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Opinion on the doctoral dissertation

“Detailed numerical modeling of solid fuels conversion processes”

by Ms. Ewa Karchniwy

PhD advisors: Assoc. Prof. Adam Klimanek, Silesian University of Technology, Gliwice, Poland;
Prof. Terese Løvås and Dr. Nils Erland L. Haugen, NTNU Trondheim, Norway

1. Actuality of the subject

The motivation of the Candidate (and her Advisors) to undertake the present PhD work is well rooted in the needs of combustion technology of pulverised coal, biomass, and alternative fuels such as RDF. It is pretty obvious to state that a better knowledge of the physical and chemical phenomena involved will help improved design of the combustion devices and the process parameters and, consequently, more efficient and environmentally friendly operation. In the PhD thesis, this far-reaching practical goal is a natural guideline for advanced study of the reactive flow thermomechanics, keeping it short. The problem involves turbulence, fuel in the form of dispersed solid particles, chemical reactions of devolatilisation and combustion in gas and solid phases (referred to in the thesis as the fuel conversion processes), as well as the heat and mass transfer phenomena ultimately linked to the fuel conversion. Therefore, the topic of the doctoral dissertation is evidently difficult and challenging in many ways. It requires an in-depth understanding of turbulent flow modelling and computation, particle-turbulence interactions (PTI), and turbulence-chemistry interactions (TCI). These issues are still open and belong to the core of fluid mechanics research, as I perceive it. Within this vast area of partly uncharted land, the ambition of the Candidate has been to gain some more insight into the role of turbulence in the fuel particle conversion processes. The PhD subject is definitely of actuality and the research problem has been correctly stated. Although the very thesis of this PhD study has not been explicitly written, it may tentatively be formulated as: turbulence of the carrier phase plays a role in the mass transfer process to fuel particles and needs to be accounted for in a physically-sound modelling of the process, at least for some range of control parameters. But there are more original aspects to the PhD findings than that, as documented in the dissertation and briefly reported in the following.

2. Methodology applied

The present work has mainly a theoretical and numerical character. The analysis of multi-physics phenomena in a geometrically simple setup, rather than focusing on complex-geometry “real-life” flow cases, is perfectly correct at this stage of developments. Notwithstanding the emphasis on more fundamental issues, the study is illustrated by a practically-relevant computation of an industrial-scale boiler. To handle turbulence, the full numerical solution of the governing equations of flow is performed; it is termed direct numerical simulation (DNS). The Navier-Stokes (N-S), the continuity, and the energy equations are solved together with mass transport equations of chemical species (reactants) for a detailed analysis of TCI, see description of Paper I below. Alternatively, the RANS turbulence modelling has been applied (Paper II). To handle PTI, which is the main difficulty of the subject, the dispersed phase has been solved in the Lagrangian approach under the point-particle approximation. When modelling the devolatilisation and char combustion (as heterogeneous surface reactions), the particles were considered as a source of mass (in the transport equations of reactants) and energy (in the carrier phase energy equation). In some of the cases, where the so-called two-way interphasial momentum coupling was accounted for, the particles were also considered as a source of momentum in the N-S equation. The fine-scale analysis of the mass transfer process was performed using the so-called particle-resolved DNS where the char particle was treated as a finite-size object in the flow. Such as approach, described in detail in Paper III, allows one to relax many of the assumptions needed in the point-particle approximation, including the drag force and Ranz-Marshall correlation for heat (and mass) transfer. Instead, the analysis at the level of resolved particle can provide closure relationships for less detailed, yet computationally efficient, point-particle simulations.

3. Brief description of the contents

The form of the PhD document differs from the standard one which is a self-contained dissertation. Instead, the Candidate has chosen to prepare a 60-page "general guide" to her work (containing introduction, methodology and summary) followed by three original research papers ("the Papers") published in *Journal of Fluid Mechanics* (2019) and *Combustion & Flame* (2021, 2022). The latter was included in the PhD document in the form of submitted manuscript (as of August 2021). The Candidate has been the first, corresponding author in all three papers; her Advisors (A. Klimanek and N.E.L. Haugen) co-authored the papers. It needs to be recalled that both JFM (IF=3.63) and C&F (IF=4.19) are renowned research journals in the subject area of fluid mechanics and combustion.

