

Interactive comment on “Testing the effects of the numerical implementation of water migration on models of subduction dynamics” by M. E. T. Quinquis and S. J. H. Buiter

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General comments

The authors present a study comparing three numerical implementations adding parametrizations of water transport to computational simulations of subduction zones. The research presented in this manuscript generally is relevant to the numerical study of the dynamics and chemistry of subduction systems. As simulations of fully coupled two-phase flow for the study of fluid transport in large-scale geodynamic situations such as subduction zones are difficult to achieve, many computational studies resort to simplified numerical parametrizations of fluid transport.

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This study compares three such parametrizations in terms of their influence on first a sinking sphere model and later on a realistically scaled subduction model. The three numerical methods are based on the same principle of fluid moving upwards at higher rates than solid deformation, thereby hydrating the material they are migrating across. The ability of local rock to de/hydrate, and thus the availability of free water for transport, is determined with the thermodynamic software *Perple_X*.

The three methods are different in what velocity is chosen to govern water migration. The first method chooses a transport rate given by the arbitrary choice of one vertical discrete grid space per discrete time step. The second method uses a given vertical fluid migration velocity combined with the local solid velocity vector, and the third method uses a buoyancy-driven Darcy velocity, again combined with local solid velocity.

After comparing the model outcomes using these three numerical parametrizations, the authors conclude that both the model evolutions and their final states do not show significant differences for the three methods tested. From this observation they draw the conclusion that the specifics of the numerical implementation of water transport in large-scale simulations are "not that important" (p. 1791, l. 27), and that even the arbitrary choices made for the first of the three methods should be "equally fine" (p. 1792, l. 4).

I see some substantial issues with both content and presentation of this research in the current form. Nevertheless, I would recommend this manuscript to be published subject to a number of revisions and technical corrections as listed below.

(1) The authors give the misleading impression of presenting a comprehensive overview over various numerical implementations of water migration coupled to de/hydration processes in subduction zone models. What the authors in fact do is comparing three very similar and rather basic parametrizations of water transport, none of which is a numerical implementation of the actual physics involved in fluid transport through a deforming solid matrix. The fundamental physics of this problem

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set are those described as thermo-chemically coupled reactive two-phase flow (i.e. conservation of mass, momentum, energy and composition). Of course, to compare parametrizations such as the ones employed here to a numerical implementation of fully coupled two-phase flow would go beyond the scope of the present study. Nevertheless, all the discussion of the presented research should be clearly put into that physical context throughout the manuscript, and necessary qualifications should be added.

(2) Based on two-phase physics, there are a number of scaling relationships, such as characteristic velocity of fluid percolation, characteristic length scales (compaction length), characteristic over-pressures produced by fluid flow, etc. To take some of these scalings into account both in justifying the model simplifications leading to the choice of parametrizations of fluid transport, as well as in a more quantitative discussion of the results, would greatly benefit this study.

(3) The chosen particle-wise treatment of distributing water content along the migration path raises the issue of mass conservation. The basic unit of discretization in finite element models is the finite element. Marker particles should only be used to track the advection of material properties along the material flow, but these particles are not themselves a consistent unit of spatial discretization, meaning that a particle does not have a defined volume or mass in such a numerical method. To treat hydration processes as particle-wise operation renders the whole treatment susceptible to particle density and thus violates conservation of mass. The issue is further complicated by the insertion/deletion scheme employed to maintaining a more uniform particle per element count. The particle-wise procedure constitutes a fundamental weakness of the water migration schemes presented in this study, which needs to be addressed. As a basis of this discussion, the authors should state a conservation equation of water content and then discuss which simplifications lead to the particular implementation and how they may be justified.

(4) In the light of the issues raised in the first comments, I would encourage the authors

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to add some strong qualifications to their conclusions. Given that the only difference between the three parametrizations is the different fluid velocity vector applied to the method, the fact that the final outcome of the results is similar is not of great surprise. This observation, however, does not in itself give rise to any conclusions about the general validity of this type of parametrization for large-scale geodynamic models. I would also argue that the use of something as arbitrary as the first of the three methods should not be condoned with the term "equally fine". Rather I would recommend the authors to deal with the question, why the final result of all three methods come to look similar at all to the first method with its frankly odd choice of one grid cell per time step for defining a fluid transport rate.

