Revised Response to Reviewer #1

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

Introduction. As a result of addressing the second reviewer's concern about my model's under-performance (my choice of words), I must revise my first response to Reviewer #1. The reason for this under-performance was that I had set the parameters of the hydraulic conductivity function (HCF) incorrectly. In fact, my original choice of parameters yielded numerical values of the HCF that were far too low and was the functional equivalent to ignoring it all together. Correcting this problem improved the model's performance significantly and also makes it easier to respond to Reviewer #1's comments. But it also required me to completely rewrite the Results and Summary Sections, add 7 more figures and about 5 more pages of text, and alter the Abstract and Introduction. It is therefore impractical to just highlight my changes to the manuscript (in the preferred manner of responding to reviewer's) because both reviewers will probably need to critically reread the interpretive sections again.

Reviewer: *Introduction- It is important to clarify that the non-equilibrium process the 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 make it clear that I am discussing the 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: I performed the same sensitivity analysis on ρ_w and soil thermal conductivity, λ_s, [and $C_s(T, \theta)$ for that matter] with the updated model as I did with the previous version of the model. The conclusions are largely the same. The functional dependency of ρ_w on temperature, T_K, is not significant and certainly is not responsible for the under-performance of previous version of my model. The sensitivity analysis of for λ_s, and $\lambda_s^{[2]}$ in particular, is now incorporated into the discussion of the model's performance on the Quincy Sand data and highlighted elsewhere in the manuscript. As it now happens $\lambda_s^{[2]}$ does contribute quite positively to the model's performance.

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 the 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 revised the manuscript to emphasize that the new functional parameterizations are more physically realistic, particularly at higher temperatures and pressures, than those I used in the 2012 paper. This is now stated in the Introduction and reiterated in the "theory section".

(B) The corrigendum is now embedded in lines 253-276 and the forgotten term has been subsumed into the Stefan factor.

(C) Reformulating the HCF obviated any need to discuss any sensitivity analysis of the Stefan factor.

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 of which was mentioned here. Suggest review of Marek, R., and J. Straub (2001), Analysis of the evaporation coefficient and the condensation coefficient of water, Int. J. Heat Mass Transf., 44, 3953.*

Author's Response:

(A) The papers discussing the temperature sensitivity of the condensation coefficient (Tsuruta and Nagayama, 2004, J Phys Chem B 108, 1736-1743; and Kon et al., 2014, Phys Fluids, 26, 072003) are now cited in the paper.

(B) As far as empiricism goes, I am satisfied with my first response; viz: 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 I admit does include an empirically adjustable parameter, but that is different from a fully empirical (or maybe semi-empirical) model such as that discussed in Smits et al. (2011). Nevertheless, the only real distinction I draw between these two "empirical" methods is that "This second approach [meaning my flux-based S_v] allows for a more physically-based parameterization of the flux". This is completely in keeping with my desire to stay as faithful to the physics of this scientific problem as I can. I clearly cannot claim that my approach 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: The Introduction now explains more fully why *Massman* [2012] needed to be revisited: lines 83-85 state "Or, more fundamentally, the calculated vapor and its attendant gradient became largely meaningless because it is impossible for water vapor to be in equilibrium with liquid water if there is no liquid water." This is basically the fundamental problem with the equilibrium model. It can never be correct or physically realistic if the soil moisture has completely evaporated.

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 dont 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 models, making it difficult to pinpoint if the improvements are solely due to the consideration of non-equilibrium behavior. The author should do a direct comparison between the two models with all else equal (including boundary conditions), that would be beneficial.*

