table 2 which is reported in Kantarelis et al. [4], therein referred to as case *S/B: 0*. All specific components of the bio oil can be found in the same paper as well as the measurements methods and more detailed descriptions of the plant.

Table 1
Biomass composition [4].

Analysis	Parameter				
	Moisture (wt%)	Volatile matter (wt%)^{db}	Ash (wt%)^{db}	Fixed carbon (wt%)^{db}	HHV (MJ/kg)
Proximate analysis	9.8	83	0.31	16.6	20.46
	C, wt%^{db}	H, wt%^{db}	O^{a}, wt%^{db}	N, wt%^{db}	S, ppm^{db}
Ultimate analysis	50.7	6.1	42.71	0.18	<120

[a] By difference.
[db] Dry basis.

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