(5) Style of language and clarity of presentation: Although the language use is generally good, the chosen register is perhaps a bit too informal at times. Most notably the frequent use of "our" relating to various parts of the research or to individual model properties perhaps sets a slightly too personal tone. Also, there are a number of sections in the text, particularly during the presentation and discussion of results, that could profit from a reorganization of the content to create a more clearly laid out logic pathway for the reader to follow (see specific comments below).

(6) Use of figures: The general quality of figures supplied along with the text is good. However, it would be generally helpful if the authors gave a short introduction to the contents of a figure when they first refer to it. Unfortunately, that is not the case in the present manuscript. The authors are strongly encouraged to add such descriptions to the text, especially throughout the results and discussion sections.

Specific comments

A list of specific comments is given below, commenting on some more specific issues.

p. 1771

Title: Given the limited spectrum of numerical parametrizations tested in this study, I

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suggest the title to be adapted to be more narrow in focus. For example: "Testing the effect of three numerical parametrizations of water migration on models of subduction dynamics."

p. 1773

Introduction: As mentioned in the general comments, some discussion of the following points should be added to the introduction: (i) Water migration is governed by two-phase flow, for which a full physical theory is available; (ii) some reasons why numerical implementation of the fully coupled two-phase physics is challenging, especially in large-scale geodynamic simulations; (iii) some justification for the choice of the three kinds of parametrized implementation of water migration to be tested; (iv) limits of the scope of this comparative study imposed by the methodological similarity of the three chosen methods.

l. 15ff: The two kinds of free water listed here seem to refer to the same thing, which is a free aqueous fluids present in, and percolating through the pore space. In two-phase physics, the porosity is traditionally understood as the volume fraction of the continuum occupied by a fluid phase inside a solid matrix, and in a granular matrix that would be naturally be the space along the grain boundaries. Please clarify your statement.

l. 20ff: This logic is difficult to follow. One of the known processes of bringing water down into the oceanic crust is the extensional stress state along the top boundary of the bending subducting plate. These bending stresses seems to be large close to the trench, so it would rather seem that these conditions would lead to decompaction bringing more free water into the oceanic crust, rather than expelling it through compaction? I suggest checking the physical argument and reformulating this section for clarity.

p. 1774

l. 9-10: This sentence suggests that water released from dehydration of the slab forms

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cold plumes, which is not the case. Rather, such cold plumes consist of mantle material hydrated by water released from the slab, thus creating weak and positively buoyant batches of mantle that may rise as cold diapirs. Please reformulate for clarity.

l. 14-15: This comment on subduction initiation seems out of context here, because water that potentially contributes to subduction initiation must be derived from a different source than the subduction fluids that are the subject of this study. I suggest to omit this statement.

l. 29: "However, exactly how water migrates in the lithosphere and the mantle is not well constrained." I disagree with this statement. The physics of this process is sufficiently well described by the two-phase flow conservation equations. It is true, however, that these physics have not yet been used to full effect in numerical simulations of subduction zone dynamics. Please correct the statement.

p. 1775

l. 2-3: See comment above (p. 1775, l. 15ff). The two types of fluid transport seem to refer to the same concept. Please reformulate for clarity.

l. 7-10: This sentence is not quite clear. The authors refer to the effect of advection of both free and bound water with the deformation field of the solid rock phase. Please clarify the statement.

l. 22-26: Both in your study as well as in the one quoted from Cagnioncle et al. (2007), Darcy flux is calculated purely from the buoyancy contrast between fluid and solid phase, and not from the actual pressure gradient. Please reformulate accordingly. Also, when referring to the influence of solid material flow on fluid migration, please use the terminology of advection along the solid flow field.

l. 13-26: As the three approaches to parametrized water migration are in fact the same as the three implementations the authors later test, it would be useful to assign some sort of identifier to each type (types A, B, C or I, II, III, or similar), which the authors then

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consistently use throughout the manuscript to refer to these types of implementation. It would greatly improve the clarity of the following presentation and discussion of model results.

l. 27 to p. 1776, l. 3: This passage is not stated clearly enough. What exactly is meant by the first sentence? The third sentence should more clearly point out that no previous study has compared the outcome of more than one of these parametrizations in comparison.

p. 1776

l. 4: Be more specific about the method of investigation, which is to take the three types of melt migration schemes introduced above and compare the outcomes of these three schemes for the two model types, sinking sphere and subduction zone.

