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Interactive comment on "The challenges of an in situ validation of a non-equilibrium model of soil heat and moisture dynamics during fires" by William J. Massman

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General comments

Note that all papers referenced in these comments and not in the manuscript are designated with an * and are in an additional list found below.

This manuscript is the third in a series on modeling soil heat and moisture dynamics under extreme surface heating associated with forest fires or prescribed slash pile burns. The first two papers (Massman, 2012, 2015) compared model results with a laboratory simulation of surface fire (Campbell et al., 1995). According to the Abstract

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the coupled heat and moisture model developed by the author is improved in two main ways: (1) the formulation for the non-equilibrium vapor source term, S_v , is modified for extremely dry soil moisture content and (2) the apparent thermal conductivity is no longer used in Fourier's law in the soil heat flow equation because that resulted in the double counting of thermal vapor transport (de Vries, 1958). Additional changes to the Massman (2015) model not highlighted in the Abstract are also detailed. The manuscript describes a slash pile burn field experiment carried out in a pine forest in Colorado and compares the latest model version to the field measurements (showing moderate to good agreement for the variables of greatest interest). Final sections discuss sensitivity analyses, the potential for future fire studies, and a summary.

Explicit formulation of an expression for S_v is required in so-called non-equilibrium versions of the Philip and de Vries (1957) theory, including those with the well-known extensions detailed in de Vries (1958, 1987*) and Milly (1982*). Until relatively recently all Philip and de Vries type theories in the soil physics literature were formulated with the assumption of local phase equilibrium between liquid water and its vapor throughout the soil domain even though it is recognized that for evaporation/condensation to occur in a soil pore such an equilibrium cannot be exactly true. In these equilibrium versions S_v is determined implicitly and only one partial differential equation, with corresponding boundary and initial conditions, is required to simulate soil moisture flow compared to two for a non-equilibrium version. Recently Smits et al. (2011) and Trautz et al. (2015) claimed significantly better simulation of cumulative evaporation and soil moisture content with similar non-equilibrium versions. Massman (2015) also made such a claim when updating the Massman (2012) model which assumed equilibrium. In the current manuscript it is indicated that the latest improvements to S_v "enhanced the stability and performance of the model" although neither the current nor the 2015 paper makes a direct comparison between equilibrium and non-equilibrium predictions.

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Novak (2019), which followed on Novak (2012), was devoted to a detailed investigation of the non-equilibrium formulation and the results of modeling moisture and heat heat flow with and without it. It was mainly prompted by the realization that if recent claims about the importance of non-equilibrium are true then all previous investigations of soil evaporation (and other phenomena in soil physics) that assumed equilibrium are invalid. The relevant Novak (2019) findings can be summarized as follows: (1) in a soil drying under natural conditions or due to fire evaporation begins at the soil surface but eventually moves steadily deeper into the soil with the phase change occurring within a very narrow frontal-type evaporation zone (at most a few mm wide), (2) a dry layer in which moisture flow is dominated by upward vapor diffusion exists above the evaporation front and relatively wet soil in which upward liquid flow dominates exists below it, (3) $S_v \approx 0$ everywhere outside the evaporation zone (especially true in the dry layer; a small amount of condensation driven by the soil thermal gradient exists in the wet layer but the values are several orders of magnitude smaller than those at the front). (4) there is no discernible difference for all dependent variables (and corresponding fluxes) between the non-equilibrium and equilibrium version models everywhere outside the narrow evaporation zone, (5) the "intrinsic resistance" (Shuttleworth, 1975*) associated with Hertz-Knudsen dynamics is 2-3 orders of magnitude smaller than the within-pore diffusion resistance that governs a proper physically-based formulation for S_v and can therefore be neglected, (6) avoiding the imposition of equilibrium at the soil surface during drying, which in principle is required within a fully non-equilibrium model, is more difficult in practice due to numerical instability; imposing equilibrium at the bottom boundary of the soil domain, if deep enough so that little change occurs, and in the initial condition is physically realistic. The Novak (2019) results show clearly that the numerical implementations of the heat and moisture transport equations in Smits et al. (2011) and Trautz et al. (2015) were flawed and their conclusions about the importance of and the necessity to use non-equilibrium models were incorrect.

Therefore, while the implementations of a non-equilibrium version of heat and mois-

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ture flow in Massman (2015) and in the new manuscript are not incorrect in principle, if done correctly, there is clearly no advantage to doing so despite the author's perception of better performance in both cases (never actually shown). True differences between the equilibrium and non-equilibrium models that do exist within the narrow evaporation zone (as shown in Novak, 2019) are unobservable and have no bearing on the objectives stated in the Introduction to the new manuscript with regard to effects of fire on soil. Furthermore a non-equilibrium model requires greater programming labor, is more complex, has longer computation times, and has greater potential for programming error and numerical instability.

The S_v formulation actually used based on the Hertz-Knudsen Equation [line 126, Eq. (8)] is incomplete since the much larger within-pore diffusive resistance that exists is neglected, implicitly resulting in a smaller resistance which would bring the non-equilibrium model used closer to the equivalent equilibrium model (Novak, 2019). Massman (2015) described two formulations for S_v , one of which was based on Novak (2012) which assumed pore diffusive resistance alone to be limiting to within-pore diffusion but the two formulations were not compared directly. An improved and fully physically-based version of the Novak (2012) model is derived in Novak (2019).