I will now briefly describe the contents of the PhD document, referring first to the Candidate's general guide (the 60-page text) and then to the original research papers.

3.1 The general guide

It is contained in Chapters 1-4 of the PhD document accompanied by the bibliography section. There is also an abstract in English and, as a separate sheet, an abstract in Polish (no Polish title, though). In Chapter 1, following a brief motivation that refers to the world energy policy, the state of the art in the subject area is presented in a comprehensive way. The bibliography includes nearly 150 entries, which is respectable for a PhD thesis. The cited literature covers important contributions to the subject, also some very recent ones. The state-of-the art overview offers a reasonably well thought, no-equation introduction to the research tasks undertaken by the Candidate. In the methodology (Chapter 2), somewhat contrary to what one would expect and to what is promised ("*…discuss selected aspects of the governing equations and numerical methods*", p.27), there is no detailed presentation of the approach. I would appreciate reading a concise one, preferably in a self-contained manner, but I understand that: (i) the very methodology is already described in detail in the respective Papers I-III and (ii) preparing it would need an extra effort. If possible, at the PhD defence I would very much appreciate such a concise presentation that would feature a unifying view on the basic points on physics and modelling, and emphasizing, whenever possible, the relationships among (and the complementarity of) the approaches applied in Papers I-III. The methodology, as it stands now, is limited to the brief mention about the software used: an open-source code `Pencil` as well as a commercial one `ANSYS-Fluent` supplemented by in-house UDFs. Then, there is some supplementary material to Paper III that, in my view, should rather belong to Sec. 3.3 in the form of Appendix or alike. Yet, this is a minor point only.

3.2 Paper I

It reports on a DNS study of particle-laden, forced isotropic turbulence. The main question that is answered in the paper is how the carrier phase turbulence affects the mass transfer among the particles and the flow. For the purpose, the role of particles preferential concentration due to their interaction with eddy structures of turbulent flow, also known as particle segregation or clustering, is analysed. This effect of two-way momentum coupling is considered as well. The paper relies on a previous publication (Haugen *et al.*, JFM 2018), yet the important extension of the work consists in the account of particle size polydispersity.

3.3 Paper II

Here again, the effect of turbulence on the mass transfer of reactants from the bulk of the carrier gas phase to the particle surface is analysed in a RANS-type study; if I understood correctly, the findings of the paper cited just above are applied here. The effect is twofold: the mass transfer may be reduced due to particle clustering or it may be enhanced because of the relative particle velocity w.r.t. the carrier phase. The net impact of turbulence depends on whether the surface combustion is controlled by chemical kinetics or by reactants diffusion, as quantified by the Damköhler number. In the paper, a particle-laden jet in co-flow is considered as benchmark example, followed by a full-scale study of an industrial coal-fed boiler.

3.4 Paper III

The main thrust of this contribution is a detailed computational study of char particle combustion. The particle is considered as finite (and not a material point as in Papers I and II), therefore an overset (or Chimera) grid is applied for fine resolution of the particle "near field". Valuable results are obtained in the study, including the sensitivity of fuel conversion rate to several control parameters of the process. The only less convincing aspect of this paper is the novelty of the observation concerning the computational accuracy, if I understood correctly. (The sound speed reduction being beneficial in weakly-compressible methods or, alternatively, that the chosen Mach number should make a reasonable compromise between the incompressibility constraint and the time step restriction).