Author's Response: Here I am still inclined to disagree somewhat with reviewer. As I just pointed out the equilibrium model cannot be correct when there is no soil moisture to be in equilibrium with. Therefore, the non-equilibrium assumption must per force improve the model's performance. Nonetheless, the revisions now make it clear that a "properly calibrated" HCF is a significant contributor to the present model's performance. The revisions also note that I do not know how much (if any) the equilibrium model could be improved with the inclusion of such a HCF. But that said even the previous version of my model, which did under-perform because of an "improperly calibrated" HCF, still outperformed my 2012 model (see Figs. 1-3 in my response to the first reviewer). Furthermore, as I mentioned in my first response and discussed in the previous manuscript, the new model requires at least one new BC. But the BCs for both the equilibrium and non-equilibrium models are largely driven by the energy input, $Q_R^{\Downarrow}(t)$, which is the same for both models. The nuances between the two models' BCs are not responsible for the improvement of the non-equilibrium model over the equilibrium model. Neither can I convince myself that the new parameterizations are responsible. I did incorporate at least the new enthalpy of vaporization into the equilibrium model and it made virtually no difference to the model simulation. It is theoretically possible that the new parameterization of $\rho_{v,sat}$ could make some difference in the equilibrium model. But the equilibrium model code was not amenable to simply substituting the new $\rho_{v,sat}$ for the old one and the non-equilibrium model became unstable with the old parameterization of $\rho_{v,sat}$. But in the final analysis neither the BCs nor the new functional parameterizations actually address the fundamental ($\theta \equiv 0$) problem intrinsic to the equilibrium assumption. I cannot conclude anything other than the non-equilibrium model is the preferred (or "correct") model.

Reviewer: *Sec 3.3 It would be helpful to have a figure or table of initial and boundary 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 understand the experiment/model comparison.*

Author's Response: My response here is largely the same as before: I must plead guilty to fearing the anti-plagiarism software. I personally have no problem repeating myself (or previous papers I have published) on key parts of any new and related paper, but these days the journals don't seem to want too much repetition. I have had a couple colleagues review this paper and 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 the paper as short as possible while focusing it on the physics of this problem. Otherwise I have no problem including a discussion of Campbell's experiments, but I would prefer the journal's approval or encouragement first. Concerning the reviewer's other suggested clarifications, I am not sure that they are sufficient to justify a longer paper (especially given the additions I have already made).

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

Author's Response: I do not fully understand the reviewer's concern. But maybe this issue has been obviated by the revisions. The new results indicate that including θ_r in the model did not improve the Quincy Sand simulation, but that it did improve the Palousse B simulation.

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

Author's Response: I believe this concern has largely been obviated by the changes to the HCF and the resulting improvement in the model's performance.

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

Author's Response: My response here is largely the same as before: I disagree that I found "that the experimental results for evaporation are flawed". As I explained in the text that the experimental techniques do not allow the same spatial and temporal resolution for the soil moisture profile as does the model solution. The model solution yields a data point every 1.2 s and every 0.001 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 data 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". (The revision now indicate that it carries an inherent uncertainty due spatial and temporal coarseness of the data.) This should not be surprising (but again I am sorry if it is confusing). I now report that I performed the same calculation on all of the other experiments. My overall (purely model-based) conclusion is that for any experimental estimate of E_{loss} there is an inherent uncertainty of $\approx \pm 0.03$ (in absolute terms) due to the limitations of the sampling techniques. I have revised the manuscript to say that the observationally-based fractional $E_{loss} = 0.31 \pm 0.03$. So all I have really done here is to use the model to estimate the under-sampling related uncertainty in the data-derived E_{loss}.

Reviewer: *Figure 6 shows condensation (increase in soil moisture) at a certain depth. 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 the water retention and K behavior rather than only the discussion. It is unclear how each formulation improves the overall results This would be especially helpful to understand the sensitivity in the dry soil region. The discussion, as written is difficult to follow.*

Author's Response: A significant portion of the reviewer's concerns should have been obviated by the "properly calibrated" HCF and attendant improvements in the models performance. Nonetheless, some of my first response is still appropriate. (A) The sparseness of the spatial and temporal resolution of the experimental observations may mean the peak does not appear in the observations because it was missed by the sampling techniques. This is not a flaw in the data, just a limitation of the measurement techniques. (B) I did not attempt to quantify the sensitivity analyses numerically, but I did attempt to visually display them in all the revised figures. (C) The revisions now include a figure (Fig. 9) of the HCF. (D) I think the revisions should answer many of the reviewer's concerns.

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 case of the Dry Quincy Sand. If the water retention model selection is properly considered, why does the author need to make these adjustments? Shouldnt the function able to be adjusted below the residual value based on physical changes such as temperature effects?*

Author's Response: The revisions should obviate the reviewer's concerns. Once the HCF was "properly calibrated" the importance of the residual soil moisture term was reduced. The updated model (and manuscript) also includes a HCF for film flow in addition to the original capillary flow HCF model. All this is fully documented in new version of the manuscript.

