Dynamic Modeling of a BioGrate Boiler

Alexandre Boriouchkine





DOCTORAL DISSERTATIONS

Dynamic Modeling of a BioGrate Boiler

Alexandre Boriouchkine

A doctoral dissertation for the degree of Doctor of Science in Technology to be presented with due permission of the Aalto University School of Chemical Technology for public examination and debate in Auditorium KE2 (Komppa Auditorium) at the Aalto University School of Chemical Technology (Espoo, Finland) on the 17th of June, 2016, at 12 noon.

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Aalto University publication series **DOCTORAL DISSERTATIONS** 92/2016

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ISBN 978-952-60-6808-4 (printed) ISBN 978-952-60-6809-1 (pdf) ISSN-L 1799-4934 ISSN 1799-4934 (printed) ISSN 1799-4942 (pdf) http://urn.fi/URN:ISBN:978-952-60-6809-1

Unigrafia Oy Helsinki 2016

Finland



441 697 Printed matter



Author

| Permission to publish grant | ad (data) 27 April 2016 | Languago English |
|-------------------------------|--------------------------|----------------------------------|
| Manuscript submitted 6 Nov | vember 2015 | Date of the defence 17 June 2016 |
| Field of research CHEM006 | 3Z Chemical Technology | |
| Series Aalto University publi | cation series DOCTORAL | DISSERTATIONS 92/2016 |
| Unit Department of Biotechno | ology and Chemical Techn | ology |
| Publisher School of Chemica | l Technology | |
| Dynamic Modeling of a BioGra | ate Boiler | |
| Name of the doctoral disse | rtation | |
| Alexandre Boriouchkine | | |
| | | |

Abstract

Biomass utilization in energy production through combustion is regarded as an efficient alternative to consuming diminishing fossil natural resources. Furthermore, biomass is not only a naturally replenishable energy source, but is also CO2 neutral, and thus it is a sustainable option to satisfy the ever-growing energy demand. Existing combustion technologies such as industrial boilers and furnaces can utilize renewable fuels to a certain degree only, mainly when blended with traditional fossil fuels. Consequently, new technologies have been developed, such as BioGrate boilers, which can fully benefit from biomass fuel.

Furthermore, future energy systems will comprise an increasing variety of energy sources for flexible energy generation. This will impose new challenges on boiler systems in terms of rapid changes in power demand and the ability to operate under low-load conditions. Thus, the development of these systems will require an insight into the combustion process for the optimal design and operation of energy boilers. Mathematical modeling allows the acquisition of important knowledge on the combustion process and underlying phenomena.

This thesis presents a mechanistic model for a BioGrate boiler developed for process phenomena investigation, including an evaluation of the effect of varying particle size and moisture content on biomass combustion and the dynamic response of the burning fuel bed to a varying primary air supply. To improve the accuracy of the developed model, appropriate pyrolysis kinetics for the debarking residue were determined and the associated reaction heats were estimated from a mechanistic model of fixed-bed pyrolysis, which was also developed in this work.

In addition, a simplification of the developed model for process control and monitoring is presented. The simplified model demonstrated acceptable accuracy in comparison with the detailed model and faster-than-real-time computational times. Both models were successfully validated with experimental data and showed the ability to predict the observed experimental trends. The results indicate that the model provides valuable information for improving the efficiency of a BioGrate boiler.

Keywords Biomass Combustion, Mechanistic Modeling, Combustion Modeling, Pyrolysis Modeling, Norway Spruce Debarking Residue, Mechanistic Model for On-line Computations

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|---------------------------------|-------------------------------|----------------------|
| ISBN (printed) 978-952-60-6808- | 4 ISBN (pdf) 978-952- | 60-6809-1 |
| ISSN-L 1799-4934 | ISSN (printed) 1799-4934 | ISSN (pdf) 1799-4942 |
| Location of publisher Helsinki | Location of printing Helsinki | Year 2016 |
| Pages 169 | urn http://urn.fi/URN:ISBN:97 | 8-952-60-6809-1 |



| Monografia | 🛛 Artikkeliväitöskirja | Esseeväitöskirja |
|---|------------------------------------|------------------------|
| Julkaisuluvan myöntä | mispäivä 27.04.2016 | Kieli Englanti |
| Käsikirjoituksen pvm | 06.11.2015 | Väitöspäivä 17.06.2016 |
| Tutkimusala CHEM00 | 6Z Kemian tekniikka | |
| Sarja Aalto University | publication series DOCTORAL DISSER | TATIONS 92/2016 |
| Yksikkö Biotekniikan j | a kemian tekniikan laitos | |
| Julkaisija Kemian tekn | iikan korkeakoulu | |
| BioGrate -kattilan dyna | aminen mallinnus | |
| Väitäekirien nimi | | |
| Tekijä Alexandre Boriouchkine | | |

Tiivistelmä

Biomassan polttoa pidetään tehokkaana energiantuotantomenetelmänä, joka mahdollistaa hupenevien fossiilisten polttoaineiden korvaamisen. Tämän lisäksi biomassa on sekä uusiutuva että CO2-neutraali luonnonvara, joka tarjoaa kestävän ratkaisun jatkuvasti kasvavalle energian kysynnälle. Olemassa olevat polttoteknologiat voivat hyödyntää biomassaa vain osittain, yleensä seoksena fossiilisten polttoaineiden kanssa. Tästä johtuen on kehitetty uusia teknologioita, kuten BioGrate-kattila, joka pystyy hyödyntämään uusiutuvia polttoaineita sellaisenaan.

Tulevaisuuden energiajärjestelmät tulevat sisältämään yhä enemmän erilaisia energialähteitä joustavaan energian tuotantoon. Tämä kohdistaa kattilaprosesseihin uusia haasteita, kuten nopeita kuorman muutoksia sekä energiatuotantoa minimiteholla. Tämän takia onkin tärkeää ymmärtää järjestelmien kehityksessä palamisprosessissa tapahtuvat ilmiöt, sillä se mahdollistaa kattiloiden optimaalisen suunnittelun ja ajon.

Tämä väitöskirja esittää Biograte-kattilalle mekanistisen mallin, joka mahdollistaa palamisilmiöiden tutkimisen. Tähän sisältyy erilaisten biomassan ominaisuuksien, kuten raekoon ja kosteuspitoisuuden vaikutuksen evaluointi sekä muuttuvan primääri-ilmansyötön vaikutuksen tutkiminen palavaan polttoainekerrokseen.. Mallin tarkkuuden parantamiseksi, BioGrate-kattilassa käytetylle polttoaineelle on määritetty pyrolyysikinetiikka ja siihen liittyvä reaktiolämpö on estimoitu tässä työssä myös kehitetyn pakattu-peti –pyrolyysimallin avulla. Kehitetty yksityiskohtainen mekanistinen malli on lisäksi yksinkertaistettu prosessin monitorointiin ja säätöön soveltuvaksi. Verrattuna yksityiskohtaiseen malliin, yksinkertaisempi malli pystyy kuvaamaan palamista riittävän tarkasti laskenta-ajan ollessa silti realiaikaa lyhyempi. Kummatkin mallit on validoitu kokeellisen data avulla ja kokeet osoittavat mallien ennustuskyvyn olevan riittävä kokeellisesti mitattujen palamisilmiöiden kuvaamisesssa.

Suoritettujen simulaatioiden avulla on tutkittu raekoon ja kosteuspitoisuuden vaikutusta biomassan palamiseen. Lisäksi on selvitetty palamisilman vaihtelun vaikutusta polttoaineen palamiseen. Yksityiskohtaisen mallin avulla on tutkittu raekoon ja kosteuspitoisuuden vaikutusta biomassan palamiseen BioGrate –kattilassa. Tämän lisäksi palamisilman vaihtelun vaikutusta polttoaineen palamiseen on selvitetty. Tulokset osoittivat, mallian avulla saadaan arvokasta tietoa BioGrate-kattilan tehokkuuden parantamiseen.

Avainsanat Biomassan poltto, Mekanistinen mallinnus, Palamisen mallinnus, Pyrolyysin mallinnus, Metsäkuusen kuoriaines, Mekanistinen malli on-line laskentaan

| ISBN (painettu) 978-952-60-0 | 3808-4 | ISBN (pdf) 978-9 | 952-60-6809-1 |
|------------------------------|------------|----------------------|----------------------|
| ISSN-L 1799-4934 | ISSN (pai | nettu) 1799-4934 | ISSN (pdf) 1799-4942 |
| Julkaisupaikka Helsinki | Painopail | ka Helsinki | Vuosi 2016 |
| Sivumäärä 169 | urn http:/ | /urn.fi/URN:ISBN:978 | -952-60-6809-1 |

Preface

The research work presented in this thesis has been carried out in the research group of process control and automation, Aalto University, School of Chemical Technology (Espoo, Finland) during the period 2010-2015. The experimental part of the work has been carried out in the University of Sheffield (Sheffield, the UK) in 2012. This work has been a part of two projects funded by the Finnish Funding Agency for Technology and Innovation: Energy boilers and separate services (Dynergia) and Integrated condition-based control and maintenance (ICBCOM). The financial support for the research received from the Fortum Foundation, Emil Aaltonen Foundation, Walter Ahlström Foundation, the Finnish Foundation for Technology Promotion, the Research Foundation of Helsinki University of Technology, and the Finnish Automation Foundation is gratefully acknowledged.

I would like to express my gratitude to Professor Sirkka-Liisa Jämsä-Jounela for the supervision of this thesis as well as for the guidance and support throughout the whole research and writing process. I am also thankful for the many opportunities that she uncovered during the work in the research group of process control and automation. Next, I wish to thank PhD Alexey Zakharov, especially, for his help with the mathematical aspects of this work and also for the help with other challenges encountered during the research. Mr. Juha Huotari is gratefully acknowledged for arranging the full scale industrial experiments and the valuable discussions on the BioGrate boiler operation. I am very grateful to Professors Vida Sharifi and Jim Swithebank for the opportunity to work as a member of SUWIC research group and to conduct my experiments in the University of Sheffield.

I had a pleasure of working with fine and cheerful colleagues like Jerri, Vesa-Matti, Jukka, Miao, Rinat, Palash and Octavio. Finally, I wish to thank my parents, relatives and friends for the support and encouragement throughout this process as well as throughout my life.

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List of Publications

This thesis consists of an overview and of the following publications which are referred to in the text by their numerals

1. Boriouchkine A., Zakharov A., Jämsä-Jounela S.-L. (2012). Dynamic modeling of combustion in a BioGrate furnace: The effect of operation parameters on biomass firing. *Chemical Engineering Science*, **69**(1), 669-678. ISSN 0009-2509, dx.doi.org/10.1016/j.ces.2011.11.032.

2. Boriouchkine A., Sharifi V., Swithenbank J., Jämsä-Jounela S.-L. (2014). A study on the dynamic combustion behavior of a biomass fuel bed. *Fuel*, **135**, 468-481. ISSN 0016-2361. dx.doi.org/10.1016/j.fuel.2014.07.015.

3. Boriouchkine A., Sharifi V., Swithenbank J., Jämsä-Jounela S.-L. (2015). Experiments and modeling of fixed-bed debarking residue pyrolysis: the effect of fuel bed properties on product yields. *Chemical Engineering Science*, **138**, 581-589. ISSN 0009-2509. dx.doi.org/10.1016/j.ces.2015.07.055.

4. Boriouchkine A., Jämsä-Jounela S.-L. Simplification of a mechanistic model of biomass combustion for on-line computations. Submitted. List of Publications

Author's Contribution

Publication 1: Dynamic modeling of combustion in a BioGrate furnace: The effect of operation parameters on biomass firing

A. Boriouchkine developed the mechanistic model of biomass combustion in a BioGrate boiler, conducted simulations, interpreted the results, and wrote the manuscript with the co-authors. A. Zakharov developed and implemented the numerical scheme for solving the model. The initial conditions for the modeling work were provided by Mr. K. Helkilinna from Wärtsilä Biopower Ltd.

Publication 2: A study on the dynamic combustion behavior of a biomass fuel bed

A. Boriouchkine designed and conducted spruce debarking residue pyrolysis experiments under the supervision of Prof. V. Sharifi and Prof. J. Swithenbank. Mr. A. Lumby assisted with the fixed-bed pyrolysis experiments and Mr. K. Penny assisted with the thermogravimetric analysis. A. Boriouchkine was responsible for estimating the kinetic parameters for the pyrolysis rate equations, further development of the model, conducting simulations, interpreting the simulation results, and writing the manuscript with the co-authors. The debarking residue samples used in the experiments were provided by Mr. R. Aronen from Finnforest Ltd., Vilppula sawmill.

Publication 3: Experiments and modeling of fixed-bed debarking residue pyrolysis: The effect of fuel bed properties on product yields

A. Boriouchkine further analyzed the results from the debarking residue pyrolysis experiments, and developed and implemented a model of fixed-bed debarking residue pyrolysis to investigate the pyrolysis behavior of the material. A. Boriouchkine validated the model, conducted simulations, interpreted the results, and wrote the manuscript with the co-authors. **Publication 4:** Simplification of a mechanistic model of biomass combustion for on-line computations

A. Boriouchkine developed the simplified dynamic model of biomass combustion in a BioGrate boiler for on-line applications, performed simulations, and wrote the manuscript. The industrial experiments and data collection for model validation were organized by J. Huotari from MW Biopower Ltd., and the experiments were conducted in co-operation with A. Boriouchkine and Dr. J. Kortela. Data on the flue gas composition, which was used to determine the biomass combustion rate, were collected during the experiments with Servomex 2500 FTIR analyzer by the personnel from Technical Research Centre of Finland.

List of Symbols

| $\varDelta H_{CO}$ | enthalpy of CO formation (kJ/mol) |
|------------------------|--|
| $\varDelta H_{CO_2}$ | enthalpy of CO ₂ formation (kJ/mol) |
| ΔH_{evap} | enthalpy of vaporization (kJ/kg) |
| $\Delta H_{p,i}$ | pyrolysis enthalpy of component i (kJ/kg) |
| μ | fluid viscosity |
| A | pre-exponential factor (s ⁻¹) |
| A_{pyr} | pre-exponential factor of a pyrolysis reaction (s-1) |
| C _{CH4} | concentration of methane (mol/cm ³) |
| C _{co} | concentration of carbon monoxide (mol/cm ³) |
| C_{H2O} | concentration of steam (mol/cm ³) |
| <i>C</i> ₀₂ | concentration of oxygen (mol/cm ³) |
| $C_{p,o2}$ | heat capacity of oxygen (J/(kg K)) |
| $C_{p,H2O,g}$ | heat capacity of water vapor (J/(kg K)) |
| $C_{p,N2}$ | heat capacity of nitrogen (J/(kg K)) |
| $C_{p,c}$ | heat capacity of char (J/(kg·K)) |
| $C_{p,G}$ | heat capacity of pyrolytic gas (J/(kg K)) |
| $C_{p,H2O}$ | heat capacity of liquid water (J/(kg·K)) |
| $C_{p,w}$ | heat capacity of wood (J/(kg·K)) |
| C_s | heat capacity of the solid phase (J/(kg·K)) |
| d_{cavity} | average cavity diameter (m) |
| $D_{g,i}$ | gas-phase diffusivity of component i in air(m ² /s) |
| $D_{i,eff}$ | effective diffusion coefficient of component i (m ² /s) |
| d_p | particle diameter (m) |
| | |

| Ε | activation energy (J/mol) |
|------------------------|--|
| ε | emissivity coefficient |
| F_{in} | total volumetric air flow to the furnace (m³/s) |
| F _{out} | total volumetric flow out of the furnace (m^3/s) |
| h | heat transfer coefficient (W m ⁻²) |
| h_{C} | fraction of char in the total amount of material on the grate |
| H_{g} | enthalpy of the gas phase (J/kg) |
| H_{G} | energy content of the gas phase (J) |
| $h_{i,eff}$ | effective mass transfer coefficient |
| I- | energy flux in a negative direction (W/m ²) |
| I^+ | energy flux in a positive direction (W/m ²) |
| Ι | identity matrix |
| k_a | absorption coefficient (m-1) |
| k_{air} | thermal conductivity of air |
| k_{bed} | effective heat conduction coefficient of the packed bed $(W/(m{\cdot}K))$ |
| k_c | reaction rate of char combustion reaction (1/s) |
| $k_{e\!f\!f,i}$ | effective reaction constant of a heterogeneous reaction i (kg/(m ³ ·s)) |
| k_{fiber} | heat conductivity of wood fiber (W/($m \cdot K$)) |
| k_g | heat conductivity of the gas $(W/(m \cdot K))$ |
| k_m | reaction rate coefficient for component m (1/s) |
| $k_{m,i}$ | mass transfer coefficient for the gaseous component i (kg/(m ³ ·s)) |
| k _{max} | maximum heat transfer coefficient (W/($m\cdot K$)) |
| k_{min} | minimal heat conduction coefficient (W/(m·K)) |
| <i>k</i> ₀₂ | mass transfer coefficient of oxygen to the char particle (m/s) |
| $k_{p,i}$ | rate constant for pyrolysis of component i |
| $k_{pyr,comb}$ | rate constant of combustion of pyrolytic gas (1/s) |
| k _{rs} | void-to-void heat conduction coefficient (W/(m·K)) |

| k_{rv} | solid surface-to-solid surface heat conduction coefficient $(W/(m\cdot K))$ |
|-------------------------|--|
| k_s | scattering coefficient (m ⁻¹) |
| $k_{r,C}$ | rate constant for the char reaction with oxygen (kg/(m_3 ·s)) |
| $k_{r,CO2}$ | rate constant for the char reaction with carbon dioxide $(kg/(m^3 \cdot s))$ |
| $k_{s,eff}$ | heat conduction coefficient of the solid matter (W/($m\cdot K$)) |
| $k_{r,H2O}$ | rate constant for the char reaction with water (kg/($m_3 \cdot s$)) |
| $k_{r,i}$ | reaction rate constant for the component i (kg/(m ³ ·s)) |
| $k_{s,rad}$ | heat radiation coefficient of the solid matter (W/($m\cdot K$)) |
| l_{wire} | wire length (cm) |
| M_{CO} | molar mass of CO (kg/mol) |
| M_{CO_2} | molar mass of CO ₂ (kg/mol) |
| $m_{\imath,k}$ | estimated mass of the first volatile component at time instance k (mg) |
| <i>m</i> _{2,k} | estimated mass of the second volatile component at time instance k (mg) |
| m _C | amount of char in the furnace (kg) |
| m _{co} | amount of carbon monoxide in the furnace (kg) |
| $m_{_{fuel}}$ | amount of fuel in the furnace (kg) |
| m _{H2O,i} | amount of moisture in the furnace (kg) |
| m _{In} | fuel feed to the furnace (kg/s) |
| m _m | predicted weight of component m (kg) |
| m _{meas} | measured mass of a biomass sample (mg) |
| <i>m</i> ₀₂ | amount of air in the furnace (kg) |
| $m_{p,G}$ | total amount of pyrolytic gas in the furnace (kg) |
| $m_{p,i}$ | amount of volatile component i in the furnace (kg) |
| m_{sample} | mass of the sample (g) |
| m _{H2O,l} | amount of moisture on the grate (kg) |
| $m_{_{H2O}}$ | amount of water vapor in the fuel layer (kg) |