4. Assessment of the original contributions

As the PhD findings have been reported in three multi-authored papers, I need to rely on the Candidate's statements about her own contribution. They are honestly reported/declared and listed in the summaries of Papers I-III, see respective first paragraphs of Sections 3.1-3.3 in "The general guide". Given the description provided there (see point 3.1 above) and the fact that the Candidate has been the first and corresponding author, these statements are definitely trustable and otherwise well correspond to the usual practice of PhD studies (and the pain & glory involved…). In my opinion, the original contributions of the Candidate refer to:

1. A comprehensive study of mass transfer involving a polydispersed particle system in turbulent flow. It nicely complements and extends a recent work of this kind referring to the monodisperse systems. The first very interesting finding, irrespective of the fuel conversion process, is the impact of the two-way momentum coupling on the preferential particle concentration and the observation that polydisperse particles cluster in correlated positions. Arguably the main result of the DNS study refers to the particle conversion processes: it is the confirmation, for the assumed polydispersity characteristics, of the complex turbulence-particle-chemistry interactions (PTI-TCI), observed earlier in monodispersed flow. They are: (i) the mass transfer reduction due to clustering and, therefore, the impact on the heterogeneous reaction rates, and (ii) the mass transfer enhancement due to turbulence. Both these effects depend on the particle inertia (quantified by the Stokes number) and the ratio of flow and chemistry time scales.

2. The modelling of turbulence impact on the fuel conversion process performed in the RANS framework. The study is related to the findings from the DNS reported above. Given that the RANS models, unlike DNS at the moment, are applicable as industrial work-horse, the large-scale simulation results of an industrial boiler are reported. In this case, the assessment is less obvious because of the flow spatial heterogeneity and variable temperature field; generally, the turbulence effect has been found to be only moderate.

3. An attempt to study the fuel conversion process in a very detailed way, following recent progress in particle-resolved DNS. The study has been performed applying a number of simplifying assumptions (see discussion below in point 4.1, item 5), yet it represents, in my opinion, a step forward w.r.t. just the dynamics on the particle-resolved level, by accounting for chemical reactions. The results refer to some aspects of the problem only but seem original and promising to provide closure relationships for simplified modelling.

4.1 Technical points, issues for discussion, remarks and questions

As a whole, the dissertation makes a rather pleasant reading: the text is carefully written in good and rich English language. As for the subject matter, there are some points that are not obvious (at least for this referee) or not sufficiently explained, so they may call for a broader explanation, trigger remarks or questions. There are also some inaccuracies or incorrect statements, etc. However, the remarks do not undermine my generally very positive opinion on the present work.

The major technical points are listed below (basically, in the order of appearance in the text). I will be grateful for a written reply and, for some of the concerns, also a discussion at the public PhD defence.

1) I appreciated the general classification of modelling approaches for dispersed flows (Fig. 1.1). Among them, the point-particle LES is mentioned, which is correct. This method has the potential to account for the larger-scale eddies and their impact on particle dynamics and combustion processes. LES becomes nowadays computationally affordable in real-life flows. I would very much welcome an opinion of the Candidate on this method, as applicable (or not) to fuel conversion processes. What has been done to date, if anything? What are the difficulties one can anticipate? How critical they are, etc.

2) At several places of the text, the notion of particle “boundary layer” (BL) is invoked. This makes me troubled, as the canonical use of the term “BL” in fluid mechanics refers to high-Re flows where the governing equations of flow and heat transfer in the near-wall region are shown to simplify to the parabolic ones (Prandtl eqs.). Is it the case in the present work? (However, Re of relative motion are typically not very high for sub-millimetre scale particles.) Or, was just the “near-field” meant instead?

3) Referring to the combustion regimes of char particle, illustrated in Fig. 1.5: Zone II is described in the text (p. 10, top) as being controlled by the reactant diffusion; however, according to the figure, it seems to be (equally) dependent both on diffusion and kinetics. Please clarify.

4) The particle clustering in turbulence which is of experimental evidence can only be retrieved in those modelling approaches that resolve instantaneous eddy structures (or at least part of them). The standard RANS method does not belong to this category (one can argue about URANS, though). The particle concentration gradients do appear in RANS-based simulations but they are due to turbulence inhomogeneity, as in the near-wall regions, and this behavior is rather referred to as “turbophoresis”. Yet, the clustering is invoked in the thesis in the RANS context (p. 39, 1st line, also Paper II). I was struggling to grasp the intended meaning of “clustering” here. Please explain.

