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Review

of the doctoral dissertation of Ms. Ewa Karchniwy on

„Detailed numerical modeling of solid fuels conversion processes"

Basis for evaluation

I reviewed the doctoral dissertation in accordance with the resolution of the Discipline Council for Environmental Engineering, Mining and Power Engineering of the Silesian University of Technology from 25/11/2021.

The presented dissertation has been prepared in the area of technical sciences, field of engineering and technical sciences. The scientific discipline chosen by the PhD student is environmental engineering, mining and energy.

The topic discussed in the thesis under consideration relates to mathematical description and numerical modelling of phenomena occurring during solid fuel conversion process. Therefore, one can conclude that the choice of discipline is undoubtedly justified.

Structure and construction of the dissertation

The dissertation consists of 143 pages (A4 format) and contains 5 Chapters. Chapter I provides an introduction to the problem, motivation, literature review and summary of the review. Moreover, in this part of the thesis, objectives have been presented.

In Chapter 2, theoretical description (mathematical formulation) of the solid fuels conversion processes have been provided. In addition, numerical methods used to predict problems under consideration have been outlined here. Chapter 3 briefly describes 3 papers that form a basis of this dissertation. In this chapter, other publications of Ms. Karchniwy have also been mentioned.

Chapter 4 contains thesis summary/ conclusions and future work. The last chapter no. 5 copies of 3 mentioned before publications have been attached.

In addition to the main part of the thesis (5 aforementioned chapters), the work contains:

- A title page with information about: an author, dissertation title, universities involved and logos of universities.
- Preface, which includes the names of the supervisors.
- Abstract, summarizing the purpose of the work and the tools, methods used as well as conclusions of the investigations.
- Acknowledgements
- Table of contents (named Contents)
- Thesis structure
- List of Figures

In the dissertation also 17 pages of bibliography (see page 47) has been included. The bibliography contains as many as 148 items (papers). Among the cited items are those from the 1930s as well as those published recently (2021).

It is worth mentioning here that among the cited papers there are also publications of Ms. Karchniwy (see position 1 and 2). They have been published in good scientific journals:

- Combustion and Flame (2021)
- Journal of Fluid Mechanics (2019)

The content of the main part (5 Chapters)

The dissertation entitled: ***„Detailed numerical modeling of solid fuels conversion processes"*** contains 5 Chapters.

In Chapter 1, the author describes the importance of solid fuels and the process of their combustion (even nowadays). She emphasizes that the numerical models developed in this work will be useful for the design and optimization of combustion systems.

The author lists the most popular approaches to modelling of solid fuel combustion:

- Euler-Euler for high solids content
- Euler-Lagrange for low solid phase content

Ms. Karchniwy describes methods of predicting the interactions between gas and solid particles. (one-way, two-way, four-way coupling). The importance of turbulence is also noticed here and models such as RANS, DNS and LES are mentioned.

In the introduction, the author also briefly describes the process of solid fuel conversion and highlights its complex nature (moisture evaporation, devolatilization, heterogeneous reactions). The author mentions the available pyrolysis models (so-called network models):

- *functional Group-Depolimerization,*

- *Vaporization and Crossling model,*

- *Flash-Distillation Chain-Statistics model,*

- *Chemical Percolation Devolatilization.*

and points a serious disadvantage of these kind of models: time-consuming calculations. The alternative here is to use so-called empirical models that are valid for selected conditions only.

The heterogeneous chemical reactions that occur at the particle surface can be largely affected by the reagents diffusion rate (form the core flow). Therefore, Ms. Karchniwy also lists the available models predicting this phenomenon:

- *Single Film Model,*
- *Two Films Model,*
- *Continuous Film Model.*

Taking into account the importance of kinetic and diffusion, the PhD student describes 3 zones (regimes) of combustion. Another important parameter for reaction/conversion rate is porosity and pore structure within the solid particle. Ms. Karchniwy also does not forget about this aspect and describes the available models:

- *Grain Model*
- *Random Pore Model*

The PhD student also refers to the purpose of the thesis and explains influence of turbulence in the process under considerations. She claims that turbulence affects the solid particle conversion process by changing transport of heat and mass. Its influence can only be observed in the combustion zone II and III where diffusion affects the total reaction rate.

