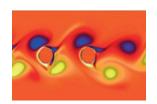
# **GrateCFD** — Enabling optimum Grate fired woody biomass and waste to energy plant operation through Computational Fluid Dynamics



### Newsletter 2-2020

### Progress in 2020

Simulations using the developed CFD toolbox have been in focus in 2020, representative of up to large-scale WtE grate combustion units. In parallel a simulation approach based on using stochastic reactors for both the bed and the freeboard is used. These two approaches both forms potential powerful packages for simulations of grate combustion plants. The ultimate goal is to study concept improvements using these simulations tools.

# GrateCFD workshop and steering committee meeting by web, again

Due to the Covid-19 virus, also the second workshop and steering committee meeting in 2020 was arranged online, 2 December. Also this time the event went smooth, but the physical meeting is surely missed.

# GrateCFD workshop and steering committee meeting by web

Due to the Covid-19 virus, the first workshop and steering committee meeting in 2020 was arranged online, 4 June. The event went smooth, showing that it is possible to carry out such events online, if it is required.

### PostDoc work

The PostDoc position within "NOx modelling and simulation" is ongoing. Corinna Netzer from Germany started her work January 2019 and the work is in good progress, focusing on the use of stochastic reactor networks as a tool to model grate furnaces, including the fuel bed. Her first paper from this work is now published in Energy & Fuels.

### PhD work

The PhD position within "Computational fluid dynamics (CFD) modeling of biomass and waste to energy plants" is ongoing. <u>Jingyuan Zhang</u> from

China, the PhD candidate, is progressing well, focusing on particle and fuel bed modelling and the use of OpenFOAM for modelling the fuel bed decomposition in grate furnaces. His first scientific paper from the work is now published in Chemical Engineering Journal.

### **GrateCFD in EERA Bioenergy Newsletter**

An article entitled "Circular economy and value chain thinking - The future of Waste-to-Energy" presented GrateCFD as well as WtE 2030 (Waste-to-Energy 2030) in an EERA (European Energy Research Alliance) Bioenergy newsletter.

### GrateCFD in IEA Bioenergy Task 36 Newsletter

An article entitled "Computational Fluid Dynamics for improving large-scale woody biomass and Municipal Solid Waste combustion units" in the IEA Bioenergy Task 36 newsletter presented GrateCFD as well as mention several other R&D projects (WtE 2030, CapeWaste, NEWEST-CCUS) at SINTEF working with key WtE actors towards a more circular economy.

### **GrateCFD in Energy & Fuels**

One GrateCFD work has been published in Energy & Fuels:

Corinna Netzer, Tian Li, Lars Seidel, Fabian Mauß, Terese Løvås (2020). <u>Stochastic Reactor-Based Fuel Bed Model for Grate Furnaces</u>. The abstract is given below.

"Biomass devolatilization and incineration in grate-fired plants are characterized by heterogeneous fuel mixtures, often incompletely mixed, dynamical processes in the fuel bed and on the particle scale, as well as heterogeneous and homogeneous chemistry. This makes modeling using detailed kinetics favorable but computationally expensive. Therefore, a computationally efficient model based on zero-dimensional stochastic reactors and reduced chemistry schemes, consisting of 83 gas-phase species and 18 species for surface reactions, is developed. Each reactor is enabled to account for the

GrateCFD

http://www.sintef.no/GrateCFD

- a Knowledge-building Project for Industry (KPN) co-funded by the Research Council of Norway through the ENERGIX-programme. Contact: oyvind.skreiberg@sintef.no

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three phases: the solid phase, pore gas surrounding the solid, and the bulk gas. The stochastic reactors are connected to build a reactor network that represents the fuel bed in grate-fired furnaces. The use of stochastic reactors allows us to account for incompletely mixed fuel feeds, distributions of local temperature and local equivalence ratio within each reactor and the fuel bed. This allows us to predict the released gases and emission precursors more accurately than if a homogeneous reactor network approach was employed. The model approach is demonstrated by predicting pyrolysis conditions and two fuel beds of grate-fired plants from the literature. The developed approach can predict global operating parameters, such as the fuel bed length, species release to the freeboard, and species distributions within the fuel bed to a high degree of accuracy when compared to experiments."

### GrateCFD in Fuel

One GrateCFD connected work has been published in Fuel:

Shuai Wang, Yanqing Niu, Tian Li, Denghui Wang, Shi'en Hui (2020). Experimental and kinetic study on the transformation of coal nitrogen in the preheating stage of preheating-combustion coupling process. The abstract is given below.

"Preheating-combustion of pulverized coal has been demonstrated as an effective low NOx combustion technology. This method preheats a coal stream to high temperatures before the coal stream is injected into a utility boiler for combustion. Considering the complex mechanisms during the preheating, the effects of the preheating parameters, including temperature, residence time and excess air ratio are studied in a drop-tube furnace in detail. Meanwhile, a kinetics analysis on the transformation of coal-N in gas phase is also performed by means of Chemkin-Pro coupled with mature NOx reduction mechanisms. The experimental results show that the yield of coal-N converted to NO decreases at first and then increases with increasing excess air ratio. The lowest NO yield after preheating is achieved at excess air ratio of 0.1. To reduce NOx formation effectively, the preheating zone should be under high temperature and long residence time. Kinetic modeling indicates that NO was reduced into N<sub>2</sub> by both hydrocarbon radical and HCN. Also, the modeling results show that the increasing excess air ratio weakens the effect of hydrocarbon radical reduction, and the mole ratio of NO<sub>HCN</sub>/NO<sub>HCN+CiHj</sub> decreases from 1.99 to 1.17 with the increasing excess air ratio from 0.1 to 0.6."

