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Interactive comment on "A non-equilibrium model for soil heating and moisture transport during extreme surface heating" *by* W. J. Massman

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First, my thanks to the reviewer for his/her comments.

Reviewer: Introduction- It is important to clarify that the non-equilibrium process th author is discussing is non-equilibrium phase change between the liquid and vapor phases. This is not clear here, nor at certain points in the introduction and could be confusing to the reader.

Author's Response: I agree. The revisions will make clear that I am discussing th non-equilibrium phase change and that I am assuming thermal equilibrium.

Reviewer: Sensitivity analysis on the rho water as a function of temperature. Does this make any difference? Same for thermal conductivity.

Author's Response: All the following model sensitivity analyses were performed w the version of the model that included θ_r and $\lambda_s^{(2)}$.

(A) I varied ρ_w by $\pm$10%. Changes in the model performance were negligible. Also a much earlier version of the model I did include the $\partial \rho_w / \partial t$ term. Those previous model runs indicated that $\partial \rho_w / \partial t$ could be safely ignored. Consequently I am disinclined to revise the manuscript very much concerning the variations in ρ_w, unle the reviewer knows of or can suggest some physically meaningful way of including parameterizing the possible increase in ρ_w associated with bound water (which is a more involved effort).

(B) I varied λ_s by $\pm 10\%$, with very little consequence to the results presented in the current manuscript. Next, I varied λ_s by $\pm$0.2 Wm^{-1}K^{-1}, which changes the minimu value of λ_s (dry soil value) by about $\pm$80% and the maximum value of λ_s by about $\pm$6%. The model simulations of $T = T(t)$ (Manuscript Figure 1) and $\theta = \theta(t)$ (Manuscript Figure 2) were noticeably (and I would claim significantly) improved for $\lambda_s + 0.2$ and equally noticeably degraded for $\lambda_s - 0.2$. But $\lambda_s + 0.2$ caused the final profiles for ρ_v (Manuscript Figure 7) and e_v (Manuscript Figure 8) to increase substantially with exactly the opposite effect for $\lambda_s - 0.2$. In general, these results a very similar to those I have already reported in the current manuscript when discussing the sensitivity analysis associated with $\lambda_s^{(2)}$. Combining both types of sensitivity analyses for λ_s suggests that the significant improvements to the model's performance are primarily the result of increasing the dry-soil value of λ_s, which allows more heat to penetrate faster into the soil, thereby evaporating soil moisture faster and allowing the model to evaporate more soil moisture. Upon some reflectio further realized that the same sort of model improvement should be possible by decreasing the soil's volumetric specific heat $C_s(T, \theta)$. I tested this by decreasing b slope parameter c_{s1} as well as changing the (monotonically increasing) linear dependency of $c_s(T)$ to one that asymptotes to a smaller dry-soil value as the soil temperature increases. And indeed the model results were similar to (but not as go as) the $\lambda_s + 0.2$ case. In addition, these $c_s(T)$-related improvements were further diminished by the need to reduce the radiant forcing (surface boundary condition) s as to maintain the objective of matching the behavior of the experimentally-observe 5 mm temperatures. I will include these discussions in the revisions, but I must also include a caveat: This sensitivity analysis of λ_s is not particularly meaningful becau improving (at least some metrics of) model performance could only be achieved wit physically unrealistic values for $\lambda_s^{(2)}$ and/or the dry-soil value for $\lambda_s^{(1)}$. Therefore, all that can really be concluded from this λ_s sensitivity analysis is that data-based (or physically realistic) models of λ_s are quite good and that they are unlikely to be a source for any possible model inadequacies.

Reviewer: Theory section - It is unclear why the author selects specific functional parameterizations over other parameterizations. There is no justification listed as to their performance in soil heating environments compared to other functional parameterizations. Suggest that the author provide some justification/rationale for t selection of each parameterization.

Author's Response: By theory section I am assuming the reviewer is referring to section 2.2 (Functional parameterizations).

