Comment on gmd-2021-224

Anonymous Referee #2

Referee comment on "MagmaFOAM-1.0: a modular framework for the simulation of magmatic systems" by Federico Brogi et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-224-RC2, 2021

The paper by Brogi et al. develops a modular framework, MagmaFOAM, for simulating multiphase, multicomponent flow in magmatic systems based on the open-source software package OpenFOAM. The main addition to OpenFOAM are parametrizations of the magma properties, such as density and viscosity, which depend themselves on pressure, temperature and composition. The authors have designed a modular framework that allows users to select and combine model components. I expect that users in the magma-dynamics community will find this approach helpful given that magmatic properties vary dramatically between systems.

Overall, the study is a valuable contribution to the toolboxes available in magma dynamics and I appreciate that the authors provide multiple benchmark computations for their model. However, I think it is important to more clearly explain what this model "is good at" and where its limits lie, particularly since the goal here seems to be to empower a potentially broad community of users to work with models. Upon taking a closer look at the literature (some referenced below), I think the authors will find that the constitutive models they have integrated are more limiting than it might seem at first. In my opinion, an introduction that critically discusses different model approaches, their merits for understanding magma dynamics problems, but also how they relate to work beyond the magma dynamics community strictly defined would be valuable. I have provided some specific suggestions for relevant papers below.

Major concerns:

As the authors point out in the introduction, MagmaFOAM is a mixture model. There is nothing wrong with that. Mixture models have their place and their importance, but particularly since this is a modeling tool that will hopefully be useful for a diverse community of scientists, not all of which think primarily about models, I think it is important to explain very clearly what both the strengths and the limitations of a mixture approximation are. In the paragraph starting on line 33, the authors motivate mixture models as "convenient". I agree that they are, but surely (hopefully?) that is not the primary metric we want to focus on to guide model development.

I suggest that the reviewers rethink and rewrite the paragraph starting on line 33. Currently, it is a very general overview of different modeling techniques, mostly by describing what problems they have been applied to, but less information is provided about the key strengths and weaknesses of different approaches. I think it would be valuable to add that so that readers can make an informed choice about whether this model is useful for what they are trying to understand.

Specific suggestions:

The discussion of direct numerical simulations in the paragraph starting on line 33 could be improved. As the authors well know, the method originated in turbulence research and I would argue that the main claim of fame of this kind of technique is to capture emergent phenomenon in flow. That can be done in the turbulent context and it can be done in a multiphase context, where the long-range hydrodynamic interactions break the symmetry of the flow. The approach can be combined with an interface tracker (and other things), but the main added value is really to better understand emerging behavior that is difficult to parametrize a-priori.

I think it's misleading to classify Lattice-Boltzmann models (e.g., Huber et al., 2014; Parmigiani et al., 2014) as direct numerical simulations. There is no doubt that Lattice-Boltzmann methods are a valuable approach for mimicking common fluid behavior, particularly in porous media. They are also much less computationally expensive, because they do not solve the Navier-Stokes equation directly and often imply large interface

thicknesses. The method itself is completely different from a direct numerical simulation, though.

The authors seem to suggest that mixture models are particularly valuable for small particles and/or high fluid viscosities. The text in its current form seems to suggest that the size of the crystal/bubble/interface determines whether a mixture approach can be adopted or not, but there are several other considerations and there is strong evidence that a mixture approximation is quite problematic in this limit. Over the last two decades, several studies (Segre et al., An effective gravitational temperature for sedimentation, 2001 would be a good starting point to look deeper into that literature) have shown that the behavior of suspensions is particularly complex at low Reynolds number, because interfaces interact over very long distances, leading to surprising emergent behavior. They have shown that these long-range hydrodynamic interactions lead to behavior reminiscent of turbulence even at zero Reynolds number (e.g., Tong et al., Analogies between colloidal sedimentation and turbulent convection at high Prandtl numbers, 1998 etc.). The consequences on the flow field can be dramatic, particularly in the presence of shear (e.g., Qin and Suckale, Flow-to-Sliding Transition in Crystal-Bearing Magma, JGR 2019).

Minor suggestions:

Line 33: I suggest a figure or illustration to convey how drastic the simplification of a multiphase medium through the interpenetrating continuum idea really is to explain this key point to the readers. There is a rich literature on this type of approach with plenty illustrations that they authors might find inspiring.

Line 47 "average forms of the flow equations can be adopted and the need of tracking the

exact position of the interface is avoided": Many mixture models (including in this paper) do track interfaces. The most famous example is probably the two-fluid model, which the authors might want to reference for context.

Line 49 "The so-called multi-fluid Eulerian approach": I don't really know what the authors are referring to here. To me, "Eulerian" is a reference system that governing equations can be formulated in (as compared to Lagrangian) rather than an approach. I think it would be valuable to separate the two as many other methods in this paragraph are Eulerian to (e.g., our papers that are cited here, e.g. Suckale et al., 2010a).