l. 13: "slow flow" is a slightly unusual expression in this context. Please use "Stokes flow" instead, which is the traditional terminology used for this set of equations.

p. 1777:

l. 4: This quantity $\dot{\epsilon}'_e$ is in fact the second invariant of the deviatoric strain rate tensor and should be labelled as such for clarity. Accordingly, I would recommend to use the symbol $\dot{\epsilon}'_{II}$ or perhaps $\dot{\epsilon}'_2$ instead. Please propagate this terminology throughout the manuscript.

l. 11: "...only bound water influences the viscosity...". This is an odd choice. The presence of any fluid phase, be it water or melt, certainly weakens the solid matrix significantly, as the authors state elsewhere. This choice needs some justification, or else models should be rerun with free water weakening added to the method.

l. 16: The need of a minimum viscosity condition as well as the value of $10^{18} Pa s$ needs some more discussion. Why is it necessary, and why is this specific value chosen? How would a different (lower) value potentially influence the model outcome?

C896

l. 17-18: This restriction of C_{OH} to 4000 ppm is not clear enough. Does this only relate to the effect of water content on viscosity or is water content limited generally? Why is this cutoff necessary to the modelling approach?

l. 21ff, Eq. (6): As commented on above in the context of strain rates, I strongly suggest to consistently use the terminology of second invariants, especially in the case of shear stresses. The terminology of effective stress usually refers to the effective stress principle after Terzaghi (1923) or Skempton (1960), which is an entirely different matter. Therefore, I again suggest to use a symbol of the type σ'_{II} or σ'_2 , rather than σ'_e . Another useful way of referring to second invariants of stress or strain rate tensors is in terms of magnitudes, as their physical meaning is the magnitude of a tensorial quantity apart from their directionality.

l. 23: For the strain-weakening of the friction angle, do the authors use the full accumulated strain or only the component caused by plastic failure? I believe the latter option is more frequently used and makes more sense physically. Please clarify.

p. 1778:

l. 12-13: Please give some more information on the particle advection scheme. Presumably all material properties are defined on markers and these markers are then advected along with the solid flow field? As this is an important feature of the modelling approach it necessary to elaborate some more.

p. 1779

l. 10-12: First, what exactly is meant by the term "maximum water content"? Is it the maximum allowed by your method in the sense of a cutoff value, or is it the physical saturation level? If it is the latter, I think saturation water content is the better terminology. Second, the limit of maximum water content to 0.2 wt% is not clear. Why is any such imposed limit needed?

l. 13: To mention the conversion rate between wt% and ppm seems to be stating

C897

the obvious, so the sentence could be removed. However, the question arises, why the authors don't use one consistent unit for water content throughout the manuscript instead. I would suggest doing so to avoid confusion.

l. 15-16: Omit "In our models", as the advection of bound water content by material flow is a feature of the fundamental physics, not of the model. Please also explain what is meant by "material identifier". If I understand correctly, the bound water content is stored on marker particles and thus advected along with the flow field of the rock. Please clarify this passage.

l. 17-18: Perhaps "element-wise vertical transport" would be a better description for the first type of migration scheme.

l. 19ff: Again, does maximum allowed water content mean saturation water content at given PT conditions? If I understand the procedure correctly, what happens in step (2) is not so much the moving of free water, but the determining of the migration path, along which in step (3) the free water is distributed. Please clarify the three steps.

l. 21ff: It would be helpful to the reader, if in the following detailed explanation of the procedures involved in the three migration schemes would be rearranged such that they reflect the order of the three steps of procedure introduced above. That would give an improved logic sequence to the following text: (1) description of how saturation water contents are calculated for each particle; (2) description of how free water migration pathways are determined for each of the three migration scheme; (3) description of how free water is distributed along the migration path to hydrate material where possible, and how any left-over free water is treated.

p. 1780

l. 6-10: This passage is not written clearly enough. Additionally, the point that irregular grid spacing should be avoided in order to keep a constant water migration velocity is nonsensical. Rather, a water transport velocity linked to the grid spacing should be

C898

avoided, as it is a purely arbitrary, non-physical choice that renders any model outcome grid-dependent, which generally is not a favourable condition.