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 better capture the evaporation behavior for dry soils rather than wet initial soil conditions, but provides little reasoning for this. Based on others works on evaporation behavior, it is 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 more 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 the overall model performance.*
Author's Response: My response here is about the same as my first response:
(A) Yes the basic assumption is that the initial soil moisture is uniformly distributed (constant) throughout the entire column.
(B) I do not quite understand the reviewer's comment or his/her impression of how my model does or does not improve 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. On the other hand, my revisions to the previous manuscript may have obviated the reviewer's concerns.

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 water retention function and others and how this applies to fire burn models.*
Author's Response: The study has been expanded to include much more detail on the model's performance on other laboratory experiments performed by *Campbell et al.* [1995]. And, yes, the reviewer is correct that my principal purpose of the present modeling study is to explore what are the important physical processes and related parameters and parameterizations that I need to best describe the heat and moisture dynamics during these type of events. In that regard, the present study is like *Massman* [2012] and is intended to be exploratory. But present revisions now give me much more hope that I am on the right track with the non-equilibrium model, which I definitely was not with the equilibrium model. Nonetheless, I have just started working on adapting my model to wild fires and prescribed burns, so I would like to defer discussion of this point until I have more experience and a better understanding of the associated problems.

<u>Response to Reviewer#2</u>

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

Reviewer: *In this manuscript the author has developed and evaluated the model that takes a non-equilibrium process into account during evaporation and condensation of soil water. This topic fits well to the scope of Geoscientific Model Development. I think, however, there is a major flaw that needs to be addressed prior to considering publication.*
Author's Response:
(A) I agree that GMD is a good choice for this paper.
(B) But I disagree that the model is flawed (at least not in the way I believe the reviewer means flawed). Nevertheless, I do agree that the model's performance was not as good as is detailed in the revised version of my manuscript. The reason for the model's original under-performance was that I had set the parameters of the hydraulic conductivity function (HCF) incorrectly. In fact, my original choice of parameters yielded numerical values of the HCF that were far too low and was the functional equivalent to ignoring it all together. Correcting this problem improved the model's performance significantly. But it also required me to completely rewrite the Results and Summary Sections, add 7 more figures and about 5 more pages of text, and alter the Abstract and Introduction.

Reviewer: *My major concern is the performance of the non-equilibrium model. Neither soil temperatures nor soil moisture contents were well predicted using the model developed by the author as can be seen in Figs. 1-6. Discrepancies between observed and simulated values are just too large. For example, in Figure 1, differences between observed and simulated temperatures at some given times are greater than 100 degree C. Changes in soil moisture contents depicted in Figure 2 also show that the model cannot reproduce observations at all. At some depths, they are not even close. This kind of simulation is simply not acceptable in my opinion.*
Author's Response:
(A) I think the reviewer's concerns should be obviated by the improvements in the model's performance, which are now detailed in the revised manuscript.
(B) But given that the reviewer does not provide any metric or measure of what constitutes an "acceptable" model simulation with his/her opinion, I cannot be certain that even what I may view is a significantly improved performance is adequate to meet the reviewer's expectations or standards. This is a non-trivial issue because no model is ever completely faithful to data. Taking the present revisions as an example, the new figures 6 and 15 indicate the model cannot capture the observed moisture profile within the top 40 mm or so of the soil column. But I have spent the last 3 years looking at simulations of many similar and different models applied to very similar and very different settings and to

my knowledge no existing model has ever been able of capture this observed behavior. This issue is even more extreme with Stefan (or moving boundary condition) models, of which there are many, because they completely obviate any possibility of being able to capture this observed residual moisture at the top of the soil column.
(C) Overall, my basic concern here is that the reviewer may set too high a standard and may judge the present model solely on its inability to capture observations that have eluded the scientific community's efforts for at least the last 50 years or so. In general, phase change problems are (it seems to me) extraordinarily complex and may still harbor some unknown physics.