| n | total number of measurements |
|--------------------|---|
| Pr | Prandatl number |
| $Q_{g,i}$ | energy produced or consumed by a gas phase reaction i (J/(m ³ ·s)) |
| Q_s | energy released through radiation and convection (W) |
| $Q_{s,i}$ | energy produced or consumed by a solid phase reaction i (J/(m ³ ·s)) |
| Q_C | energy from char combustion (J/s) |
| Q_{in} | energy contained in primary air (J/s) |
| Qout | energy of outflowing gas (J/s) |
| r | cylindrical coordinate (m) |
| r_{c} | reaction rate of char (kg/s) |
| Re | Reynolds number |
| r_{evap} | drying rate (kg/(m ³ ·s)) |
| $r_{evap,conv}$ | rate of moisture evaporation due to the heat transfer between gas and solid |
| $r_{evap,rad}$ | rate of moisture evaporation due to the radiative heat transfer from char layer |
| $r_{g,CH4}$ | oxidation rate of methane (kg/(m ³ ·s)) |
| $r_{g,CO}$ | oxidation rate of the carbon monoxide $(kg/(m^{3}\cdot s))$ |
| $r_{g,H2}$ | oxidation rate of hydrogen (kg/($m_3 \cdot s$)) |
| $r_{g,i}$ | reaction rate of the gaseous component i (kg/(m ³ ·s)) |
| $r_{p,i}$ | rate of pyrolysis of component i (kg/s) |
| r_{pyr} | rate of pyrolysis reaction (kg/s) |
| $r_{pyr,comb}$ | rate of combustion of pyrolytic gas (kg/s) |
| r _{s,H2O} | drying rate of fuel (kg/(m³·s)) |
| $r_{s,j}$ | rate of reaction of the solid component j (kg/(m ³ ·s)) |
| r _{s,pyr} | reaction rate of pyrolysis (kg/(m³·s)) |
| S | density number (m-1) |
| Sc | Schmidt number |
| \mathbf{S}_i | mass source (kg/m ³ s) |

| Т | temperature (K) |
|--------------------|--|
| T_g | temperature of the gas phase (K) |
| T_{In} | temperature of the fed air flow (K) |
| T_s | temperature of the solid (K) |
| t | time variable (s) |
| t_k | time instance k (s) |
| u | velocity vector |
| V | volume of the material on the grate (m ³) |
| v_g | gas flow velocity (m/s) |
| X | degree of conversion of char |
| X_C | char fraction in the pyrolysis products |
| $X_{\rm H2O}$ | moisture content of the fuel |
| X_m | moisture content of the fuel in the furnace |
| $X_{p,G}$ | fraction of pyrolysis gas in the wood pyrolysis |
| $\mathbf{X}_{t,I}$ | fraction of the reactant converting to tar component i |
| \mathbf{X}_k | molar fraction |
| x | vertical coordinate (m) |
| $Y_{g,i}$ | mass fraction of the gaseous component i |
| α | mass fraction of the first volatile component in a biomass sample |
| \mathcal{E}_b | bed porosity |
| $arepsilon_p$ | particle porosity |
| κ_{conv} | heat convection coefficient (W/(m^2K)) |
| $\kappa_{s,eff}$ | effective heat conduction coefficient of the solid matter $(W/(m\cdot K))$ |
| ρ | density of the fluid (kg/m ³) |
| $ ho_{Air}$ | density of air (kg/m ³) |
| $ ho_{C}$ | mass concentration of char (kg/m ³) |
| $ ho_{CO}$ | mass concentration of carbon monoxide (kg/m ³) |
| $ ho_g$ | mass concentration of the gas phase (kg/m³) |

List of Symbols

| $ ho_{_{H2}}$ | mass concentration of hydrogen (kg/m ³) |
|--------------------------|--|
| $ ho_{m,i}$ | mass concentration of component i (kg/m ³) |
| $ ho_{O2}$ | mass concentration of oxygen (kg/m ³) |
| $ ho_s$ | total mass concentration of the solid phase (kg/m ³) |
| $ ho_{s,j}$ | mass concentration of the solid component $j\ (kg/m^3)$ |
| $ ho_{t,i}$ | mass concentration of tar component i (kg/m ³) |
| ρ_v | mass concentration of volatiles (kg/m ³) |
| $ ho_w$ | mass concentration of water (kg/m ³) |
| $ ho_{fuel \ bed \ dry}$ | density of the dry fuel bed (kg/m ³) |
| $\rho_{char \ bed}$ | density of the char bed (kg/m^3) |
| σ | Stefan-Boltzman constant (W/(m²·K4)) |
| σ_{c} | pore constriction factor |
| τ | tortuosity |
| φ | Void fraction of the fuel bed |
| Ω | Ratio of carbon monoxide to carbon dioxide |
| $arOmega_{pyr}$ | Stoichiometric coefficient of pyrolytic gas combustion |
| ω | mass fraction of component <i>i</i> |

1. Introduction

1.1 Background

Increasing biomass utilization in energy production through combustion is regarded as an efficient alternative to consuming diminishing fossil natural resources. Furthermore, biomass is not only a naturally replenishable energy source, but is also CO_2 neutral, and thus it is a sustainable option to satisfy the ever-growing energy demand. Existing combustion technologies such as industrial boilers and furnaces can utilize renewable fuels to a certain degree, mainly when blended with traditional fossil fuels. Consequently, new technologies that can fully benefit from biomass fuel have been developed. One such technology is the BioGrate boiler that can utilize biomass with a moisture content of up to 65 wt%.

The development of this advanced technology enables further increase in the overall efficiency of biomass firing. However, this development requires a good understanding of the underlying phenomena in a combustion process, especially because biomass is a challenging fuel owing to the varying properties of biomass, including moisture content, calorific value, particle size and shape, chemical composition, and inorganic content.

A detailed mechanistic mathematical model validated against experimental data can provide the necessary level of insight required for efficient optimization of a combustion process. Furthermore, model-based process design, control, and optimization greatly improve the process efficiency. Owing to the benefits of mathematical modeling, several models have been developed for biomass combustion in grate boilers. Studies by Shin and Choi (2000a), Ashtana et al. (2010), and Yang et al. (2004a) investigated the combustion of municipal solid waste (MSW) in boilers to identify the effects of the main fuel parameters on biomass combustion for design and operation optimization. Straw combustion in a grate boiler was studied by Van der Lans et al. (2000) with the aim of determining the main factor that controls combustion. With a similar purpose, Zhang et al. (2010) developed a dynamic model for wood combustion in a grate boiler. These studies have provided valuable information on the effect of the key biomass properties on boiler operation. However, no model has been developed thus far for combustion phenomena investigation that considers conical grate geometry of a BioGrate boiler.

1.2 Research problem and the asserted hypothesis

The BioGrate technology is designed to utilize various types of solid biomass, including woody residue and MSW. However, biomass utilized in power and heat production has different compositions and varying quality that depends on the moisture and volatile content, wood species, particle size, porosity, density of the material, and ash content. These variations in the fuel create challenges in power production and emissions control. Nevertheless, mathematical modeling allows investigation of underlying phenomena that affect combustion behavior, and gives insight into the requirements for improved process operation and decreased pollutant emissions. Furthermore, the burning fuel bed is the main source of energy for boiler operation, and the identification of combustible components leaving the bed is important. Thus, modeling the fuel bed provides crucial information on the underlying process phenomena and the tools for process improvement and optimization.

This work focuses on the development of a dynamic mechanistic model of biomass combustion in a BioGrate boiler. The main motivation of the work is to develop a mathematical model that can predict the effect of fuel parameters such as particle size, moisture, density, and process variables (e.g., air flow and air distribution) on grate combustion of biomass. To provide an accurate description of the biomass combustion process operation, the model must be able to predict gas and solid temperatures, as well as the composition of the gas released during the combustion. Furthermore, for improved accuracy, the model must also consider fuel-specific parameters, including pyrolysis kinetics, pyrolysis reaction heats, as well as volatile and fixed carbon content.

The hypothesis asserted in this thesis is:

The enhanced mechanistic combustion model of a BioGrate boiler provides essential information on the combustion phenomena that can be utilized to evaluate the effects of process parameter variation on the performance of the energy boiler.

The enhanced combustion model can be simplified for on-line computations to provide fast computational times while retaining sufficient accuracy in describing combustion phenomena in a BioGrate boiler.

To prove the hypothesis, the following tasks were performed:

Task 1. Development of a mechanistic model for biomass combustion in a BioGrate boiler, testing of the model with the industrial data and performing a detailed analysis of the key fuel properties on biomass firing in a BioGrate boiler.

Task 2. Improvement of the model with fuel specific kinetic parameters. Conducting experiments of Norway spruce debarking residue pyrolysis and the kinetic parameter estimation for the dynamic model. Performing model validation and an analysis on the combustion behavior of fuel in a BioGrate boiler under varying primary air flows.

Task 4. Simplified model development for on-line computations of biomass combustion in a BioGrate boiler. Conducting experiments for parameter estimation and estimation of the parameters for the simplified model and performing model validation.

Task 5. The performance evaluation of the simplified model against the enhanced model and an autoregressive model with exogenous inputs (ARX).

1.3 Scope and significance of the thesis

Owing to the significant influence of biomass properties on combustion, insight into the conversion process allows further improvement of energy generation efficiency. The main focus of this thesis is the development of a mechanistic model of biomass combustion in a BioGrate boiler. The focus also covers the development of a dynamic model of biomass combustion for on-line computations through the simplification of the mechanistic model.

The development of the dynamic model for a BioGrate boiler comprises the establishment of the modelling framework based on the information provided in literature and the improvement of the model with fuel specific pyrolysis rate equations. For the estimation of the fuel specific rate equations, experiments were conducted and the equations were estimated form the experimental data with an appropriate mathematical method. The developed model was validated and the analysis on dynamic combustion phenomena performed.

For the development of the simplified model, a general approach for enhanced model simplification is defined. Based on the approach, the model is simplified and a mathematical formulation for the simplified model is presented. The successful simplified model implementation requires several parameters to be determined. For this purpose, experiments on debarking residue pyrolysis are conducted and parameters are estimated using appropriate methods. Finally, the simplified model is validated with industrial data from a BioGrate boiler. To ensure that the simplified model performs as expected its performance is evaluated against the dynamic model of a BioGrate boiler and a linear ARX model.

The contribution of the thesis is also demonstrated in the scientific articles that investigate various aspects of biomass firing. Publication 1 presents a novel dynamic mechanistic model of biomass combustion in a BioGrate boiler and investigates the effect of the main fuel parameters on biomass combustion. In Publication 2, the model is further developed and experimental information is incorporated into it. Subsequently, the publication investigates the dynamic response of the burning fuel bed to changes in the primary air flow to define the optimal location for the primary air feed. Publication 3 presents a detailed dynamic model of fixed-bed debarking residue pyrolysis. The model is used to estimate the pyrolysis reaction heats and investigate the effect of the fuel properties on biomass devolatilization. A simplified model of biomass firing in a BioGrate boiler for on-line applications is developed and validated in Publication 4.

Outside the scope of this thesis is the development of control and monitoring methods for a BioGrate boiler.

1.4 Outline of the thesis

Chapter 2 gives a detailed description of the process structure of a BioGrate boiler and its control strategy. The state of the art in combustion modeling is presented in Chapter 3. Chapter 4 describes the dynamic model of a BioGrate boiler and presents a study of the effect of fuel properties on biomass combustion. Chapter 5 presents the improvements to the model through the inclusion of fuel specific pyrolysis rates and analyses the dynamic combustion phenomena that occur in the burning fuel bed of a BioGrate boiler. Chapter 6 presents the development of a simplified combustion model, including the general approach for model simplification, the mathematical formulation, parameter estimation for the model and its validation. In Chapter 7, the simplified model is compared with the enhanced model and a linear model. Chapter 8 discusses the perspectives on the use of the developed models for efficiency improvements to BioGrate boiler operations and considerations of their industrial implementation. Chapter 9 presents the conclusions from this work.

2. Process Description of a BioGrate Boiler

A BioGrate boiler comprises two major parts: a furnace (BioGrate) and a water-steam circuit. The energy for steam generation is produced by burning debarking residue or alternatively saw dust and pellets. The energy contained in the flue gas formed by biomass combustion is transferred to water and steam through a series of heat exchangers in the steam-water circuit.

Fuel is fed into the center of the grate from below. To improve fuel distribution in the combustion chamber, the grate consists of several ring zones, which are further divided into two types of rings: rotating and fixed. Half of the rotating rings rotate clockwise, the rest counterclockwise. The fixed rings are located between the rotating rings. The surface of the fuel starts to dry in the center of the cone as a result of heat radiation, which is emitted by the combusting flue gas and reflected back to the grate by the grate walls. This design provides enough heat to start fuel drying so that no air preheating is needed. The dry fuel then proceeds to the outer shell of the grate where pyrolysis, char gasification, and combustion occur. The ash and carbon residues fall off the edge of the grate into the water-filled annular ash space. Figure 2.1 shows a sketch of a BioGrate furnace.



Figure 2.1. Conical grate furnace of a BioGrate boiler (Anon, 2015)

The air required for gasification and combustion is distributed via annular primary air registers below the grate through nozzles in each grate plate (primary air) and through nozzles in the combustion chamber wall (secondary air). In addition, to ensure clean combustion, additional air can be fed through nozzles at the top of the combustion chamber (tertiary air) and in the boiler walls.

Burning produces heat that is absorbed in several steps. First, the saturated water evaporator and water-tube walls of the boiler absorb energy from the flue gases. Next, part of the flue gas energy is transferred to steam superheaters. In the third phase, heat is transferred to the convective evaporator. Finally, economizers remove the remaining flue gas energy. However, to prevent condensation of sulfuric acid, the flue gas temperature must be maintained above its dew point. An overall flow chart of the boiler process is presented in Figure 2.2.

The control strategy of a power plant aims to ensure that the demand for the energy production is met at all times. Stable energy generation requires the steam pressure and temperature to be within the specified limits. The temperature of the steam is regulated with attemperators situated in the superheaters that spray water to decrease excessively high steam temperatures. The steam pressure is regulated by adjusting the drum pressure, which is determined by the combustion intensity of the fuel in the furnace. The combustion intensity is adjusted with the primary air flow rate by regulating the primary air fan. At the same time, to ensure a sufficient amount of fuel on the grate, the stoker speed is increased or decreased according to the primary air feed rate. The stoker rotation speed is determined from a look-up table value specified for each air flow rate. A constant water level in the drum is maintained by feeding water according to the level height setpoint.

To maintain clean combustion and minimize possible energy losses, the secondary air flow rate is altered based on the flue gas oxygen content and primary air flow rate, such that the residual oxygen content in the flue gas remains at a desired value. However, as the additional air affects the biomass combustion rate, the stoker speed is consequently corrected by a predetermined amount.

The flue gas formed by combustion is removed from the boiler unit with a flue gas fan, so that a small constant negative pressure is maintained inside the furnace to avoid flue gas leakages to the plant environment. In addition, to regulate the furnace temperature, the flue gas can be recirculated back to the furnace by adjusting the recirculation channel valve opening and recirculation fan rotation speed according to the desired temperature.



Figure 2.2. Flow chart of a BioGrate boiler process (Anon, 2007)

Process Description of a BioGrate Boiler

3. State-of-the-Art in Modeling of a Boiler Process

The inherent properties of biomass have a significant influence on the combustion behavior of the material, and this influence has been widely researched by the scientific community. One of the groundbreaking models developed to investigate the combustion properties of biomass was presented by Shin and Choi (2000a). The authors utilized modeling to determine the effect of different parameters on the combustion of municipal waste. With the model, the authors identified three air supply-dependent combustion regimes, namely, oxygen-limited and reaction limited combustion, as well as flame extinction by convection, which occurs at high flow rates. Goh et al. (2001) developed a model to predict waste combustion in a grate boiler and validated it using laboratory experiments. The model demonstrated satisfactory agreement with the experimental measurements. The model allowed a more detailed investigation of phenomena including drying and pyrolysis as the experiments provided only limited possibilities for investigating these processes. The first two-dimensional model of solid fuel combustion on the grate, which considered gradients in not only the vertical, but also the horizontal direction, was developed by Yang et al. (2002). In contrast to the previously developed models, this model also included the mixing effect of volatiles and oxygen in the fuel layer. The simulations revealed that the width of the reaction fronts, including combustion and moisture evaporation, was limited to approximately 60 mm. The mass loss from the fuel bed mainly occurred due to moisture evaporation and devolatilization reactions. In addition, the authors found that discrepancies between measured and predicted combustion behavior were due to channeling of air through the fuel bed and the resultant poor mixing of volatiles with air.

A study by Kær (2004) on the modeling of a straw-fired boiler suggested that poor mixing of flue gases and secondary air results in high CO concentrations and unburnt carbon in fly ash. The combustion of simulated fuel was characterized by two fronts: a devolatilization front moving from the top towards the grate and a char oxidation zone proceeding in the opposite direction. Similarly, Ashtana et al. (2010) developed a static model to describe grate combustion in an MSW boiler. The modeling work revealed the presence of two combustion fronts, above which char reduction reactions occur. Furthermore, it was shown that in an oxygen free environment, char gasification reactions can play a significant role. Girgis and Hallett (2010) used a mathematical model and experiments to analyze combustion in an overfed packed bed of wood. The study demonstrated that the rate equation and product yields for pyrolysis have to be fitted to the experiments to obtain results with satisfactory accuracy. It was found that the higher the rate of pyrolysis, the wider the pyrolysis front.

The issue of air channeling has been identified as one of the most important problems in biomass combustion (Yang et al., 2002). Channeling greatly decreases the efficiency of a combustion process because of poor mixing of the material on the grate with air. This issue has been investigated by several authors, including Yang et al. (2003), who simulated channel growth in a fuel bed to investigate overall combustion behavior in the presence of a channel. The channeling effect causes fast propagation of the combustion front in the center of the bed; however, owing to poor mixing of fuel and air, the total combustion of the fuel bed occurs significantly later (t = 60 min) compared with the case of a uniform air distribution (t = 41 min). Hermansson and Thunman (2011) investigated channeling phenomena in a bed of char particle; however, in contrast to the study by Yang et al. (2003), they also modeled fuel bed collapse due to fuel consumption. As a solution to air channeling in the fuel bed, the authors suggested improving the mixing of the materials with a sufficient spread of the fuel on a grate. As another solution to the channeling problem, Duffy and Eaton (2013) proposed using grate plates that improve the distribution of primary air, thus avoiding channeling. Yang et al. (2005a) proposed a statistical model analogous to the Markov chain to describe material mixing on the grate. The modeling and experimental results indicated that grate mixing can be mathematically modeled with a procedure based on swap probability, e.g., the probability for a particle to swap places with adjacent particles. The probability of particle swapping in the center of the grate was higher than that at locations near the walls.

