[ChemEngineering] Manuscript ID: ChemEngineering-755598 - Submission Received

From:Editorial Office (chemengineering@mdpi.com)
To:halimits@yahoo.com
Cc:iwanh@petra.ac.id; a.alexiadis@bham.ac.uk; m.j.adams@bham.ac.uk
Date:Tuesday, March 10, 2020 at 05:08 PM GMT+7

Dear Dr. Sahputra,

Thank you very much for uploading the following manuscript to the MDPI submission system. One of our editors will be in touch with you soon.

Journal name: ChemEngineering
Manuscript ID: ChemEngineering-755598
Type of manuscript: Article
Title: A coarse grained model for viscoelastic solids in Discrete Multiphysics simulations
Authors: Iwan Sahputra *, Alessio Alexiadis, Michael Adams
Received: 10 March 2020
E-mails: iwanh@petra.ac.id, a.alexiadis@bham.ac.uk, m.j.adams@bham.ac.uk
Discrete Multiphysics: Modelling Complex Systems with Particle Methods
https://www.mdpi.com/journal/ChemEngineering/special_issues/Particle_Methods

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will provide email addresses for all authors and an institutional e-mail address for at least one of the co-authors, and specify the name, address and e-mail for invoicing purposes.

If you have any questions, please do not hesitate to contact the ChemEngineering editorial office at chemengineering@mdpi.com

Kind regards,

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[ChemEngineering] Manuscript ID: ChemEngineering-755598 - Major Revisions

From:Gaetan Tang (gaetan.tang@mdpi.com)
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Cc:iwanh@petra.ac.id; a.alexiadis@bham.ac.uk; m.j.adams@bham.ac.uk; chemengineering@mdpi.com
Date:Monday, April 6, 2020 at 08:40 PM GMT+7

Dear Dr. Sahputra,

Thank you for submitting the following manuscript to ChemEngineering:

Manuscript ID: ChemEngineering-755598
Type of manuscript: Article
Title: A coarse grained model for viscoelastic solids in Discrete Multiphysics simulations
Authors: Iwan Sahputra *, Alessio Alexiadis, Michael Adams
Received: 10 March 2020
E-mails: iwanh@petra.ac.id, a.alexiadis@bham.ac.uk, m.j.adams@bham.ac.uk
Discrete Multiphysics: Modelling Complex Systems with Particle Methods
https://www.mdpi.com/journal/ChemEngineering/special_issues/Particle_Methods

It has been reviewed by experts in the field and we request that you make major revisions before it is processed further. Please find your manuscript and the review reports at the following link:
https://susy.mdpi.com/user/manuscripts/resubmit/56b90ce677788844b175f722b44f0455

Your co-authors can also view this link if they have an account in our submission system using the e-mail address in this message.

Please revise the manuscript according to the reviewers' comments and upload the revised file within 10 days. Use the version of your manuscript found at the above link for your revisions, as the editorial office may have made formatting changes to your original submission. Any revisions should be clearly highlighted, so that changes are easily visible to the editors and reviewers. Please provide a cover letter to explain point-by-point the details of the revisions in the manuscript and your responses to the reviewers' comments. Please include in your rebuttal if you found it impossible to address certain comments. The revised version will be inspected by the editors and reviewers. Please detail the revisions that have been made, citing the line number and exact change, so that the editor can check the changes expeditiously. Simple statements like ‘done’ or ‘revised as requested’ will not be accepted unless the change is simply a typographical error.

Please carefully read the guidelines outlined in the 'Instructions for Authors' on the journal website https://www.mdpi.com/journal/ChemEngineering/instructions and ensure that your manuscript resubmission adheres to these guidelines. In particular, please ensure that abbreviations have been defined in parentheses the first time they appear in the abstract, main text, and in figure or table captions; citations within the text are in the correct format; references at the end of the text are in the correct format; figures and/or tables are placed at appropriate positions within the text and are of suitable quality; tables are prepared in MS Word table format, not as images; and permission has been obtained and there are no copyright issues.