### GrateCFD in Chemical Engineering Journal

One GrateCFD work has been published in Chemical Engineering Journal:

Jingyuan Zhang, Tian Li, Henrik Ström, Terese Løvås (2020). <u>Grid-independent</u> <u>Eulerian-Lagrangian approaches for simulations of solid fuel particle combustion</u>. The abstract is given below.

"In this study, a computational fluid dynamics (CFD) model with three coarse graining algorithms is developed with the implementation of a layer based thermally thick particle model. Three additional coupling methods, cube averaging method (CAM), two-grid method (TGM) and diffusion-based method (DBM), are implemented. These coupling methods are validated and compared with the widely used particle centroid method (PCM) for combustion of a biomass particle in a single particle combustor. It is shown that the PCM has a strong dependence on the grid size, whereas the CAM and TGM are not only grid independent but also improve the predictability of the simulations. Meanwhile, a new parameter, the coupling length, is introduced. This parameter affects the sampling of the gas phase properties required for the particle model and the distribution of the solid phase properties. A method to estimate the coupling length by using empirical correlations is given. In general, it is found that a too small coupling length underestimates the heating-up rate and devolatilization rate, while a too large coupling length overestimates the O2 concentration at the particle surface. The coupling length also has an influence on the distribution of the gas phase products"

### Other news

### WtE 2030 in good progress, and is in its final year

The competence building project WtE 2030 is in good progress. It is as GrateCFD funded by the Research Council of Norway and industry partners. It strengthens the research efforts within the Waste-to-Energy area, and it is a complementary project to GrateCFD. Both projects have several industry partners in common. WtE 2030 runs for three years, 2018-20, and is now in its final year. For more info about the project and achievements: www.sintef.no/projectweb/wte\_2030/

A follow-up competence building project to WtE 2030 has been applied for and has been granted funding from the Research Council of Norway. The project, CircWtE - Waste-to-Energy and Municipal Solid Waste management systems in Circular Economy, is scheduled to run for four years, 2021-24, with SINTEF Energy Research as project leader.

### New competence building project on wood stoves has been granted financing

A competence building project on wood stoves has been applied for and has been granted funding from the Research Council of Norway. The project, SusWoodStoves - Sustainable wood stoves through stove, building integration and value chain optimisation, is scheduled to run for four years, 2021-24, with SINTEF Energy Research as project leader. The topic of the project is relevant also for IEA Task 32 Biomass Combustion, in light of its significant focus on wood stoves. SusWoodStoves follows the earlier competence building projects WoodCFD and StableWood.

In addition, the Research Council granted financing to an innovation project in the industry on use of phase change material for heat storage in wood stoves: PCM-STOVE - Innovative PCM-based heat storage integrated in wood stoves.

### **IEA Task 32 Biomass Combustion**

The first <u>IEA Bioenergy Task 32</u> meeting in 2019, the first year of the current triennium, was arranged in June in Hurdal, Norway. The meeting was combined with a field trip to a 56 MW wood powder fired heating plant at Haraldrud and the Arbaflame steam explosion plant at Grasmo.

The main activities are:

- Testing methods and real-life performance of pellet stoves
- Technical guidelines for design of low emission stoves
- Survey of national strategies for reducing the impact on air quality from residential and commercial wood combustion
- Biomass for process heat in industry
- Biomass-based CHP for balancing an energy system with a large portion of uncontrollable production (intertask project)
- Workshop on improved combustion in stoves and small biomass boilers
- Workshop on experiences with combustion of pulverised non-woody solid biofuels
- Workshop on experiences with wood chips for large scale CHP production

In the previous triennium, relevant deliverables were:

- Aerosols from biomass combustion
- Advanced test methods for firewood stoves
- Particle emission measurement techniques
- State of the art on innovative CHP concepts
- Strategic study for renewable heat
- Bioenergy for heat the Hot Cases
- Workshop on Solid Recovered Fuels
- Workshop on Biomass Combustion Generated Nanoparticles

### - Workshop on New Emission Measurement Methods

The second IEA Task 32 meeting in the current triennium was arranged 21-24 January 2020 in Graz, Austria, in connection with the 6th Central European Biomass Conference. In connection with the meeting a workshop was arranged on residential wood combustion. The third meeting was arranged in June as a virtual task meeting due to Covid-19. In the fall the fourth meeting was planned to be arranged in Copenhagen together with a workshop, but the Covid-19 situation made that impossible. Therefore, a new digital meeting was arranged in December, where in addition to the progress of the activities of the current triennium, there were also discussions about possible activities in the next triennium (2022-24).

For information about IEA Bioenergy Task 32 activities, see the webpage and newsletters, and for IEA Bioenergy news, see the <u>newsletters</u>. Øyvind Skreiberg from SINTEF Energy Research is the Norwegian participant in IEA Bioenergy Task 32.

### **EERA Bioenergy – SP5 Stationary Bioenergy**

The effort last year was focused on revising the SP focus and the description of work, and this work is now finalized. A recently updated <a href="Strategic Research">Strategic Research</a> and Innovation Agenda (SRIA) has been made for the whole EERA Bioenergy. For more info on EERA Bioenergy, visit the <a href="website">website</a>, and see the <a href="newsletters">newsletters</a>. Julien Blondeau from the Free University of Brussels in Belgium is the leader of SP5 Stationary Bioenergy in EERA Bioenergy, following Berta Matas Güell from SINTEF Energy Research who led SP5 for about 5 years.