l. 16-17: "...does not necessarily eliminate it totally". This statement is not entirely correct. The change from element-wise vertical transport to an imposed vertical transport velocity removes the grid-dependence of the velocity, but does not remove the grid-dependence of the hydrated migration pathway, which in very high spatial resolution would be close to a straight line, whereas in coarser resolutions, the "staircase" character of the hydration path is much more pronounced. Please clarify the statement.

p. 1781

l. 4: "...pressures are mainly lithostatic". Especially in the mantle wedge dynamic pressures are certainly not negligible. Even in the simplest possible model setup, the corner flow forced by the subducting slab leads to substantial dynamic pressure variation in the mantle wedge, especially close to the corner. I do not quite understand why the authors chose not to use the full pressure solution to determine the Darcy velocity, as it would be straight-forward to do so. I suggest to state Darcy's law in it's full form in the text before making the assumption of lithostatic pressure.

Eq. (8): Traditionally, the symbol v_f is used to refer to fluid velocity, which may be expressed as a combination of the solid velocity v_s and the Darcy velocity q as $v_f = v_s + q/\phi$. This is found from rearranging the definition of Darcy velocity, which is $q = \phi(v_f - v_s)$. Would the authors please clarify their notation and add an equation of how they combine their Darcy velocity with the solid flow field to obtain the water migration pathway. Also, it would benefit the clarity to separate the definition of permeability out of Eq. (8), so that it becomes $q = \omega \frac{k_\phi}{\eta_f} \Delta \rho g$, which is more in tune with traditional notation of Darcy's law. The permeability then becomes $k_\phi = \frac{d^2 \phi^2}{270}$. Please also supply a reference for your choice of a geometrical factor of 270.

l. 12-14: The question of how much of the water is present in interconnected pore

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space is certainly not straight forward to quantify. However, it is well known that fluids can form interconnected pore networks already at very small volume fractions of below 1%. It seems that the main function of the introduced factor ω is to impose a variation on permeability, thus reducing or increasing the speed of water migration. Please clarify the use of ω .

I. 19-20: The last sentence of this paragraph should be reformulated in the context of the fluid velocity defined by the statement $v_f = v_s + q/\phi$, as it follows from standard two-phase flow theory. Darcy's law defines a relative flux q of fluid material with respect to solid material flow v_s . Please reformulate and clarify.

I. 21ff: I have some concerns about the criteria by which the authors mean to quantify the model results. First, it certainly makes sense to track the topmost extent of the hydrated zone, however the information gained from it does not quantify an "effective water migration velocity", but rather the rate of advancement of the hydration front. These two concepts are not the same. Second, these criteria only quantify the vertical extent of the hydrated zone, but not its structure or its geometry. The author seem to not take quantitative account of such factors. Third, the quantity a root-mean-square water content is not entirely clear. How is it calculated? Why do the authors not use a more physical quantity like the total water mass or volume integrated over those parts of the domain?

p. 1782

I. 7: Please choose a different name for this type of model setup. "Stokes model" is a term often used for any flow model described by Stokes equations. Perhaps "sinking sphere model" would be an alternative option. Please propagate this change to all following passages, where this model type is referred to.

I. 13: What do the authors mean by "...do not couple the thermal and mechanical aspects of the models."? As temperature advection is taken into account, there already is a coupling between thermal and mechanical aspects of the model. Do the authors

C900

mean to say, that no T-dependent viscosity is employed here?

p. 1783:

I. 10: The values chosen for the vertical migration velocity should be based on some scaling argument derived from two-phase physics. Please elaborate your choice.

p. 1784

I. 4: From the context I assume that the symbol OH_{rms} refers to the quantity of root-mean-square water content. I could, however, not find any passage in the manuscript where the symbol is defined. Please check and correct if necessary.

p. 1785

I. 15-17: The meaning of this sentence is not clear to me. Please reformulate the idea.

I. 27 to p. 1786, I. 1: The meaning of this sentence is not entirely clear. Please reformulate your conclusion.

p. 1788

I. 4-6: This short discussion of vertical grid size variation illuminates the fundamental flaw of the element-wise vertical water migration scheme. Since the authors decide to use the scheme despite its obvious flaw for the sake of comparison, the inherent grid-dependence of the scheme should be pointed out clearly as a reason not to use it in future studies.

I. 8-13: The authors run the first and third scheme with and without water-weakened rheology, but not the second. This choice is not obvious, please explain.