If the reviewers have suggested that your manuscript should undergo extensive English editing, please address this during revision. We suggest that you

have your manuscript checked by a native English speaking colleague or use a professional English editing service. Alternatively, MDPI provides an English editing service checking grammar, spelling, punctuation and some improvement of style where necessary for an additional charge (extensive re-writing is not included), see details at https://www.mdpi.com/authors/english.

Do not hesitate to contact us if you have any questions regarding the revision of your manuscript or if you need more time. We look forward to hearing from you soon.

Kind regards,
Mr. Gaetan Tang
Assistant Editor
E-Mail: gaetan.tang@mdpi.com
The First World Energies Forum - Current and Future Energy Issues
14-16 Sept 2020, Rome, Italy
https://wef.sciforum.net/

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E-Mail: ChemEngineering@mdpi.com
http://www.mdpi.com/journal/ChemEngineering/

[ChemEngineering] Manuscript ID: ChemEngineering-755598 - Accepted for Publication

From:Gaetan Tang (gaetan.tang@mdpi.com)
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Date:Saturday, April 25, 2020 at 05:22 AM GMT+7

Dear Dr. Sahputra,

We are pleased to inform you that the following paper has been officially accepted for publication:

Manuscript ID: ChemEngineering-755598
Type of manuscript: Article
Title: A coarse grained model for viscoelastic solids in Discrete Multiphysics simulations
Authors: Iwan Sahputra *, Alessio Alexiadis, Michael Adams
Received: 10 March 2020
E-mails: iwanh@petra.ac.id, a.alexiadis@bham.ac.uk, m.j.adams@bham.ac.uk
Discrete Multiphysics: Modelling Complex Systems with Particle Methods
https://www.mdpi.com/journal/ChemEngineering/special_issues/Particle_Methods
https://susy.mdpi.com/user/manuscripts/review_info/56b90ce677788844b175f722b44f0455

We will now make the final preparations for publication, then return the manuscript to you for your approval.

If, however, extensive English edits are required to your manuscript, we will need to return the paper requesting improvements throughout.

We encourage you to set up your profile at SciProfiles.com, MDPI's researcher network platform. Articles you publish with MDPI will be linked to your SciProfiles page, where colleagues and peers will be able to see all of your publications, citations, as well as your other academic contributions.

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Kind regards,
Mr. Gaetan Tang
Assistant Editor
E-Mail: gaetan.tang@mdpi.com
The First World Energies Forum - Current and Future Energy Issues
14-16 Sept 2020, Rome, Italy
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E-Mail: ChemEngineering@mdpi.com
http://www.mdpi.com/journal/ChemEngineering/

Journal ChemEngineering (ISSN 2305-7084)
Manuscript ID ChemEngineering-755598
Type Article
Title A Coarse Grained Model for Viscoelastic Solids in Discrete Multiphysics Simulations
Authors Iwan H. Sahputra * , Alessio Alexiadis , Michael J. Adams
Special Issue Discrete Multiphysics: Modelling Complex Systems with Particle Methods
Abstract Viscoelastic bonds intended for Discrete Multiphysics (DMP) models are developed to allow the study of viscoelastic particles with arbitrary shape and mechanical inhomogeneity that are relevant to the pharmaceutical sector and which has not been addressed by the Discrete Element Method (DEM). The model is applied to encapsulate particles with a soft outer shell due, for example, by the partial ingress of moisture. It was validated by simulation of spherical homogeneous linear elastic and viscoelastic particles. The method is based on forming a particle from an assembly of beads connected by springs or springs and dashpots that allow the sub-surface stress fields to be computed, and hence an accurate description of the gross deformation. It is computationally more expensive than DEM but could be used to define effective interaction laws.