### RHC technology and innovation platform

The European Technology and Innovation Platform on Renewable Heating & Cooling (RHC-ETIP) brings together stakeholders from the biomass, geothermal and solar thermal sector - including related industries such as District Heating and Cooling, Thermal Energy Storage, Hybrid Systems and Heat Pumps to define a common Research, Development and Innovation strategy for increasing the use of renewable energy technologies for heating and cooling. Previously concrete work has been carried out by the Biomass Panel in the RHC-ETIP connected to giving input to the SET-plan issues paper on renewable fuels and bioenergy, as well as work connected to the Implementation of the biomass technology roadmap of the Biomass Panel. The aim of the latter was to update the progress in R&I priorities identified by the Biomass technology roadmap. This work continues through different efforts. Øyvind Skreiberg from SINTEF Energy

Research is a member of the Biomass Panel Steering Committee.

For the three years period 2019-21 there is a special focus on work to be carried out in horizontal working groups (HWG) that focus on contributing to 1) vision (finalized in 2019), 2) research and innovation priorities (finalized in 2020) and 3) deployment and implementation strategy (in 2021) documents. Øyvind Skreiberg chairs the HWG 100% Renewable Buildings, where a number of members from the different RHC-ETIP panels are contributing to the HWG. The work progressed well and HWG 100% Renewable Buildings submitted in 2019 their contribution to HWG Vision 2050, which finalized the Vision 2050 based on input from all the HWGs, including also 100% Renewable Districts, 100% Renewable Cities and 100% Renewable Industry. In 2020, focus has been on defining research and innovation priorities, and a Strategic Research and Innovation Agenda (SRIA) has now been finalized. In 2021, the focus will be on developing an Implementation and deployment strategy.

As a continuation of the SET-Plan work, workgroups were established to provide specific input to the SET-Plan work, e.g. Action 5 Energy Efficiency in Buildings with the sub-action 5.2 Heating and Cooling Technologies for Buildings and Action 8 Renewable Fuels and Bioenergy. The work and an endorsed implementation plan were finalized. Øyvind Skreiberg was involved in the Action 5 work, representing the Biomass Panel. The work is now continued, focusing on the implementation of the SET-Plan, both for Action 5 and 8.

See the RHC-ETIP news webpage for other news.

#### **Recent events**

Bioenergidagene 2020, 23-24 November 2020, econference.

http://www.bioenergidagene.no/

Energigienvinning av avfall 2020, 11 November 2020, e-seminar.

https://www.avfallnorge.no/kurs-ogarrangementer/energigienvinning-av-avfall-2020

IRRC Waste - to - Energy, 15-16 October 2020, Vienna, Austria. - Changed to e-conference due to Covid-19

http://www.vivis.de/veranstaltungen/irrc

28th European Biomass Conference & Exhibition, 27-30 April 2020, Marseille, France. - Changed to econference due to Covid-19, 6-9 July

#### **Upcoming events**

29th European Biomass Conference & Exhibition, 26-29 April 2021, Marseille, France. + e-conference http://www.eubce.com/

10th CEWEP Waste-to-Energy Congress in Prague, 24-25 September 2020, Prague, Chechia. -Postponed to 23-24 September 2021 due to Covid-19 https://www.cewep.eu/cewep-congress-2020-prague/

ISWA World Congress 2021, 4-7 October 2021, Athens, Greece.

https://www.iswa.org/

**Links** (click on the links or logos to get there)

WoodCFD

SKOG22

Energi21

Renewable Heating and Cooling ETIP

**EERA Bioenergy** 

IEA Task32 Biomass Combustion

IEA Task 36 Material and Energy valorisation of waste in a Circular Economy



















# Project information and past achievements

### **About the project**

The main objective of GrateCFD is development of CFD aided design tools and operational guidelines for optimum grate fired BtE and WtE plant operation through:

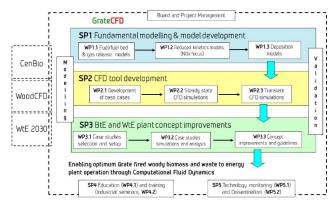
- Model development: improved fuel/fuel bed and gas release models, heat-exchanger deposition models and reduced kinetics models (NOx); and validation of these
- **Simulations**: transient and steady state CFD simulations of BtE and WtE plants; and validation
- Concept improvements: BtE and WtE plant case studies selection, setup, simulations and analysis, giving design and operational guidelines

### The sub-objectives are:

- Develop improved fuel, gas and particle submodels to be included in the CFD simulations
- Develop numerical tools that are tailored to study concept improvements for grate fired BtE and WtE plants, with focus on emission reduction, combustion performance, energy efficiency and availability
- Obtain operational and retrofitting guidelines for optimum operation of grate fired BtE and WtE plants through CFD simulation case studies
- Education of highly skilled candidates within this area and training of industry partners
- Monitoring of activities and state-of-the-art within this area and dissemination of knowledge to the industry partners, and other interested parties when applicable

Main anticipated results of the project are guidelines that will be aimed at improving combustion conditions, obtaining optimum operation over a wide range of thermal loads, decreasing emission levels at significant variations in fuel composition and production demand and increasing combustion and plant efficiency and availability.