Several studies explored the effect of various variables on combustion. These studies investigated the effect of modeling parameters, including fuel moisture content, combustion air feed, and particle size. Van der Lans et al. (2000) described straw combustion in a moving bed with a two-dimensional homogeneous (temperature of solid and gas are assumed equal) steady-state model, and studied the effect of the combustion parameters, including particle size, heat capacities of straw and volatiles, and bed porosity on the burning of the fuel bed. The authors found that with a twofold increase in the straw char outer surface area, the thermal conductivity of the bed or the mass transfer coefficient increases the ignition rate by approximately 30% and results in ~100 K lower bed temperatures. A 10% increase in heat capacity decreases the ignition rate by 10%; however, a 10% increase in combustion front propagation velocity can be achieved by decreasing the bed porosity from 0.58 to 0.48.

Johansson et al. (2007) conducted a sensitivity analysis of biomass combustion in a fixed-bed with a mathematical model. The sensitivity analysis revealed that the hydrogen fraction in volatile gases strongly influences the ignition rate. It was also observed that no parameters, with the exception of the mixing rate of gaseous species and the heat and mass transfer coefficients, influence the solid and gas temperatures by more than 10%. In addition, a comparison of alternative values of the model parameters, including the volatile mixing rate, heat and mass transfer coefficients, and the effective area of a char surface, showed a difference of up to 25% in the released gas concentrations. Zhou et al. (2005) investigated the combustion of a straw bed using a mathematical model. Their work suggested that variables, including the effective heat conductivity of the bed, straw heat capacity, and bed packing, have the most influence on the model predictions.

Yang et al. (2004b) investigated the effect of moisture content and air flow on the burning behavior of biomass. The following trends were established: First, the higher the moisture content, the lower the combustion rate. For example, a decrease in moisture from 50 to 10 wt% resulted in a four-fold increase in the biomass combustion rate. A similar effect is observed for the devolatilization rate, which increased three-fold with a four-fold decrease in the moisture content. Second, an increase in the air flow rate increases the evaporation rate; however, an increase beyond a critical point decreases the rate of drying. Finally, char combustion is affected by both the moisture content and primary air flow. An increase in the air flow increases the char burning rate by a similar amount for all moisture contents; however, drier fuel can sustain combustion at higher air flow rates than wetter ones.

The investigations of the effect of fuel particle size were based on models in which particles are modeled separately in the fuel bed for an accurate description of the underlying processes. Peters (2002) proposed a discrete particle model (DPM) to simulate combustion of biomass fuel in packed beds. The approach of describing the fuel as an ensemble of separate particles demonstrated high accuracy in the prediction of temperature and gas evolution. Furthermore, this approach did not need any empirical correlations. Thunman and Leckner (2002) investigated fixed-bed combustion of thermally large particles, e.g., particles with significant internal temperature gradients with a model. The results suggest that the continuous media approximation for large particles yields poor accuracy in combustion modeling. Bruch et al. (2003) modeled fixed-bed combustion of wood as an ensemble of single particles, which were modeled separately. This approach demonstrated acceptable accuracy in modeling the overall mass loss rate of the fuel bed. An investigation of the effect of particle size on combustion was conducted by Yang et al. (2005b) using a model where fuel particles were resolved separately. The study indicated that an increase in particle size decreases the combustion rate, shifts the combustion from fuel lean to fuel reach combustion, and increases burning temperatures. Similarly, Thunman et al. (2002) proposed a simplified model of a particle for comprehensive fuel bed modeling. The results implied that drying and devolatilization significantly reduce the size of the particle, and combined with char combustion on the surface of the particle, greatly reduce the time of complete drying and devolatilization.

Studies considering the whole boiler, including a furnace and a convective section, have focused on the analysis of overall boiler operation. Yang et al. (2007) modeled straw combustion in a 38 MW grate boiler using a solid biomass model coupled with a FLUENT model of the convective section of the

boiler. The results demonstrated that most NO formed above the fuel bed. In addition, the radiation shaft was not efficiently used, and a large part of the shaft was occupied by weak flows. Full-scale boiler modeling was used by Yin et al. (2008) to investigate combustion in a 108 MW grate boiler. The researchers suggested that a more reliable fuel bed model is required to match the experimental data with the model predictions. Nevertheless, the model was a good tool for process design and optimization. Based on the model predictions, the authors suggested attenuation of high-speed, high-oxygen flow at the front wall of the boiler and increased mixing in the burnout zone. Combustion in a small-scale boiler with a moving grate was modeled by Zhang et al. (2010). The study found that although secondary air jets provide adequate mixing of volatiles with oxygen, high temperature zones form in close vicinity to the secondary air jets. Simsek et al. (2009) employed the discrete element method (DEM) to model wood combustion in a grate boiler. The model was coupled with a computational fluid dynamics (CFD) model to simulate the whole boiler process. The results indicated the feasibility of such an approach. Yu et al. (2010) used the model previously developed by Yang et al. (2002) to simulate straw combustion in an oxygen-enriched atmosphere and found that the NO concentration increased because of the higher oxygen concentration. Similarly, Liang and Ma (2010) used the model of Yang et al. (2002) and observed results similar to those of Yu et al. (2010). Kurz et al. (2012) modeled the combustion of wood chips in a 240 kW boiler, and the combustion of wood chips and volatiles in the convective section of the boiler was described with a single three-dimensional steady-state model that demonstrated good agreement with the measurements. The researchers suggested, based on a comparison of the measurements with model predictions, that unsteady process phenomena, including the formation and collapse of channels in the fuel bed as well as air leaking into the boiler, can cause disturbances in the process operation.

Although the aforementioned models provide valuable information on combustion process phenomena and allow investigations of the effects of various process parameters on biomass firing, these complex and computationally demanding models are not suitable for applications such as process control and monitoring. Consequently, several computationally light models have been presented in the literature.

Gray-box modeling, which comprises ordinary differential equations (ODEs) with parameters identified in order to fit a particular boiler system, is a rather popular modeling technique for on-line applications. For instance, Hogg and El-Rabaie (1991) utilized a gray-box coal combustion model to develop a generalized predictive control strategy for a 200 MW boiler. Similarly, the most recent applications of this technique discuss modeling of boilers of various scales. Gölles et al. (2014) modeled combustion in a 30 kW boiler using a gray-box model to describe the key states present in the boiler. Similarly, Kortela and Jämsä-Jounela (2014) used gray-box modeling to model biomass firing in a 16 MW BioGrate boiler. On the other hand, Flynn and O'Malley (1999) constructed a model based on air/mass flows and adiabatic flame temperature to predict the key process variables.

Fuzzy logic-neural networks have also been proposed for modeling of energy boilers (Liu et al., 2013). For instance, Peng et al. (2007) used a Gaussian radial basis function (RBF) autoregressive model with exogenous inputs (ARX) to describe combustion in a coal-fired boiler and develop a nonlinear model predictive control strategy for efficiency improvement of the de-NOx reaction. This approach proved to be effective in minimizing ammonia consumption in the de-NOx reaction. The main approach of describing fuel combustion in ARX models relates fuel and air flows to boiler power output (Havlena and Findejs, 2005) or to steam production (Leskens et al., 2002;Leskens et al., 2005).

The computationally light models can be divided into two categories based on the degree of involvement of the identification methods: 1) fully data-based methods, e.g., ARX, ANN-ARX, and ANN-Fuzzy, and 2) models based on ODEs with identified parameter functions. Nevertheless, models in both of these categories suffer from limitations such as data-overfitting and insufficient reproducibility of nonlinear process behavior. In addition, industrial processes tend to operate in a limited number of regimes; thus, the identification of less common operational conditions is inherently difficult. Moreover, these models lack variables such as gas and solid temperatures and fuel composition on the grate, which are the key parameters for predicting pollutant emissions and the ability of the boiler to react to rapidly changing power demand.

Modern energy systems utilize a combination of various energy sources for energy productions and, thus, a deep understanding of the underlying combustion phenomena and the effect of fuel properties on the firing efficiency of renewable fuel is essential for further development of these systems. Furthermore, the development of energy systems will rely on smart coordination of various sources and thus will require fast transitions between various operation regimes of a boiler process. Therefore, model-aided boiler design, operation, and control offer an opportunity in the development and efficient operation of sophisticated smart energy systems. State-of-the-Art in Modeling of a Boiler Process

4. Dynamic Modeling of a BioGrate Boiler

This chapter presents modeling of biomass combustion in a BioGrate boiler. First, the mechanistic model developed by the author, along with the assumptions and the solving algorithm are presented. Next, the results on the effects of the fuel variables on biomass combustion are presented and discussed.

4.1 Dynamic model of a BioGrate boiler

In a BioGrate boiler, biomass reacts through the three main reactions that occur either in parallel or sequentially: drying, pyrolysis, and char conversion. The mechanistic modeling of the BioGrate boiler considers these three stages of biomass combustion. The model accounts for mass and energy conservation and considers a solid and a gaseous phase. The burning fuel bed in a BioGrate boiler is modeled in one dimension using the walking grate concept. The walking grate approach divides the fuel layer into vertical one-dimensional sections; thus, this concept assumes that fuel movement on the grate resembles that on a traveling grate. The structure of the model is presented in Figure 4.1 and that of the simulated fuel layer is presented in Figure 4.2.


Figure 4.1. Model structure and the solving procedure



Figure 4.2. Structure of the simulated fuel layer

4.1.1 Modeling of solid phase mass conservation

The solid phase reactions considered by the model include drying and pyrolysis, as well as char oxidation and gasification, which, in general, can be described by Equation (4.1). The reactions considered in the solid phase are presented in Table 4.1

$$\frac{\partial \rho_{s,j}}{\partial t} = -r_{s,j} \tag{4.1}$$

where $\rho_{s,j}$ and $r_{s,j}$ are the mass concentration and the reaction rate of solid component *j*, respectively.

Table 4.1. Solid phase reactions

 $\begin{aligned} H_2O(l) &\longrightarrow H_2O(g) \\ Wood &\longrightarrow Gas, Tar, Char \\ C(s) + \alpha O_2(g) &\longrightarrow 2(1-\alpha)CO(g) + (2\alpha - 1)CO_2(g) \\ C(s) + CO_2(g) &\longrightarrow 2CO(g) \\ C(s) + H_2O(g) &\longrightarrow CO(g) + H_2(g) \end{aligned}$

The rate of drying, Equation (4.2), is defined by the energy available for evaporation.

$$r_{s,H2O} = \max\left(0, \frac{\rho_{H_2O}}{\max(\rho_{H_2O})} \frac{C_s(T_s - 378K)}{\Delta t \Delta H_{vap}}\right)$$
(4.2)

where $r_{s,H2O}$ and ρ_{H2O} are the drying rate and the mass concentration of water in fuel, respectively, C_p is the heat capacity of fuel, T_s is the temperature of fuel, ΔH_{vap} is the heat of vaporization and Δt is the time step.

The pyrolysis reaction rates are described by an Arrhenius expression (Equation (4.3) and (4.4)).

$$r_{p,1} = -2 \cdot 10^9 \exp(-146[kJ/mol]/(RT))\rho_{p,1}$$
(4.3)

$$r_{p,2} = -7 \cdot 10^4 \exp(-83[kJ/mol]/(RT))\rho_{p,2}$$
(4.4)

where $\rho_{p,i}$ and $r_{p,i}$ are the mass concentration and the reaction rate of volatile component *i* = 1, 2, respectively

The rates for the char reactions are calculated using Equation (4.5). In this work, it is assumed that the rate of char oxidation only depends on the concentration of oxygen, as suggested by Pomerantsev (1986).

$$r_{s,j} = k_{eff,i} \rho_{g,i} \tag{4.5}$$

where $\rho_{g,i}$ is the mass concentration of gaseous reactant in a heterogeneous reaction with char and $k_{eff,i}$ is the effective reaction rate.

For each heterogeneous reaction between char and O_2 , H_2O , or CO_2 , an effective reaction constant, - given by Equation (4.6), - is then calculated as follows:

$$k_{eff,i} = \frac{Sk_{m,i}k_{r,i}}{Sk_{m,i} + k_{r,i}}$$
(4.6)

where *S* is the density number (the particle surface area per unit volume, Equation (4.7)), $k_{m,i}$ is the mass transfer coefficient (Equation (4.8)) (Wakao et al., 1979), and $k_{r,i}$ is the reaction constant.

$$S = \frac{6(1 - \varepsilon_b)}{d_p} \tag{4.7}$$

where ε_b is the fuel bed void fraction and d_p is the particle diameter

$$k_{m,i} = D_{g,i} / d_p \left(2 + \operatorname{Re}^{1/2} S c^{1/3} \right)$$
(4.8)

where $D_{g,i}$ is the diffusion coefficient of component *i* in air, Re is Reynolds and Sc is the Schmidt number

The reaction constants, k_r , are computed for oxidation (Equation (4.9)) (Branca and Di Blasi, 2003), with the associated CO/CO₂ ratio (Equation (4.10)) (Evans and Emmons, 1977), and reduction with H₂O, Equation (4.11) (Matsumoto et al., 2009), and CO₂ (Equation (4.12)) (Matsumoto et al., 2009). In the case of the reactions with H₂O and CO₂, a random pore model is used that also depends on the conversion degree of char because, unlike to the oxidation reaction, the slow rates of these reactions allow reactants to enter the pores.

$$k_{r,C} = 1.1 \cdot 10^6 \cdot \exp(-114.5[kJ/mol]/R/T_s)$$
(4.9)

$$CO/CO_2 = 4.3 \exp(-3390/T_s)$$
 (4.10)

$$k_{r,H_2O} = 9.99 \cdot 10^4 \cdot \exp\left(-136\left[kJ / mol\right]/R / T_s\right) (1 - X) \sqrt{1 - 10\ln(1 - X)}$$
(4.11)

$$k_{r,CO_2} = 1.1 \cdot 10^9 \exp\left(-260[kJ/mol]/R/T_s\right) X$$
(4.12)

where X is the conversion degree of char

4.1.2 Modeling of gas phase mass conservation

The gaseous components considered by the model include water vapor, tar, oxygen, carbon monoxide, carbon dioxide, nitrogen, methane, and hydrogen. The concentration of each component is modeled considering gas convection (Equation (4.13)) and relevant reactions, including combustion of carbon monoxide, methane, and hydrogen, as well as gas formation in the pyrolysis reaction.

$$\frac{\partial}{\partial t}(\rho_{g,i}\varepsilon_b) - \frac{\partial}{\partial x}(v_g\rho_{g,i}\varepsilon_b) = -r_{g,i} + Y_{g,i}r_{s,pyr}$$
(4.13)

where $r_{s,pyr}$ is the pyrolysis reaction rate and $Y_{g,i}$ is the mass fraction of the gaseous pyrolysis product.

The reaction rates for the combustion of carbon monoxide, methane, and hydrogen are presented in Equations (4.14)–(4.16) (Babushok and Dakdancha, 1993;Pomerantsev, 1986):

$$r_{g,CO} = 1.3 \cdot 10^{14} \exp(-125.5[kJ/mol]/R/T_g) C_{CO} C_{O_2}^{0.5} C_{H_2O}^{0.5}$$
(4.14)

$$r_{g,CH_4} = 5.6 \cdot 10^{12} \exp(-103.8[J/mol]/R/T_g) C_{O_2}$$
(4.15)

$$r_{g,H_2} = 2.14 \cdot 10^{14} \exp(-129[J/mol]/R/T_g)C_{O_2}$$
(4.16)

The momentum equation is omitted because the Ergun equation only predicts a 2.5% velocity increase owing to the pressure loss over a 1 m high fuel layer with 0.6 porosity and packed with particles 20 mm in diameter. Similarly, the effect of gas diffusion was considered negligible compared with convection.

4.1.3 Modeling of solid phase energy conservation

The energy conservation equation for the solid phase (Equation (4.17)) considers heat conduction, heat exchange between the phases, energy consumed in the drying and pyrolysis, and energy received during char combustion. In addition, the radiative heat transfer is included in the continuity equation.

$$\frac{\partial T_s}{\partial t}C_s\rho_s = \frac{\partial}{\partial x} \left(\kappa_{s,eff} \frac{\partial T_s}{\partial x}\right) + \kappa_{conv}S(T_g - T_s) + \sum \mathcal{Q}_{s,i} + k_a(I^+ + I^-) - k_a\sigma T_s^4$$
(4.17)

where C_s and ρ_s are the heat capacity and mass concentration of fuel, respectively. $\kappa_{s,eff}$ is the effective heat conductivity inside fuel particles, κ_{conv} is the convective heat transfer coefficient. $Q_{s,i}$ is the energy generated in a solid phase reaction. k_a is the heat radiation absorption coefficient, I^+ and I^- are the radiative heat fluxes towards the grate and towards the fuel layer surface, σ is Stefan-Boltzmann constant.

Heat conduction in solid particles is described by Equations (4.18) - (4.22). Equation (4.18) describes the effective heat conductivity of wood (Janssens, 2004), Equation (4.21) describes radiative heat transfer within the wood pores. Equation (4.22) correlates the particle porosity to the pore diameter.

 $k_{s.eff} = \varepsilon_p k_{max} + (1 - \varepsilon_p) k_{min} + k_{s.rad}$ (4.18) where ε_p is the particle void fraction, k_{min} and k_{max} are the heat conductivities of wood across and along the fiber, respectively. $k_{s,rad}$ is the radiative heat conductivity inside a particle.

Equations (4.19) and (4.20) define the heat conductivity of wood across and along the fiber, respectively (Janssens, 2004).

$$k_{\min} = \frac{k_g k_{fiber}}{\varepsilon_p k_{fiber} + (1 - \varepsilon_p) k_g}$$
(4.19)

$$k_{\max} = \varepsilon_p k_g + (1 - \varepsilon_p) k_{fiber}$$
(4.20)

 k_g is the heat conductivity of the gas in the particle voids, k_{fiber} is the heat conductivity of wood fiber

$$k_{s,rad} = \frac{4\varepsilon_p \sigma T_s^{\ 3} d_{cavity}}{1 - \varepsilon_p} \tag{4.21}$$

$$d_{cavity} = 3.5 \cdot 10^{-5} \sqrt{\varepsilon_p} \tag{4.22}$$

where d_{cavitu} is the size of particle voids

The particle porosity is calculated according to Equation (4.23), which is a function of the mass concentrations of wood, char, and moisture (Bryden and Hagge, 2003).

$$\varepsilon_p = 1 - (\rho_v + \rho_c) / 1500 - \rho_w / 1000 \tag{4.23}$$

where ρ_v is the mass concentration of volatiles, ρ_c is the mass concentration of char and ρ_w mass concentration of water in fuel.