5) p. 39, also Paper III: “cylindrical grid”. It is not immediately clear that the particle-resolved DNS is performed in 2D only. I think this point should have been explicitly stated in the abstract of the paper and in the preview of its contents. Otherwise, have there been no 3D studies of the problem so far? More important: when referring to the experimental data for validation purposes, a special care is needed as the 2D and 3D cases may considerably differ. Also, using the term “DNS” sounds a bit like an overstatement as laminar flow only is solved. Please comment on all these concerns.

6) the thesis summary, p. 43: why “the effect of turbulence” on St? The Stokes number St as a non-dimensional measure of particle inertia is fixed beforehand, right? (unless the char particle shrinks because of ongoing combustion process). Please clarify.

7) Paper I, Eq. 2.5 and below: it is unclear to me why isothermal sound speed is used. Please explain.

8) Paper I: the analysis of the role of polydispersity is very interesting. In the case considered, the particle size distribution (PSD) is determined by its various PDFs (Fig. 2) where the minimum and maximum diameters are not set independently but rather directly related to the largest and smallest

turbulent eddies, right? I was wondering whether, apart from the mean particle diameter \overline{d_p}, yet another measure of the PDF which, naturally, is the r.m.s. of d_p (the second-order central moment) can/should enter the description? A trace of this idea can be spotted in Eq. A9 where two higher-order moments of d_p appear. This way, perhaps, one could ultimately be able to prescribe the PSD and its effect independently of the length scales that determine the turbulence spectrum. A comment on this issue would be welcome.

9) Paper I, the text in p. 1159 referring to Fig. 5: is there any quantitative measure available concerning the cluster "strength" or "sharpness"? Or does this term rather refer to a "naked-eye" inspection only? (The results are otherwise very interesting.)

10) Paper I, Fig. 7: it would be instructive to know why *C(r)* does not asymptotically decrease to zero: is it a numerical artefact or is there a physical reason to it?

11) Paper II, Eq. 8 & the text below it; also the discussion on turbulent dispersion modelling in RANS: I understand that this is not the main issue of the paper but information provided here is imprecise. Generally, discrete random walk models are known to be deficient, yet they are amply used *faute de mieux*, especially in commercial software. Equation 8 does not account for possible anisotropy of turbulence, and even less for its inhomogeneity (the case illustrated in Fig. 8 does represent inhomogeneous turbulence). Then, if the formula is used every time step Δt, then the time scale of the Lagrangian correlation of the fluctuating velocity generated this way is implicitly introduced as Δt/2, which is erroneous. Next, the relative velocity will indeed be "exaggerated" as the Authors put it. Generally, stochastic models based on the Langevin equation for the fluid velocity along the particle trajectories are free of these drawbacks and satisfy the correct limiting behavior of zero relative velocity when St → 0. A comprehensive paper by J.-P. Minier [*Prog. Energy Combust. Sci.*, 2015] may serve as an authoritative reference to the topic;

12) Paper III, the sound speed reduction: please be more detailed about this aspect. Is it just because of the weakly-compressible approach applied to solve the flow? Or is the case considered indeed compressible? If not, does the Pencil code feature a truly-incompressible solver option as well?

4.2 Minor remarks, some misprints, etc.

These remarks refer to the points where more explanation is suggested for the sake of a better clarity, or misprints/mistakes have been spotted. There is no obligation for the Candidate to reply.

