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Review of the doctoral dissertation by Ms Eleonora Spricigo entitled *"Application of smoothed particle hydrodynamics method to interfacial two-phase flows"*

This review has been prepared on the request of the Scientific Council of the Institute of Fluid-Flow Machinery of the Polish Academy of Sciences (IMP PAN) in Gdańsk, in response to the letter signed by Prof. Grzegorz Żywica, Deputy Director for Research, dated 05 July 2024 (ref. no. RN-421-4/23), followed by a contract signed on 16 July 2024.

1. Introduction

The submitted doctoral thesis by Ms Eleonora Spricigo, MSc Eng., prepared under the supervision of Prof. Jacek Pozorski from IMP PAN, deals with the application of the smoothed particle hydrodynamics (SPH) method to the numerical analysis of the problems involving two-phase flows with interfacial surfaces. A so-called weakly compressible (WCSPH) variant of the method has been used. The PhD Candidate has proposed a new formulation for the viscosity force term in the fluid momentum equation, and implemented it in the SPH computer code that has been developed at IMP PAN for over a decade now. The principal objective of the research discussed in the thesis was to analyse the effectiveness and numerical performance of the new formulation in the simulations of a range of two-phase flows. In particular, the problems of a plane two-fluid Poiseuille flow, of a rising gas bubble in a liquid, and of water sloshing in a moon pool were investigated. As for the latter sloshing problem, the Author has coupled the SPH code with a commercial optimization tool in order to develop a predictive mathematical model that can be used for optimizing a moon pool geometry for given flow (water wave) conditions.

The dissertation by Ms Eleonora Spricigo is written in good English, and consists of six numbered chapters, supplemented by a bibliography list and three appendices. The main text is preceded by acknowledgements, thesis abstracts in English and Polish, and the lists of figures, tables, acronyms and mathematical symbols. In total, the work comprises xi + 134 numbered pages, and 12 unnumbered pages (containing the above-mentioned lists).

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The first, introductory chapter, starts with a short overview of discrete methods that are currently in use to model multi-phase flows, then introduces the SPH method, together with a brief history of its development since the method was conceived in year 1977. This is followed by a concise presentation of the motivation, main objectives and the scope of the research undertaken by the PhD Candidate. The next Chapter 2 presents, on 26 pages, the details of the SPH approach applied in the thesis, starting from the concept of the method, followed by the discussion of numerical issues characteristic of this approach, related approximation techniques, presentation of discrete forms of the continuity and momentum equations, and the methods for the implementation of boundary conditions. Chapter 3 presents the proposed novel SPH formulation (called mVER by the Author) of the viscosity force term in the momentum equation, and then shows the examples of the validation of the new SPH model against the analytic and numerical results known from the literature. This is followed by Chapter 4, devoted to the numerical analysis of water sloshing in a moon pool. First, the proposed mVER model is applied to simulate the sloshing mechanism in a simple rectangular tank to validate the SPH model, and then a more complex problem of water sloshing in a moon pool with a recess is investigated. Chapter 5 is concerned with the presentation of an optimization technique developed by the Candidate, which can be used to optimize a moon pool shape to minimize the height of a water wave generated in the pool for given external surface wave conditions. The concluding, three-page-long Chapter 6, summarizes the content of the thesis and the main results achieved. The Bibliography list is very extensive, since it includes as many as 204 references (most recent from year 2023). Finally, the three appendices at the end of the main text contain technical details which may be of interest to those directly involved in computer programming of the SPH method.

2. Comments on the contents of the thesis

The text of the thesis is well organized and appropriately divided into self-contained chapters. The level of English used by the Author is satisfactory – I have spotted about three dozens of obvious errors, typos and missing words throughout the whole manuscript, but I do not consider this as a dramatically large number. All the plots are carefully prepared and their number is sufficient to follow the Author's considerations and illustrate the results achieved. Perhaps with the exception of the pressure fields in Fig. 3.8, 3.10, 4.11, 4.12 and 4.13 that could have been plotted as contour line plots for their better readability.

