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Review Report on the doctoral thesis for the degree of Philosophiae Doctor submitted to Silesian University of Technology and Norwegian University of Science and Technology

Thesis Title: "Detailed numerical modeling of solid fuels conversion processes"
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Project background and relevance.
The thesis is dedicated to the problem of solid fuel conversion, specifically pulverised coal. Since many years we observe the decarbonization trend in different fields of industry. Research conducted by The World Health Organization indicates that carbon dioxide emissions associated with burning primarily coal contributes to the intensification of climate change, such as heat waves and violent weather phenomena, which will undoubtedly affect the deterioration of the quality of life for future generations. Out of available fossil fuels, it is coal that contributes to the highest carbon dioxide production. It is worth mentioning that coal consumption decreases in the developed countries but increases in emerging economies. On of the most attractive options to gradually mitigate CO_2 emissions is to design highly efficient and low-emission technologies and optimize the existing ones. Currently the numerical simulations became a standard tool used at the design or optimization stage of solid fuel combustion systems. Further study of fundamental phenomena occurring during solid

fuel conversion and development of associated new modelling approaches needed to be conducted.

General description of the thesis

The manuscript is fully completed with original work that represents an interesting advancement in the field of solid fuel conversion simulation focusing on the impact of turbulence on the conversion rate as well as combustion behaviour of a resolved carbon particle at different scales.

The thesis comprises 158 pages and follows often met structure of a PhD thesis in science. It begins with abstract, acknowledgments, section introducing the thesis structure followed by introduction, which directly leads to a list of objectives, followed by chapters dedicated to methodology, contributions and thesis summary. Finally the three scientific papers are attached.

Chapter 1 "Introduction" described the motivation and relevance of the research subject. A comprehensive classification of particulate flows modelling is described and different scales at which solid fuel conversion can be modelled. Component processes occurring during solid fuel conversion are also analysed. An important part of the thesis is to asses the impact of turbulence on the solid fuel conversion rate is introduced. This part of the thesis contains a literature review on the numerical studies of solid fuels conversion. The discussion of this part is carefully referenced (148 references) and a comprehensive bibliography contains all the relevant papers for the discussed field.

The thesis demonstrates a solid understanding of the state-of-the-art in the research area and the knowledge of the most important and current literature. An in-depth analysis of the literature and the existing state of knowledge on the discussed issue allowed the author to correctly identify the gap in the current research and define the thesis objectives. The main objectives of these studies are:

- employing point particle DNS to study the effect of turbulence on the mass transfer rate in polydisperse particle systems,
- investigating the effect of turbulence on the conversion rate in practical, large-scale systems through RANS simulations,
- estimating a sensitivity of this effect to relevant parameters,
- developing an efficient resolved particle DNS model for a single particle combustion,
- gaining a thorough comprehension of the behaviour of the reacting char particle

Chapter 2 "Methodology" describes selected aspects of the governing equations and numerical methods devoted to solid fuel conversion considered at different scales is described in this section. The smallest one is a two-dimensional resolved carbon particle that undergoes conversion in a laminar flow. The medium one was a DNS of isotropic and homogeneous turbulence with reacting Lagrangian particles. The largest ones, are practical turbulent systems of an industrial-scale boiler modeled using the Euler-Lagrange approach and RANS equations in their incompressible form. The numerical models were formulated based on Pencil Code adopted to perform point particles DNS. Large-scale simulations have been performed using the commercial software ANSYS-Fluent with User Defined Functions describing particle reaction rate accounting for the effect of turbulence.

Chapter 3 "Contributions" summarizes the author's publications. The thesis is in the form of a collection of 3 papers submitted to high quality peer-reviewed international journals. Two of the papers have already been published and the third one was still under consideration at the time of preparing this report.

Chapter 4 summarises the most crucial conclusions of the work. Chapter 5 contains the 3 research papers.

The title of the doctoral dissertation corresponds to the subject of the analyzed publications, and the total value of IF is 12. Such a high IF proves that the work represents a high scientific level and the research was carried out properly, which was positively assessed by the reviewers of these journals. All these works are collective works in which the PhD student is the first author. The author responsibility was to set-up and perform simulations, post-process the results and prepare the manuscript. The candidate contribution is clearly stated in the thesis. Additionally PhD candidate has a minor contribution to 10 papers and conference publications or presentations that describes her activity.

I have deeply investigated the work and my impression is that the thesis and the publications are written with high quality and clarity. They are relatively easy to follow, despite the fact that the subject of the research is very complex. Within the whole thesis the writing is clear and excellent and no major faults have been found. In editorial terms the thesis should receive high notes. The layout and structure of the work is clear and logical. The graphical content was very carefully prepared. The language is comprehensive and coherent while errors and inaccuracies are relatively rare.

The presented objective of the work is consistent with the subject of the dissertation and the described scope discusses the subject matter exhaustively. Reading the work as a whole allows to state that the specific objectives have been achieved and current results pave the way to far reaching research objectives for the future.