Reviewer: *If observed data are not well predicted, how can we know that the theory behind the model is correct?*
Author's Response:
(A) The ability to reproduce data does not "prove" any theory correct. The case I am attempting to make with the present manuscript, as well as the previous version, is that the non-equilibrium model is an improvement over the equilibrium model, not that the non-equilibrium model is necessarily "correct" (at least in any final sense of this scientific problem). To me the improvements in the present model's performance demonstrates an undeniably clear step in the right direction. And it is definitely a much more obvious step in the right direction than outlined in previous version of this manuscript. Nonetheless, the previous solution is still an improvement over my equilibrium model [*Massman* 2012] and (just for the fun of it) I am including the following three figures in my response to the reviewer that compare my former solution (previous version of the manuscript) to the now newly "recalibrated" equilibrium model.
(B) By "theory" I am assuming that the reviewer is referring to my source term, S_v (Equations (10) and (11) of the present manuscript). Otherwise I am not quite sure what the reviewer means by "theory". Nonetheless, I do not know if my source term is "correct" or not, there are no data anywhere on which to base any model of S_v, just hypotheses and theoretical ideas about S_v as I discuss in the present paper and as discussed in the papers I cite. But I was quite explicit on how I constructed it, the assumptions I made, and the physics behind those assumptions. My conclusion regarding the present model of S_v is that it is physically plausible and, given the dearth of experimental knowledge of S_v, reasonably realistic. There may be better models available for S_v, I just don't know of them.