The importance of changes to the S_v formulation [lines 144–154, including Eqs. (9) and (10)] to model behavior is difficult to assess because no information about the depth of and water content within the modeled evaporation zone is reported. The changes were apparently confined to $\theta \leq 0.01$ (based on $S_w \leq 0.02$ and porosity of 0.51) which if confined to the dry layer above the evaporation front would have no effect since $S_v \approx 0$ there. The temperature measurements and model calculations (Figure 6) show values well above boiling for the upper 5 cm of soil at least and the soil in that part of the dry layer has essentially zero water content. Line 150 indicates that S_v is changed only when at most a mono-layer of water exists on the soil particle surfaces. I would expect that little evaporation can occur from such surfaces and they must have been

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located in the dry layer. If this is true then explanation of the better model stability and performance due to the changes in S_v indicated in the Abstract is difficult to understand because the changes would have negligible effect.

There is no recognition of the issue of not imposing equilibrium at the soil surface (lines 236–243) in the most general version of a non-equilibrium model which requires a Robin type boundary condition for vapor density (see Novak, 2019, for a detailed discussion).

It is likely that the small effect that was found upon elimination of the double counting of vapor "distillation" (lines 155–196), reported in the Abstract as a major improvement to the Massman (2015) model, is due to the fact that the double counting was guantitatively important only within the narrow evaporation zone. Therefore soil temperatures in most of the domain are not affected very much. Other changes to soil thermal conductivity include accounting for a large effect (as much as a 70% decrease) of temperature on the thermal conductivity of the mineral component based on that of α -quartz although there is no discussion about the mineral fractions in the soil and whether they are dominated by quartz sand. The soil is reported to be 60-65% sand, 20-25% silt, and 10-15% clay. Do any other soil mineral components behave similarly to quartz? In Massman (2012) the large effect of temperature on volumetric heat capacity (due to both mineral and water component variations) is included. For thermal conductivity apparently only the dependencies of the water and air components on temperature are accounted for but not that of the mineral component. This is maintained in Massman (2015). For normal conditions these dependencies on temperature are usually small enough to be neglected but under fire they appear to be significant especially given that the thermal regime is of greatest interest. Modification of R_n in the Bauer term is reported but it is also indicated that the thermal infrared contribution to heat flow is negligible anyway.

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The large model complexity in this paper, which often requires referral to Massman (2012, 2015) to fully understand, makes it difficult to read and the meaning of the results somewhat incomprehensible. The physics of the various components is generally not new except for perhaps the non-equilibrium part which has been shown to be unnecessary. I wonder whether including every process imaginable in such a model is warranted and even helpful given the uncertainties of fire under field conditions and associated measurement difficulties. Despite the many processes the model still reguired a number of tuning parameters. Under normal field conditions many processes, e.g., storage of water vapor, advection of heat by air and water flow and water vapor by air flow, and heat of wetting are known to be of negligible importance and do not have to be included in coupled heat and moisture flow models (Grifoll, 2013*; Novak, 2010*, 2016*). This may not remain true under more extreme fire conditions but order-of-magnitude calculations could be used to determine this. The upper boundary conditions are especially uncertain in this paper since they require proper understanding of how the slash pile burns including analysis of air flow within and above the pile. I am skeptical about the temperature boundary condition used in the paper. According to Figure 4 sensible heat flux was positive throughout the fire experiment while the picture in Figure 2 suggests a pile with internal temperatures of about 1000° C so that there likely was a steep temperature inversion above the soil surface and therefore the sensible heat flux must have been negative (downward). Despite this the modeled soil temperatures are reasonable, presumably a testament to empirical parameter tuning. Actually since surface temperature was measured in the experiment it could just as well (or even better) have been used as the upper (Dirichlet) boundary condition to the heat flow equation.

Specific comments

What is the physics underlying Eq. (5) (line 117)? Is it Stefan flow? Grifoll (2013*) included not only Stefan flow in his heat and moisture transport study but also the mechanical dispersion associated with it. He found that this dispersion affected vapor

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flow in the dry layer although the effect on evaporation rate from the soil was small. The physics he described was sound but the effect of dispersion was probably exaggerated because the assumed longitudianal dispersivity was likely too large. Eq. (5) is similar to a differentiated form of Eq. (12) in Grifoll (2013^{*}).

It is well known that the greatest limitation to evaporation from soil is soil hydraulic conductivity (Hanks and Gardner, 1965*; Grifoll, 2013*). For the standard environmental temperature range (10–60° C) both the hydraulic conductivity and soil water retention curves vary significantly with temperature (the former through the viscosity of water and the latter through surface tension; however measured retention curve variations are usually larger than expected from surface tension alone which is not yet understood) Accounting for these temperature variations in actual modeling is not always important (Milly, 1984*). There is no indication whether the temperature dependencies of the hydraulic properties (lines 303–341) are included in the model. For the larger temperature range under surface fire it might be important.

No qualitative indication is given as to how the fire evolved over time (lines 361–374), i.e., for how long the fire burned intensively as in Figure 2. Was there a period in which just glowing ashes existed? It would be useful to the reader to have a feeling for what happened. A time series of photos would be ideal.

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