(A) I did explain several of my choices and why I used them in preference to the 20 paper. These include: the enthalpy of vaporization, H_v, the saturation vapor pressu $\rho_{v,sat}$, the saturation vapor pressure, $e_{v,sat}$, the need to include the self diffusion of water vapor, and the Stefan factor, S_F. And where I did test the differences betwee various parameterizations I usually found some (often slight) improvement in mode performance. But my overarching concern was and remains the desire for functiona parameterizations that are more physically realistic (particularly at higher

temperatures) than those I used in the 2012 paper. I am willing to revise the manuscript to point this out, but it does seem unnecessary to me.

(B) There is one corrigendum that I will need to correct. Shortly after submission I discovered an oversight in formulations for D_{vd} (page 11, line 13) and D_{vv} (page 11 line 15). The vapor pressure, e_v, was not included with the pressure term P_{ST}/P_{atm} These two diffusivities should read:

$$D_{vd} = D_{vdST}\left(\frac{P_{ST}}{e_v + P_{atmos}}\right)\left(\frac{T_K}{T_{ST}}\right)^{\alpha_{vd}}$$

and

$$D_{vv} = D_{vvST}\left(\frac{P_{ST}}{e_v + P_{atmos}}\right)\left(\frac{T_K}{T_{ST}}\right)^{\alpha_{vv}}$$

But this does not actually require any change to the model because this additional term can be subsumed into the approximation for S_F. In fact, amending S_F with thi additional term actually improves the approximation I developed for S_F.

(C) In an effort to understand the consequences of correcting this oversight I performed a sensitivity analysis on approximations to this amended S_F. And I discovered other approximations that significantly improved the model's performanc So I am also planning to revise the present manuscript to include a discussion of these results in a separate subsection under the larger section devoted to sensitivit analyses.

Reviewer: Nonequilibrum phase change approaches/formulations – I would argue that both approaches are empirical rather than truly having a physical basis. For example, the modified Hz-K approach includes a volume normalized interfacial surface area, interfacial surface transfer coefficient and equavelent pore radius, all values that are not easily determined and oftentimes used as fitting parameters. There is much work on the parameterized dynamic condensation coefficient, none o which was mentioned here. Suggest review of Marek, R., and J. Straub (2001), Analysis of the evaporation coefficient and the condensation coefficient of water, In J. Heat Mass Transf., 44, 39–53.

Author's Response:

(A) Thanks for reminding me about Marek and Straub (2001), but they mostly addre the pressure sensitivity of the evaporation and condensation coefficients, which is n really to critical for my model. But since submission I have discovered two papers th discuss the temperature sensitivity of these coefficients (Tsuruta and Nagayama, 2004, J Phys Chem B 108, 1736-1743; and Kon et al., 2014, Phys Fluids, 26, 072003). These two papers are quite germane to my model and so I am planning to revise the manuscript accordingly.

(B) As far as empiricism goes, I think the reviewer and I have a slightly different understandings of what is meant by "empirical". In my lexicon, my source term, $S_v^{(M}$ is a physically-based model of S_v, which does include an empirically adjustable parameter, but that is different from a fully empirical (or maybe semi-empirical) moc such as that discussed in Smits et al. (2011). Nevertheless, the only real distinction draw between these two "empirical" methods is that "This second approach [meani my flux-based S_v] allows for a more physically-based parameterization of the flux" (page 12, line 23-24). This is completely in keeping with my desire to stay as faithfu the physics of this scientific problem as I can. I clearly cannot claim that my approa is completely devoid of empiricism. But I do not think this distinction merits any change to the manuscript.

Reviewer: It might be helpful to discuss why Massman 2012 required revisiting/amendment more in the introduction.

Author's Response: I am not sure exactly what the reviewer's concern here is. Th basic reason I wanted to revisit the 2012 model is stated in the introduction. The 20 model did not allow the evaporated moisture to escape out of the open surface at th top of the modeling domain, which was traced back in the 2012 paper to the equilibrium assumption (largely through the performance of the Kelvin Equation at extremely low soil moistures). I will mention this aspect of the Kelvin Equation in the current manuscript, but I am not sure if this is what the reviewer has in mind.

