

Exploration of synthetic terrestrial snow mass estimation via assimilation of AMSR-E brightness temperature spectral differences using the Catchment land surface model and support vector machine regression

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Abstract

This study explores improvements in the estimation of snow water equivalent (SWE) over snow-covered terrain using an ensemble-based data assimilation (DA) framework. The NASA Catchment land surface model is used as the prognostic model in the assimilation of AMSR-E passive microwave (PMW) brightness temperature spectral differences (ΔT_b) where support vector machine (SVM) regression is employed as the observation operator. A series of synthetic twin experiments are conducted using different precipitation boundary conditions. The results show, at times, DA degrades modeled SWE estimates (compared to the land surface model without assimilation) over complex terrain. To mitigate this degradation, a physically-constrained approach using different ΔT_b for shallow-to-medium or medium-to-deep snow conditions along with a “data-thinning” strategy are explored. Overall, both strategies improve the model ability to encapsulate more of the evaluation data and mitigate model ensemble collapse. The physically-constrained DA and 3-day thinning DA strategies show marginal improvements of basin-averaged SWE in terms of reduction of bias from 10 mm (baseline DA) to -5.2 mm and -2.5 mm, respectively. When the estimated forcings are greater than the truth, the baseline DA, physically-constrained DA, and 3-day thinning DA improve SWE the most with approximately 30%, 31%, and 24% reduction of RMSE (relative to OL), respectively. Overall, these results highlight the limited utility of PMW ΔT_b observations in the estimation of snow in complex terrain, but do demonstrate that a physically-based constraint approach and data thinning strategy can add more utility to the ΔT_b observations in the estimation of SWE.

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2 **estimation via assimilation of AMSR-E brightness**
3 **temperature spectral differences using the Catchment**
4 **land surface model and support vector machine**
5 **regression**

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9 **Key Points:**

- 10 • snow estimation
11 • physically-constrained assimilation
12 • data thinning

Abstract

This study explores improvements in the estimation of snow water equivalent (SWE) over snow-covered terrain using an ensemble-based data assimilation (DA) framework. The NASA Catchment land surface model is used as the prognostic model in the assimilation of AMSR-E passive microwave (PMW) brightness temperature spectral differences (ΔT_b) where support vector machine (SVM) regression is employed as the observation operator. A series of synthetic twin experiments are conducted using different precipitation boundary conditions. The results show, at times, DA degrades modeled SWE estimates (compared to the land surface model without assimilation) over complex terrain. To mitigate this degradation, a physically-constrained approach using different ΔT_b for shallow-to-medium or medium-to-deep snow conditions along with a “data-thinning” strategy are explored. Overall, both strategies improve the model ability to encapsulate more of the evaluation data and mitigate model ensemble collapse. The physically-constrained DA and 3-day thinning DA strategies show marginal improvements of basin-averaged SWE in terms of reduction of bias from 10 mm (baseline DA) to -5.2 mm and -2.5 mm, respectively. When the estimated forcings are greater than the truth, the baseline DA, physically-constrained DA, and 3-day thinning DA improve SWE the most with approximately 30%, 31%, and 24% reduction of RMSE (relative to OL), respectively. Overall, these results highlight the limited utility of PMW ΔT_b observations in the estimation of snow in complex terrain, but do demonstrate that a physically-based constraint approach and data thinning strategy can add more utility to the ΔT_b observations in the estimation of SWE.

1 Introduction and Background

Snow is a significant contributor to the Earth’s hydrologic cycle (Liston, 1999), energy cycle (Fernandes et al., 2009), and climate system (Curry et al., 1995; Barnett et al., 2005). It accounts for a large fraction of the available freshwater resources in many parts of the northern hemisphere (Barnett et al., 2005). However, direct quantification of snow mass, or snow water equivalent (SWE), across time and space using point-scale, ground-based techniques remains challenging due to the spatial and temporal variability inherent to snow processes. Land surface models are another approach to estimate SWE across regional and continental scales. However, significant uncertainty is common place in model-derived SWE estimates due to associated model structure error, model forcing error, model parameterization error, and initial condition error (Lynch-Stieglitz, 1994; Dong et al., 2007; R. H. Reichle, 2008; R. H. Reichle et al., 2017).

