

Improved phase-field models of melting and dissolution in multi-component flows

Eric W. Hester, Louis-Alexandre Couston, Benjamin Favier, Keaton J. Burns and Geoffrey M. Vasil

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Revised submission: 18 September 2020
Final acceptance: 23 September 2020

Note: Reports are unedited and appear as submitted by the referee. The review history appears in chronological order.

Review History

RSPA-2020-0508.R0 (Original submission)

Review form: Referee 1

Is the manuscript an original and important contribution to its field?

Good

Is the paper of sufficient general interest?

Good

Is the overall quality of the paper suitable?

Good

Can the paper be shortened without overall detriment to the main message?

Yes

Do you think some of the material would be more appropriate as an electronic appendix?

No

Do you have any ethical concerns with this paper?

No

Recommendation?

Accept with minor revision (please list in comments)

Comments to the Author(s)

In this paper, Authors present an extension of the phase field approach to investigate on melting and dissolution at interfaces.

The paper is well written and well presented and pushes forward the application of the phase field method.

I am personally interested in expanding the possibilities of the Phase Field method, which should sometimes be referred to as interface capturing methods.

I have just few minor comments.

Authors refer to the thickness of the interface as epsilon. In literature, the dimensionless thickness of the interface is usually called the Cahn number (the ratio of the thickness to the system macroscopic scale).

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G.Soligo, A. Roccon, and A. Soldati, (2019) Breakage, coalescence and size distribution of surfactant-laden droplets in turbulent flow *J. Fluid Mech.*, 881, 244–282 F. Magaletti, F. Picano, M. Chinappi, L., Marino, and CM. Casciola, C. M. (2013) The sharp-interface limit of the Cahn–Hilliard/Navier–Stokes model for binary fluids. *J. Fluid Mech.* 714, 95–126.

There are not many instances in which spectral methods are used in connection with Phase Field approaches. This because tackling the space dependent behavior of fluid properties requires specific attention.

Authors could perhaps be interested in discussing Dedalus a bit better, although the code is fully described in the references.

G.Soligo, A. Roccon, and A. Soldati, (2019) Coalescence of surfactant-laden drops by Phase Field Method, *J. Comp. Physics*, 376, 1292–1311

Review form: Referee 2**Is the manuscript an original and important contribution to its field?**

Excellent

Is the paper of sufficient general interest?

Good

Is the overall quality of the paper suitable?

Excellent

Can the paper be shortened without overall detriment to the main message?

Yes

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I have one question. In general, physical meaning of the phase-field model is guaranteed by the variational formulation from Ginzburg-Landau type free energy. On the other hand, equation (2.4) in this study is given in the heuristic manner on behalf of variational formulation. It is not clear for me how the mathematical strictness guaranties the physical rigor. I would be grateful if the authors could comment on this point.

Decision letter (RSPA-2020-0508.R0)

17-Sep-2020

Dear Mr Hester,

On behalf of the Editor, I am pleased to inform you that your Manuscript RSPA-2020-0508 entitled "Improved phase-field models of melting and dissolution in multi-component flows" has been accepted for publication subject to minor revisions in Proceedings A. Please find the referees' comments below.

The reviewer(s) have recommended publication, but also suggest some minor revisions to your manuscript. Therefore, I invite you to respond to the reviewer(s)' comments and revise your manuscript. Please note that we have a strict upper limit of 28 pages for each paper. Please endeavour to incorporate any revisions while keeping the paper within journal limits. Please note that page charges are made on all papers longer than 20 pages. If you cannot pay these charges you must reduce your paper to 20 pages before submitting your revision. Your paper has been ESTIMATED to be 21 pages. We cannot proceed with typesetting your paper without your agreement to meet page charges in full should the paper exceed 20 pages when typeset. If you have any questions, please do get in touch.

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- Funding statement

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*Ensure that you include valid contact details for the lead author (institutional address, email address, telephone number).

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Once again, thank you for submitting your manuscript to Proceedings A and I look forward to receiving your revision. If you have any questions at all, please do not hesitate to get in touch.

Best wishes
Raminder Shergill
proceedingsa@royalsociety.org
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Dr Bruno Welfert
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Reviewer(s)' Comments to Author:

Referee: 1

Comments to the Author(s)

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Referee: 2

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Author's Response to Decision Letter for (RSPA-2020-0508.R0)

See Appendix A.

Decision letter (RSPA-2020-0508.R1)

23-Sep-2020

Dear Mr Hester

I am pleased to inform you that your manuscript entitled "Improved phase-field models of melting and dissolution in multi-component flows" has been accepted in its final form for publication in *Proceedings A*.

Our Production Office will be in contact with you in due course. You can expect to receive a proof of your article soon. Please contact the office to let us know if you are likely to be away from e-mail in the near future. If you do not notify us and comments are not received within 5 days of sending the proof, we may publish the paper as it stands.

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On behalf of the Editor of Proceedings A, we look forward to your continued contributions to the Journal.

Sincerely,
Raminder Shergill
proceedingsa@royalsociety.org

Appendix A

Response to Referees

Referee 1 comments

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Response to Referee 1

We thank the referee for their comments. We have added references to the Cahn number in equation 1.1, as well as to the papers suggested. We have also expanded on the numerical methods underlying Dedalus at the start of section 4.

Referee 2 comments

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Response to Referee 2

We thank the referee for their comments. We have added a small discussion of this point at the end of section 2, after introducing the phase-field equations. To summarise our addition: Phase-field models can be derived via variational formalisms, some of which we cite in our fourth bullet point in the introduction (references 34 to 38). However a variational derivation is not required. We emphasise the view of reference 31 (Beckermann et al. 1999), which states “phase-field equations are only quantitatively meaningful in the sharp-interface limit where they can be ultimately related to experiment”. It is our asymptotic derivation, combined with validation in quantitative numerical experiments, that demonstrates the physical accuracy of our model. We hope this clarifies the referees question.