Scientific content and contribution

Three publications on international peer reviewed journals (all of them first author) is a very good package for a PhD. These articles address the highly relevant areas of solid fuel conversion.

Paper I. The paper aims to study how turbulence affects the mass transfer rate between the fluid and inertial particles and how this can possibly influence the net surface reaction rate. Point particle DNS of a cubic domain with homogeneous and isotropic turbulence were performed over a range of parameters such as Damköhler (Da), (mean) Stokes (St) and Reynolds numbers. The goal was also to verify if a model formulated to account for the effect of turbulence in monodisperse particle systems is still applicable when polydisperse particles are considered. It was found that there exists a correlation between locations of clusters that are made of particles with different sizes.

Paper II. The objective of this paper was to verify theoretical predictions in real situations and apply the model that accounts for the effect of turbulence to practical, large-scale systems (tangentially fired boiler). The authors concluded that, at stoichiometric conditions, the effect of turbulence associated with particle clustering depends on the fuel type and atmospheric composition. Significant reduction of the conversion rate due to particle clustering was observed in cases with mass flow rates corresponding to around-stoichiometric and fuel-rich mixtures. On the other hand the effect of turbulence on the mass transfer rate does not directly translate into the effect on the overall conversion rate. The observation was that the particle diameter variations, can shift the combustion regime towards more kinetically or diffusion-controlled.

Paper III. This paper described the resolved particle simulations of solid fuel combustion. It is worth noticing that two unconventional aspects of the numerical model are that 1) all transport coefficients were fitted to match predictions of the kinetic theory; 2) the speed of sound was reduced to relax time step and grid size requirements. The model was validated against numerical and experimental results. Good accuracy was achieved although not all features of the experimental results were correctly predicted.

All the results are presented clearly. In my opinion the thesis generates significant new knowledge in the scientific area of particle thermal conversion process.

In her work, the author uses the Pencil Code (open-source solver for compressible flows). The code was adopted to perform resolved particle simulations and point particle DNS. Ansys Fluent was also utilised. User Defined Functions have been prepared describing the impact of turbulence on particle reaction rates. Fluent was used in the large scale simulations as well as cross code validation against the model implemented into the Pencil Code. Additionally Cantera was used to verify the implementation of the gas phase chemistry module into the Pencil Code.

The research task undertaken by the author required extensive knowledge of the theory of processes and phenomena occurring during solid fuel conversion process (heat transfer, chemical kinetics, fluid mechanics) and numerical modelling.

The topic should be considered difficult, up-to-date and filling the gap in the actual research work. The selection of the research issues is relevant and interesting from the scientific and practical point of view.

Discussion questions

1. Paper I. One of the conclusions of the paper is that there exists a correlation between locations of clusters that are made of particles with different sizes. What is your opinion on the sense of implementing a model describing char fragmentation behaviour based on the porosity? How this phenomena could interfere with particle clustering?
2. Paper III. How would you estimate the impact of dimensionality on the results? Have you considered extension from 2-D to 3-D and discusing the particle conversion rate sensitivity to the model dimensionality?
3. Can the developed models be extended to thermally thick regime particles? What is your opinion on integrating Single Particle Models with DNS?
4. Paper II. What is the impact of the particle clustering on radiative heat transfer?
5. Paper II. The papers have shown that it is relatively easy to account for the effect of turbulence on mass transfer to the reacting particle. Is it acceptable to skip particle dispersion modelling (e.g. using a stochastic tracking method) and calculate only the average particle motion? The white areas in Figures 15-18 (lack of particles) suggest such approach.
6. Paper II. It is reported in [28] that the computational mesh has 5.88 million elements (0.1m). Despite rather high resolution, Fig. 17 shows an immediate diffusion of the primary fuel-air stream. Can the numerical diffusion be responsible for that phenomena?
7. Paper II. Is it true that the pulverised coal particle conversion models are becoming more sophisticated, but the critical part of the simulation process is the resolution of the numerical mesh in the burner area? Please comment.

Concluding remarks

The analysed doctoral thesis of Ewa Karchniwy fits to the Environmental Engineering, Mining and Power Engineering Scientific Discipline. My substantive assessment of the work is high. This thesis represents a great deal of work. The research it describes is of the international standard. The objectives have been well designed and the candidate has fulfilled her aims. The present thesis fulfils all criteria for a PhD dissertation. This thesis is ready to be defended orally and certainly meets the requirements laid down for the degree of PhD by the statutes in the Journal of Laws of the Republic of Poland (Dz. U. 2018, poz. 1669 z późn. zm.).

I therefore request the Scientific Discipline Council of Environmental Engineering, Mining and Power Engineering of the Silesian University of Technology for the acceptance of the submitted doctoral dissertation and allow MSc Ewa Karchniwy to defend her thesis orally.

In my opinion the thesis can be awarded with distinction.

Name of the referee

Norbert Modliński