The literature review is sufficiently comprehensive and contains many important for the topic items (papers). The literature review is also summarized by the author. Ms. Karchniwy notes that to study turbulent combustion of pulverized coal, the most frequently used is the "point particle DNS" approach. On the other hand, the complex conversion process is examined with use of resolved particle model.

The author ends Chapter 1 with the aim of the work:

- study of the effect of turbulence on the rate of conversion
- use of point particle DNS, RANS models to study the effects of turbulence
- understanding the combustion behavior of a coke particle.

Chapter 2 (Methodology) briefly describes the models, boundary conditions and software (the Pencil Code, Ansys Fluent) used in 3 papers attached in Chapter 5.

Chapter 3 describes contribution of Ms. Karchniwy in 2 published papers and one publication under review. Ms. Karchniwy indicates that her contribution is as follows:

Paper I: conduction of the simulations , post-processing, preparation of manuscript

Paper II: setting-up simulations, post-processing, preparation of the manuscript

Paper III: conduction of simulations, post-processing, preparation of the manuscript

Chapter 4 contains the thesis summary/conclusions.

- A broad range of Stokes and Damkohler numbers has been investigated
- The back- reaction of particle momentum to fluid was observed to significantly increase clusters strength at stokes number higher than 0.1.
- The model developed in this work to predict effect of turbulence on the mass transfer rate can be used for both: monodisperse and polydisperse particles.
- in the large-scale systems it has been observed that the turbulence causes the particle to travel much further before reaching a full conversion.
- Whenever RANS simulations are involved in the design and optimization process one cannot forget about the particle clustering.
- Effect of turbulence is clearly visible in systems with relatively large particles and high mass flow rates.
- In the boiler under consideration the influence of turbulence is significant in some regions of the combustion chamber (mass transfer rate decreased by 20%). However, conversion is reduced by 2% only

Chapter 5 contains 3 papers (2 already published) that are basis of the dissertation.

First paper (I) „Effect of turbulence on mass transfer rates between inertial polydisperse particles and fluid" has been published in Journal of Fluid Mechanics.

In this paper authors investigate how turbulence affects the mass transfer rate between inertial particles and fluid in a dilute, polydisperse particle system. During simulations DNS model and Euler -Lagrange approach have been used.

One of the conclusion is that particle clustering decreases mass transfer rate between phases. This occurs when the flow time scale is long relative to chemical time scale.

Paper no. 2 "the effect of turbulence on mass transfer in solid fuels combustion: RANS model" has been published in Combustion and Flame Journal. In this paper, a kinetic-diffusion surface combustion model is modified to introduce effect of turbulence on mass transfer rate. This modification takes into consideration:

- an influence of gas-paticle relative velocity increase on mass transfer rate

- an influence of turbulence-induced particle clustering on mass transfer rate

Moreover, a simplified numerical model of combustion chamber has been developed and applied to simulations of real industrial-scale boiler. The conclusion is that the effect of turbulence on combustion rate is minor.

Paper 3 "A numerical study on the combustion of a resolved carbon particle" was submitted to Combustion and Flame Journal and is currently under review. The paper describes completely different approach compared to models shown in Papers no. 1 and 2. Here, so-called resolved particle model is used. Using the Pencil software a novel numerical discretization is utilized: an overset grid. Moreover, compressible DNS model is used to predict fluid flow. The paper demonstrates ability of the model developed to predict carbon conversion. Results of the simulations are validated against experimental and numerical data. In addition, a sensitivity analysis of carbon conversion for selected parameters is described. One of the main conclusion is that the oxygen diffusivity change has a strong influence on reaction rate of heterogenous reactions.