a) Abstract and several other occurrences in the text: the phrase "particle back-reaction" may be misleading in the context of reacting flows (fuel conversion processes). Why not use, depending on the context, "two-way coupling" or "turbulence modulation" instead?
b) p. 1, bottom: "relies of" → "relies on";
c) p. 4, the phrase "exchange from fluid to particles only" sounds misfortune as "exchange" is reciprocal by nature;
d) p. 4: rigorously, the account for four-way coupling is conditioned on the volume fraction of the dispersed phase being sufficiently large, rather than the high mass loading;
e) p. 6, bottom: devolatalize or devolatilize?
f) p. 16, 2nd paragraph: "turbulent domain" sounds rather awkward;
g) p. 31, top: "particle which interior" → "whose";
h) References, p. 47ff: the bibliographic data of Refs. [39], [64]-[66], [70] are incomplete;
i) Paper I, line below Eq.2.2: D/Dt is preferably called the material derivative to discern it from the advective term;
j) Paper I, Sec. 2.2, 1st line: I suggest to use the term "point-particles" or "material points" here (as their Lagrangian dynamics is referred to just below the text) rather than "point sources" (which basically refers to their role in the Eulerian equations of the carrier phase);
k) Paper I, text below Eq. 2.10: usually it is ($1+f_i$) that is referred to as the drag correction factor;
l) Paper I, Tab. 1 and Fig. 2: are the particle diameters provided in non-dimensional units?
m) Paper II, p. 77 line 9: what is "turbulence particle dissipation model"?
n) Paper III, line above Eq. 16 and below (twice): "kinetic viscosity".

4.3 Brief description and assessment of the PhD thesis
(according to the formal requirements communicated by Silesian University of Technology)

- **a)** **The title** is fine and informative. Perhaps, one could make it even a bit more descriptive by adding the words “particle” or “disperse medium/flow”, then “devolatilisation” and “combustion” (instead of “conversion”?).
- **b)** **Structure** of thesis is not the one of a classical PhD document, since the main part of the original research is reported in the journal articles, but it is fine in general (see only a remark on the methodology in point 3.1 above).
- **c)** **Bibliography** is rich and adequately covers the state of the art.
- **d)** **Aim of the work** is clearly specified in Sec. 1.6 of the thesis.
- **e)** **Methodology** is correct. It refers to mathematical modelling and numerical simulation of reactive flow thermomechanics. The use of point-particle DNS and particle-resolved analysis is appreciated. Also, the RANS-type industrial scale computations have been documented.
- **f)** **Assessment of results** is provided in the first part of point 4 of this review. The scope and quality of results are appreciable for a PhD work.
- **g)** **Applicability of findings.** Although the PhD dissertation mainly addresses fundamental issues in particle-laden reactive turbulent flows, the results may evidently have a practical significance, not only for fossil fuel particles, but also for biomass or RDF; possibly, there may exist other relevant applications in the context of chemical or process engineering involving reactive particle systems in turbulence;
- **h)** **Imperfections, suggestions for improvements, questions.** Imperfections any not many (some are listed in point 4.2 above) – generally, the PhD document is carefully written and the Candidate has to be congratulated on the effort and its outcome. Concerning the questions related to the research work itself, some are formulated in point 4.1 above, mainly as an invitation for the Candidate to look beyond and as a support for discussion at the PhD defence.
- **i)** **General assessment about the solution of the research problem and its originality.** As argued in point 1 of this review, the problem is clearly of actuality, the tasks for the PhD research have been correctly identified and solved. The originality of research has been confirmed through publications in scientific journals of international reputation.
- **j)** **General assessment of the Candidate’s background and expertise in the subject area.** The expertise in the area of environmental engineering and energy (also mechanical engineering) is appreciated. My general assessment is undoubtedly positive, as reiterated just below.

5. Final conclusion

The doctoral dissertation presented by Ms. Ewa Karchniwy provides a proof of her good knowledge of fluid thermomechanics and combustion phenomena in their theoretical aspects, the use of computational fluid dynamics tools, and applications to several flow problems including those of practical relevance. The Candidate has demonstrated her capabilities to critically scrutinize the bibliography of the subject as well as various variants of computational approaches to turbulent flows. The thesis contains original analyses and novel findings beyond the state of the art. Judging by the PhD document, the Candidate has proven her good knowledge of the subject area, the professional skills, as well as the ability to think and work creatively.

Given all the above, **my final conclusion about Ms. Ewa Karchniwy being a doctoral candidate is positive and I recommend that she orally defends the PhD dissertation with no reserve at all**. Moreover, given (i) the degree of difficulty of the thesis subject, (ii) the quality findings reported in the PhD work, listed in this review and published in renowned research journals **I propose that the PhD thesis of Ms. Ewa Karchniwy be awarded distinction** (*summa cum laude*).