At combustion temperatures, the radiative heat transfer becomes significant, and in the model, it is considered using the two-flux model given by Equations (4.24) and (4.25).

$$\frac{dI^{+}}{dx} = -(k_a + k_s)I^{+} + k_sI^{-} + \frac{1}{2}k_a\sigma T_s^4$$
(4.24)

$$-\frac{dI^{-}}{dx} = -(k_a + k_s)I^{-} + k_sI^{+} + \frac{1}{2}k_a\sigma T_s^{4}$$
(4.25)

The absorption and scattering coefficients are calculated according to Equation (4.26). The heat radiation from the freeboard is included in the two-flux model as a boundary condition equal to 7.8×10^4 (W·m⁻²).

$$k_a = -\frac{1}{d_p} \ln(\varepsilon_b), k_s = 0 \tag{4.26}$$

4.1.4 Modeling of gas phase energy conservation

The energy continuity equation for the gas phase (Equation (4.27)) includes heat exchange between the gas and solid phases, energy received through gas convection, and energy gained from carbon monoxide, methane, and hydrogen oxidation.

$$\frac{\partial H_g \varepsilon_b}{\partial t} \rho_g = -\frac{\partial}{\partial x} \left(\varepsilon_b v_g H_g \right) - \kappa_{conv} S(T_g - T_s) + \sum \mathcal{Q}_{g,i}$$
(4.27)

where H_g and ρ_g are the enthalpy and the density of the gas phase, v_g is the fluid velocity, $Q_{a,i}$ is the reaction heat of gas phase reaction *i*

4.1.5 Numerical methods for solving the model and the description of the simulation environment

The conservation equations were solved using numerical methods which were selected based on the properties of each equation (as summarized in Figure 4.1.). The equations can be divided into three categories based on the order of the spatial derivative, for example the solid phase continuity equation belongs to the category that is independent of the spatial coordinate. Category two describes equations with convection like the gas phase mass and energy continuity equations. The last category comprises the solid phase energy continuity equation that includes the heat conduction term.

The solid mass continuity equations were discretized with implicit and semiimplicit Euler methods. The implicit method was utilized for the case related to the water and the volatile components. In contrast, the semi-implicit method was used to discretize the equation describing the evolution of the char content, since its reaction rate depends on the oxygen, water vapor and carbon dioxide contents. The equations for the gas phase concentrations and the enthalpy were spatially discretized using the three-point upwind finite difference method (linear upwind difference scheme) while the time discretization was obtained with the explicit Euler method.

The solid energy continuity equation was discretized spatially with the central difference scheme, whereas, the time derivative was discretized via the implicit Euler method. In general, the methods selected for the spatial discretization were second-order accurate, however, it should be noted that the discretization of the time derivative was performed with first order-accurate methods. This was carried out in order to avoid non-physical oscillations at discontinuities and once fully discretized the model was implemented in MATLAB.

4.2 Results of the Dynamic Modeling of a BioGrate Boiler: Effects of the operation parameters on biomass firing

The simulation results show that the bed comprising the smallest particle size ignites most rapidly. The ignition time increases as the particle size increases (Table 4.2), and the largest particles take twice as long to ignite compared with smaller diameter particles; however, smaller particles are more prone to cooling by the primary air. In contrast, large particles resist cooling more efficiently owing to their smaller heat transfer area. Larger particles enhance heat transfer inside the bed and allow the heat to spread more efficiently across the bed. This phenomenon results in lower temperature gradients in the bed. Consequently, the improved heat transfer increases moisture evaporation inside the fuel bed but due to lower temperatures inside the fuel layer, the pyrolysis and char combustion times increase.

| Particle diameter, mm | Mean front propagation rate kg/m²/s |
|-----------------------|-------------------------------------|
| 15 | 0.0224 |
| 25 | 0.0218 |
| 30 | 0.0209 |
| 40 | 0.0202 |
| 50 | 0.0197 |

Table 4.2. Mean combustion front propagation rates for different particle sizes

The simulation concerning the moisture content effect, Figure 4.3, shows that fuels with 60 and 70 wt% moisture content exhibit a rapid increase in gas production after being subjected to the furnace environment. The fuels with the two highest moisture contents show noticeably larger initial gas production rates. Subsequently, after the fuel layer surface has achieved a stable drying rate, the production rate of combustibles begins to increase, suggesting that the fuel has ignited. The results suggest that drier fuel ignites much more rapidly than wet fuel. However, the fuel with the highest moisture content, 70 wt%, does not seem to burn properly, as it demonstrates a rather low increase in the gas production rate. However, after ignition, all the fuels achieve a relatively constant combustion front propagation rate: $0.03 \text{ kg/m}^2 \text{ s}$ for the driest fuel (40 wt%) and $0.02 \text{ kg/m}^2 \text{ s}$ for the wettest one (70 wt%), with the values for the other fuels in between. A more detailed analysis on the effect of fuel parameters on biomass combustion is presented in Publication 1.



Figure 4.3. a) The overview of gas production rates of fuels with different moisture content b) the gas production rates, a close up

Dynamic Modeling of a BioGrate Boiler

5. Enhanced Dynamic Model of a BioGrate Boiler and Analysis of the Fuel Bed Combustion Dynamics

The dynamic model provides a valuable insight into the phenomena occurring inside the burning fuel layer. However, the biomass combustion is susceptible to variations in fuel composition and primary air flow. The dynamic behavior of the dry fuel thermal decomposition is mainly determined by pyrolysis kinetics. Thus, a higher model accuracy with respect to biomass pyrolysis is especially beneficial in the evaluation of combustion dynamics. In the enhanced model, the kinetic parameters used in the original model (Equations (4.3) and (4.4)) are replaced with the parameters estimated here. The kinetic parameters are estimated from the experimental data on the devolatilization of Norway spruce debarking residue. After the estimation, the model with the estimated parameters is validated. Finally, the results on the analysis of dynamic fuel combustion phenomena are presented and discussed.

5.1 Estimation of the pyrolysis kinetic parameters for the enhanced model

The kinetic parameters are approximated by fitting the estimated mass loss curve to the mass loss curve measured in the thermogravimetric experiments of debarking residue pyrolysis. Firstly, this section presents the material used in the experiments and its pretreatment. Secondly, the thermogravimetric (TG) experiments of debarking residue pyrolysis are described. Thirdly, mathematical methods used for the parameter estimation are presented and the parameters are estimated.

5.1.1 Material

The fuel samples used in the experiments were a mixture of spruce bark and wood residue with an approximate ratio of spruce stem wood residue to wood bark of 3:7. The particles were thin with irregular shapes and had the following approximate size range: 0.1 - 4 cm x 0.5 - 2 cm x 0.01 - 0.03 cm. The material was collected from Metsä Wood Sawmill in Vilppula, Finland and dried prior to the experiments. Composition of fuel samples from the same sawmill site was analyzed by the accredited (EN ISO/IEC 17025) laboratory ENAS LTD, Finland, and the reported material properties are presented.

Enhanced Dynamic Model of a BioGrate Boiler and Analysis of the Fuel Bed Combustion Dynamics

5.1.2 Description of the experimental setup

Reaction rates were determined by thermogravimetry, with a Perkin Elmer TGA 4000. The thermogravimetric analysis (TGA) was performed on samples air-dried overnight at room temperature and on ones that were dried in an oven at 90 °C for two weeks. The air-dried material which included wood and bark samples were cut into small pieces prior to the TGA tests, whereas, the oven-dried samples were crushed in a Retsch PM100 ball mill and the powder obtained was sieved. Oven-dried material was screened and separated into two batches, one with particles smaller than 500 μ m and another with particles larger than 500 μ m. The batch with particles > 500 μ m consisted of needle-shaped pure wood particles while the other batch contained both bark and wood powder. TGA was then performed on both batches and on a mixture of them with a 2:5 ratio, in addition, TGA was also run on the air-dried wood and bark samples. For the analysis, 8-12 mg of a sample was loaded in to a ceramic crucible and heated at a rate of 80 °C/min in a nitrogen atmosphere (20 ml/min).

5.1.3 Mathematical method for kinetic parameter estimation

The estimation of the parameters is formulated as an optimization problem which is solved with a sequential quadratic programming (SQP) algorithm. The problem is defined by the objective function, Equation (5.1) which is minimized with respect to the kinetic parameters. The objective function expresses the sums of squares (RSS), between the measured and the calculated mass loss curve. The calculated mass loss curve - which is modelled with Arrhenius equations - is assumed to comprise two parallel reactions with the respective pre-exponential factors and activation energies: A1, A2, E1 and E2. Pomerantsev (1986) has demonstrated that a satisfactory accuracy can be achieved in approximating the overall pyrolysis reaction by dividing it in to two parallel subreactions. Each subreaction describes the pyrolysis of volatile components with distinct reaction kinetics, for instance, holocellulose and lignin. Nevertheless, it is likely that each subreaction will capture pyrolysis characteristics of various wood constituents, but in different proportions. To account for the two separate wood components and their respective reactions a parameter α , which defines the initial mass fraction of these components, is estimated along with the kinetic parameters.

$$F(m_1, m_2, m_{meas}) = \sum_{k=1}^{N} (m_{1,k}(\alpha, A_1, E_1, t_k) + m_{2,k}(\alpha, A_2, E_2, t_k) - m_{meas}(t_k))^2$$
(5.1)

where m_1 and m_2 is the mass of volatile component 1 and 2, m_{meas} is the measured sample mass, respectively, k is the discretized time step, a is the mass fraction of a volatile component

In the objective function, the mass of a sample at each time step is given as the sum of masses of volatile component one, Equation (5.2), and two, Equation

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(5.4). For both components, the reaction rate constant, k_i , is defined by Equation (5.3).

$$m_{1,k} = m_{1,k-1} \exp(-k_1(t_k - t_{k-1}))$$
(5.2)

where $m_{i,k}$ and $m_{2,k}$ is the predicted sample weight at time instance k

$$k_i = A_i \exp(-E_i/(RT)) \tag{5.3}$$

$$m_{2',k} = m_{2,k-1} \exp(-k_2(t_k - t_{k-1}))$$
(5.4)

where k_i , A_i and E_i are the reaction rate constant, pre-exponential factor and activation energy, respectively for a volatile component *i* pyrolysis

The initial conditions for the optimization are given by Equations (5.5) and (5.6) which define the mass fraction of each volatile component through parameter α .

$$m_{1,k=0} = \alpha (m_{meas,t=0} - m_{char+ash})$$
(5.5)

$$m_{2',k=0} = (1 - \alpha)(m_{meas,t=0} - m_{char+ash})$$
(5.6)

where A_i , [1/s], i = 1,2 and the temperature is a function of time.

The estimated kinetic parameters and R^2 are summarized in Table 5.1. The results indicate that the parameter estimation was successful as the R^2 index is above 99%.

Table 5.1. Comparison between the measured combustion front propagation velocities and the ones predicted by the model

| | A ₁ , 1/s | A ₂ | E ₁ , J/mol | E ₂ | α | R ² |
|-------------|----------------------|----------------|------------------------|----------------|--------|----------------|
| Spruce Bark | 0.2739 | 1.109e+03 | 2.586e+04 | 6.208e+04 | 0.2982 | 99.98% |
| Spruce Wood | 4.4355e+04 | 1.681e+05 | 1.145e+05 | 8.907e+04 | 0.0743 | 99.96% |
| < 500 µm | 0.4409 | 2.087e+05 | 2.905e+04 | 8.990e+04 | 0.2454 | 99.91% |
| >500 µm | 5.637e+05 | 2.295e+05 | 1.369e+05 | 9.273e+04 | 0.0708 | 99.94% |
| Mixture | 3.156e+02 | 2.205e+04 | 8.008e+04 | 7.838e+04 | 0.1539 | 99.92% |

The set of kinetic parameters estimated for "Mixture" was substituted into the model (Equation (4.3)) and the model was validated.

5.2 Validation of the enhanced model

The model was validated against the ignition front propagation velocities reported by Saastamoinen et al. (2000) for the fixed-bed combustion of spruce wood chips. Secondly, the simulated gas compositions were compared to the Enhanced Dynamic Model of a BioGrate Boiler and Analysis of the Fuel Bed Combustion Dynamics

values reported by Girgis and Hallett (2010). The parameters used for the validation are given in Table 5.2 and the results of the model validation in Table 5.3.

The overall model performance is acceptable, and the predicted values correspond to those acquired experimentally. The model also predicts satisfactorily the propagation velocities for all combinations of moisture content and air flow.

| | Saastamoinen et | al. (2000) | This s | study | |
|---------------|-----------------------|-----------------------|----------------------------|-----------------------|--|
| Particle size | 5-20 mn | n | 20 mm/12.5 mm | | |
| | moisture content, wt% | bed density, kg/m3 | moisture con- tent, wt% | bed density, kg/m3 | |
| Bed densities | 10.8 | 157 | 10.8 | 157 | |
| | 18.8 | 145 | 18.8 | 145 | |
| | 33.4 | 140 | 33.4 | 140 | |

Table 5.2. Parameters for the mechanistic model validation

Table 5.3. Comparison between the measured combustion front propagation velocities and the ones predicted by the model

| Moisture content | Air flow | Saastamoinen et al. (2000) mm/s | Model prediction mm/s 20 mm/ 12.5 mm |
|------------------|----------|------------------------------------|---|
| | 0.07 | 0.42 | 0.468/0.476 |
| 10.8 | 0.15 | 0.58 | 0.519/0.571 |
| | 0.23 | 0.47 | 0.476/0.529 |
| | 0.07 | 0.34 | 0.380/0.391 |
| 18.8 | 0.15 | 0.47 | 0.420/0.484 |
| | 0.23 | 0.39 | 0.414/0.426 |
| | 0.07 | 0.28 | 0.257/0.244 |
| 33.4 | 0.15 | 0.25 | 0.268/0.292 |
| | 0.23 | 0.27 | 0.277/0.260 |

The comparison was performed for a simulated reaction front propagating approximately 10 cm above the grate. The following parameters were used for the simulation: air flow, 108 kg/(m²h); overall bed density, 150 kg/m³; gas temperature above the fuel bed, 900 °C; particle diameter, 2.8 cm; and bed porosity, 0.6. The simulated gas profile of the fixed-bed combustion is presented in Figure 5.1.

As demonstrated by the results presented in Figure 5.1, the model is able to reproduce satisfactorily the measured gas evolution profile in the burning fuel bed. The model predicted the gas formation during the char combustion phase, which occurs between 0 and 4 cm above the grate particularly well. Nevertheless, due to the differences in the compositions of material used in the experiments and the simulated one, some discrepancies are noticeable in the gas formation were also significant between different experiments. Nevertheless, the qualitative trend of tar and CO observed in the results matches the measured one satisfactorily.

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Figure 5.1. Simulated countercurrent combustion of a fuel bed comprising spruce debarking material

5.3 Analysis of fuel bed combustion dynamics

The efficiency of a boiler largely depends on the combustion dynamics, as the burning fuel bed is the source of energy for plant operation. Thus, the combustion dynamics were analyzed with the mechanistic model by varying the rate of the primary air flow fed into the burning fuel bed and observing the effects on moisture evaporation, devolatilization, and char consumption. The flows and the responses are presented in Figures 5.2-5.5. In the simulations, the fuel bed density was assumed as 150 kg/m3 on a dry basis, the moisture content was kept at 55 wt%, the initial fuel layer height was 0.5 m, the freeboard temperature was 900 °C, and the fuel speed was 1.5 mm/s. The air flow was varied between 3 m³/s (0.039 m/s) and 5 m³/s (0.064 m/s), which is the typical air flow range for BioGrate boiler operation.

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Figure 5.2. Gas phase composition during the simulation with a constant air flow



Figure 5.3. Gas phase composition during the simulation with large steps in the air flow

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Figure 5.4. Gas phase composition during the simulation with small steps in the air flow



Figure 5.5. Gas phase composition during the simulation with a gradual increase in the air flow

The results shown in Figures 5.2–5.5 demonstrate that the gas compositions in all cases are similar: the gas comprises a large amount of water from moisture evaporation, as well as tar, carbon monoxide, and carbon dioxide formed in pyrolysis and char combustion. All cases showed a dramatic change in gas composition when the fuel finished drying. The end of the drying increases the energy flux to the dry wood and, thus, forces the devolatilization of the remaining volatiles, which causes a spike in gas formation and a notable change in composition.

The fuel bed responses presented in Figures 5.2–5.5 indicate that changes in air flow have a substantial effect on the fuel bed behavior, as large changes are observable in the gas release rates. The interaction between the air flow and

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drying is demonstrated by the reaction rates presented in Figures 5.6–5.9 (the air flows used are presented in Figures 5.2–5.5), as the drying rate shown in Figures 5.6 and 5.8 has an observable effect from the induced air flow changes. The time of complete moisture evaporation depends on the average air flow rate. For instance, the drying times for varying and constant air flows were the same because the average air flow rate was the same. The simulation with a gradual increase in the air flow indicated a significantly shorter drying time due to a larger average air flow. The larger air flow resulted in more intensive char combustion and thus increased energy transfer to the drying fuel, which increased the drying rate.

In a similar fashion, the pyrolysis reaction rates also showed a dependence on the air flow; however, the influence was slightly smaller than that for the drying rate. Changes in the pyrolysis rate also affect the calorific value of the released gas (Figure 5.10), as the release of CO, H_2 , and CH_4 is proportional to the devolatilization rate. Furthermore, the calorific value also depends on the location of the fuel on the grate and consequently its stage of conversion. Close to the grate center, the effect of air flow on the calorific value was minor; the change in the air flow velocity, which occurred between 0.5 and 1 m, increased the heat content by 20%, while the step changes, which occurred between 1.5 and 2 m from the center, resulted in a 70% increase in the gas calorific value. The step changes during the char combustion phase, between 3.5 and 4 m from the center, increased the energy release by 90%. In contrast to the calorific value, the temperature of the gas leaving the bed was not affected by the air flow because all excessive energy was absorbed by the drying fuel. However, among all the reactions, char combustion (Figure 5.11) demonstrated the highest dependence on the air flow.

The simulations suggest that moisture evaporation controls the pyrolysis rate by absorbing the energy produced by char combustion. Due to this phenomenon, the pyrolysis rate has a lower dependence on primary air flow compared with moisture evaporation.