The introductory Chapter 1 is nine pages long and presents, with an adequate level of detail, the development of numerical methods applied to multi-phase flows, and places the SPH method used by the Candidate against the background of other, mesh-based and mesh-free approaches. Next, in Section 1.2, the origin and early development of the SPH method is briefly described, followed by the discussion of the literature that is the

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most relevant in the context of the research undertaken in the submitted dissertation. Further, again briefly, the contributions of the former PhD students supervised by Prof. Jacek Pozorski are mentioned. The chapter is concluded with the presentation of the motivation, the goals and the scope of the research carried out by the Author. Although the statement *"the goal is to demonstrate the capabilities of our code to simulating the new model"* sounds awkward, since the code is a computer representation of a model rather than a tool for its simulating. In overall, I find this introductory chapter useful for understanding what one can expect in the following parts of the thesis.

Chapter 2 contains, on 26 pages, an exhaustive presentation, of the theory of the Smoothed Particle Hydrodynamics method. First, the fundamental idea of interpolating any field function in terms of its values given at a number of discrete material points by means of a continuous and smooth function called a kernel is presented, and the required properties of such kernel functions are discussed. Then, the specific forms of the kernels are presented, including those implemented in the computer code that has been developed at IMP PAN for about 20 years and was used by the Candidate for her calculations. Subsequently, the formulae for the calculation of the first and second order differential operators of the kernel functions are shown. In particular, it is argued why an antisymmetric form (2.19) for the gradient operator is preferred to a symmetric one. Given the approximate formulae for the differential operators, in Section 2.2 the expressions for the fluid density, equivalent to the continuity equation, and for the momentum balance and energy conservation are presented. This leads to discretized forms of the continuity and linear momentum equations in Section 2.3) supplemented by the physical (constitutive) equations relating pressure to the fluid density. The last section of the chapter concisely presents a few methods that are applied to implement boundary conditions in the SPH modelling, including the so-called ghost-particle approach adopted by the Author.

Throughout this chapter the PhD Candidate has demonstrated good knowledge of the theoretical and practical aspects of the SPH method. No doubt that some of the considerations presented Chapter 2 may be difficult to follow for those not familiar with the intricacies of the SPH, but, nevertheless, I think they are necessary for the completeness of the thesis.

Having presented the mathematical apparatus of the SPH in the previous chapter, the Author proceeds to the validation of her discrete model in Chapter 3 (which is 16 pages long). The chapter starts with the critical discussion of the viscous force term in the approximate SPH equation for the momentum balance. Based on the literature review, the Candidate proposes in Section 3.1 a new formula for the inter-particle viscosity $\bar{\mu}_{ab}$, which replaces an arithmetic mean of the viscosities of two neighbouring particles (an approach used in the past) by a harmonic one, resulting in equation (3.11) for the viscous force term. This is a novel element regarding the numerics of SPH and is a central point of the submitted dissertation. However, I think that, for consistency of the text, this

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Section 3.1 would find a better place in Chapter 2, which is entirely devoted to the theory of SPH, restricting Chapter 3 to the sole analysis of the results from the computations.

In Section 3.2, in order to validate the results produced by the Author's modified model, called mVER, single- and two-fluid steady-state Poiseuille flows in the plane geometry are examined. In case of the single-fluid flow, a very good agreement between analytical and numerical results has been achieved, as convincingly demonstrated in Fig. 3.2. Regarding the two-fluid flow, also very good agreement between the theory and numerics has been presented in Fig. 3.3, showing a clear improvement on the original approach (i.e., with the arithmetic mean of the viscosity) by Violeau (2012). However, the results obtained by Hu and Adams (2006) are very close to those obtained by the Author with her modified model. A more challenging problem, that of a gas bubble rising in a liquid, is investigated in Section 3.3. Two regimes, distinguished by the combination of the Reynolds and Eotvos (Bond) numbers, or the final shapes of the originally circular bubble, are considered. In the first regime, called the 'ellipsoidal bubble' case, the results obtained by the Author compare favourably with those from the literature when the current vertical position of a bubble centre is analysed (Fig. 3.7a); however, the time variation of the buble vertical velocity exhibits oscillations (Fig. 3.7c). Essentially, in the more demanding second regime, called the 'skirted bubble' case, very similar conclusions, with the oscillating bubble velocity, can be drawn (Fig. 3.11a). The Author attributes the observed fluctuations in the velocity to the fact, that so-called weakly compressible variant of the method (WCSPH) has been adopted, in which an artificial speed of sound is introduced to the model. I wonder, if the Author has tested the effect of different values of the sound speed s on the numerical results, to see if increasing s leads to smaller oscillations? If so, I think it would be a good point for the discussion during the public defence of the dissertation. Another point of my interest is whether the model by Hu and Adams (2006) would perform better than the Author's model? (this question is prompted by the close similarity between this model results and the Author's ones as observed for the two-phase Poiseuille flow, as seen in Fig. 3.3). And finally, on page 51, the Author suggests that the form of a kernel may contribute to inaccurate results. Honestly, I would be surprised if any modification in a smoothing kernel function (a mathematical concept) could help to significantly reduce the oscillations in the bubble rising velocity (a physical effect). But, perhaps, the Candidate does have some thoughts and ideas on this topic which she could share during the public discussion over the thesis?