Alternatively, characterizing the amount of SWE across regional and continental scales has been attempted using remotely-sensed measurements from space-borne instrumentation, primarily in the form of passive microwave (PMW) brightness temperature, T_b , measurements (e.g., Advanced Microwave Scanning Radiometer for EOS; AMSR-E) (Derksen et al., 2005; Dong et al., 2005; Brucker et al., 2011). However, the accuracy of satellite-based SWE retrievals are adversely impacted by snow morphology (Kelly et al., 2003), stratigraphy (Derksen et al., 2005), snow grain size (Armstrong et al., 1993), ice crusts (Rees et al., 2010), depth hoar (Brucker et al., 2011), and sub-grid scale lake effects (Derksen et al., 2010). PMW T_b -based SWE retrievals are also affected by forest and atmospheric attenuation (Wilheit et al., 1980; Derksen et al., 2005; Savoie et al., 2009), signal attenuation in deep snow (Clifford, 2010), and the assumed (quasi-) linear relationship between the electromagnetic response of the snowpack and the physical characteristics of SWE (Chang et al., 1996; Clifford, 2010). Figure 1 shows a simple comparison of *in situ* measurements of snow depth from the SNOwpack TELEmetry (SNOTEL) network along with AMSR-E PMW spectral difference ($\Delta T_{b18V-36V}$, see notations in Equation 1). Although PMW $\Delta T_{b18V-36V}$, in general, captures the accumulation and ablation phase of the snow season, significant high-frequency noise exists and must be carefully considered.

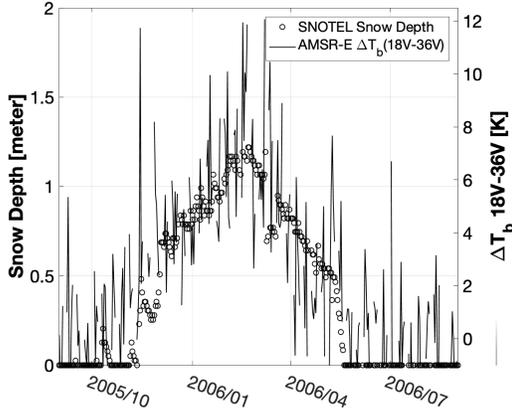


Figure 1. Comparison between AMSR-E $\Delta T_{b18V-36V}$ observations and SNOTEL snow depth measurements for a location in Western Colorado ($40.31^\circ N$, $105.65^\circ W$) from 1 September 2005 to 1 September 2006. Note how ΔT_b captures the general features of snow depth and SWE, but contains more signals (e.g., snow temperature) not related to snow mass as well as the presence of high-frequency noise.

65 Fortunately, data assimilation (DA) is an effective approach to optimally combine
 66 information from both observations and model predictions to generate high-quality es-
 67 timates that are superior to the observations or to the model alone (McLaughlin, 2002;
 68 R. H. Reichle, 2008; Forman & Margulis, 2010; Draper & Reichle, 2015). Instead of as-
 69 assimilating snow retrievals, such as SWE or snow depth (SD), PMW T_b or ΔT_b observa-
 70 tions (spectral differences, computed as the difference between two T_b s, Equation 1) can
 71 be directly assimilated into a land surface model in order to improve model-derived snow
 72 mass estimates. Satellite-based PMW T_b observations are sensitive to snow volume scat-
 73 tering, and therefore, contain snow information applicable during all-weather and night-
 74 time conditions.

75 Multifrequency T_b assimilation was first performed for improvement of point-scale
 76 SWE estimation (Durand & Margulis, 2006). Spectral difference (ΔT_b) was first assi-
 77 milated by Pulliainen (2006) that reduced SWE and SD estimation systematic errors. A
 78 follow-on study conducted by Durand et al. (2009) improved SD estimates via assimi-
 79 lation of vertically-polarized T_b ground-based measurements at 18.7 GHz and 36.5 GHz
 80 over a snow-covered region. Similarly encouraging results were demonstrated for continen-
 81 tal-scale snow storage estimates using T_b assimilation (Kwon et al., 2016, 2017).