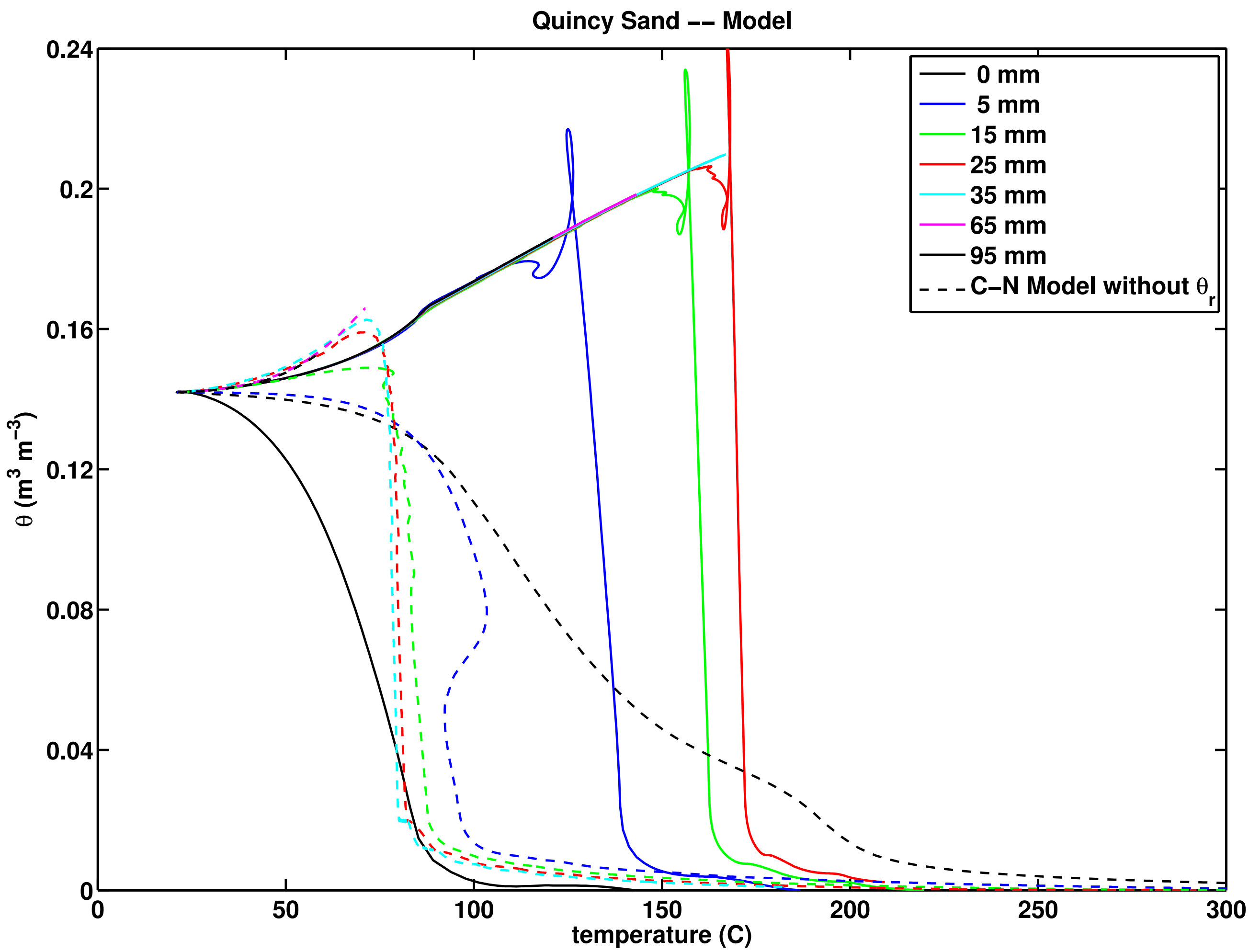
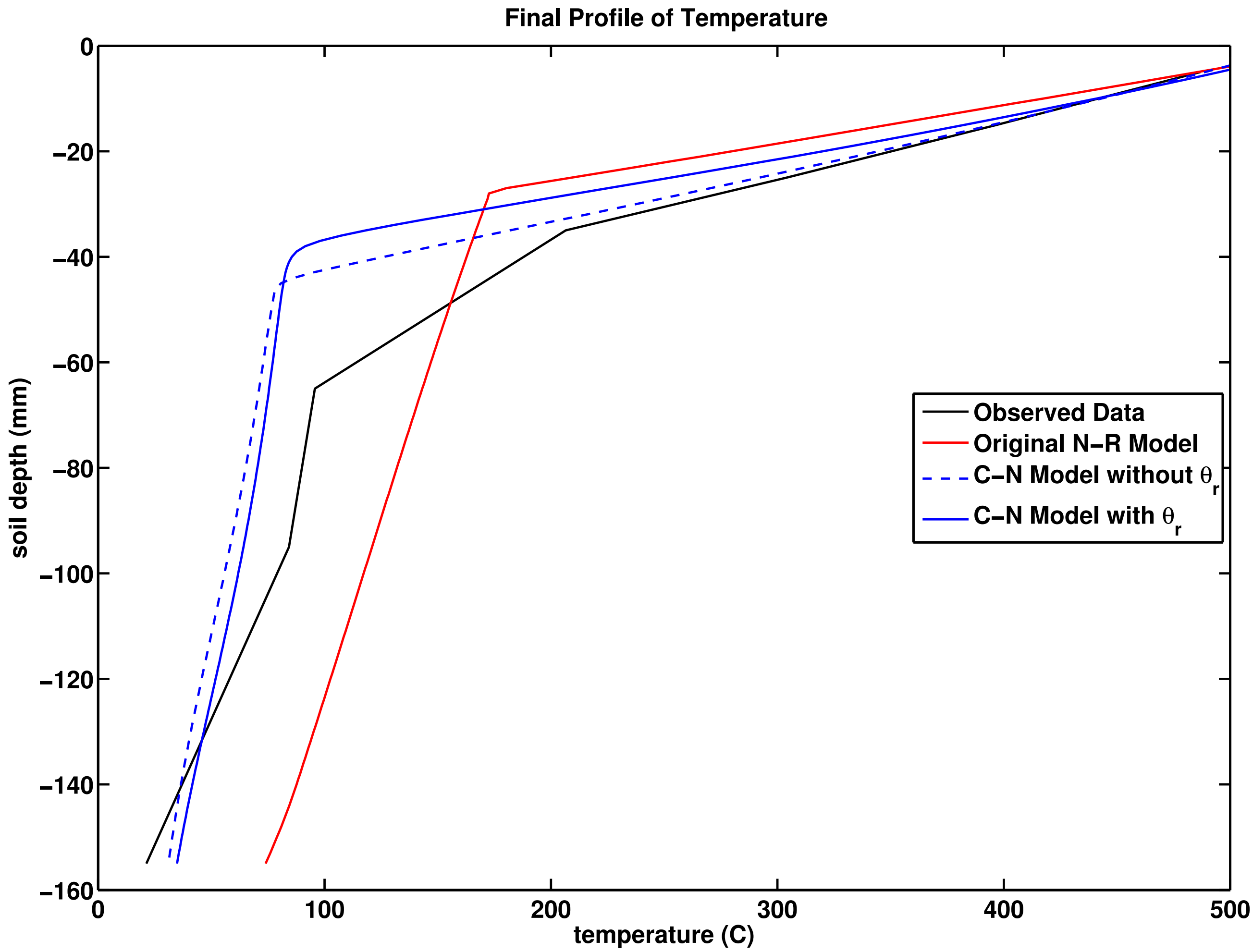