I. 16: Is this really "trench migration" if it occurs at the beginning of the run, before stress accumulation leads to brittle failure? Maybe I did not understand the description correctly, please reformulate for clarity.

p. 1789

C901

In general the description of results is rather vague and too phenomenological ("migration schemes cause small differences", "effects...are more substantial", "distribution...is similar", "Larger variations occur..."). Please reformulate with better structuring and more quantitative analysis of results. Introduce each figure before referring to results displayed in it.

p. 1790

2nd paragraph: This whole paragraph is too vague and not very clear. Also, consider if a longer simulation run time might give more room for water-weakened rheology to show greater effect, especially as water starts penetrating the overriding plate. Also, one of the main influences of free water is to facilitate melting, which has a significant influence on the dynamics of subduction. Furthermore, a water-weakened rheology may lead to cold diapirism, which again influences the dynamics and the overall water transport in the subduction zone (why do these models not develop cold diapirs?). Please restructure your argument for clarity and include some more factors, perhaps along with some scaling arguments to underline your findings.

l. 19-20: "free water does not affect the rheology of the mantle materials". However, it certainly does in reality, so the question remains why the authors did not choose to include the rheological weakening by free water, especially as it constitutes a fairly straight-forward addition to any numerical method.

l. 20: "speculate". I suggest making an informed statement in place of speculation.

l. 26: "This would then decrease the potential effects of free water on pore pressures". Yes, but melt would then build up pore pressure instead of the free water it has dissolved, so the potential weakening effect would remain.

p. 1791

l. 20-22: The logic of the last sentence in this paragraph is not quite obvious. How does a stronger corner flow due to water-weakened rheology lead to more hydrated mate-

C902

rial being entrained downwards by the slab? It would be more obvious, if the water-weakening would lead to stronger mechanical decoupling between slab and mantle wedge and thus less entrainment of hydrated mantle? Please elaborate.

l. 24: "Stokes flow model". As mentioned above, the term Stokes flow is traditionally used for any flow problem described by Stokes equations. Please use another identifier for your first series of model runs, such as "sinking sphere models" or similar.

Technical corrections

A number of technical corrections are listed below, mainly relating to form and language of the manuscript.

Title: In order to be a bit more specific about the content, I suggest to adapt the title to: "Testing three numerical implementations of water migration in models of subduction dynamics".

p. 1772

l. 1. Add definite article: "...brings water into [the] Earth's upper mantle."

l. 5. Add definite article: "localisation of deformation in [the] lithosphere and mantle."

l. 8. Be more specific: "Therefore, [computational] models use..."

l. 15. "...the material flow field also moves the free water..." By material flow field, I assume you refer to the flow of the solid rock phase? Please clarify the statement.

l. 22. Consider changing expression to: "Our models [demonstrate that] the bound water..."

l. 25. Add coma: "in the mantle wedge[,] which..."

l. 26. Consider reformulating as: "[This finding underlines the importance of employing] dynamic time evolution models..."

C903

p. 1773

l. 14: Add "[oceanic] crust" to be more specific of the context.

l. 18: Set expression to plural form: "mineralogically bound fluids in the form of [hydroxyl complexes]."

l. 24: Consider reformulating the sentence for better clarity: "It has been well documented that mineralogically bound water is released when [hydrated minerals undergo certain phase transitions]"

p. 1774

l. 1: Correct spelling: "... even [greater] depths."

l. 21: Change expression: "...the subduction slab [may in turn] increase ..."

p. 1775

l. 2: Change terminology to "interconnected [pore space]"

p. 1776

l. 3-4: Reformulate to avoid close repetition of "investigate".

p. 1780

l. Correct spelling: "the [remaining] water".

p. 1784

l. 25: Correct spelling: "can locally [increase]".

p. 1786

l. 16: Change expression to: "(1) a 7 [and] 8 km crustal layer..., respectively."

p. 1787

C904

l. 6: Reverse order of words: "16 particles per element are [used initially]".

p. 1788

l. 20: Change expression: "...but not [significantly]".

p. 1790

l. Change expression: "...free water could reduce [the] plastic yield stress, [thereby] reducing ..."

p. 1791

l. 13-15: Reformulate to avoid close repetition of sentences starting with "this".

Interactive comment on Solid Earth Discuss., 5, 1771, 2013.

C905