The results indicate that the fuel bed has rapid combustion dynamics. Figures 5.12 and 5.13 demonstrate the normalized (mean removed and scaled by standard deviation) drying and pyrolysis rates and air flows, respectively. As can be observed, the air flow instantly affects the drying and pyrolysis rates. After the change in the flow rate, the reaction rate stabilizes after 30 s, but the rate only becomes constant after ~500 s. At the char combustion stage, the increase in the air flow rate also dramatically increased the content of carbon monoxide in the released gas. The simulated gas profiles in Figures 5.2–5.5 clearly follow this trend.

The simulations suggest that different fuels have different combustion dynamics, and the most prominent differences between the fuels are observed during the pyrolysis phase. Furthermore, bark showed a more rapid drying rate compared with the other fuels, which is a result of its lower devolatilization temperature. The results from the analysis are discussed in more detail in Publication 2.

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Figure 5.6. Reaction dynamics during the simulation with a constant air flow; (∇) wood, (\circ) bark, (–) mixture



Figure 5.7. Reaction dynamics during the simulation with large steps in the air flow; (∇) wood, (\circ) bark, (–) mixture

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Figure 5.8. Reaction dynamics during the simulation with small steps in the air flow; (∇) wood, (\circ) bark, (–) mixture



Figure 5.9. Reaction dynamics during the simulation with a gradual increase in the air flow; (∇) wood, (\circ) bark, (–) mixture

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Figure 5.10. Calorific values of gas under different air flows



Figure 5.11. Rate of char combustion under different air flows

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Figure 5.12. Normalized drying rate and air flow



Figure 5.13. Normalized pyrolysis rate and air flow

The efficiency of advanced process control methods, for instance, model predictive control (MPC), requires high accuracy of dynamic modeling, which can be achieved through mechanistic modeling. However, the full enhanced model developed in this thesis for a BioGrate boiler cannot be utilized due to its complexity. Therefore, this chapter proposes a simplification of the mechanistic model suitable for these tasks. The purpose of the simplified model development is to minimize the computational time but, at the same time, to retain sufficient accuracy in describing combustion phenomena.

The main idea of the simplification is to divide the fuel layer into zones located between the reaction fronts and to assume uniform conditions within each zone. This strategy is based on the observation that large temperature and composition gradients exist at the reaction fronts, whereas the degree of variation is limited between the fronts. Such an approach allows to significantly reduce the number of variables by neglecting those that are not critical in the mathematical description of a combustion process.

This chapter is structured as follows: First, the simplification approach is presented. Second, the mathematical formulation of the model is introduced. Third, the parameters required for the successful implementation of the model are estimated. Finally, the model with the estimated parameters is validated.

6.1 General approach for simplification of the enhanced model

The simplification of the model developed in this thesis involves three main phases. The purpose of the first phase is to divide the fuel layer into zones to reduce computational burden. This is performed based on the simulation results from the enhanced model by identifying largest gradients with respect to the char, volatile and moisture content which indicate the end of each respective zone.

In the second phase, the reaction-limiting factors are determined among oxygen concentration, convective, radiative and conductive heat transfer, such that non-restrictive factors can be omitted from the model. This is done by comparing the magnitude of each heat transfer mechanism with respect to each other and by removing the least significant ones. The char oxidation reac-

tion is generally known to be limited by the primary air feed, since almost all oxygen is consumed close to the grate (as shown in Figure 5.1) and hence the propagation of the front is limited by oxygen supply. The area on top of the fuel layer is not included into the consideration, since it does not receive oxygen from below. With the absence of oxygen, the low heat conductivity of char can be assumed to prevent the heat flux downwards and to effectively stop the front from propagating. In case of pyrolysis and drying, the front propagation of these reactions is limited by heat transfer from hotter areas as these reactions require sufficient temperature to become active. Thus, the identification of the reaction limiting factors can be done based on the gradients in the temperature profile as well as on the radiative heat flux profile.

These considerations result in a significant simplification of the temperature profile as only the temperature of the char layer is assumed to be a variable. Instead, concentration wise the fuel layer is divided into three zones.

Finally, the detailed description of the third phase of the simplification approach, namely, the mathematical formulation of the model, is provided in the following.

6.2 Mathematical formulation of the simplified model

This section presents the development of a simplified dynamic model for online computations. First, based on the simulation results from the enhanced model, the reaction-limiting factors are identified (Section (6.2.1)). Then, the equations of the enhanced model are simplified by considering these factors. In Section (6.2.2), the parameters required for the successful implementation of the model are determined and in Section (6.3) the model is validated. The simplified model was implemented in the MATLAB computation environment and solved with the implicit Euler method. An overview of the model structure is presented in Figure 6.1.



Dynamic Model Development for On-line Computations through Simplification of the Enhanced Mechanistic Model

Figure 6.1. Overview of the model structure

6.2.1 Mathematical formulation of the dynamic model for on-line computations

In the first phase, the reaction-limiting factors have to be identified, which is done based on simulations of the enhanced mechanistic model. The results from the enhanced model (Figure 6.2) suggest the presence of three reaction fronts corresponding to each major reaction: char combustion, pyrolysis, and evaporation zones. This means that the walking grate concept, which described fuel movement on the grate as well as temperature and concentration gradients in the horizontal direction in the dynamic model, has to be omitted because of the assumption of uniform conditions inside each zone.

In the second phase, the reaction-limiting factors are identified from the simulation results presented in Figure 6.2 starting from char oxidation zone. In that zone, oxygen is consumed almost completely by the reaction. However, the primary air flow initially decreases the temperature of char as it enters the furnace. This effect is shown in Figure 6.2 as a decrease in temperature which becomes more significant towards the surface of the grate. Thus, in addition to the oxidation reaction also the heat exchange between char and the primary air is significant and can be up to 1000 $^{\circ}$ C close to the grate.

The pyrolysis zone, which lies above the char oxidation zone, is rather thin and, thus, the temperature of the reacting fuel is close to the char combustion temperature. The simulation results in Figure 6.2 indicate that the char oxidation and pyrolysis zones overlap since char forms during the devolatilization reaction. Thus, it is assumed that the temperature of the pyrolysis zone equals that of the char oxidation zone.

Moisture evaporation, being an endothermic reaction, is limited by the radiative as well as by the convective heat transfer from the char combustion zone. Heat conduction is neglected due to its low contribution since, the conductive heat flux over one char particle and 100 °C temperature gradient is 670 W/m² while in case of radiative heat transfer it is nine times higher (calculated by differentiating the heat flux over the interface between the drying and pyrolysis zones over one particle diameter). In addition, conduction contributes only slightly to the evaporation due to low heat conductivity of char and thus its effect is neglected. The contribution of the radiative heat transfer mechanism is significant at the interface of the pyrolysis and the drying zones where temperature exceeds 500 °C. Another significant mechanism is convection, as it facilitates drying by allowing heat transfer from the hot gas from the oxidation zone to the colder fuel layer. Thus, both the radiative and the convective heat transfer mechanisms can be assumed to contribute significantly to the moisture evaporation. Next, mathematical equations based on these considerations are presented for each zone, in accordance with the phase three of the approach.



Figure 6.2. Simulation results from the enhanced model

6.2.1.1 Char combustion zone

In char combustion zone, both the mass and energy are considered in accordance with the general simplification approach.

Mass conservation

Char forms during the pyrolysis phase and is subsequently consumed by the oxidation reaction:

$$\frac{dm_{c}}{dt} = X_{c} \sum_{i=1}^{3} r_{p,i} - r_{c}$$
(6.1)

where m_c is the amount of char on the grate, X_c is the char yield from wood pyrolysis and r_c is the char reaction rate.

The effective char consumption rate is described by Equation (6.2) and, depending on the conditions, char oxidation is kinetically or mass transfer controlled. Owing to the omission of the spatial coordinates, the term h_cSV was introduced to model the effect of the char layer thickness on the consumption of oxygen. Thus, Equation (4.6), which describes the effective rate constant of char combustion in the enhanced model, is modified as:

$$k_{eff,C} = h_C SV k_{O2} k_C / (k_C + h_C SV k_{O2})$$
(6.2)

where $k_{eff,C}$ is the effective reaction rate of char, *V* is the fuel layer volume, k_{o_2} is the mass transfer coefficient of oxygen onto the surface of char particle, h_c is the mass fraction of char on the grate

where the mass transfer coefficient is calculated from the Sherwood number:

$$k_{o2} = D_g / d_p \left(2 + \text{Re}^{1/2} S c^{1/3} \right)$$
(6.3)
where D_q is the oxygen diffusivity in air and d_p is the particle size

The volume of the fuel layer is defined by Equation (6.4):

$$V = \frac{m_{fuel}}{\rho_{fuel \ bed \ dry}} + \frac{m_C}{\rho_{char \ bed}}$$
(6.4)

 $ho_{fuel \ bed \ dry}$ is the density of dry fuel, $ho_{char \ bed}$ is the density of char bed

Parameter S is the density number:

$$S = \frac{6(1 - \varepsilon_b)}{d_p} \tag{6.5}$$

where ε_b is the porosity of fuel bed

and h_c is the mass fraction of char:

$$h_C = m_C / (m_{fuel} + m_{H2O,l} + m_C)$$
(6.6)

where m_{C} , m_{fuel} and $m_{H2O,l}$ are the amounts of char, fuel and water.

The char combustion kinetics are defined by Equation (6.7) (Branca et al., 2005):

$$k_{c} = 1.1 \cdot 10^{6} \exp(-114.5[kJ/mol]/(RT_{s}))$$
(6.7)

Char has a large impact on both mass and energy balances, therefore, the yield of char from pyrolysis must also be properly defined. Furthermore, the calorific value of char has to be determined to define whether the residual volatiles affect the energy balance.

Energy conservation

The energy balance of the solid phase, as outlined in Equation (6.8), mainly includes energy stored in char and minute amounts of volatile components. A fraction of the energy of the solid phase is transferred with the gases formed in pyrolysis and oxidation reactions. Moreover, the enthalpy of the solid phase is affected by oxidation reactions and the heat released or consumed by pyrolysis reactions. As the air is supplied from under the grate, it is heated by the burning char layer, such that:

$$\frac{dH_{s}}{dt} = Q_{in} - Q_{out} - \Delta H_{evap} r_{evap,rad} + \sum_{i=1}^{3} (\Delta H_{p,i} - C_{p,w}T) r_{p,i} + Q_{C} - Ah(T_{S} - T_{G,In})$$
(6.8)

where Q_{in} is the energy contained in primary air and Q_{out} is the energy of the gas out flow, ΔH_s is the enthalpy of the solid phase, $\Delta H_{p,i}$ is the pyrolysis heat of wood component *i*, $C_{p,w}$ is the heat capacity of wood, Q_C is the energy form char combustion. *A* is the total outer surface of the fuel and *h* is the heat transfer coefficient.

It is evident from the Equation (6.9) that depending on the intensity of thermal decomposition, the effect of pyrolysis heat can have a significant effect on the energy balance and thus needs to be estimated.

$$Q_{C} = \left(\frac{\Delta H_{CO}}{M_{CO}} \frac{2(\Omega - 1)}{\Omega} r_{C} + \frac{\Delta H_{CO2}}{M_{CO2}} \frac{2 - \Omega}{\Omega} - C_{p,C} T_{S}\right) r_{C}$$
(6.9)

where ΔH_{CO} and ΔH_{CO2} is the reaction enthalpy of char oxidation to carbon monoxide and carbon dioxide, respectively, $C_{p,c}$ is the heat capacity of char, Ω is the stoichiometric coefficient defined as follows (Evans and Emmons, 1977):

$$\Omega = \frac{2 + 2 \cdot 4.3 \exp(-3390/T_s)}{2 + 4.3 \exp(-3390/T_s)}$$
(6.10)

The temperature of the gas phase can be calculated by dividing the energy content of the char by its enthalpy:

$$T = \frac{H_S}{m_C C_{p,c} + C_{p,w} \sum_{i}^{3} m_{p,i}}$$
(6.11)

6.2.1.2 Fuel pyrolysis zone

For each volatile component of the fuel (cellulose, hemicellulose, and lignin), the following mass conservation equation is devised:

$$\frac{dm_{p,i}}{dt} = r_{evap} \frac{X_{p,i}(1-X_m)}{X_m} - r_{p,i}$$
(6.12)

where $X_{p,i}$ is the fraction of cellulose, hemicellulose and lignin, X_m , the moisture content of the fuel in the furnace, is defined by Equation (6.13). Fuel moisture content is calculated as follows:

$$X_m = \frac{m_{H2O,l}}{m_{fuel} + m_{H2O,l}}$$
(6.13)

Wood pyrolysis (Equation (6.14)) consists of the individual devolatilization reactions of cellulose, lignin, and hemicellulose. Thus, for the modelling of pyrolysis it is important to determine the content of each wood polymer $(X_{p,i})$ in the fuel.

$$r_{p,i} = k_{p,i} m_{p,i} \tag{6.14}$$

$$k_{p,i} = A \exp\left(-E_{pyr}/(RT_s)\right) \tag{6.15}$$

where T_s is the temperature of pyrolysis, according to the simplification approach it is assumed to be equal to the char combustion temperature.

Due to partial overlapping between char and pyrolysis zones, char combustion and volatile gas combustion might compete if the temperature in char oxidation zone will become excessively low:

$$k_{pyr,comb} = T_g / T_s k_C \tag{6.16}$$

6.2.1.3 Fuel drying zone

Evaporation of moisture is most active at temperatures exceeding 100 °C. However, according to the simplification approach, the temperature profile described by Equation (4.17) is omitted and the heat flux becomes the determinant factor of moisture evaporation rather than local temperature. Therefore, instead of temperature, the evaporation rate (Equation (6.17)) is now determined by radiative heat transfer from burning char (Equation (6.18)) and by convective heat transfer from the gas phase (Equation (6.19)).

$$\frac{dm_{H_2O,l}}{dt} = X_m \dot{m}_{ln} - r_{evap,conv} - r_{evap,rad}$$
(6.17)

Walking grate concept which described fuel movement on the grate is replaced with a continuous fuel input, the term $X_m m_{In}$, which describes the moisture content in the fuel feed. $r_{\text{evap, conv}}$ and $r_{\text{evap,rad}}$ are the drying rates due to convective (Equation (6.18)) and radiative heat transfer (Equation (6.19)), respectively

$$r_{evap,rad} = \sigma A_{moist} \left(T_s^4 - 373^4 \right) / \Delta H_{evap}$$
(6.18)

where σ is the Stefan-Boltzmann constant and ΔH_{evap} is the heat of evaporation

$$r_{evap,conv} = hA_{moist} (T_g - 373) / \Delta H_{evap}$$
(6.19)

where *h* is the heat transfer coefficient (Wakao et al., 1979):

$$h = \frac{2 + 1.1 \operatorname{Pr}^{1/3} \operatorname{Re}^{3/5}}{d_p} k_{air}$$
(6.20)

where D_p is the particle diameter.

 A_{moist} is the area of moist fuel:

$$A_{moist} = A_{moist,0} \frac{m_{H2O}}{m_{H2O} + m_C + m_{fuel}}$$
(6.21)

The amount of wet fuel (Equation (6.22)) depends on the fuel drying and pyrolysis rates, as described by Equation (6.12). However, since walking grate concept is omitted, a variable, m_{In} , describing fuel feeding rate has to be introduced.

$$\frac{dm_{fuel}}{dt} = (1 - X_m)\dot{m}_{ln} - \sum_{i=1}^3 r_{p,i}$$
(6.22)

where m_{fuel} is the amount of dry fuel on the grate, X_{H2O} is the moisture content of fuel, m_{In} is the feed of the dry fuel, $r_{p,i}$ is the reaction rate of the individual wood component (cellulose, hemicellulose and lignin).

6.2.1.4 Mass conservation equations in the gas phase

The amount of oxygen in the fuel layer comprises the oxygen supplied by the primary and secondary air flows, as well as the char reaction rate and the flow of oxygen out of the layer:

$$\frac{dm_{O2}}{dt} = 0.23\rho_{Air}F_{In} - (k_{eff,c} + k_{pyr,comb} + F_{Out}/V)m_{O2}$$
(6.23)

where ρ_{Air} is the density of air at normal pressure at 20 °C, F_{In} and F_{Out} are the flows into and from the furnace, respectively

It is assumed that the gas density depends only on the temperature. Therefore, the outflow of gas from the fuel layer depends on the gas expansion, as outlined in Equation (6.24):

$$F_{Out} = F_{in} \frac{\rho_G(T_G)}{\rho_G(T_{in})}$$
(6.24)
where $\rho_G(T)$ is the gas density at the temperature of gas T and $\rho_G(T)$ is the

where $\rho_G(T_G)$ is the gas density at the temperature of gas, T_G and $\rho_G(T_{in})$ is the gas density at 20 °C

The amount of carbon monoxide, dioxide and pyrolytic gas are described by Equations (6.25), (6.26) and (6.27), respectively:

$$\frac{dm_{CO}}{dt} = \frac{2(\Omega - 1)}{\Omega} r_C - (F_{Out} / V) m_{CO}$$
(6.25)

$$\frac{dm_{CO2}}{dt} = \frac{2-\Omega}{\Omega} r_C + \Omega_{pyr} r_{pyr,comb} - (F_{Out} / V) m_{CO2}$$
(6.26)

The transport equations of the pyrolytic components (Equation (4.13)) were combined into one equation to describe the evolution of volatiles - Equation (6.27):

$$\frac{dm_{p,G}}{dt} = X_{p,G}m_{p,G} - \Omega_{pyr}r_{pyr,comb} - (F_{Out}/V)m_{p,G}$$

$$(6.27)$$

where Ω_{pyr} is the stoichiometric coefficient of pyrolytic gas combustion

$$\frac{dm_{H2O}}{dt} = r_{evap} - (F_{Out} / V)m_{H2O}$$
(6.28)

6.2.1.5 Energy conservation equations in the gas phase

The enthalpy of the gas phase, defined by Equation (6.29), is affected by the flow of the primary air and the flow of the reacted gas out of the fuel layer. In addition, the energy is consumed to heat the inflowing primary air and in the heat transfer between the gas and the drying fuel. The enthalpy is increased by evaporated moisture, gases formed in the oxidation reaction, and energy gained by heat transfer between gas and char:

$$\frac{dH_G}{dt} = Q_{In} - Q_{Out} + T_s C_{p,c} r_C + \sum_{i=1}^3 (C_W T_S) r_{p,i} + 373 C_{p,H2O,g} r_{evap} - Ah(T_s - T_{g,In}) - \Delta H_{evap} r_{evap,conv}$$
(6.29)

where Q_{in} is the enthalpy of the primary air, Q_{out} is the enthalpy of gas flowing out of the fuel layer.