The Work Breakdown Structure of GrateCFD is:



GrateCFD management and work break down structure and project links and information flow. (WoodCFD: Clean and efficient wood stoves through improved batch combustion models and CFD modelling approaches, <a href="http://www.sintef.no/woodcfd">http://www.sintef.no/woodcfd</a>; CenBio: The Norwegian Bioenergy Innovation Centre, <a href="http://www.cenbio.no">http://www.cenbio.no</a>; <a href="http://www.cenbio.no">WtE 2030</a>: KPN project started in 2018)

GrateCFD will run for four and a half years (2017-2021) and has a total cash budget of 24 million NOK, which is 80% financed by the Research Council of Norway through the ENERGIX program and 20% financed by the industrial partners.

### The GrateCFD consortium

The project consortium covers all the necessary aspects, and includes large and central industrial players in the biomass to energy (BtE) and waste to energy (WtE) areas in Norway, Sweden and Switzerland.

SINTEF Energy Research leads the project and focus on both modelling and experimental activities.

NTNU (Norwegian University of Science and Technology) supervise the PhD, the PostDoc and Master candidates, and lead specific modelling activities.

The industrial partners contribute with finances as well as access to plants and their extensive industrial knowledge generated through their commercial activities within the BtE and WtE areas: Statkraft Varme AS, Oslo EGE, Returkraft AS, Vattenfall AB, Hitachi Zosen Inova AG.

The constellation of project partners is very strong, bringing together leading research organisations within the field and major industrial players.

### **Project background**

Biomass to energy (BtE) and waste to energy (WtE) plants in Norway need to comply with stricter emission limits and/or adjust to tighter profit margins. EU has for example recently adopted a further reduction of emission limits from medium (scale) biomass combustion plants through the so-called

MCP Directive. Tighter profit margins mean that poorer/cheaper fuel qualities become interesting, as well as operational optimization with respect to efficiency and capacity maximization. particulate and CO emissions are special concerns, as well as the operational challenges following particle deposition on heat transfer surfaces. The majority of the operational BtE and WtE plants in Norway are grate fired plants, and even though different grate technologies have been developed, they suffer from both variations in fuel quality and changing operating conditions, resulting in nonoptimum operating conditions. The most costeffective measure to abate the resulting operational challenges, including increased emission levels, are with primary measures.

Computational Fluid Dynamics (CFD) is the ultimate design tool for BtE and WtE plant combustion and heat transfer sections, however, cost-effective sub-models need to be developed, implemented and used in an optimum way. Moreover, the CFD simulations need to be carried out for transient conditions, to study the effect of changing operating conditions, and minimize the impact of these through improved plant operation and operational guidelines.

GrateCFD therefore focuses on enabling optimum grate fired BtE and WtE plant operation through CFD aided design and operational guidelines. Improved models and modelling approaches, in combination with targeted experiments/measurement campaigns, are keys for future's increased sustainable BtE and WtE plants. This will have a significant impact on two of the most important renewable value chains in Norway today, the BtE and WtE value chains.

#### **Project overview**

The project is divided into 5 subprojects (SP), each subproject is itself divided into several work packages (WP).

- Fundamental modelling & model development -SP1
- CFD tool development SP2
- BtE and WtE plant concept improvements SP3
- Education and training SP4
- Technology monitoring and dissemination SP5

### Fundamental modelling & model development - SP1

The main objective of SP1 is to develop improved fuel, gas and particle sub-models to be included in the CFD simulations in SP2 and SP3.

SP1 leader: Senior Research Scientist Nils Erland Haugen, SINTEF Energy Research

#### CFD tool development - SP2

The major objectives of SP2 are to develop a numerical tool that is tailored to study concept improvements for grate fired BtE and WtE plants, with focus on emission reduction, combustion performance, energy efficiency and availability. SP2 leader: Research Scientist Mette Bugge, SINTEF Energy Research

### BtE and WtE plant concept improvements - SP3

The major objective of SP3 is to obtain operational and retrofitting guidelines of grate fired BtE and WtE plants through CFD simulation case studies.

SP3 leader: Senior Business Developer Per

Carlsson, SINTEF Energy Research

### **Education and training - SP4**

The major objective of SP4 is to strengthen the education within this field through MSc and PhD students, and a PostDoc candidate. The objective is also to increase the competence level in the industry. The long-term goal is competence building and strengthening of the education within combustion of biomass and biomass residues in BtE plants and MSW in WtE plants.

SP4 leader: Professor Terese Løvås, NTNU

### Technology monitoring and dissemination - SP5

The major objectives of SP5 are to monitor the latest research and technological developments and to disseminate research results.

SP5 leader: Chief Scientist <u>Øyvind Skreiberg</u>, SINTEF Energy Research, who also is the GrateCFD project leader

### Earlier progress

In 2019 NOx reduction was an important topic in GrateCFD, and several studies connected to NOx have been carried out, where one of the goals has been to arrive at a reduced kinetics mechanism that includes NOx, which can be used in CFD simulations. The mechanism is ready and was published in 2019. Simulations of full scale plants are important in GrateCFD, and three plants have been chosen and plant data and drawings have been collected to set up the simulation cases geometrically, including air addition system below the grate and the grate itself, where after the different developed models will be used in simulations the last two years of the project. Initial simulations have been carried out in 2019, as a basis for choice of further detailed simulations. In June 2019 a measurement campaign was carried out at the Vattenfall WtE plant in Uppsala. Further in 2019 focus has been on validation and completion of models and simulation tools, which in 2020 will be used for simulation of plants.