The following Chapter 4 (19 pages in length) is devoted to a problem of practical importance; namely, that of liquid sloshing in a moon pool (an opening in a vessel's hull base giving access to the water below to enable engineering activities). As first, to validate the SPH model, an academic problem is investigated, in which the liquid sloshing mechanism is analysed in a simple, rectangular tank (Fig. 4.1), when one phase is water, while the other is air. A very good agreement between the simulations and the

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theory has been achieved in terms of the water wave height, as illustrated in Fig. 4.2a. On the other hand, the quantitative differences between the simulated and theoretical values of the sloshing forces are very large, as at some instants of time they exceed 50% (Fig. 4.2b), which must be a disappointing outcome. The Author tries to explain these discrepancies by 'the presence of the viscous force' (the sentence above Fig. 4.2). I would like to ask the Candidate to say more on this issue during the thesis defence. The real moon pool case is analysed in Section 4.2. A large part of this section (over five pages) is devoted to presenting the background of the original concept of moon pools and the historic overview of their further development, whereas the discussion of the SPH results (Subsection 4.2.4) is presented on only about two pages of the text (not counting the plots), which is a bit disappointing. A moon pool with the so-called recess has been simulated as a two-dimensional problem, and the calculations have been conducted for two different particle grid resolutions. The results for the wave height time-variation at three selected points (virtual gauges) are presented in Fig. 4.9, for one selected frequency. It is a pity that there is no analysis how the changes in the frequency of oscillations (i.e. in the length of a surface wave) affect the wave height in the pool. As can be noticed in Fig. 4.10, the effect of the mesh resolution increase is moderate. It is also seen in the latter figure that the predicted resonant frequencies compare satisfactorily with those known from the literature. On the other hand, the wave heights predicted by the SPH model are considerably smaller (by a factor of two and more) than the results of experimental measurements; so again a moderate success. The chapter is concluded with a series of plots illustrating the time-variation of the distribution of discrete particles and the corresponding pressure fields.

Certainly, Chapter 5 (with 28 pages being the longest in the thesis) stands out from the previous four chapters and is loosely connected to them, since it is concerned with the problem of mathematical optimization, whereas the principal topic of the thesis is the modelling of two-phase flows. The Author states in the opening paragraph of the chapter that the goal is to find an optimal shape (dimensions) of the pool recess that will minimize the height of wave generating in the moon pool. So I wonder whether it is technically viable to adapt the pool geometry to current sea conditions which can be highly variable.

The first section of the chapter introduces basic ideas of optimization, presents a brief history of the development of this discipline, and describes different optimization approaches and algorithms that have been developed over the years. I am not a specialist in optimization methods, therefore this section presented some information that is new to me. Similarly, the next Section 5.2 dealing with some aspects of the proper design of statistical experiments contains some useful, though general, information as well. Yet, I am not fully convinced whether the work devoted to the SPH modelling should contain these two sections, distracting the reader from the main thread of the thesis. The following Section 5.3 describes the application of the commercial software *modelFRONTIER* to the