82 The studies mentioned above employed a physically-based microwave radiative trans-
 83 fer model (RTM) as the observation operator to map the relevant land surface model state
 84 variables (e.g., SWE or SD) into the corresponding observation space (i.e., T_b). However,
 85 it is difficult to apply a RTM over a large-scale snow region due to the nontrivial com-
 86 putational demand (Kwon et al., 2016). In addition, most global land surface models lack
 87 the fidelity to accurately represent the snow microstructure (e.g., snow grain size, snow
 88 grain shape, internal ice layers) to fulfill the RTM requirements (Kukkonen et al., 2012).
 89 Alternatively, a machine learning technique in the form of physically-constrained sup-
 90 port vector machine (SVM) regression can be employed (Forman et al., 2014; Forman
 91 & Reichle, 2015; Xue & Forman, 2015; Forman & Xue, 2016; Xue & Forman, 2017a, 2017b;
 92 Xue et al., 2018; Kwon et al., 2019; Ahmad et al., 2019). It has been shown that a SVM
 93 was able to accurately capture the temporal and spatial variability in the modeled T_b
 94 or ΔT_b , and thus, holds potential to improve snow estimates across large spatial scales.

95 Recently, Xue et al. (2018) used SVM regression as the PMW ΔT_b observation opera-
 96 tor over North America in the context of snow data assimilation within a land surface
 97 model. Xue et al. (2018) showed improvements in snow mass estimation under certain
 98 conditions such as shallow, dry snow in the absence of forest cover.

99 Despite the improvements in snow estimation via radiance assimilation, there are
 100 still many deficiencies that must be overcome in order to better optimize its use. For ex-
 101 ample, snow mass estimation using PMW radiometry is fundamentally an ill-posed, un-
 102 derdetermined system (Durand & Margulis, 2006). That is, there are numerous combi-
 103 nations of snow depth, snow density, snow temperature, snow grain size, and other snow
 104 characteristics that collectively yield the same ΔT_b observation. Therefore, the task of
 105 assimilating only the snow mass-related portion of the PMW ΔT_b signal from all of the
 106 other signals inherent therein (e.g., vegetation, atmosphere, snow temperature, and snow
 107 liquid water content) is a challenge. In addition, the efficacy of SVM-based PMW ΔT_b
 108 assimilation is often limited by the controllability and reachability of SVM regression (Kwon
 109 et al., 2019). All of these issues motivate this study and help answer the question: How
 110 can we further improve snow estimation with SVM-based PMW ΔT_b assimilation us-
 111 ing a physically-constrained approach? To this end, synthetic AMSR-E PMW ΔT_b ob-
 112 servations are assimilated into the Catchment Land Surface Model (i.e., Catchment) (Koster
 113 et al., 2000) using SVM regression as the observation operator over snow-covered ter-
 114 rain in Russia.

115 Unlike previous works that simultaneously assimilating a fixed number of ΔT_b chan-
 116 nels (Xue et al., 2018; Kwon et al., 2019), *a priori* modeled SWE is used as an indica-
 117 tor to determine which ΔT_b channels should be assimilated into the model. In addition,
 118 a simple “data-thinning” strategy is also explored to help mitigate high-frequency er-
 119 ror (e.g., changes in snow temperature *not* related to snow mass) embedded in the syn-
 120 thetic AMSR-E PMW ΔT_b observations. Given the fact that ground-based snow obser-
 121 vations of sufficient density and quality are not available in the study area, there is no
 122 way to determine the observational baseline for quantifying improvement in snow esti-
 123 mation using real-world measurements. Therefore, a synthetic, identical twin experiment
 124 (R. H. Reichle & Koster, 2003) is employed in this study (further discussion in Section
 125 4) in order to provide a systematic means of evaluating land surface model improvements
 126 via ΔT_b assimilation.