In 2018 the work on model development and establishment of the CFD toolbox continued, including lab-scale and full-scale validation activity, in a biomass combustion plant. In the last half of 2018 special focus was on finalising the bed model for the handling of the fuel conversion on the grate and as well base case (transient and stationary). The bed model is part of the base case, and a number of experiments have been carried out in a laboratory reactor for base case validation. For validation and for input to simulations on full scale plants it has in 2018 been carried out an experimental campaign on a grate fired Statkraft bioenergy plant, and in 2019 follows a MSW combustion plant experimental campaign.

In **2017** the work was mainly focused on model development, establishment of the CFD toolbox, and preparations for experimental validation of models and CFD simulations.

### **Earlier publications**

### GrateCFD in Fuel

One GrateCFD work has been published in Fuel: Tian Li, Øyvind Skreiberg, Terese Løvås, Peter Glarborg (2019). Skeletal mechanisms for prediction of NOx emission in solid fuel combustion. The abstract is given below.

"Emission of nitrogen oxides (NOx) is a major challenge for combustion of solid fuels. Strategies for emission control can be developed from computational fluid dynamics (CFD) simulation. This, furthermore, requires a computational efficient kinetic model that is able to capture both formation and destruction of NOx in a wide range of conditions. In this work, three skeletal mechanisms with varying degrees of reduction were developed based on a detailed kinetics model proposed recently (148 species and 2764 reactions). By preserving all major reaction pathways of NO formation, the most comprehensive skeletal mechanism Li45 (45 species and 788 reactions) behaved very similar compared to the base mechanism with regard to the prediction of NO. The more compact skeletal mechanism Li37 (37) species and 303 reactions) was generated specifically for the conditions relevant to large scale industrial combustion of solid fuels. The Li37 mechanism is capable of predicting NO formation as well as simulating common measures of NOx reduction such as the staged combustion and selective non-catalytic reduction (SNCR). Without the consideration of SNCR, the smallest skeletal mechanism Li32 (32 species and 255 reactions) still maintained a good predictability over broad temperature and excess air ratio ranges. Compared to the base mechanism, the skeletal mechanisms achieved over 70% reduction in species. Furthermore, the computational cost was lowered to a large extent, particularly with Li37 and Li32. This makes the developed skeletal mechanisms very suitable to be implemented in CFD simulations."

### GrateCFD in Chemical Engineering Transactions

One GrateCFD work has been published in Chemical Engineering Transactions:

Øyvind Skreiberg, Tian Li, Liang Wang, Mette Bugge, Terese Løvås (2019). An evaluation of effects of fuel parameters and flue gas recirculation on NOx emissions through detailed chemical kinetics simulations. The abstract is given below.

"In this work the effects of fuel parameters and under grate flue gas recirculation (FGR) are investigated when applying staged air combustion of solid fuel for the purpose of NOx reduction. In addition to temperatures, residence times and primary and overall excess air ratio, the fuel-N content and speciation, the relative fuel-C, fuel-H and fuel-O contents, the fuel moisture content, the fuel gas composition from the dry fuel and the use of FGR (in the primary and/or secondary combustion zone) influence the NOx reduction potential to a larger or smaller extent. To assess the influence of different parameters, a simulation matrix using one ideal plug flow reactor representing only the primary zone and a recent detailed chemical kinetics mechanism was carried out. The results show a large influence of the fuel-N content and speciation on the NOx reduction potential in the primary zone, and a significant influence of the fuel moisture content due to its fuel gas dilution effect. At the close to optimum NOx reduction conditions studied in this work (973 K, primary excess air ratio of 0.9), the influence of the fuel gas composition from the dry fuel on the achievable total fixed nitrogen reduction in the primary zone is relatively small, as well as its influence on the radical pool available for the fuel-N chemistry. The influence of the relative content of C, H and O in the fuel at a constant primary excess air ratio is also relatively small. From a kinetics point of view, there is a positive effect of applying under grate flue gas recirculation if the residence time is sufficiently long, however, the effect is relatively low compared to the other main influencing parameters. At higher temperatures the importance of the radical pool availability as well as its speciation increases, and a more significant part of the NH<sub>3</sub> and especially HCN reduction in the primary zone results in increasing NO formation with increasing temperature."

# GrateCFD in International Journal of Multiphase Flow

One GrateCFD work has been published in International Journal of Multiphase Flow:

Jørgen R. Aarnes, Nils E. L. Haugen, Helge I. Andersson (2019). <u>Inertial particle impaction on a cylinder in turbulent cross-flow at modest Reynolds numbers</u>. The abstract is given below.

"Particle impaction on a cylinder in a cross-flow is investigated with the use of Direct Numerical Simulations, with focus on the effect of free-stream turbulence on the front-side impaction efficiency. The turbulence considered is high-intensity homogeneous isotropic turbulence, introduced upstream of the cylinder in moderate Reynolds number flows. It is found that the free-stream turbulence leads to a significant increase in the number of particles that impact the cylinder for certain Stokes numbers (St). The peak amplification of impaction is observed at St=0.3, for different integral scales and Reynolds numbers. This peak is related to a change in impaction mechanism, from boundary stopping to boundary interception, and it will therefore depend on the size of the particles as well as on the Stokes number. Using statistical analysis, an expectation value of predicted effects of free-stream turbulence on particle impaction is derived. This expression predicts the observed impaction amplification to a good degree, particularly in terms of which Stokes numbers that are affected by the turbulence."

# GrateCFD in International Journal of Computational Fluid Dynamics

One GrateCFD connected work has been published in International Journal of Computational Fluid Dynamics:

Jørgen R. Aarnes, Nils E. L. Haugen, Helge I. Andersson (2019). <u>High-order overset grid method</u> for detecting particle impaction on a cylinder in a cross flow. The abstract is given below.