Line 55-60: I don't understand which approach/set of governing equations the authors are talking about in this segment. The comment about dispersed phase relaxation is rather generic to me as is the general issue about computational cost, which I would argue is always a constraint, one way or another. The degree to which relaxation is an issue or not depends on so many things including discretization etc.? And why bring in the pseudo fluid approach and which one are we talking about here specifically? Neither am I convinced that strong thermo-mechanical coupling is the main issue.

Line 98: I agree that the interplay between pressure, temperature, composition and physical processes is the key challenge in modeling volcanic systems. I suggest being more careful with the statement that constitutive models alone can solve the problem, though. Ultimately, constitutive models can only be as good as the equation that they are plugged into, but we do not currently have a continuum equation that applies over the broad range of conditions that volcanic systems traverse with issues arising both in the suspension limit (see the Segre paper I had mentioned above) and in the mush limit, though progress has been made in the context of the mu(I) rheology (e.g., Midi et al., On dense granular flows, 2004; Henann, D. L. & Kamrin, K. A predictive, size-dependent continuum model for dense granular flows, 2013). Needless to say, these complexities would be further amplified by thermal and geochemical effects. Let me emphasize that I do not object to the usage of the constitutive models themselves as that part is unavoidable in a mixture formulation, but with how this path is presented in the text.

Line 164: I appreciate that the authors call out the strong assumptions behind representing bubbles in melt as a monodisperse periodic array of static spheres, but I do not think that the monodisperse size distribution is necessarily the main crime here. Bubbles are not static, not even when they are so small that they do not move very fast themselves, because of the long-range hydrodynamic interactions connecting them and leading to self-organization, as manifested in bubble waves (e.g., Manga, Waves of bubbles in basaltic magmas and lavas, JGR, 1996). I have no problem with this component being integrated into the model, but I do not think that the claim that it

represents "an accurate representation of the coupled momentum balance and diffusive transport of volatiles" is warranted. Similarly, I'm not convinced that the method produces "accurate results especially at low vesicularity". That is a rather strong statement. I'd be happy to be convinced if similarly strong evidence is provided to back this up.

Line 180: The trick with these interface tracking techniques is of course what to do with the mass enclosed in an interface that drops below the grid resolution. The momentum equation is no longer off help in that case, because flow is not resolved at the subgrid scale. So yes, VOF methods are generally conservative, because they redistribute the subgrid mass, but significant error in the interface position can arise from that approach (I am guessing that is what the authors mean by "numerical blur"). I like the term "numerical blur", but in the interest of enabling users to understand the capabilities of this software as much as possible, I think it's worth not only mentioning it, but actually explaining where it comes from. In addition to the blur aspect, thought, it's also worth keeping in mind that distortions to the interface can build up, leading to seemingly sharp interface features, similar to particle-tracking of interfaces or marker chains, e.g., Van Keken et al., A comparison of methods for the modeling of thermochemical convection, JGR, 1997). I think it's worth adding a bit more explanation of the method, how it conserves mass, and what the potential drawbacks of that approach are.

Line 188: I think it would be useful for the authors to refer to an actual figure or test case here, before concluding that they find "remarkably good agreement". That would make it easier for the reader to assess whether they are convinced of the statement. I do realize that the testcases are presented in the next sections, but it's a bit odd to present the conclusion prior to showing the benchmark results.

Line 196: I entirely agree that the Rayleigh-Taylor instability is a great benchmark for fluid solvers, but I am not sure that I would present it as a benchmark of "magma mixing". The specific growth rate referred to in this section assumes two immiscible fluids, and only holds strictly in that specific limit. To me, it's a touch odd to describe the overturn dynamics of two immiscible fluids as mixing.

Line 233: Are these melts assumed to be immiscible or miscible? In other words, are they separated by a sharp interface or is there a compositional field variable that may start as sharp but can diffuse over time? Not entirely clear to me.

Line 260: I would be careful with the statement that "Reynolds number mainly controls bubble stability and breakup". There is no doubt that Reynolds is very important here, because the stagnation pressure at finite Re strongly deforms the bubble and deformation will be further amplified when turbulence kicks in. My concern with the statement is that a cursory reader could interpret this as "bubbles at low Reynolds number do not break up". That's obviously not true and I do not think that the authors want to insinuate that (as their later statement clarifies). The explanation provided at the end of the paragraph (based on Eo and Re) is much more clear.

Line 273: There is an issue in the typesetting here (line break needs removing).

Line 395: I struggle with this last paragraph. The authors make big promises here, e.g., "the inclusion of Lagrangian tracers will result in a more detailed description of the micro-physics", but do not offer a lot of evidence to back up this claim. Yes, population balance equation and Lagrangian tracers are convenient, but also have many drawbacks and it is not clear to me how they specifically advance our understanding of the micro-physics as I think of them as limited that way (after all, the "micro-physics" is largely thrown out of these very approaches). For these reasons, this last paragraph strikes me as rather speculative and a bit vague.

Overall, I think MagmaFOAM is a valuable contribution to the models available in the volcanological community. I hope my comments are helpful and I would be happy to clarify and/or discuss these suggestions if the authors want.

Jenny Suckale

Please also note the supplement to this comment:
https://gmd.copernicus.org/preprints/gmd-2021-224/gmd-2021-224-RC2-supplement.pdf