127 2 Study Domain

128 The study domain for this synthetic experiment is the East European Plain span-
 129 ning from 45°N to 64°N and from 30°E to 62°E (Figure 2), which encompasses the Volga
 130 River basin in Russia. The Volga River Basin has an area of 1,390,000 km^2 and occu-
 131 pies about one-third of the East European Plain, and ultimately discharges into the Caspian
 132 Sea. The main parts of the basin as delineated in Figure 2 are the upper Volga basin (430,000
 133 km^2), the Moskva Oka River basin (237,000 km^2), the Kama River basin (500,000 km^2),
 134 and the lower Volga River basin (223,000 km^2). The relatively large size of the study
 135 region allows for an investigation across a range of regional and snow climatologies. The
 136 upper and middle parts of the basin are covered by forest and steppe; the lower part of
 137 the basin is covered by steppe and desert. The mean annual temperature increases from
 138 the north (approximately 3°C) to the south (approximately 9°C), whereas annual pre-
 139 cipitation decreases from 750 to 150 mm in the same direction. Average depth of snow
 140 cover decreases from 60 cm in the north to about 3 cm in the south and the duration
 141 of its persistence is from 240 to 30 days moving from the north to south (Golosov & Belyaev,
 142 2016; Sidorchuk et al., 2009).

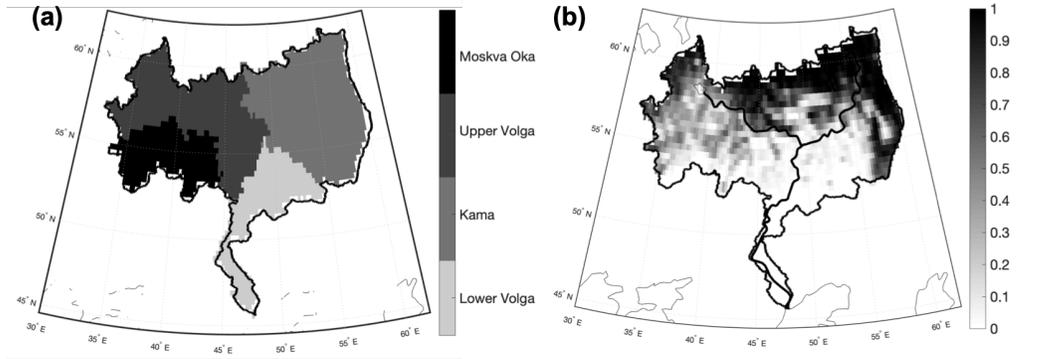


Figure 2. General maps of (a) Volga Basin and four sub-basins (Moskva Oka river basin, upper Volga river basin, lower Volga river basin, and Kama river basin) and (b) forest cover fraction as derived from the Moderate Resolution Imaging Spectroradiometer (Friedl et al., 2002).

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3 Prognostic Land Surface Model

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Following Xue et al. (2018), this work employs the Catchment Land Surface Model (a.k.a. Catchment) (Koster et al., 2000). The basic modeling unit in Catchment is based on the topographic statistics of each hydrologic catchment (or watershed) forced by gridded meteorological forcings that serve as the model boundary conditions (Zaitchik et al., 2008; Kumar, Zaitchik, et al., 2016). Catchment employs three prognostic variables (i.e., surface excess, root zone excess, and catchment deficit) in order to account for soil moisture and shallow groundwater. Snow conditions on the land surface, including snowpack consolidation and metamorphosis, are represented with a three-layer snow model (Stieglitz et al., 2001). One hydraulic limitation in Catchment is the lack of surface water impoundments (e.g., lakes and rivers) along with that of dynamic river routing. In the absence of these hydrologic processes, however, Catchment remains an excellent testbed to explore methods related to the remote sensing and modeling of terrestrial snow.