Opinion on the PhD dissertation

PhD dissertation of Ms. Ewa Karchniwy touches on a very interesting subject; also for the reviewer of this work.

The PhD student undertook the theoretical and computational analysis of solid fuel conversion process. The detailed models developed in cooperation with the Ms. Karchniwy (point particle approach, resolved particle model) are aimed at examining the influence of turbulence on the fuel conversion process and on particle clustering.

In this work Ms. Karchniwy carries out her analyzes using innovative (and often advanced) numerical / mathematical / statistical methods. Therefore, I am convinced that the conducted investigations required many hours of self-studying in mathematics and numerical methods from the PhD student.

Her work on development of models, Ms. Karchniwy, preceded by a really in-depth literature review. In the end she summarize the current state of knowledge in this topic.

The simulations described in this thesis have been conducted mainly using 2 software: Ansys Fluent and The Pencil Code.

From the editorial point of view, the text (a brief summary of the work) (4 Chapters) and the publications (Chapter no. 5) are prepared very carefully. The summary is written logically and correctly in technical language. The construction is also correct. Two publications contained in Chapter 5, published in 2019 and 2021 in the *Journal of Fluid Mechanics* and *Combustion and Flame*, respectively are of really high quality. The third publication, thematically different from the previous papers was submitted to the *Combustion and Flame* journal. Unfortunately, there is no information whether the work has been accepted for publication.

Critical remarks

It can already be concluded from the description above that, the overall assessment of the doctoral dissertation is positive. Nevertheless, in my opinion, it is the duty of the reviewer to point out the imperfections of the work done and to clarify some ambiguities and doubts. Some of them are listed below:

- why does the citation of the papers in the main text start with number [5]? (see Page 1)

- it should be considered whether the objective of the work deserves a separate Chapter. Currently, it is in Chapter 1 (introduction)

- units are very often (almost always) not given in the text (below formulas under consideration). This makes it difficult to understand and spot any errors in formulas.

- are we dealing with a spherical coordinate system in equation 2.1? If so, the diffusion element should have a different form.

- please provide more details about Figure 3.1 (more explanation)

- Fig. 3.3 Does the graph show a transient model solution? If so, for what time are the results presented?

- the calculations (Chapter 2, Paper 3) are made for laminar flow. So why do you use DNS, RANS models, here?

- does the model (Paper 3) describe conversion of a pure carbon particle (without ash?). The ash existence and behavior has a significant influence on the total conversion rate.

- could you explain the overset grid approach? What are its advantages and disadvantages?

- why (Paper 3) uses the compressible solver?

- in my opinion, the results obtained with the RANS and DNS models should be compared. I mean the influence of both variants on the temperature field and the gas composition while the combustion process (when used for optimization purposes of an industrial plant).

- at what level is the error we make when replacing DNS with RANS? This would be important information for engineers which optimize combustion systems.

- what is the computation time of the problems using DNS and RANS? Is it practical for engineers to use DNS ?

- are there any problems with convergence in any of the models developed and (if) where? - How were they solved?

- Damkohler number is not by default calculated by Fluent solver. How did You reproduce Fig.3.2? Have you used Eq. in Paper I (page 1164)? This is not default definition. How did You get this formula?

- did the PhD student take part in any experimental investigations aimed at validating the models created in this thesis? I have found Fig.6 in Paper no. 3. What kind of measurements are these? What about the other models?

- the conclusions do not state whether it is worth considering the influence of turbulence (or not?) when simulating/optimizing units fired with solid fuels (computation time, stability vs. improvement in accuracy). Why?

In my opinion, the dissertation meets the requirements set out in art. 13 of the Act from March 14, 2003 on academic degrees and title as well as on degrees and title in the field of art (Dz.U.2003.65.595 with changes). Therefore, I am applying to the Discipline Council of Environmental Engineering, Mining and Power Engineering of the Silesian University of Technology for admission Ms. Ewa Karchniwy for further proceedings as part of the doctoral dissertation.

Moreover, I would like to apply for a distinction for her work.

Rafał Buczyński