Reviewer: The author directly compares the models of Massman 2012 and this model, concluding that the new nonequilibrium based model is a better fit/improvement. I don't think Massman 2012 and this model make for a good direct comparison and allow for the conclusion that the nonequilibrium formulation is the reason the model works better. There are many differences between the two mode making it difficult to pinpoint if the improvements are solely due to the consideration non-equilibrium behavior. The author should do a direct comparison between the tw models with all else equal (including boundary conditions), that would be beneficial

Author's Response: The basis for my claim of improved performance is that the n model allows the evaporated moisture to escape out of the open surface at the top the modeling domain, whereas the 2012 model did not. I cannot attribute this to anything other than the equilibrium vs the non-equilibrium assumption. Yes I did change (and improve upon) some of the functional parameterizations and yes I had change some of the boundary conditions (two model variables in the 2012 model vs three model variables in the current model), but I don't see how any of these could have contributed significantly to the failure of the 2012 model and the success of th present 2015 model. As I mentioned in the preceding response, the main culprit behind the failure of the 2012 model seems to be the use of the Kelvin Equation wh $\theta = 0$, where the equilibrium assumption must by necessity fail. I do compare the results of the two models with the intent of showing how all the modeling diagnostic are fairly consistent with each of the model's performances, but this seems appropriate. When all is said and done I suppose that it is possible (however unlikel seems to me) that I am incorrect on this point, but at this point in time I have not fou sufficient justification for exploring this issue.

Reviewer: Sec 3.3 It would be helpful to have a figure or table of initial and bounda conditions as some of them are unclear from the discussion. In addition, the author refers the reader to another paper to better understand the boundary conditions (as well as many other things throughout this work). In addition, in section 4.1, the experiments of Campbell are not well explained, making it more difficult to understa the experiment/model comparison.

Author's Response: Here I must plead guilty to fearing the anti-plagiarism softwar I personally have no problem repeating myself (or previous papers I have publishec on key parts of any new (but similar) paper, but sometimes nowadays the journals don't want too much repetition. I have had a couple colleagues review this paper ar at least one said that there was enough content and description in the present manuscript to reproduce my model, which is what I had hoped. I do want to keep th paper as short as possible while focusing it on the physics of this problem. Otherwi I have no problem including a discussion of Campbell's experiments, but the paper get longer. Concerning the reviewer's other suggested clarifications, I am not sure t they are sufficient to justify a longer paper (especially given the changes I am alrea planning).

Reviewer: Sec 4.2 need to be clear on the definition of dynamic residual soil moist in this context

Author's Response: I do not fully understand the reviewer's concern. I will insert a sentence in the middle of line 18, page 25 that states that improved performance of the model in describing the moisture dynamic (Figure 2) results primarily from its inclusion in the WRC, rather than in the HCF. But I am not sure that this is what the reviewer has in mind.

Reviewer: Figure 2- the model's performance (ability to capture soil moisture and temperature behavior) decreases with depth. What is the reason for this?

Author's Response: The reviewer's concern here is basically the same as asking why the model does not do a better job. I think this is because the model allows toc much evaporated water to diffuse downward and then recondense ahead of the dry front. This in turn causes the temperatures to be underestimated because the therr energy, instead of increasing the soil temperatures at the observed rate, is used to re-evaporate the recondensed moisture. The model performance degrades with de because this effect propagates downward through the column. There are a couple explanations for all this: (1) The vertical transport is too weak. As I mentioned abov plan to discuss the model's sensitivity to the Stefan factor, S_F. Increasing S_F basica causes the diffusion rate to increase, but the net effect is that more water is allowec escape out the top boundary rather than diffusing downward and recondensing ahe of the drying front. This increased diffusion yields a better simulation of the soil moisture and temperature with depth, as well as more realistic vapor density and vapor pressure profiles, so I may include some additional figures. It does not completely remove the degradation with depth (at least according to my conservativ sensitivity analysis), but it does remove some of the problem. (2) I suppose this typ of model behavior may also be the result from assuming thermal equilibrium. Had I included another model variable (temperature of the evaporated and diffusing vapo then the model would have included heat transfer between the cool liquid phase ahead of the drying front and the warmer downward diffusing vapor. (I should like to thank a colleague, who reminded me that this is sort of behavior could be modeled like a cooling tower.) This would cause a more rapid downward heat transfer, which presume would improve the model's simulation of temperature ahead of the drying front. In turn then this might produce different phase change and vapor transport dynamics. I would be happy to revise the manuscript to include these thoughts or a thoughts the reviewer may have. But beyond this I really cannot say much more. To me the thermal non-equilibrium model is an interesting hypothesis, which I would lil to test. But it is not possible to do so with the present model and I hesitate to specul much more on an even more complex non-linear problem than the present one.