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In the present study, the spatial resolution of the model grid is 25 km on an Equal Area Scalable Earth (EASE version 2) grid (M. J. Brodzik et al., 2012). Realistic initial conditions in the subsurface are generated by looping the model five times over the same 10-year period from 1 September 1992 to 1 September 2002. The model is then initialized and propagated forward from 1 September 2002 in order to initialize the model with minimized initial snowpack and runoff errors. The experiment period covers 1 September 2002 to 1 September 2011, which coincides with the majority of the AMSR-E observation record that is used to train the SVM-based observation operator that is subsequently used to generate the synthetic ΔT_b observations used during assimilation (see section 4.1).

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4 Synthetic Identical Twin Experiment Setup

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As mentioned in section 1, the lack of available *in-situ* snow, soil moisture, groundwater, and runoff observations in the study region necessitates the use of a simulated version of the synthetic “truth” that serves as a reasonable proxy for the real-world system variability. The synthetic experiment starts with the generation of a synthetic “truth” followed by the generation of synthetic observations (section 4.1). Next, synthetic observations are assimilated (section 4.4) into a degraded version of the same modeling system that is forced by a different (imperfect) set of meteorological boundary conditions (section 4.3).

This type of synthetic experiment is often referred to as an “identical” twin in the sense that the same land surface model is used in all aspects of the experiment. The use of an identical twin implicitly assumes that the majority of errors encountered by a “real-world” system arise from the boundary conditions rather than from the model structure errors, parameter errors, or initial condition errors (Günther et al., 2019). In the context of snow modeling, this assumption is reasonable given the large degree of precipitation error are often found in remote, mountainous terrain such as that as the Volga basin (Rasmussen et al., 2012). Alternatively, a “fraternal” twin could be employed in which different land surface models are used during different phases of the experiment, but this is avoided in this current study in order to focus on model improvements to terrestrial snow (and its subsequent ablation and runoff) associated with erroneous precipitation in the terrestrial environment. The following discussion highlights the different components used in the synthetic identical twin experimental setup.

4.1 Synthetic Truth and Synthetic Observations

The synthetic “truth” is a single replicate simulated by Catchment using boundary conditions defined by the Modern-Era Retrospective analysis for Research and Applications, version 2 (MERRA-2) product with an hourly temporal resolution and $0.5^\circ \times 0.625^\circ$ (latitude/longitude) spatial resolution (Gelaro et al., 2017). Hydrologic states and fluxes, including SWE, snow depth, soil moisture, runoff, and surface energy fluxes, from the synthetic “truth” simulation serve as the best Catchment-based representation of the natural environment. It is important to note that the “truth” need not identically match the observed reality. Rather, the “truth” needs to adequately capture the space-time variability of the real-world system.

The synthetic “truth” ΔT_b s are generated using a well-trained SVM (see Appendix A) that maps relevant model states (e.g., SWE, snow temperature) derived from the synthetic truth into the corresponding observation space (i.e., ΔT_b). The synthetic ΔT_b truth, including spectral difference between 10.65 and 36.5 GHz, 10.65 and 18.7 GHz, and 18.7 and 36.5 GHz for both horizontal and vertical polarization (Xue & Forman, 2015, 2017a, 2017b; Xue et al., 2018), is easily expressed as:

$$\Delta T_{b18V-36V} = T_{b18V} - T_{b36V} \quad (1)$$

where T_{b18} represents T_b at 18.7 GHz; T_{b36} represents T_b at 36.5 GHz; and the subscript V represents vertical polarization with a similar equation for horizontal (H) polarization.

The synthetic ΔT_b observations, including $\Delta T_{b10H-36H}$, $\Delta T_{b10V-36V}$, $\Delta T_{b10H-18H}$, $\Delta T_{b10V-18V}$, $\Delta T_{b18H-36H}$, and $\Delta T_{b18V-36V}$, are generated by corrupting the synthetic ΔT_b truth through the inclusion of additive, Gaussian observation noise that is temporally and spatially uncorrelated. The observation noise is assumed to be Gaussian-distributed with zero mean and a standard deviation of 3 K (Burgers et al., 1998; Durand & Margulis, 2007; Kwon et al., 2016; Xue et al., 2018).