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Authors' Responses to Reviewer's Comments (Reviewer 1)

Author's Notes Please see the attachment

Author's Notes File Report Notes

Review Report Form

English language and style
( ) English very difficult to understand/incomprehensible
( ) Extensive editing of English language and style required
( ) Moderate English changes required
(x) English language and style are fine/minor spell check required
( ) I don't feel qualified to judge about the English language and style

	Yes	Can be improved	Must be improved	Not applicable
Does the introduction provide sufficient background and include all relevant references?	( )	(x)	( )	( )
Is the research design appropriate?	(x)	( )	( )	( )
Are the methods adequately described?	( )	(x)	( )	( )
Are the results clearly presented?	( )	(x)	( )	( )
Are the conclusions supported by the results?	(x)	( )	( )	( )

Comments and Suggestions for Authors

The current study presents a Discrete Multiphysics model to study deformation of viscoelastic particles. The authors applied the model to elastic and viscoelastic spherical particles under diametrical loading. Then, the model is applied to an inhomogeneous system by considering spherical particles composed of core and shell regions with different properties.

In my view, the paper is well-written. With appropriate consideration to the suggested comments, as well as other reviewers' comments, I find this paper appropriate for publication in *ChemEngineering* journal.

In line 237: it is mentioned that two parallel solid planes were used for diametric compression. I would recommend showing the planes in Fig. 5.

What are the boundary conditions in the simulations?

What is the criteria of simulation stability? What was the criteria to apply time step of

1e-11. Time step is a very critical parameter in particle based models.

Please explain how shear stress in Fig. 7 is calculated and add it to the manuscript.

Please explain why the disorder model is computationally more efficient than the cubic model?

In my view, the introduction should be more enriched by comparing the present work with other existing models in the literature, such as:

Computer simulation of the effect of deformation on the morphology and flow properties of porous media

peer-review-6790344.v1.pdf

Submission Date 10 March 2020

Date of this review 29 Mar 2020 21:01:37

Journal ChemEngineering (ISSN 2305-7084)
Manuscript ID ChemEngineering-755598
Type Article

Title A Coarse Grained Model for Viscoelastic Solids in Discrete Multiphysics Simulations

Authors Iwan H. Sahputra * , Alessio Alexiadis , Michael J. Adams

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Authors' Responses to Reviewer's Comments (Reviewer 2)

Author's Notes Please see the attachment

Author's Notes File Report Notes

Review Report Form

English language and style
( ) English very difficult to understand/incomprehensible
( ) Extensive editing of English language and style required
( ) Moderate English changes required
(x) English language and style are fine/minor spell check required
( ) I don't feel qualified to judge about the English language and style

	Yes	Can be improved	Must be improved	Not applicable
Does the introduction provide sufficient background and include all relevant references?	(x)	( )	( )	( )
Is the research design appropriate?	( )	(x)	( )	( )
Are the methods adequately described?	(x)	( )	( )	( )
Are the results clearly presented?	( )	(x)	( )	( )
Are the conclusions supported by the results?	( )	(x)	( )	( )

Comments and Suggestions for Authors

The article „A coarse grained model for viscoelastic solids in Discrete Multiphysics simulations“ by Iwan H. Sahputra, Alessio Alexiadis, and Michael J. Adams reports on the implementation of viscoelastic bonds for Discrete Multiphysics (DMP) models. Deformation of particles including sub-surface stress can be modeled in the LSM framework for elastic and viscoelastic particles, if linear springs are substituted with Kelvin-Voigt (KV) bonds. The manuscript is well organized and written in a clear way. The authors present first a simple validation case of the KV bond and extend their study to a perfectly elastic spherical particle, a viscoelastic spherical particle, and finally to a hard-core-soft-shell and soft-core-hard-shell sphere under compression. This fundamental work is of interest to the modeling and simulation community in several different engineering fields. However, this manuscript could be improved by considering the following comments:

Major comments

Several times, you mention computational cost efficiency being a factor pro DEM. However, there are no hints or comparisons or numbers concerning computational costs. This is especially interesting for judging on the performance of the cubic lattice model and the disorder model. Please, include an appropriate discussion.

In the conclusion section, you mention that this method can be easily transferred to more complex particle shape. I, and probably future readers, would love to see that. Please, run and show such simulations for at least one non-spherical geometry, like a ring, cylinder, or cone. This would make your manuscript really strong.

Please, include a discussion about the spatial discretization. In other words, how to judge on the number of isotropic or irregularly ordered beads? I guess, something like a “mesh” study should be presented. Did you carry out such studies?

Minor comments

Please, add a nomenclature for completeness including all symbols and abbreviations used.