Quincy Sand -- Model
0.24
0.2
0.16
0.12
0.08
0.04
0
θ (m3 m-3)
0
50
100
150
200
250
300
temperature (C)
0 mm
5 mm
15 mm
25 mm
35 mm
65 mm
95 mm
C–N Model without θr

Figure 1:



Final Profile of Temperature
0
−20
−40
−60
−80
−100
−120
−140
−160
soil depth (mm)
0
100
200
300
400
500
temperature (C)
Observed Data
Original N−R Model
C−N Model without θr
C−N Model with θr

Figure 2:

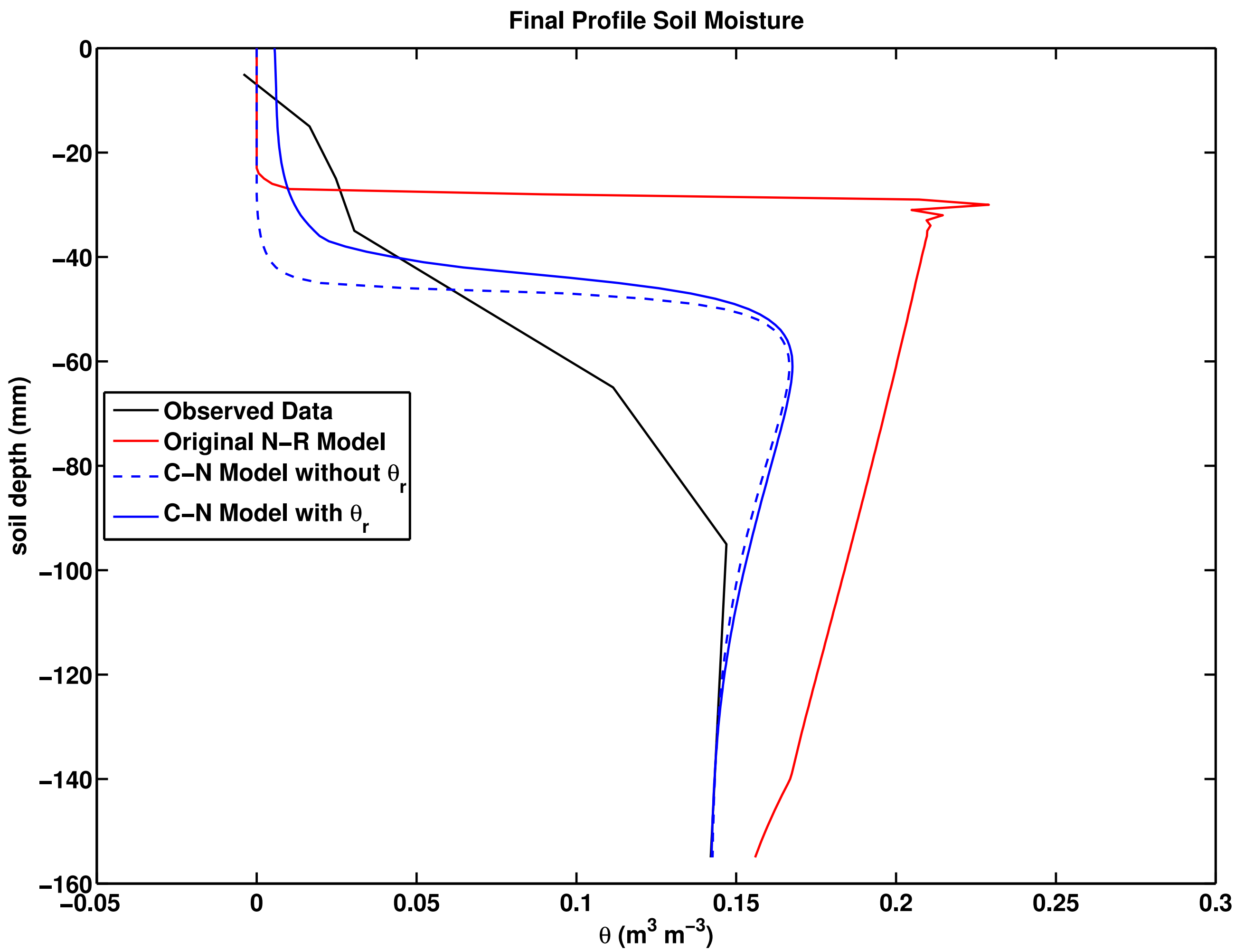

Final Profile Soil Moisture
0
−20
−40
−60
−80
−100
−120
−140
−160
soil depth (mm)
−0.05
0
0.05
0.1
0.15
0.2
0.25
0.3
θ (m3 m−3)
Observed Data
Original N−R Model
C−N Model without θr
C−N Model with θr