The temperature of the gas phase is calculated as follows:

$$T_{G} = \frac{H_{G}}{m_{CO}C_{p,CO} + m_{CO2}C_{p,CO2} + m_{p,G}C_{p,G} + m_{H2O,G}C_{p,H2O,G} + m_{O2}C_{p,O2} + m_{N2}C_{p,N2}}$$
(6.30)

The successful implementation of the model requires the following information: the content of volatile components, $X_{p,i}$, the respective devolatilization heats, $\Delta H_{p,i}$, the char yield from pyrolysis X_c , the calorific value of char.

6.2.2 The experimental set-up and methods for determination of the required modelling parameters

This section presents the estimation of pyrolysis reaction heats, mass fractions of wood constituents, char yield from pyrolysis and its calorific value.

The pyrolysis heats are determined by fitting the temperature predicted by the model to the measured temperature profile obtained during the fixed-bed pyrolysis experiments. Char yield from pyrolysis is determined from TGA, which is conducted on the solid product obtained at the end of the fixed-bed pyrolysis experiments. Calorific values for char are determined by analyzing the pyrolysis residue from fixed-bed experiments with a bomb calorimeter. In the following, the experiments, the experimental procedure, and the equipment for the fixed-bed and TGA experiments are described. Then mathematical model used in the determination of pyrolysis heats is presented and reaction heats are determined.

6.2.2.1 Experimental set-up

The parameters for the rate equations and reaction heats were determined by fitting the temperature profiles measured in fixed-bed pyrolysis experiments to the model predictions. Fixed-bed experiments were also used to determine the solid, liquid, and gaseous product yields from debarking residue pyrolysis. Thermogravimetric (TGA) experiments were used to analyze the composition of solid residue from fixed-bed pyrolysis experiments. Fixed-bed and TGA experiments are discussed in the following section.

6.2.2.2 Fixed-bed experiments

Prior to the fixed-bed experiments, the material was dried for two weeks at room temperature. In each experiment, approximately 100 g of material was used. The sample was loaded into a sample basket, which was then inserted into the reactor comprising a metal cylinder surrounded by a temperature-controlled furnace. The temperature measurements were obtained inside the fuel bed using three M-type thermocouples located 11, 15, and 20 cm from the top of the reactor with data logged every 4-5 s.

In the first two experiments, the samples were heated to a target temperature of 500 °C, in the third and fourth to 700 °C, and in the final to 600 °C. All samples were heated at a pre-programmed wall heating rate of 6 °C/min, and the material was held for 1 h at the specified temperature with the exception of the first sample, which was held at the final temperature for 3 h prior to switching off the furnace. To collect the condensable gases, the products from the pyrolysis reaction were directed into a water-cooled condenser with an exit connected to a glass flask immersed in ice water. This set-up allowed liquid phase samples to be collected in a glass bottle throughout the experiment. The hose from the bottle outlet was connected to a diverter T valve, and its two other outlets were connected to an extraction hood and a gas collection bottle.

The gas sample was collected only after the pyrolyzing material reached the target temperature. Nitrogen was used to purge the pyrolytic gas from the reactor at a rate of 2 L/min. The reactor set-up used in the experiments is presented in Figure 6.3. Figure 6.4 presents the obtained solid and liquid yields.



Figure 6.3. Schematic of the small scale pyrolyser



Figure 6.4. Liquid and solid product yields as a function of temperature

6.2.2.3 TGA experiments

The purpose of the TGA experiments was to investigate the volatile, char, ash, and moisture content of the samples obtained from the fixed-bed pyrolysis experiments. In each TGA experiment, the sample was heated to 900 °C at a heating rate of 80 °C /min. The char yield was calculated as the ratio between the ash free sample weights at 900 and 110 °C. Similarly, the moisture content was calculated as the ratio between the sample weight at 110 °C and the initial sample weight. The TG device used was a Perkin Elmer TGA 4000, and the experiments were performed under a nitrogen atmosphere (20 mL/min) with

approximately 10 mg of material used in each experiment. After the fixed-bed experiments, the pyrolytic residue was collected and its volatile and fixed carbon fractions were determined. The char, volatile, and ash contents of the pyrolytic residue from experiments conducted at different temperatures are presented in Figure 6.5.

6.2.2.4 Determination of char and volatile fractions

The experimental results indicate a strong dependence of the liquid yield on temperature, namely, the higher the temperature, the lower the yield (Figure 6.4). This behavior suggests that at higher temperatures, the magnitude of volatile cracking reactions increases, which further decomposes tar fractions that are unreactive at lower temperatures. The solid yield, which comprises char and residual volatile matter, as presented in Figure 6.5, demonstrates a weaker dependence on temperature. The char yield is independent of temperature, and the weight fraction of fixed carbon is approximately 0.26 in all experiments.



Figure 6.5. Volatile content of the pyrolyzed residue

6.2.2.5 Calorific value determination

For the determination of calorific value (CV), a Parr 6200 bomb calorimeter was used. In each analysis of CV, approximately 1 g of material was used. The sample was loaded in a holder and a wire for the ignition of material was adjusted to touch the surface of the sample to ensure proper combustion of the material in the bomb. The bomb was pressurized with pure oxygen at 40 bar. The amount of water into which the bomb was immersed was carefully quantified. The calorific value was calculated according to Equation (6.31).

$$CV = \left(9866.4 \frac{{}^{o}C}{J} \cdot \Delta T - 1.20 \frac{J}{cm} \cdot l_{wire}\right) / m_{sample}$$
(6.31)

where ΔT is the measured temperature rise in water, l_{wire} is the wire length and m_{sample} is the sample mass.

6.2.2.6 Calorific values of the virgin wood and pyrolyzed samples

The main trend observed in the calorific analysis of the samples implied the dependence of the higher heating value on the stem wood and bark content and Table 6.1 compares the calorific values for the pyrolyzed solids and the virgin wood samples. The samples containing more bark had lower calorific values than the ones containing more stem wood; such tendency was also observed by Ingram et al. (2008) for pine wood and bark. As a result, the > 500 μ m sample had the highest calorific value, despite having the highest moisture content among the three milled samples. The mixture of the two milled samples had the second largest calorific content while the sample comprising the finest particles had the lowest. As expected, moisture content had a significant effect on the heating values: the samples with 7 wt% moisture content had the lowest calorific values, 15-17 MJ/kg, while the samples with 2 wt% moisture had an energy density of approximately 20 MJ/kg.

Table 6.1. Calorific values of the pyrolysis residues and virgin wood samples

| Sample | Bark | Wood | Wood < 500 µm | Wood > 500 µm | Mix- ture | EXP1/ 500 °C | EXP2/ 500 °C | EXP3/ 700 °C | EXP4/ 700 °C | EXP5/ 600 °C |
|----------------|------|------|------------------|------------------|--------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| HHV (MJ/kg) | 16,9 | 19,0 | 19,8 | 21,1 | 20,5 | 31,3 | 30,5 | 32,2 | 31,6 | 32,2 |

Compared to the virgin wood, the pyrolyzed samples had higher calorific values (31–32 MJ/kg) which are similar to the calorific value of pure carbon, graphite. Despite the differences in the volatile content among pyrolyzed residue, depicted in Figure 6.5, the difference in calorific content were rather insignificant. Thus, it can be assumed that pyrolysis of fuel which occurred above 500 °C produces char whose calorific value is very similar to carbon.

$\bf 6.2.2.7$ Mathematical model and determination of reaction enthalpies and associated reaction rates

In this work, the pyrolysis reaction enthalpies and associated reaction rates and are determined by fitting the predictions for temperature profile from a model to the temperature profile measured in the fixed-bed experiments (Grieco and Baldi, 2011;Park et al., 2010). However, since the model of wood pyrolysis is complex and requires long computational times the fitting cannot be done directly. This problem is circumvented by defining combinations of the following reaction heats: for hemicellulose 0, -100 and -200 kJ/kg, for cellulose 0 and -100 kJ/kg and for lignin -400, -600 and -1000 kJ/kg and then selecting the combination producing the best prediction of the temperature profile. Therefore, this section is divided into two parts: the first presents the model fixed-bed pyrolysis used to predict temperature profile; the second presents the determination of the reaction rates and enthalpies.

6.2.2.8 Mathematical model of debarking residue pyrolysis

The fixed-bed pyrolysis model describes the mass loss rate of the fuel in a small-scale cylindrical pyrolysis reactor. It was shown in Publication 3 that fuel used in a BioGrate boiler is thermally thin and the pyrolysis is kinetically controlled (Biot number << 1 and pyrolysis numbers (Py^I and Py^{II}) >> 1).

Therefore, it is assumed that pyrolysis of the debarking residue can be approximated by a continuous media approach, i.e., treating the fuel layer as a porous media. In the model, the heat and mass transfer are governed by mass, energy, and momentum continuity equations, while the overall pyrolysis reaction is divided into pseudo-components that capture the pyrolysis kinetics of hemicellulose, cellulose, and lignin. The model parameters are given in Table 6.2 while the main equations of the model are presented in Table 6.3. These include mass and energy conservation equations for the solid phase, described by Equations (6.32) and (6.33), and for the gas phase, described by Equations (6.43) and (6.50). In the gas phase, momentum conservation is described by Equation (6.42). The density of the gas phase only depends on temperature, as shown by Equation (6.48), whereas the mass fractions of nitrogen and the gaseous pyrolysis products are dependent on the rate of wood decomposition and tar cracking (Equation (6.44)).

| Wood heat capacity | 2400 kJ/kg/K | (Shin and Choi, 2000) |
|------------------------|--|----------------------------|
| Char heat capacity | -0.0038T ² + 5.98T - 795.28 | (Gupta et al., 2003) |
| Wood heat conductivity | 0.35 W/m/K | (Grønli and Melaaen, 2000) |
| Char heat conductivity | 0.1 W/m/K | (Grønli and Melaaen, 2000) |
| Bed porosity | 0.82 | |
| Wood emissivity | 0.7 | (Corbetta et al., 2014) |
| Char emissivity | 0.92 | (Corbetta et al., 2014) |
| σc | 0.01 | |
| τ | 15 | |

Table 6.2. Parameters used in the model

The overall heat conductivity of the bed is described by a function proposed by Yagi and Kunii (1957), which includes heat conduction between particles (Equation (6.35)), heat radiation between voids and particles (Equation (6.36)), and void-to-void heat radiation (Equation (6.37)). The heat conductivity of the solid phase (Equation (6.35)) is assumed to comprise heat conduction (Equations (6.37) and (6.39)), and heat radiation (Equations (6.40)).

Based on studies by Garcia-Pérez et al. (2007) and Oasmaa et al. (2003) and by assuming that fuel comprises bark and wood in 3:7 proportion, the following composition of the material was calculated: cellulose 36 wt%, hemicellulose 24 wt% and lignin 40 wt% A more detailed description of the model is presented in Publication 3.

The model, based on the finite element method, was implemented in the COMSOL 5.0 software package, and the time dependent kinetic and continuity equations were solved using the backward difference method (BDF).

| Solid phase | | | | | |
|---|--|------------------|--|--------|--------------|
| Mass continuity equation | | | | (6.32) | (Anon, |
| $\frac{\partial \rho_{s,i}}{\partial t} = -k_{s,i}\rho_{s,i}$ | | | | | 2014) |
| Energy continuity equation | | | | (6.33) | (Anon, |
| $(2C_{s})\frac{\partial T_{s}}{\partial T_{s}} = \nabla_{s}(k_{s} \nabla T_{s}) + O_{s}$ | | | | () | 2014) |
| $(pC_{p,w}) \frac{\partial l}{\partial t} = \sqrt{(\kappa_{bed} \sqrt{T_S}) + Q}$ | | | | | |
| Effective heat conductivity of the bed | (6.34) | (Yaqi | Effective heat con- | (6.35) | (Janss |
| | (0.0.1) | and | duction coefficient | (0.00) | ens |
| $\frac{k_{bed}}{l} = \frac{\beta(1-\varepsilon_b)}{1-\varepsilon_b} + \varepsilon_b \beta \frac{d_p k_{rv}}{l}$ | | Kunii, | $k_{s.eff} = \varepsilon_p k_{max} + (1 - \varepsilon_p) k_{min}$ | | and |
| $k_g = \gamma \left(\frac{k_g}{L} \right) + \frac{1}{(1 + 1)^2} \qquad k_g$ | | 1957) | $+ k_{s, rad}$ | | Doug- |
| $\begin{pmatrix} \kappa_{s,eff} \end{pmatrix}$ $(1/\varphi) + a_p \kappa_{rs} / \kappa_g$ | | | | | 2004) |
| | (6.36) | (Yaqi | k k a | (6.37) | (Janss |
| $0.1952 1-\varepsilon \left(T \right)^{3}$ | (0.00) | and | $k_{\min} = \frac{\kappa_g \kappa_{fiber}}{\varepsilon_p k_{fiber} + (1 - \varepsilon_p) k_g}$ | (0.07) | ens |
| $k_{rv} = \left \frac{\varepsilon_{rv} \varepsilon_2}{\varepsilon_b} \frac{1}{\varepsilon} \right \left \frac{1}{100} \right $ | | Kunii, | | | and |
| $\left(1+\frac{1}{2(1-\varepsilon_b)}\right)$ | | 1957) | | | Doug- |
| | | | | | 2004) |
| $I = 0.1052 \left(\varepsilon \right) \left(T \right)^3$ | (6.38) | (Yagi | $k_{\max} = \varepsilon_p k_g + (1-\varepsilon_p) k_{fiber}$ | (6.39) | (Janss |
| $k_{rs} = 0.1952 \left(\frac{1}{1 - \varepsilon} \right) \left(\frac{100}{100} \right)$ | | and Kunii | | | ens |
| | | 1957) | | | Doug- |
| | | , | | | las, |
| Padiative beat conductivity of wood | (6.40) | (lane | Particla diamator | (6.41) | 2004) |
| particles | (0.40) | sens | $d_{p} = d_{p,0}(\rho_{c} + \rho_{w})/\rho_{w,0}$ | (0.41) | |
| $4\varepsilon_p \sigma T_s^3 d_{cavity}$ | | and | p p,00 c 1 m 1 m,0 | | |
| $k_{s,rad} = \frac{1}{1 - \varepsilon_p}$ | | Doug- | | | |
| | | 2004) | | | |
| Gas phase | | | | | |
| Momentum conservation in the packed be | t | | | (6.42) | (Anon, |
| $\frac{\rho\left(\partial \vec{u} + (\vec{u} \cdot \nabla) \cdot \vec{u}\right) - \nabla \left[-pI + \frac{\mu}{(\nabla \vec{u} + (\nabla \vec{u})^T) - (\nabla \vec{u} - \nabla \vec{u})^T\right]}{\rho\left(\partial \vec{u} + (\nabla \vec{u})^T\right) - (\nabla \vec{u} - \nabla \vec{u})^T}$ | $\frac{2\mu}{(\nabla,\vec{u})I}$ | $-(ur^{-1} + l)$ | $\left \vec{u}\right + \frac{Q_{br}}{\vec{u}}$ | | 2014) |
| $\varepsilon_b \left(\partial t + (u + v) \varepsilon_b \right)^{-1} \left[-\frac{p_1}{\varepsilon_b} + \varepsilon_b \right]^{-1} \left[-\frac{p_2}{\varepsilon_b} + \frac{p_1}{\varepsilon_b} + \frac{p_2}{\varepsilon_b} \right]^{-1} \left[-\frac{p_1}{\varepsilon_b} + \frac{p_2}{\varepsilon_b} + \frac{p_2}{\varepsilon_b} + \frac{p_2}{\varepsilon_b} \right]^{-1} \left[-\frac{p_2}{\varepsilon_b} + \frac{p_2}{\varepsilon_b} + \frac{p_2}{\varepsilon_b}$ | $3\varepsilon_b$ | (444 - 14 | \mathcal{E}_{b}^{r} | | |
| Gas phase mass continuity equation | | | | (6.43) | (Anon, |
| $\varepsilon_{i}\rho \frac{\partial \omega_{i}}{\partial \omega_{i}} - \nabla \cdot \left(\rho D_{i,\sigma}^{m} \nabla \omega_{i} + \rho \omega_{i} D_{i,\sigma}^{m} \frac{\nabla M_{n}}{\partial \omega_{i}} + D_{i,\sigma}^{T} \frac{\nabla T}{\partial \omega_{i}}\right)$ | $\left(- \right) + \rho(\vec{u} \cdot \nabla)_{\theta}$ | $\omega_i = S_i$ | | | 2014) |
| $\partial t = \begin{pmatrix} \cdot & \cdot, sy \end{pmatrix} \cdot \begin{pmatrix} \cdot & \cdot, sy \end{pmatrix} M_n & \cdot, sy \end{pmatrix} T$ |) | | - | | |
| Source term | (6.44) | (Anon | $D_{i,eff} = \varepsilon_{b}^{3/2} D_{i}$ | (6.45) | (Anon, 2014) |
| $S_i = -A_i \exp(-E/(RT))\omega_i \rho + n_{i,eff} S(\rho_{i,s} - \omega_i \rho)$ | | , 2014) | | | 2014) |
| Mass transfer coefficient | (6.46) | | Average molar mass | (6.47) | (Anon, |
| $h_{eff,i} = (2 + 0.6 \cdot (\mu_{\rm f}/{\rm D_e})^{1/3} {\rm Re}^{0.5})/{\rm d_p} \cdot {\rm D_e}$ | | | of the fluid | | 2014) |
| | | | $M_n = \left(\sum_i \frac{\omega_i}{M_i}\right)$ | | |
| Mass conservation of the fluid | (6.48) | (Anon | Diffusion coefficient | (6.49) | (Anon, |
| $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$ | | , 2014) | $D_{i} = \frac{1-\omega_{i}}{\omega_{i}}$ | | 2014) |
| CI | | 2014) | $D_i = \frac{x_k}{\sum x_k}$ | | |
| | | | $\sum_{k \neq i} \overline{D_{ik}}$ | | |
| Energy continuity equation | (6.50) | (Anon | Effective diffusion | (6.51) | (Fogler |
| $\rho C_n \frac{\partial T_g}{\partial x} + \rho C_n \vec{u} \cdot \nabla T_a = \nabla \cdot (k \nabla T_a) + O$ | | , 2014) | coefficient | | , 2006) |
| $r \partial t$ $r' g g z z$ | | 2017) | $D_e = \frac{D_i \varepsilon_p O_c}{\widetilde{\tau}}$ | | |

| Table 6.3. Modeling | equations of | of fixed-bed | pyrolysis |
|---------------------|--------------|--------------|-----------|
|---------------------|--------------|--------------|-----------|

6.2.2.9 Selection of reaction rates and the determination of reaction heats During devolatilization, wood is decomposed through thermal conversion of its constituents, namely cellulose, hemicellulose, and lignin. The literature reports considerably different values for the activation energies of the wood constituents. For instance, Roberts (1971) reported values for the activation energies of the pyrolysis reaction under practical conditions (cellulose: 126
kJ/mol and lignin: 38 kJ/mol). Grønli et al. (2002) reported markedly different values (cellulose: 236 kJ/mol and lignin: 46 kJ/mol). Values reported by Grønli et al. (2002) for cellulose are supported by a large number of studies, for instance Várhegyi et al. (1994), obtained an activation energy of 238 kJ/mol by using ash free cellulose.