Fig. 7: top and bottom center position. The shear stress at the two top/bottom positions seems a bit odd to me. Can you explain the contours more thoroughly?

There might be a typo in the 3.3 title.

A visualization of the shell-thickness-to-radius-ratio would be beneficial.

In the abstract, you mention: “The model is applied to encapsulate particles with a soft outer shell due, for example, by the partial ingress of moisture.” Can you elaborate a little bit more on how to model such an encapsulated particle with emphasis on the model parameters and shell thicknesses? In a real system, are you able to find all the necessary parameters?

Submission Date 10 March 2020

Date of this review 25 Mar 2020 15:42:05

Journal ChemEngineering (ISSN 2305-7084)
Manuscript ID ChemEngineering-755598
Type Article

Title A Coarse Grained Model for Viscoelastic Solids in Discrete Multiphysics Simulations

Authors Iwan H. Sahputra * , Alessio Alexiadis , Michael J. Adams

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Authors' Responses to Reviewer's Comments (Reviewer 3)

Author's Notes Please see the attachment

Author's Notes File Report Notes

Review Report Form

English language and style
( ) English very difficult to understand/incomprehensible
( ) Extensive editing of English language and style required
( ) Moderate English changes required
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	Yes	Can be improved	Must be improved	Not applicable
Does the introduction provide sufficient background and include all relevant references?	(x)	( )	( )	( )
Is the research design appropriate?	(x)	( )	( )	( )
Are the methods adequately described?	(x)	( )	( )	( )
Are the results clearly presented?	(x)	( )	( )	( )
Are the conclusions supported by the results?	(x)	( )	( )	( )

Comments and Suggestions for Authors revision attached

peer-review-6791465.v2.pdf

Submission Date 10 March 2020

Date of this review 24 Mar 2020 16:28:54

The current study presents a Discrete Multiphysics model to study deformation of viscoelastic particles. The authors applied the model to elastic and viscoelastic spherical particles under diametrical loading. Then, the model is applied to an inhomogeneous system by considering spherical particles composed of core and shell regions with different properties.

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- What is the criteria of simulation stability? What was the criteria to apply time step of 1e-11. Time step is a very critical parameter in particle based models.
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- In my view, the introduction should be more enriched by comparing the present work with other existing models in the literature, such as:
  Computer simulation of the effect of deformation on the morphology and flow properties of porous media

Reviewer's comment on manuscript ChemEngineering-755598

The manuscript entitled "A coarse grained model for viscoelastic solids in Discrete Multiphysics simulations" by I.H. Sahputra, A. Alexiadis and M.J. Adams presents the particle model including multiple bonds for modelling viscoelastic particles with arbitrary shapes and mechanical heterogeneity. The model allows for modelling particles composed of core and shell regions with different mechanical properties, resembling real objects, such as seeds or grains. Two different ways of constructing spheres were presented and analysis of the force-displacement characteristics for these two constructions was done. A good agreement between numerical and theoretical results has shown a high applicability of the proposed approaches to model viscoelastic particles heterogeneous in shape and mechanical properties.

The topic of manuscript is interesting and the problem undertaken is very important. A searching for methods of modelling particles with arbitrary shapes and mechanical heterogeneity in a reasonable period of time is a crucial issue for engineering design process, agriculture, design of food processes and manufacturing *et al.* .

Paper has a high scientific value and it is well organized. Therefore, I recommend the publication of the manuscript on ChemEngineering, provided that Authors consider corrections, as detailed below.

Minor issues:

1. Line 161: Phrase "the red line are calculated" should be changed into "the red line is calculated".
2. Line 185: "displacements ~~are~~ calculated".
3. Line 228: A dot at the end of sentence is missing.
4. Figures 12 and 13: Units "Nm^{-1}" are missing after k(core) = ……, k(shell) = …..
5. Line 450: Symbol δ is missing in the bracket (/2r).
6. Discussion of results presented in figures 12 and 13 is pure. I suggest to extend it.
7. Figures 14 and 15: Title of x axis should be k, not K.
8. Line 496: "fields not only ~~of~~ for elastic particles".