Figure 3:

Reviewer: *The idea of considering the non-equilibrium processes may be a significant step to understand coupled water and heat transfer in soils during fire. However unless the author shows much better simulation result, it will be difficult for readers to be convinced that the non-equilibrium process has to be taken into account or plays an important role.*
Author's Response:
(A) Again I cannot tell exactly what the reviewer means by a "much better simulation result" or what standards apply by which to evaluate such performance. But maybe the revisions will have obviated his/her concerns.
(B) But, I can assure the reviewer and any potential reader that the non-equilibrium process has been taken into account at least in terms of a model that includes S_v. On the other hand, as to whether the non-equilibrium process (S_v) plays an important role in the model's solution (performance), which I think is the reviewer's real point, that is something of a different issue. Here the reviewer may be expressing some of the same concern that the first reviewer expressed, only based on a somewhat different metric. My basic argument concerning why the equilibrium model is better than the non-equilibrium model is more than just improved performance. I believe the non-equilibrium assumption is just better and more realistic physics that the equilibrium model. The Introduction now includes the following: "He [Massman referring of his 2012 equilibrium model] further traced the cause of this anomalous behavior to the inapplicability of the equilibrium evaporation assumption, which allowed the soil vapor gradient behind the drying front to become so small that the soil vapor could not escape (diffuse) out of the soil. Or, more fundamentally, the calculated vapor and its attendant gradient became largely meaningless because it is impossible for water vapor to be in equilibrium with liquid water if there is no liquid water.", which is intended to clarify to the reader that the equilibrium model must (at some point as $\theta \to 0$) fail because it does not have the correct physics.

Reviewer: *If simulation can be improved by calibrating some parameters, I think the author should consider doing that. By doing that, the author may be able to discuss sensitivity of each parameter.*
Author's Response: The model's performance was significantly enhanced by altering the parameters of the HCF.

Reviewer: *Unless the author shows much better simulation results, I do not think the manuscript should be accepted.*
Author's Response: I believe I have obviated the reviewer's concerns.

Reviewer: *I have some specific comments as well. 1. Recently there have been many studies to model soil water retention curves and unsaturated hydraulic conductivities in very dry range (low potential) to account for, for example, film-type flow. This may be triggered as we now have some new devices to measure soil water potential in very dry* *range. I am wondering if a HCF model which considers film-type flow may improve the simulation result under fire as non-capillary-type residual water seems to play an important role here. 2. Related to the comment above, it is well accepted that soil water and heat transfer simulation performance strongly relies on how WRC and HCF are modeled. The author therefore needs to show soil hydraulic data used in this study and models fit in a figure. 3. It is not necessary to show synchronized model profiles in Figs 5 & 6. There is also typo in both figures: Synchronized not Synchonized*

Author's Response:

1. The model now includes film flow and its contribution to the present model's performance is negligible.

2. I agree: the present model's performance strongly relies on how WRC and HCF are modeled. Comparing the previous and present versions of the manuscript, as well as the newly revised section 4.3.2, clearly demonstrate this. The revisions now explain that the soil samples used in this experiment were destroyed long ago and that their hydraulic properties were never determined. And except for the low moisture end of the WRC, the WRCs of these soils have never been studied either. But the principal WRC used here, Equation (15), is discussed at some length by *Massman* [2012], who supports it with the appropriate justifications and citations. On the other hand, the data void created by the present HCF, Equation (17), was filled by calibrating it against the observed temperature and moisture data (see section 4.2.2 of the manuscript for further details). The revisions now include figure 9, which shows the various terms associated with the model HCF, Equations (17)-(19) of the present manuscript, as functions of soil moisture.

3. Thanks for pointing out the misspelling. Including the synchronized model helps make the point that the data are potentially biased due to the spatial and temporal coarseness of the sampling. (Also see my response to the first reviewer on this issue.) There is little overhead to including the synchronized model profiles (figures 5 & 6, plus new figures 14 & 15) and I see no benefit to eliminating them from these figures.