"An overset grid method was developed to investigate the interaction between a particle-laden flow and a circular cylinder. The method is implemented in the Pencil Code, a high-order finite-difference code for compressible flow simulation. High-order summation-by-parts operators were used at the cylinder boundary, and both bi-linear Lagrangian and bi-quadratic spline interpolation were used to communicate between the Cartesian background grid and the body-conformal cylindrical grid. The performance of the overset grid method was assessed to benchmark cases of steady and unsteady flows past a cylinder. Results show high-order accuracy and good agreement to the literature.

Particle-laden flow simulations were performed, with inertial point particles impacting on a cylinder. The simulations reproduced results from the literature at a significantly reduced cost. Further, an investigation into blockage effects on particle impaction revealing that the previously published DNS data is less accurate than assumed for particles with very small Stokes numbers."

### **GrateCFD in Energy Procedia**

One GrateCFD work has been published in Energy Procedia:

Øyvind Skreiberg, Tian Li, Elettra Vantaggiato, Liang Wang, Mette Bugge, Terese Løvås (2019). An evaluation of effects of operational parameters on NOx emissions through detailed chemical kinetics simulations. The abstract is given below.

"NOx emissions from biomass and Municipal Solid Waste (MSW) combustion is a great concern. Technologies for reducing NOx emissions based on flue gas cleaning using e.g. Selective Non-Catalytic Reduction (SNCR) or Selective Catalytic Reduction (SCR) are well known. However, limiting NOx emissions by primary measures is an attractive opportunity, avoiding or limiting the use of costly secondary measures. Many factors influence the NOx emission level from biomass and MSW combustion plants, like fuel-N content and speciation, and operating parameters as air distribution and staging, flue gas recirculation, temperature and residence time. In this work a recent detailed chemical kinetics mechanism is used to investigate the NOx reduction potential by staged air combustion at different operational conditions, using two ideal plug flow reactors connected in series. This enables revealing a kinetics limited reduction potential, as a guideline for further detailed studies at targeted conditions using stochastic reactor networks or Computational Fluid Dynamics (CFD). The results show, for demolition wood as fuel, a large NOx reduction potential, as high as above 95% total fixed reduction at theoretically nitrogen optimum conditions. Through reaction path analyses the main reaction pathways and reactions are identified. Comparison with experimental results from grate combustion units is made. Finally, a comparison with earlier and less extensive detailed chemical kinetics mechanisms is made, to check for significant differences and assess the reasons for those. The final goal would be to arrive at computationally effective reduced chemical kinetics mechanisms that could be applied in CFD simulations of real biomass and MSW combustion plants, to arrive at improved operational conditions or improved design."

# **GrateCFD in Geophysical & Astrophysical Fluid Dynamics**

One GrateCFD connected work has been published in Geophysical & Astrophysical Fluid Dynamics: Jørgen R. Aarnes, Tai Jin, Chaoli Mao, Nils E. L. Haugen, Kun Luo, Helge I. Andersson (2018). Treatment of solid objects in the Pencil Code using an immersed boundary method and overset grids. The abstract is given below.

"Two methods for solid body representation in flow simulations available in the Pencil Code are the immersed boundary method and overset grids. These methods are quite different in terms of computational cost, flexibility and numerical accuracy. We present here an investigation of the use of the different methods with the purpose of assessing their strengths and weaknesses. At present, the overset grid method in the Pencil Code can only be used for representing cylinders in the flow. For this task, it surpasses the immersed boundary method in yielding highly accurate solutions at moderate computational costs. This is partly due to local grid stretching and a body-conformal grid, and partly due to the possibility of working with local time step restrictions on different grids. The immersed boundary method makes up the lack of computational efficiency with flexibility in regard to application to complex geometries, due to a recent extension of the method that allows our implementation of it to represent arbitrarily shaped objects in the flow."

### GrateCFD at 7th IWMRRF

One GrateCFD work was presented at 7th International Workshop on Model Reduction in Reactive Flow (IWMRRF), 18-21 June 2019, Trondheim, Norway:

Tian Li, Øyvind Skreiberg, Terese Løvås, Peter Glarborg. Reduced mechanisms for emission control in solid fuel combustion with SNCR.

#### GrateCFD at ICheaP14

One GrateCFD work was presented at ICheaP14 in Bologna, Italy, 26-29 May 2019:

Øyvind Skreiberg, Tian Li, Liang Wang, Mette Bugge, Terese Løvås. An evaluation of effects of fuel parameters and flue gas recirculation on NOx emissions through detailed chemical kinetics simulations.

A <u>corresponding article</u> has been published in Chemical Engineering Transactions.

### GrateCFD at 17th International Conference on Numerical Combustion

Two GrateCFD works were presented at 17th International Conference on Numerical Combustion, 6-8 May 2019, Aachen, Germany:

- 1. Corinna Netzer, Tian Li, Terese Løvås, Lars Seidel, Fabian Mauß (2019). A Reactor Network Approach for Grate Combustion Plants based on Detailed Chemistry.
- 2. Jingyuan Zhang, Tian Li, Henrik Ström, Terese Løvås (2019). Simulation of thermally thick wood particles combustion with an Eulerian–Lagrangian method.

### **GrateCFD at ICAE 2018**

One GrateCFD work was presented at 10th International Conference on Applied Energy, 22-25 August 2018, Hong Kong, China:

Øyvind Skreiberg, Tian Li, Elettra Vantaggiato, Liang Wang, Mette Bugge, Terese Løvås. An evaluation of effects of operational parameters on NOx emissions through detailed chemical kinetics simulations.