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problem mentioned above, which is finding the optimal shape of the moon pool recess for given water wave conditions. My impression is that the text on eight pages (83 to 90) is a typical user manual giving instructions how to work with a specific piece of computer software. Therefore, I think that the best place for this part of the thesis would be in an appendix. The Author says that the optimization has been performed by applying the method known as RSM (Response Surface Method). It is not clear to me why just this particular method has been selected for application? What are the advantages of this method over other optimization methods available? The results of the moon pool shape optimization are illustrated in Figures 5.12 to 5.18. Honestly, given the length and the amount of details presented in the preceding part of this chapter, the final outcome seems to be quite modest. Especially after the Author's remark that 'The investigation done in this chapter must be regarded as qualitative' (the first line below Fig. 5.17). On the other hand, the PhD Candidate must have spent a lot of effort to first learn the methods of mathematical optimization, then to get familiar with the computer software adopted, and finally to couple the SPH code with the optimization software, which certainly deserves appreciation.

The final Chapter 6 summarizes the content of the dissertation, and reiterates the conclusions following from the numerical simulations carried out by using the modified SPH code for solving a number of problems of theoretical and engineering importance.

3. Minor remarks

(a) The list of acronyms before the main part of the work is useful, though I have noticed that some, appearing in the text, are missing (LHS, PDF, SSH). Similarly, some mathematical symbols (e.g. σ in eq. (2.86), $\boldsymbol{u}_{ab}$ in eq. (3.9), U_g on p. 45) are also missing in the respective list.

(b) The meaning of the operator $< \cdot >$ is not explained, neither in the text nor the list of symbols.

(c) page 15, line 2 from the bottom: is the value of the normalization constant $C' = 9\pi$ for $d = 3$ correct? (the value in Table 2.1 is $C' = 21/2\pi$).

(d) Some text is missing in the sentence immediately preceding eq. (2.17).

(e) page 23, the two lines after eq. (2.41): there are no subscripts b in the above equation.

(f) page 26, the two lines after eq. (2.62): formulations cannot be summed up (but formulae can).

(g) page 29, line 8 after eq. (2.68): conservation of what?

(h) page 31, the first line after eq. (2.75): why the particular threshold value $h/100$ has been adopted?

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(i) page 33, line 1: reference for the Tait equation would be useful.

(j) page 37, unnumbered equation: throughout the work the pressure is denoted by P, whereas here it is p.

(k) page 38, eq. (3.3): one of the right parentheses in the brackets is superfluous.

(l) page 41, caption to Fig. 3.1: one-fluid, or two-fluid Poiseuille flow?

(m) page 45, unnumbered equation for Re and Eo numbers: the equations include the velocity U_g, but in the line below we see v_0.

(n) page 57: in eq. (4.1) the quantity $a_0(t)$ has a unit of force, while in eq. (4.4) it seems to have a different unit.

(o) page 73, line 6 from the bottom: mathematical definition cannot be maximized or minimized!

4. Final evaluation of the thesis

I am sure that the results of Ms Eleonora Spricigo's research which are discussed in the submitted doctoral thesis are an original and significant contribution to the field of computational fluid dynamics, and help us to better understand the complex mechanism of two-phase flows with interfacial surfaces. The improved SPH model constructed by the Candidate can be readily applied to simulate the phenomena which are of importance to both theoreticians involved in solving fundamental problems of hydrodynamics of two-phase flows as well as to engineers designing and operating vessels with moon pools.

The thesis is clearly and understandably written and appropriately organized. The objectives of the research undertaken by the PhD Candidate have been achieved, and all the conclusions are supported by the results presented in the work. Part of the results obtained has already been published in a peer-reviewed paper. Throughout the thesis, Ms Eleonora Spricigo has convincingly demonstrated her thorough theoretical knowledge and the ability to solve independently complex problems of fluid dynamics and to properly analyse and interpret the results of numerical simulations.

5. Recommendation

Based on my evaluation presented above in this review, I recommend the acceptance of the submitted doctoral dissertation for its public defence by the Candidate. In my opinion, providing that the defence is successful and all necessary formal requirements are fulfilled, Ms Eleonora Spricigo, MSc Eng., deserves a PhD degree in the discipline of Mechanical Engineering.

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