Reviewer: Figure 5 discussion – The author discusses the experimental results of Campbell compared to numerical results, concluding that the experimental results f evaporation are flawed. This discussion is confusing and needs to be better clarifie Need to be consistent with terminology throughout – model referred to as sub-sampled synchronized, synchronized model etc. Please select one.

Author's Response: I disagree that I found “that the experimental results for evaporation are flawed". As I explained in the text that the experimental techniques not allow the same spatial and temporal resolution for the soil moisture profile as do the model solution. The model solution yields a data point every 1.2 s and every 0.0 m. The experimental is much coarser in both space and time. So I sub-sampled the fully sampled model solution to match each of the experimental data points at the times and locations at which they were obtained. I called this sub-sampled solution the synchronized model (meaning synchronized in space and time with the observations). Then I computed the evaporative loss, E_{loss}, using both forms of the model output. The results were different. I do not conclude from this test that the da are flawed, but rather given the different model estimates of E_{loss}, I conclude that there a real possibility that any experimentally-based estimate of E_{loss} is “biased" (maybe I should have said that it carries an inherent uncertainty due spatial and temporal coarseness of the data.) This should not be surprising (but I am sorry if it confusing). I did not report that I performed the same calculation on all of the other experiments. My overall (purely model-based) conclusion is that for any experiment estimate of E_{loss} there is an inherent uncertainty of $\approx \pm 0.05$ (in absolute terms) due the limitations of the sampling techniques. I can revise the manuscript to say that th observationally-based fractional E_{loss} = 0.31 $\pm$ 0.05. All I have really done here is t use the model to estimate the uncertainty in the data-derived E_{loss}.

Reviewer: Figure 6 shows condensation (increase in soil moisture) at a certain dep This needs to be discussed in the paper as this behavior is not seen in the experimental results. Sensitivity analysis – there is no quantifiable results, only statements like slightly sensitive, weak role etc. Suggest more quantitative descriptions of sensitivity. Water retention curve and hydraulic conductivity function sensitivity analysis discussion – it would be beneficial to show a figure that shows th water retention and K behavior rather than only the discussion. It is unclear how ea formulation improves the overall results This would be especially helpful to understa the sensitivity in the dry soil region. The discussion, as written is difficult to follow.