A <u>corresponding article</u> has been published in Energy Procedia.

# GrateCFD at 37th International Symposium on Combustion

One GrateCFD work was presented at 37th International Symposium on Combustion, 29 July - 3 August, Dublin, Ireland:

Jingyuan Zhang, Tian Li, Terese Løvås. Simulating thermochemical conversion of thermally thick wood particles with an Eulerian-Lagrangian method.

### **GrateCFD at EUBCE 2018**

One GrateCFD connected work was presented at EUBCE 2018 in Copenhagen, Denmark, 14-17 May 2018:

Geir Skjevrak, Liang Wang, Tore Filbakk, Øyvind Skreiberg, Henrik Kofoed Nielsen, Johan E. Hustad. Effects of Fuel Additives on Quality of Agricultural Wastes Pellets.

### GrateCFD in Energy & Fuels

A GrateCFD connected work entitled "Investigation on Ash Slagging Characteristics during Combustion of Biomass Pellets and Effect of Additives" was published in Energy & Fuels. The abstract is given below.

"This study reports a systematic investigation into ash slagging behavior during combustion of barley straw and barley husk pellets with or without additives in a residential pellet burner. The slagging tendencies of the pellets were evaluated based on the amount, chemistry, mineralogy, and morphology of inlet ash formed as slag and sintering degrees of

residual ash. The barley straw and husk pellets showed high slagging tendencies with 39 and 54 wt % ingoing ash formed as slag. Analyses using X-ray fluorescence and scanning electron microcopy combined with energy-dispersive X-ray spectroscopy revealed high concentrations of K, Si, and Ca but a minor amount of P in barley straw slag. The slag mainly contained melted potassium silicates directly observed by X-ray diffraction. For the barley husk, high ash slagging tendency was observed and mainly attributed to the formation and melting of potassium phosphates, potassium silicates, and complex mixtures of the two mineral phases. Addition of marble sludge completely eliminated ash slagging during combustion of barley straw and husk pellets because it led to the formation of high temperature melting calcium potassium phosphates, calcium rich potassium silicates, and oxides. Addition of calcium lignosulfonate showed a less pronounced ability to mitigate ash slagging issues during combustion, although it promoted the formation of calcium-rich silicates and phosphates (both with highmelting points) in barley straw and husk ash, respectively. This process was accompanied by considerable reduction in the amount and sintering degree of the formed barley straw and husk slag."

### GrateCFD at 6th Sino-Australian Symposium on Advanced Coal and Biomass Utilisation Technologies

One GrateCFD connected work was presented at 6th Sino-Australian Symposium on Advanced Coal and Biomass Utilisation Technologies, 4-8 December 2017, Perth, Australia:

Liang Wang, Geir Skjevrak, Øyvind Skreiberg, HongWei Wu, Henrik Kofoed Nielsen, Johan E. Hustad. Investigation on Ash Slagging Characteristics during Combustion of Biomass Pellets and Effect of Additives.

## **GrateCFD in Progress in Energy and Combustion Science**

A comprehensive review paper with the WoodCFD PhD candidate Inge Haberle as first author has been published in Progress in Energy and Combustion Science:

Inge Haberle, Øyvind Skreiberg, Joanna Lazar, Nils Erland L. Haugen (2017). Numerical models for thermochemical degradation of thermally thick woody biomass, and their application in domestic wood heating appliances and grate furnaces. Progress in Energy and Combustion Science 63:204-252. The abstract is given below.

"This paper reviews the current state-of-the-art of numerical models used for thermochemical

degradation and combustion of thermally thick woody biomass particles. The focus is on the theory of drying, devolatilization and char conversion with respect to their implementation in numerical simulation tools. An introduction to wood chemistry, as well as the physical characteristics of wood, is also given in order to facilitate the discussion of simplifying assumptions in current models. Current research on single, densified or non-compressed, wood particle modeling is presented, and modeling approaches are compared. The different modeling approaches are categorized by the dimensionality of the model (1D, 2D or 3D), and the one-dimensional models are separated into mesh-based and interfacebased models. Additionally, the applicability of the models for wood stoves is discussed, and an overview of the existing literature on numerical simulations of small-scale wood stoves and domestic boilers is given. Furthermore, current bed modeling approaches in large-scale grate furnaces are presented and compared against single particle models."

### **GrateCFD in EERA Bioenergy Newsletter**

An article entitled "Computational Fluid Dynamics for improving micro- to large-scale woody biomass and municipal solid waste combustion units" presented GrateCFD as well as WoodCFD (Clean and efficient wood stoves through improved batch combustion models and CFD modelling approaches) in an EERA (European Energy Research Alliance) Bioenergy newsletter.

### **Publication list**

Corinna Netzer, Tian Li, Lars Seidel, Fabian Mauß, Terese Løvås (2020). <u>Stochastic Reactor-Based Fuel Bed Model for Grate Furnaces</u>. Energy & Fuels 34(12):16599-16612.

Shuai Wang, Yanqing Niu, Tian Li, Denghui Wang, Shi'en Hui (2020). Experimental and kinetic study on the transformation of coal nitrogen in the preheating stage of preheating-combustion coupling process. Fuel 275, 117924.

Øyvind Skreiberg, Michael Becidan (2020). <u>Circular economy and value chain thinking - The future of Waste-to-Energy</u>. EERA Bioenergy News 13:8-9.

Øyvind Skreiberg (2020). Computational Fluid Dynamics for improving large-scale woody biomass and Municipal Solid Waste combustion units. IEA Bioenergy Task 36 June 2020 newsletter.