A large spread in the kinetic parameters is common for other wood constituents, although values of 80–100 kJ/mol (Rao and Sharma, 1998) for hemicellulose are most commonly reported in the literature. A wider range of values are commonly reported for the activation energy of lignin estimated from the TGA curves of wood samples: 20 kJ/mol (Orfão et al., 1999)), 30 kJ/mol (Várhegyi et al., 1994), 19–40 kJ/mol (Domínguez et al., 2008), 46 kJ/mol (Butterman and Castaldi, 2010; Grønli et al., 2002), 35–65 kJ/mol (Várhegyi et al., 1997), and 70–80 kJ/mol (Barneto et al., 2009; Rao and Sharma, 1998).

Based on the literature values for devolatilization, two sets of kinetic parameters were selected to describe the pyrolysis kinetics of the spruce debarking residue (Table 6.4). The first set was measured for softwood bark and the second for spruce stem wood. As can be observed from the parameters of these sets, the kinetics of bark and stem wood are similar. However, the simulations with the fixed-bed pyrolysis model indicated that reaction set one better describes the debarking residue decomposition at higher temperatures and, therefore, this was selected for the model.

| Parameter set | Reaction | | А | E (kJ/kg) | n | |
|---------------|----------------------------|---------------------|--|-----------|------|--------------------------------|
| 1 | Cellulose pyrol- ysis | k _{cell} | 8.75x10 ¹⁸ (min ⁻¹) | 233 | 1 | (Garcìa-Pérez et al., 2007) |
| | Hemicellulose pyrolysis | k _{hcell} | 5x10 ⁸ (min ⁻¹) | 105 | 1 | (Garcìa-Pérez et al., 2007) |
| | Lignin pyrolysis | k _{lignin} | 25 (min ⁻¹) | 30 | 1.12 | (Garcìa-Pérez et al., 2007) |
| 2 | Cellulose pyrol- ysis | k _{cell} | 4.17x10 ¹⁵ (s ⁻¹) | 213.1 | 1 | (Broström et al., 2012) |
| | Hemicellulose pyrolysis | k _{hcell} | 3.6x10 ⁶ (s ⁻¹) | 100.6 | 1 | (Broström et al., 2012) |
| | Lignin pyrolysis | k _{lignin} | 1 (s ⁻¹) | 38.6 | 1 | (Broström et al., 2012) |

Table 6.4. Kinetic parameters used in the model

The selection of the reaction heat ranges for individual wood components was based on findings according to which pyrolysis of unmilled wood samples is an exothermic process. For instance, Beall (1971) determined that at temperatures exceeding 400 °C, wood pyrolysis becomes an exothermic reaction with overall exothermic reaction heats of 446 and 254 J/g for the unextracted softwood and hardwood samples, respectively. Similarly, Roberts (1971) reported typical heats of reactions in the range between -160 and -240 J/g for wood samples heated to temperatures higher than 320 °C. Arseneau (1971) investigated the heat of pyrolysis of cellulose and noted that the pyrolysis of thick cellulose samples and cellulose samples overlaid with Al2O3 were characterized by an exothermic reaction whereas pyrolysis of thin cellulose samples resulted in an endothermic reaction heats. Roberts (1971) also concluded that the exothermic reaction heat can be explained solely by primary pyrolysis

which under practical conditions proceeds through a dehydration reaction that favors char formation. Sadhukhan et al. (2008) found that an enthalpy of pyrolysis of -245 kJ/kg represents the overall heat of reaction of a large wood cylinder.

The simulations with neutral pyrolysis heat indeed demonstrated that pyrolysis of debarking residue is an exothermic process. Thus, the range for the overall reaction heat was selected to be -160 – -480 kJ/kg. This range corresponded to the following individual reaction heats of the components: lignin: -400, -600, and -1000 kJ/kg; cellulose: 0 and -100 kJ/kg; and hemicellulose: 0, -100, and -200 kJ/kg. The RSS index for each combination is reported in Figure 6.6, which also presents a comparison of the combination with the smallest RSS (-600, -100, and -200 kJ/kg) with the measured temperature of the second thermocouple.



Figure 6.6. a) Comparison of the measured and simulated temperature profile; b) RSE indexes for the combinations of reaction heats for primary pyrolysis

6.2.3 Validation of the model with the selected reaction rates and determined enthalpies

The value obtained for the pyrolysis enthalpy was incorporated into the model, and the subsequent prediction was validated against the measurements of the three thermocouples obtained in all experiments. Overall, the model demonstrated satisfactory accuracy; however, some discrepancies were observed for the thermocouple 3 (T3) owing to varying gas flow patterns in the fuel bed in different experiments. Figure 6.7 (a) presents the validation results against all experimental measurements and Figure 6.7 (b) visualizes the deviations of the model predictions from the measured temperatures because of flow variation

and particle re-orientation. To demonstrate the effect of flow patterns, additional gas temperatures, located one particle diameter away from the T3, were included in Figure 6.7 (b).

6.2.4 Summary of the parameters for the simplified dynamic model

Based on the results from this section the following values were determined for the model. Pyrolysis heats for cellulose, hemicellulose and lignin were estimated to be -100, -200 and -600 kJ/kg, respectively. Wood composition was calculated to be: 36 wt% cellulose, 24 wt% hemicellulose and 40 wt% lignin. Kinetic parameters presented in Table 6.4 as Set 1 were found appropriate for describing pyrolysis of the debarking residue. Char yield from pyrolysis 26 wt% and its composition is assumed to be pure carbon, because residual volatiles had only a slight effect on the calorific value.



Figure 6.7. a) Measured and predicted temperature profiles of the fixed-bed experiments, experiment at 500 °C (solid), 600 °C (dash-dot) and 700 °C (dashed line), measurements TC3 (+), TC2 (o) and TC1 no marker. Simulated TC3 (x), TC2 (\Box) and TC1 solid thick line. b) The comparison of measured temperatures TC3, (500, 600 and 700 °C) and simulated gas temperatures at the coordinates of TC3 \pm 1D_p.

6.3 Validation of the simplified model with industrial data from a BioGrate boiler

The parameters values estimated in the previous section were included into the simplified model. In addition, the fuel-feeding rate was resolved in order to convert the stoker rotation speed (%) to material flow (kg/s) by calculating the conversion constant from plant data. This constant was determined by using approximately two-thirds of the data while the final third was used for validation. The model was implemented in MathWorks MATLAB (2014b), solved with the implicit Euler scheme and validated.

The validation was performed against industrial data obtained during fullscale plant experiments at Biopower 5 16 MW CHP (an energy boiler based on

the BioGrate boiler technology) located at Mänttä-Vilppula, Finland. The aim of the experiments was to analyze the effect of variations in fuel moisture content on the combustion behavior of the boiler. For this purpose, three changes in the fuel moisture content of different magnitudes were induced by switching the fuel feed to an auxiliary fuel bunker loaded with 5, 10, or 25 m³ wood chips with approximately 22 wt% moisture content. After the bunker contents were fully discharged, the fuel feed was switched back to the typical fuel, which has 55 wt% moisture content. The data were collected with a 1 s sampling interval during this period, and then utilized for validation purposes along with the measured primary and secondary air flow rates, stoker speed, and moisture content.

The model inputs used for the validation were the same as in the experiments, and are presented in Figures 6.8. In the beginning of the simulation, it was assumed that furnace contained 2000 kg of moist fuel and 400 kg of burning char, particle diameter was assumed to be 2 cm and the heat exchange area between the char and the fuel was calculated to be 30 m². The model predictions are presented in Figure 6.9.

The comparison of the simulated and measured fuel burning and moisture evaporation rate suggested a good ability of the model to predict biomass combustion. The effects of step changes in the moisture content on the combustion of biomass are well described by the model. Furthermore, the model also described well the smaller variations caused by primary and secondary air flow disturbances. The results indicate that the primary air did not affect the combustion rate alone, but that there is also a contribution from the secondary air. This is shown particularly well at the time instance at 90000th sample, where a large increase in the secondary air flow increased the combustion rate.



Figure 6.8. Inputs: fuel feed, fuel moisture, primary air, secondary air



Figure 6.9. Measured and predicted outputs: moisture evaporation rate, fuel burning rate and flue gas content

In this chapter, the performance of the simplified dynamic model is evaluated by comparing the predicted fuel combustion rates against the rates calculated from the enhanced dynamic model. The simplified model is also compared against an ARX model to demonstrate the benefits of including mechanistic description of process phenomena into the model

7.1 Comparison of the simplified dynamic model against the enhanced model

For the performance evaluation of the simplified dynamic model, a comparison of the model predictions against the predictions from the enhanced model was performed. Both models were simulated using primary air, fuel moisture content and fuel feed rate measured during the industrial experiments which were described in Section 6.3.

The results indicated that the decrease in the fuel combustion rate caused by the fuel moisture content decrease was equally well reproduced by both models: the predicted combustion rate started decreasing with the increased content of drier fuel on the grate. Similarly, as the moisture content of the fuel begun increasing, the predicted combustion rate increased due to the increase in the moisture evaporation rate of the fuel. This is visible in the period that occurred at the time instance of 800 seconds from the beginning of the simulation.

In conclusion, the simplified model reacted sufficiently well to changes in the primary air; however, the prediction of the simplified model was smoother as it reacted less significantly to the variations in fuel properties than the enhanced model. Nevertheless, the computational time for simulation of the simplified model was 38000 times shorter than that for the full model. Thus, it can be concluded that the simplified model is sufficiently accurate and fast for on-line computations of biomass combustion. The comparison is presented in Figure 7.1.



Figure 7.1. Comparison of the predictions from the enhanced and simplified models

7.2 Comparison of the simplified dynamic model against a linear ARX model

To compare the performance of the simplified model against a linear databased model, which is widely used for on-line computations, a comparison with a linear ARX model was performed. For the comparison, two ARX submodels were identified: one for the moisture evaporation rate and the other for predicting the fuel burning rate. The same inputs were used for ARX model identification as for the simplified model simulation, including both the primary and secondary air flows, stoker speed and fuel moisture content as shown in Figure 6.8. The data, measured at one-second intervals, provided the required amount of information for the models. The first two experiments enabled model identification, while the data from the third experiment allowed validation. All model predictions outlined in the thesis were obtained using pure or open-loop simulation and thus none of the models require measured outputs. The residuals from ARX models were tested for autocorrelation, as well as for cross-correlation with model inputs, to ensure that the model order was sufficient: both models were of the fourth order with respect to both the inputs and the output. Although, the autocorrelation of residuals for fuel combustion rate violated limits, increasing or decreasing model orders from order four only worsened the violation. Nevertheless, for the purpose of simulating combustion rate, the model was found sufficient as the absolute values of the autocorrelation were rather low. Autocorrelations of residuals and the highest cross-correlation of residuals and inputs for both models are

presented in Figure 7.2. In both models, the highest cross-correlation values were observed between the primary air flow (u_1) and the output residual.



Figure 7.2. Autocorrelation and cross correlation of residuals for ARX models predicting moisture evaporation and fuel combustion rates

The comparison indicated that both models are able to predict the fuel combustion rate due to a linear relation between fuel consumption and the primary and secondary air flow. In contrast to the fuel burning rate (Figure 7.3), the evaporation rate, presented in Figure 7.4, was predicted sufficiently well only by the simplified dynamic model. The ARX model demonstrated only a minor ability to follow the steady-state variations observed in the evaporation rate.

The comparison of the mean square prediction error of the model predictions, presented in Table 7.1 suggest a similar trend as was previously observed in Figure 7.3 and 7.4. The comparison indicates that the moisture evaporation rate predicted by the simplified model is closer to the measured value when compared to that of the ARX model. In the case of the fuel burning rate prediction, both models demonstrate a minor prediction error, although, the prediction by the ARX model is slightly more accurate.

Table 7.1. Mean square prediction error of the ARX and of the simplified model

| Model | Variable | Mean squared error | |
|------------------|----------------------|--------------------|--|
| | Fuel burning rate | 0.0052 | |
| ARA | Moisture evaporation | 0.0572 | |
| Simplified model | Fuel burning rate | 0.0078 | |
| Simplified model | Moisture evaporation | 0.0449 | |

In summary, the ARX model was able to predict the combustion rate which was directly proportional to the air feed, however, the prediction of the drying rate was less accurate since it is controlled by nonlinear phenomena such as heat radiation. Moreover, the possibility for the identification of such databased models is limited due to lack of required measurements, for example, for the moisture content of the flue gas. Thus, mechanistic model offers an attractive alternative for on-line computations of combustion processes as it not only predicts the reaction rates but also the internal states such as fuel bed composition. Publication 4 provides more information on the identification of databased models for predicting the fuel combustion and drying rate.



Figure 7.3. Comparison of burning rates predicted by the simplified dynamic model and the ARX model



Figure 7.4. Comparison of evaporation rates predicted by the simplified dynamic model and the ARX model

The models - including the mechanistic model, simplified model and ARX models - were compared in terms of their run times and the results are presented in Table 7.2 while the associated computer configurations are shown in Table 7.3. The computational times of the mechanistic model largely benefit from the parallel computations in Matlab versions below R2015b and both clock frequency and the number of CPU cores. A larger number of processor cores and higher clock frequencies allowed Desktop-1 to perform almost three times faster compared to the laptop computer. On these two computers, computational times of ARX and the simplified model benefitted less from a larger core number and higher clock frequencies. Matlab version R2015b demonstrated significantly longer computational times for the mechanistic model and were almost six times longer when compared to the simulation time obtained on computer Desktop-1 running R2014b, possibly due to some deficiencies in the parallel computing toolbox. Nevertheless, the computational times of the simplified model on the newer Matlab version on Desktop-1 were almost two times faster than on Desktop-1 running an older version. Furthermore, the Desktop-2 demonstrated even further improvements in computational times due to the upgrades in the CPU architecture and these advancements resulted in faster computational times of the ARX model.

Table 7.2. Run times of different models on different computer configurations

| | Mechanistic (s / simu- lated second) | Simplified | ARX |
|--------------------|---|------------|-----------|
| Computer | | | |
| Laptop | 14.173497 | 6.23E-04 | 7.21E-07 |
| Desktop-1 (R2014b) | 5.403695 | 5.34E-04 | 6.477E-07 |
| Desktop-1 (R2015b) | 31.443311 | 2.81E-04 | 7.066E-07 |
| Desktop-2 | 28.240536 | 2.11E-04 | 5.927E-07 |

Table 7.3. Computer configurations

| Computer | Matlab version | RAM (GB) | CPU Model | Frequency (GHz) | # of Cores | # of Threads |
|-----------|----------------|-------------|------------------------|--------------------|---------------|-----------------|
| Laptop | R2015a | 8 | Intel i5-3340M | 2.7 | 2 | 4 |
| Desktop-1 | R2014b | 12 | Intel i7 920 | 3.6 | 4 | 8 |
| Desktop-2 | R2015b | 8 | Intel Xeon E3- 1230 | 3.2 | 4 | 8 |

8. Perspectives on the use of the developed models for efficiency improvements to BioGrate boiler operations and considerations of their industrial implementation

Bio-power plants are increasingly shifting their role from providing base-load power to dispatchable, highly flexible power generation. Such a shift implies that power plants are able to operate over wide load ranges with rapid changes in load levels. Thus, flexible power generation requires determining the highest and the lowest load at which power plant remains operational and the maximum rate of changes allowed. The determination of the aforementioned operational parameters is largely affected by inherently variant fuel properties, such as moisture, volatile and ash content, particle size distribution as well as the material type.

Fuel properties are strongly related to both, the range of the load change and to the transition rates between the power production levels. The results presented in Section 5 demonstrated that the rate of response of the burning fuel bed is material dependent and suggest that material type has to be considered via process control during the transition. As suggested by the results from Section 4, fuel moisture content is another variable which largely affects the combustion behavior as a high moisture content leads to increased fuel ignition delays. Nevertheless, the beneficial effect of flue gas recirculation on fuel drying was ascertained in Section 4, hence, the full mechanistic model can be employed to evaluate the ability of the flue gas recirculation to facilitate the ignition of very wet fuels. Furthermore, the model allows the evaluation of the forming combustible gases and thus presents a possibility to prevent any excessive pollution caused by the load changes.

Wide operational load range and fast transition rates require optimal combustion conditions and in this regard, the primary air flow and its distribution between the grate rings are the most important parameters to consider. The results from Section 4 indicate that the primary air has the strongest impact on the combustion process, as an inappropriate air flow slows down burning through the insufficient supply of oxygen or excessive cooling of the fuel layer. The full mechanistic model can be employed to determine the combustion intensity in the fuel layer located on different rings and to optimize the primary air distribution, as demonstrated in Section 5. Next, the secondary air, which completes the combustion of pyrolytic gases released by the burning fuel layer, has to be directed to the area with intensive formation of the pyrolytic gases. Therefore, the formation of the pyrolytic gases predicted by the full mechanistic models allows for the optimization of their combustion.

At maximum power production, incomplete fuel combustion becomes a major limiting factor, since the fuel feed to the furnace has to be increased and that can lead to some material leaving the grate unburnt. In addition, as was shown by the results in Publication 1, the temperature of the combustion can also become a critical factor and in order to avoid any equipment damage, it has to be investigated with the model as well.

Model based control such as model predictive control (MPC) is an excellent technique to achieve optimal load transitions. This technique, however, requires that the underlying model is able to describe the combustion phenomena. As a result, the implementation of the simplified model for improved control has several benefits for power production flexibility, which stem from its ability to describe combustion phenomena and to predict variable values that are otherwise unavailable. Furthermore, the simplified model allows the monitoring of the state of the furnace, more specifically, fuel amount and composition, temperatures as well as the composition of the forming flue gas. Additionally, the deep insights into the process conditions provided by the model ensure that prerequisites such as a sufficient amount of fuel required for the load transition are fulfilled. Thus, based on these model predictions, the minimum and maximum load and the transition rate between these two can be established online for flexible control of power generation.

The successful implementation of the simplified model in an industrial environment requires the determination of power plant dependent variables, such as fuel feed rate as well as surface area and volume of the fuel layer. However, the accuracy of the simplified model is essentially dependent on the rate of pyrolysis gas combustion, which competes for the available oxygen with the char combustion reaction at the interface of the char burning zone. Publication 4 explores the possibility of including an adaptive coefficient in the model to account for the uncertainties associated with the competitive nature of char and pyrolytic gas combustion. This is done by including a PI controller that adjusts the value of Equation (6.49) in the following way, as presented in Equation (8.1) :

$$k_{pyr,comb} = u(t)T_g / T_s k_C$$
(8.1)

where u(t) is the controller output. The error used as the controller input is calculated as a difference between the measured and predicted flue gas oxygen content. This arrangement allows for an improvement in the model accuracy by predicting both fuel burning rate and moisture evaporation.