Author's Response: (A) Here the reviewer's concern about Figure 6 reinforces the point I just made about the sparseness of the spatial and temporal resolution of the experimental observations. I think the peak does not appear in the observations because it was missed by the sampling techniques. This is not a flaw in the data, ju a limitation of the measurement techniques. But clearly by missing the additional water that has accumulated in the profile, E_{loss} must be overestimated (biased) for t experiment. (B) I do not think quantifying the sensitivity analyses is particularly insightful. There are really only 3 categories (relative to the control run that is discussed in the present manuscript): (1) Small enough not to offer much insight, fo which I used “weak", “slightly sensitive", etc. (2) Caused the model to become unstable and fail, which suggests that the model has probably slipped over into a hyperbolic PDE. Again for diagnosing the present model performance this yields rather limited physical insight. (3) A significant improvement or significant degradati such as discussed above with λ_s and now more importantly with S_F (also discusse above). Including figures of the new model solution for the new parameterization fo S_F is in my mind a much more useful sensitivity analysis than a table of numbers. (I could include more figures of the behavior of the WRC and HCF, but again I think do so misses the point a bit. Neither Campbell et al. (1995) nor Massman (2012) included the HCF, because the assumption is that the soil heating and resulting evaporation are so fast that including liquid soil moisture movement (HFC) was probably unnecessary. I wanted to test this assumption with this new model and basically I confirmed it. But I cannot be certain that for field application that this assumption is valid because the heating and evaporation rates are likely to be at le: 2 orders of magnitude slower than Campbell's laboratory experiments (Massman 2012). Meaning that in the field liquid soil moisture movement is a real possibility. E given the plethora of WRCs and HCFs I also wanted to try some other combination of them (just in case). Some combinations made only slight (positive or negative) differences in the solution, but others produced instabilities. Again the degree of change was not large, but the failures are worth noting. But I don't think a detailed analysis of the WRCs and HCFs is warranted here because they are only secondaı to the model's performance in the present case. But for a field application, then I would agree it could be quite insightful to have a detailed look at the performance o the various WRCs and HCFs. (D) I will attempt to include the above discussion in tl revisions.

Reviewer: The discussion of the importance of residual soil moisture and values lower than the residual value is very important to this work. This is confusing to me when the author then states that they artificially lowered the residual value in the ca of the Dry Quincy Sand. If the water retention model selection is properly considere why does the author need to make these adjustments? Shouldn't the function able be adjusted below the residual value based on physical changes such as temperatu effects?

Author's Response: After several tests I can now assure the reviewer (as well as myself) that there was no need to make any adjustments to θ_{r*}. After reassigning θ to 0.03 and increasing b_1 (to keep the model stable), the model was able to capture much of the observed soil moisture dynamics for dry Quincy Sand. But unlike the moister Quincy Sand test case discussed in the present manuscript, it is very difficu to determine if including θ_r improved the simulation or not because the two simulations (with and without θ_r) for dry initial conditions were very similar. I will rev

the manuscript to reflect these new results.

Reviewer: 4.3.3 Are the initial soil moisture conditions for the entire column (i.e. constant soil moisture throughout)? The author discusses how the model can bette capture the evaporation behavior for dry soils rather than wet initial soil conditions, provides little reasoning for this. Based on others works on evaporation behavior, it difficult to capture the different stages of evaporation (e.g. atmospheric controlled stage 1, dominated by capillary action and diffusion controlled stage 2, which is mo influenced by the soil properties rather than the atmosphere conditions). Even more difficult is capturing the transition between the stages. It seems that this model is better able to capture the stage 2 dynamics but this leads to a lot of questions on th overall model performance.

Author's Response: (A) Yes the basic assumption is that the initial soil moisture is uniformly distributed (constant) throughout the entire column (see page 24, lines 2- (B) I am simply noting my observation about the model's performance of moist vs d samples. I have long had the impression that it is more difficult to accurately model soil evaporation and transport than it is to accurately model temperatures and heat flux. Therefore, my model's performance (vis-a-vis moist vs dry initial conditions) basically confirmed my expectations. Otherwise I do not quite understand the reviewer's comment or his/her impression of how my model does or does not impro upon modeling the dynamics of stage 1 and stage 2 drying. If the reviewer would provide some references and elaborate more on his comment I would be happy to consider how to revise the manuscript.

Reviewer: The author should discuss the applicability of this model to different scenarios, to include fire burn environments. More of the contribution of this work seems to be the investigation of the specific parameterizations, such as the soil wa retention function and others and how this applies to fire burn models.

Author's Response: I am expecting (and looking forward to) quite a few opportunities in the near future to field test this model. At this point I do not see any reasons why the model should not be broadly applicable at least to bare soil (i.e., th model does not include a plant transpiration component). But I hesitate to speculat further about a problem that I have not yet tackled. Otherwise I need further clarification from the reviewer about his/her comment.