Jingyuan Zhang, Tian Li, Henrik Ström, Terese Løvås (2020). <u>Grid-independent Eulerian-Lagrangian approaches for simulations of solid fuel particle combustion</u>. Chemical Engineering Journal 387, 1 May 2020, 123964.

Sondre Relling (2019). Development of a low-dissipation solver for large eddy simulation based on OpenFOAM. NTNU Master thesis. Main supervisor: Terese Løvås, Cosupervisor: Tian Li

Tian Li, Øyvind Skreiberg, Terese Løvås, Peter Glarborg (2019). Reduced mechanisms for emission control in solid fuel combustion with SNCR. 7th International Workshop on Model Reduction in Reactive Flow (IWMRRF), 18-21 June 2019, Trondheim, Norway.

Tian Li, Øyvind Skreiberg, Terese Løvås, Peter Glarborg (2019). Skeletal mechanisms for prediction of NOx emission in solid fuel combustion. Fuel 254, 15 October 2019, 115569.

Øyvind Skreiberg, Tian Li, Liang Wang, Mette Bugge, Terese Løvås (2019). An evaluation of effects of fuel parameters and flue gas recirculation on NOx emissions through detailed chemical kinetics simulations. Chemical Engineering Transactions 74:217-222.

Corinna Netzer, Tian Li, Terese Løvås, Lars Seidel, Fabian Mauß (2019). A Reactor Network Approach for Grate Combustion Plants based on Detailed Chemistry. 17th International Conference on Numerical Combustion, 6-8 May 2019, Aachen, Germany.

Jingyuan Zhang, Tian Li, Henrik Ström, Terese Løvås (2019). Simulation of thermally thick wood particles combustion with an Eulerian–Lagrangian method. 17th International Conference on Numerical Combustion, 6-8 May 2019, Aachen, Germany.

Jørgen R. Aarnes, Nils E. L. Haugen, Helge I. Andersson (2019). <u>Inertial particle impaction on a cylinder in turbulent cross-flow at modest Reynolds numbers</u>. International Journal of Multiphase Flow 111:53-61.

Jørgen R. Aarnes, Nils E. L. Haugen, Helge I. Andersson (2019). High-order overset grid method for detecting particle impaction on a cylinder in a cross flow. International Journal of Computational Fluid Dynamics 33(1-2):43-58.

Øyvind Skreiberg, Tian Li, Elettra Vantaggiato, Liang Wang, Mette Bugge, Terese Løvås (2019). An evaluation of effects of operational parameters on NOx emissions through detailed chemical kinetics simulations. Energy Procedia 158:103-110.

Jørgen R. Aarnes, Tai Jin, Chaoli Mao, Nils E. L. Haugen, Kun Luo, Helge I. Andersson (2020). <u>Treatment of solid objects in the Pencil Code using an immersed boundary method and overset grids</u>. Geophysical & Astrophysical Fluid Dynamics 114(1-2):35-57.

Fredrik Buvarp (2018). Experimental development of combustion models. SINTEF Summer Job Project report. Main supervisor: Per Carlsson, Co-supervisors: Mette Bugge, Judit Sandquist

Jingyuan Zhang, Tian Li, Terese Løvås (2018). Simulating thermochemical conversion of thermally thick wood particles with an Eulerian-Lagrangian method. 37th International Symposium on Combustion, 29 July - 3 August, Dublin, Ireland.

Nguyen Cong Thanh (2018). A thermogravimetric and kinetic study on devolatilization of biomass. NTNU Master thesis. Main supervisor: Terese Løvås, Co-supervisor: Liang Wang

Elettra Vantaggiato (2018). Reduced chemical model development for grate fired biomass application. NTNU Project thesis. Main supervisor: Terese Løvås, Cosupervisor: Tian Li

Geir Skjevrak, Liang Wang, Tore Filbakk, Øyvind Skreiberg, Henrik Kofoed Nielsen, Johan E. Hustad (2018). Effects of Fuel Additives on Quality of Agricultural Wastes Pellets. 26th EUBCE, 14-17 May 2018, Copenhagen, Denmark.

Liang Wang, Geir Skjevrak, Øyvind Skreiberg, Hongwei Wu, Henrik Kofoed Nielsen, Johan E. Hustad (2018). Investigation on Ash Slagging Characteristics during Combustion of Biomass Pellets and Effect of Additives. Energy & Fuels 32(4):4442-4452.

Liang Wang, Geir Skjevrak, Øyvind Skreiberg, Hongwei Wu, Henrik Kofoed Nielsen, Johan E. Hustad (2017). Investigation on Ash Slagging Characteristics during Combustion of Biomass Pellets and Effect of Additives. 6th Sino-Australian Symposium on Advanced Coal and Biomass Utilisation Technologies, 4-8 December 2017, Perth, Australia.

Inge Haberle, Øyvind Skreiberg, Joanna Lazar, Nils Erland L. Haugen (2017). Numerical models for thermochemical degradation of thermally thick woody biomass, and their application in domestic wood heating appliances and grate furnaces. Progress in Energy and Combustion Science 63:204-252.

Øyvind Skreiberg (2017). Computational Fluid Dynamics for improving micro- to large-scale woody biomass and municipal solid waste combustion units. EERA Bioenergy Newsletter 2017 (7), p. 5.

Øyvind Skreiberg (2017). <u>Modellering og numeriske simuleringer for økt bærekraft</u> (in Norwegian). SINTEF blog article.