Next, the simplified model, which comprises differential-algebraic equations (DAEs), has to be linearized and converted to a state-space form. This is due to the fact that a state-space model allows for the most straightforward imple-

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mentation of MPC and Kalman filter. The linearization of the model can be performed in two ways: In the first alternative, the linearized model is obtained by approximating the nonlinear terms, such as evaporation rate due to heat radiation, in the model by using Taylor series. However, obtaining the analytical derivatives of the model functions is time consuming, which in some cases, is infeasible. The second method involves the numerical linearization of the model. The major advantage of numerical differentiation is its simplicity, as it does not require any special considerations for the algebraic part of the model, which is otherwise compulsory for the implementation of the control methods. The disadvantage of this method is somewhat lower accuracy of the approximation when compared to that obtained in the first alternative.

In conclusion, the utilization of the simplified model in MPC presents an excellent opportunity to achieve highly flexible power production through the ability of the model to describe the internal combustion phenomena. Such a detailed description of the biomass combustion not only allows to establish the efficient transition trajectory between different loads but it also allows to expand the operational limits of a power plant. Perspectives on the use of the developed models for efficiency improvements to BioGrate boiler operations and considerations of their industrial implementation

9. Conclusions

This thesis presented dynamic modeling of a BioGrate boiler for process phenomena investigation and for on-line computations. The process phenomena investigation was based on the enhanced mechanistic model that comprised mass and energy continuity equations for the solid and gaseous phases and considered drying, pyrolysis, char combustion, and gasification, which are the main reactions observed during biomass combustion. Similarly, the simplified model considered the gaseous and solid phases and the major combustion reactions, including drying, pyrolysis, and char oxidation.

The results of the work demonstrated that the model provides important insight into the thermal conversion of biomass. The simulations indicated that particle size has a major effect on both heat and mass transfer and consequently on the chemical reactions. Small particle sizes tend to increase mass transfer of gaseous compounds out of particles and consequently decrease the residual volatile content in the solid phase. Furthermore, smaller particles result in higher temperatures in the fuel layer, which increase solid phase reaction rates. However, these particles are more affected by the cooling effect from the primary air compared with larger particles, which may lead to combustion extinction. Similarly, moisture content is another important variable that affects the calorific value and the ignition time.

The investigation of the effect of combustion air demonstrated that the fuel layer combustion dynamics are rather quick, especially the response of char combustion, which is instantaneous. The changes in char combustion also majorly affect the drying rate and, to some extent, the devolatilization reaction. The results indicated that the magnitude of the gas formation response increases with its calorific value towards the outer rings of the grate.

Moist fuel consisting of small particles is more prone to flame extinction and, therefore, the primary air flow has to be regulated accurately. In addition, small particles require less primary air because the small size decreases the amount of volatile components in the solid phase, and more secondary air has to be used to improve volatile burnout. Nevertheless, primary air can be used for fast and efficient regulation of the burning process, as the fuel bed combustion dynamics are fast. However, to achieve more significant changes in the combustion process, air has to be directed to the fuel on the outer rings of the grate.

A simplified model was successfully developed and validated. This model demonstrated acceptable accuracy in describing the behavior of the burning fuel layer. The computational time of the simplified model was significantly faster than that of the enhanced model and allowed faster than real time simulations. As a result, the simplified dynamic model can be utilized in the development of model-based methods that require fast computation times.

The results obtained in this thesis successfully prove the hypothesis presented in Chapter 1, as the model was able to provide essential information on the combustion phenomena. The effects of the most important fuel properties, as well as a varying primary air flow, were studied and improvements were proposed. Furthermore, the simplified model demonstrated satisfactory accuracy in describing biomass combustion in a BioGrate boiler and superior accuracy compared with an ARX model.

This thesis provides valuable information for the development of smart energy systems. The share of these systems in energy production will inevitably increase due to challenges imposed by climate change, diminishing reserves of fossil fuels, and demands for increased flexibility of energy production. In particular, the flexibility of future energy production can be increased by utilizing the understanding of combustion reactions and the underlying phenomena in the design of novel processes. In addition, the enhanced mechanistic model allows further improvements in process operation through personnel training and plant auditing. Furthermore, the proposed simplified model allows the development of advanced model-based control and monitoring methods for efficient operation of future energy systems.

Future work includes the development and implementation of advanced process control and monitoring methods and process optimization for efficient and flexible power production. Furthermore, both models allow for the development of a simulator that is especially useful for the operator training.

References

- Anon, 2015. BioPower combustion technology, http://www.manbw.ru/analitycs/biopower.html 2015(9/25).
- Anon, 2014. Manual, Version 5.0. Burlington, USA: Comsol Multiphysics.
- Anon, 2007. http://news.mongabay.com/bioenergy/2007/05/wrtsil-wins-order-forsix-biomass-power.html 2015(09/25).
- Antal, M. J. J., Várhegyi, G., 1995. Cellulose Pyrolysis Kinetics: The Current State of Knowledge, Industrial & Engineering Chemistry Research 34(3), 703-717.
- Antal, M. J., Várhegyi, G., Jakab, E., 1998. Cellulose Pyrolysis Kinetics: Revisited, Industrial & Engineering Chemistry Research 37(4), 1267-1275.
- Arseneau, D. F., 1971. Competitive Reactions in the Thermal Decomposition of Cellulose, Canadian Journal of Chemistry 49(4), 632-638.
- Asthana, A., Ménard, Y., Sessiecq, P., Patisson, F., 2010. Modeling on-grate MSW incineration with experimental validation in a batch incinerator, Industrial & Engineering Chemistry Research 49(16), 7597-7604.
- Babushok, V., Dakdancha, A., 1993. Global kinetic parameters for high-temperature gas-phase reactions, Combustion, Explosion and Shock Waves 29(4), 464-489.
- Barneto, A. G., Carmona, J. A., Alfonso, J. E. M., Alcaide, L. J., 2009. Use of autocatalytic kinetics to obtain composition of lignocellulosic materials, Bioresource technology 100(17), 3963-3973.
- Branca, C., Di Blasi, C., 2003. Devolatilization and combustion kinetics of wood chars, Energy Fuels 17, 1609-1615.
- Branca, C., Blasi, C. D., Elefante, R., 2005. Devolatilization and Heterogeneous Combustion of Wood Fast Pyrolysis Oils, Industrial & Engineering Chemistry Research 44(4), 799-810.
- Broström, M., Nordin, A., Pommer, L., Branca, C., Di Blasi, C., 2012. Influence of torrefaction on the devolatilization and oxidation kinetics of wood, Journal of Analytical and Applied Pyrolysis 96, 100-109.
- Bruch, C., Peters, B., Nussbaumer, T., 2003. Modelling wood combustion under fixed bed conditions☆, Fuel 82(6), 729-738.
- Bryden, K. M., Hagge, M. J., 2003. Modeling the combined impact of moisture and char shrinkage on the pyrolysis of a biomass particle☆, Fuel 82(13), 1633-1644.
- Butterman, H. C., Castaldi, M. J., 2010. Biomass to fuels: Impact of reaction medium and heating rate, Environmental Engineering Science 27(7), 539-555.
- Cho, J., Davis, J. M., Huber, G. W., 2010. The Intrinsic Kinetics and Heats of Reactions for Cellulose Pyrolysis and Char Formation, ChemSusChem 3(10), 1162-1165.
- Corbetta, M., Frassoldati, A., Bennadji, H., Smith, K., Serapiglia, M. J., Gauthier, G., Melkior, T., Ranzi, E., Fisher, E. M., 2014. Pyrolysis of Centimeter-Scale Woody Biomass Particles: Kinetic Modeling and Experimental Validation, Energy Fuels 28(6), 3884-3898.
- Domínguez, J. C., Oliet, M., Alonso, M. V., Gilarranz, M. A., Rodríguez, F., 2008. Thermal stability and pyrolysis kinetics of organosolv lignins obtained from Eucalyptus globulus, Industrial Crops and Products 27(2), 150-156.

- Duffy, N. T., Eaton, J. A., 2013. Investigation of factors affecting channelling in fixedbed solid fuel combustion using CFD, Combustion and Flame 160(10), 2204-2220.
- Evans, D. D., Emmons, H., 1977. Combustion of wood charcoal, Fire Safety Journal 1(1), 57-66.
- Flynn, M., O'Malley, M., 1999. A drum boiler model for long term power system dynamic simulation, Power Systems, IEEE Transactions on 14(1), 209-217.
- Fogler, S., 2006. Elements of Chemical Reaction Engineering, 4. Ed. Upper Saddle River, USA: Pearson Educations.
- Garcia-Perez, M., Chaala, A., Pakdel, H., Kretschmer, D., Roy, C., 2007. Vacuum pyrolysis of softwood and hardwood biomass: comparison between product yields and bio-oil properties, Journal of Analytical and Applied Pyrolysis 78(1), 104-116.
- Girgis, E., Hallett, W. L., 2010. Wood combustion in an overfeed packed bed, including detailed measurements within the bed, Energy & Fuels 24(3), 1584-1591.
- GOH, Y. R., YANG, Y. B., ZAKARIA, R., SIDDALL, R. G., NASSERZADEH, V., SWITHENBANK, J., 2001. Development of an Incinerator Bed Model for Municipal Solid Waste Incineration, Combustion Science and Technology 162(1), 37-58.
- Gölles, M., Reiter, S., Brunner, T., Dourdoumas, N., Obernberger, I., 2014. Model based control of a small-scale biomass boiler, Control Engineering Practice 22, 94-102.
- Grieco, E., Baldi, G., 2011. Analysis and modelling of wood pyrolysis, Chemical Engineering Science 66(4), 650-660.
- Grønli, M. G., Varhegyi, G., Di Blasi, C., 2002. Thermogravimetric analysis and devolatilization kinetics of wood, Industrial & Engineering Chemistry Research 41(17), 4201-4208.
- Havlena, V., Findejs, J., 2005. Application of model predictive control to advanced combustion control, Control Engineering Practice 13(6), 671-680.
- Hermansson, S., Thunman, H., 2011. CFD modelling of bed shrinkage and channelling in fixed-bed combustion, Combustion and Flame 158(5), 988-999.
- Hogg, B., El-Rabaie, N., 1991. Multivariable generalized predictive control of a boiler system, Energy Conversion, IEEE Transactions on 6(2), 282-288.
- Janssens, M., 2004. Douglas B, Wood and wood products.In: Harper CA, editor.Handbook of building materials for fire protection.New York: McGraw-Hill , 7.1-7.58.
- Janssens, M., Douglas, B., 2004. Wood and wood products, in: Harper, C. (Ed), Handbook of Building Materials for Fire Protection. New-York, McGraw-Hill, pp. 1-58.
- Johansson, R., Thunman, H., Leckner, B., 2007. Influence of intraparticle gradients in modeling of fixed bed combustion, Combustion and Flame 149(1–2), 49-62.
- Kær, S. K., 2004. Numerical modelling of a straw-fired grate boiler, Fuel 83(9), 1183-1190.
- Kortela, J., Jämsä-Jounela, S. -., 2014. Model predictive control utilizing fuel and moisture soft-sensors for the BioPower 5 combined heat and power (CHP) plant, Applied Energy 131(0), 189-200.
- Kurz, D., Schnell, U., Scheffknecht, G., 2012. CFD simulation of wood chip combustion on a grate using an Euler–Euler approach, Combustion Theory and Modelling 16(2), 251-273.

- Leskens, M., Van Kessel, L., Bosgra, O., 2005. Model predictive control as a tool for improving the process operation of MSW combustion plants, Waste Management 25(8), 788-798.
- Leskens, M., Van Kessel, L., Van den Hof, P., 2002. MIMO closed-loop identification of an MSW incinerator, Control Engineering Practice 10(3), 315-326.
- Liang, Z., Ma, X., 2010. Mathematical modeling of MSW combustion and SNCR in a full-scale municipal incinerator and effects of grate speed and oxygen-enriched atmospheres on operating conditions, Waste Management 30(12), 2520-2529.
- Liu, X., Kong, X., Hou, G., Wang, J., 2013. Modeling of a 1000MW power plant ultra super-critical boiler system using fuzzy-neural network methods, Energy Conversion and Management 65, 518-527.
- Matsumoto, K., Takeno, K., Ichinose, T., Ogi, T., Nakanishi, M., 2009. Gasification reaction kinetics on biomass char obtained as a by-product of gasification in an entrained-flow gasifier with steam and oxygen at 900–1000 C, Fuel 88(3), 519-527.
- Orfão, J. J. M., Antunes, F. J. A., Figueiredo, J. L., 1999. Pyrolysis kinetics of lignocellulosic materials—three independent reactions model, Fuel 78(3), 349-358.
- Park, W. C., Atreya, A., Baum, H. R., 2010. Experimental and theoretical investigation of heat and mass transfer processes during wood pyrolysis, Combustion and Flame 157(3), 481-494.
- Peng, H., Nakano, K., Shioya, H., 2007. Nonlinear predictive control using neural nets-based local linearization ARX model—Stability and industrial application, Control Systems Technology, IEEE Transactions on 15(1), 130-143.
- Peters, B., 2002. Measurements and application of a discrete particle model (DPM) to simulate combustion of a packed bed of individual fuel particles, Combustion and Flame 131(1–2), 132-146.
- Pomerantsev, V., 1986. Fundamentals of Applied Combustion Theory. Leningrad, USSR: Energoatomizdat.
- Rao, T. R., Sharma, A., 1998. Pyrolysis rates of biomass materials, Energy 23(11), 973-978.
- Roberts, A. F., 1971. The heat of reaction during the pyrolysis of wood, Combustion and Flame 17(1), 79-86.
- Saastamoinen, J., Taipale, R., Horttanainen, M., Sarkomaa, P., 2000. Propagation of the ignition front in beds of wood particles, Combustion and Flame 123(1), 214-226.
- Shin, D., Choi, S., 2000a. The combustion of simulated waste particles in a fixed bed, Combustion and Flame 121(1), 167-180.
- Shin, D., Choi, S., 2000b. The combustion of simulated waste particles in a fixed bed, Combustion and Flame 121(1–2), 167-180.
- Simsek, E., Brosch, B., Wirtz, S., Scherer, V., Krüll, F., 2009. Numerical simulation of grate firing systems using a coupled CFD/discrete element method (DEM), Powder Technology 193(3), 266-273.
- Thunman, H., Leckner, B., Niklasson, F., Johnsson, F., 2002. Combustion of wood particles—a particle model for eulerian calculations, Combustion and Flame 129(1–2), 30-46.
- Thunman, H., Leckner, B., 2002. Modeling of the combustion front in a countercurrent fuel converter, Proceedings of the Combustion Institute 29(1), 511-518.
- Van der Lans, R., Pedersen, L., Jensen, A., Glarborg, P., Dam-Johansen, K., 2000. Modelling and experiments of straw combustion in a grate furnace, Biomass and Bioenergy 19(3), 199-208.

- Várhegyi, G., Antal Jr., M. J., Jakab, E., Szabó, P., 1997. Kinetic modeling of biomass pyrolysis, Journal of Analytical and Applied Pyrolysis 42(1), 73-87.
- Varhegyi, G., Jakab, E., Antal, M. J., 1994. Is the Broido-Shafizadeh Model for Cellulose Pyrolysis True? Energy Fuels 8(6), 1345-1352.
- Wakao, N., Kaguei, S., Funazkri, T., 1979. Effect of fluid dispersion coefficients on particle-to-fluid heat transfer coefficients in packed beds: Correlation of nusselt numbers, Chemical Engineering Science 34(3), 325-336.
- Yagi, S., Kunii, D., 1957. Studies on effective thermal conductivities in packed beds, AIChE Journal 3(3), 373-381.
- Yang, Y. B., Newman, R., Sharifi, V., Swithenbank, J., Ariss, J., 2007. Mathematical modelling of straw combustion in a 38MWe power plant furnace and effect of operating conditions, Fuel 86(1), 129-142.
- Yang, Y., Nasserzadeh, V., Goodfellow, J., Swithenbank, J., 2003. Simulation of channel growth in a burning bed of solids, Chemical Engineering Research and Design 81(2), 221-232.
- Yang, Y. B., Goh, Y. R., Zakaria, R., Nasserzadeh, V., Swithenbank, J., 2002. Mathematical modelling of MSW incineration on a travelling bed, Waste Management 22(4), 369-380.
- Yang, Y. B., Lim, C. N., Goodfellow, J., Sharifi, V. N., Swithenbank, J., 2005a. A diffusion model for particle mixing in a packed bed of burning solids, Fuel 84(2–3), 213-225.
- Yang, Y. B., Ryu, C., Goodfellow, J., Sharifi, V. N., Swithenbank, J., 2004a. Modelling Waste Combustion in Grate Furnaces, Process Safety and Environmental Protection 82(3), 208-222.
- Yang, Y. B., Sharifi, V. N., Swithenbank, J., 2004b. Effect of air flow rate and fuel moisture on the burning behaviours of biomass and simulated municipal solid wastes in packed beds, Fuel 83(11–12), 1553-1562.
- Yang, Y. B., Ryu, C., Khor, A., Sharifi, V. N., Swithenbank, J., 2005b. Fuel size effect on pinewood combustion in a packed bed, Fuel 84(16), 2026-2038.
- Yin, C., Rosendahl, L., Kær, S. K., Clausen, S., Hvid, S. L., Hille, T., 2008. Mathematical modeling and experimental study of biomass combustion in a thermal 108 MW grate-fired boiler, Energy & Fuels 22(2), 1380-1390.
- Yu, Z., Ma, X., Liao, Y., 2010. Mathematical modeling of combustion in a grate-fired boiler burning straw and effect of operating conditions under air- and oxygenenriched atmospheres, Renewable Energy 35(5), 895-903.
- Zhang, X., Chen, Q., Bradford, R., Sharifi, V., Swithenbank, J., 2010. Experimental investigation and mathematical modelling of wood combustion in a moving grate boiler, Fuel Processing Technology 91(11), 1491-1499.
- Zhou, H., Jensen, A. D., Glarborg, P., Jensen, P. A., Kavaliauskas, A., 2005. Numerical modeling of straw combustion in a fixed bed, Fuel 84(4), 389-403.



ISBN 978-952-60-6808-4 (printed) ISBN 978-952-60-6809-1 (pdf) ISSN-L 1799-4934 ISSN 1799-4934 (printed) ISSN 1799-4942 (pdf)

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