4.2 Boundary Condition Correction

Meteorological boundary conditions (a.k.a., forcings) are an important component for snow model simulations in the context of a synthetic, identical twin experiment. Therefore, it is critical to first characterize the boundary condition (precipitation) errors. Boundary condition errors often result in bias or random errors that can be considered representative of the “real-world” errors that could be encountered in an operational assimilation system (Günther et al., 2019). Precipitation (snow) measurement errors frequently range from 20% to 50% in windy conditions (Clifford, 2010). Hence, an error characterization strategy is employed here such that the difference between MERRA-2 forcings (synthetic truth) and GLDAS forcings used in both the open loop (section 4.3) and data assimilation (section 4.4) runs serves as a reasonable proxy for a range of plausible pre-

Table 1. Summary of GLDAS precipitation correction factor γ

Forcing	Neutral	Positively-biased	Negatively-biased
γ	1.9	2.9	1.0

224 precipitation error scenarios. That is, the cumulative, domain-averaged GLDAS precipita-
 225 tion over the study period is rescaled to match 50% (negatively-biased), 100% (neutral),
 226 and 150% (positively-biased) of the MERRA-2 precipitation by multiplying a fixed factor
 227 (γ , Table 1) computed as:

$$228 \quad \gamma = \frac{\alpha \times \sum Precipitation_{(MERRA-2)}}{\sum Precipitation_{(GLDAS)}} \quad (2)$$

229 where $\sum Precipitation_{(MERRA-2)}$ and $\sum Precipitation_{(GLDAS)}$ are the cumulative, domain-
 230 averaged MERRA-2 and GLDAS precipitation over the course of the entire study pe-
 231 riod, respectively, where α set to 50%, 100% , and 150% to yield the rescaled GLDAS
 232 scenarios for negatively-biased, neutral, and positively-biased relative to MERRA-2 (syn-
 233 thetic truth) precipitation, respectively.

234 These three different scenarios will help explore how data assimilation can improve
 235 terrestrial snow estimation where the total amount of precipitation in the study domain
 236 is over-, well-, or under-estimated. In addition, the shortwave and longwave radiation
 237 boundary conditions are also rescaled proportionally (not shown). This last step is con-
 238 ducted in order to more carefully focus on the first-order control of precipitation (and
 239 its error) on snow mass assimilation.

240 As shown in Figure 3a) and 3b), there is a strong precipitation gradient from the
 241 north to south across the study domain where the highest precipitation is in the north-
 242 west of the domain for both MERRA-2 and GLDAS. Under the positively-biased sce-
 243 nario (Figure 3d), the “true” precipitation (i.e., MERRA-2) is less than the precipita-
 244 tion forcing field used in both OL and DA (i.e., positively-biased precipitation) with a
 245 gradient from the southeast to northwest. A similar pattern is seen for the negatively-
 246 biased scenario (Figure 3e) but with more “true” precipitation relative to the OL and
 247 DA precipitation. Even though the 9-year cumulative amount of precipitation across the
 248 domain is identical between MERRA-2 and the neutral precipitation scenarios, differ-
 249 ences still exist at different locations between these two data sets as shown in Figure 3f).
 250 As a result, the amount of SWE could be significantly different at different locations due
 251 to the nonlinear hydrologic response of forcing even though the domain-averaged pre-
 252 cipitation is identical between the two.

253 4.3 Ensemble Open Loop

254 As mentioned previously, an ensemble open-loop (OL) simulation is conducted with-
 255 out the assimilation of synthetic observations. The “imperfect” boundary conditions are
 256 established using the Global Land Data Assimilation System (GLDAS) product with 3-
 257 hourly temporal and $2.0^\circ \times 2.5^\circ$ (latitude/longitude) spatial resolution (Rodell et al.,
 258 2004). In this study, the difference between the “truth” and the OL ensemble mean is
 259 representative of the system errors. One key in the success of data assimilation (section 4.4)
 260 is the appropriate characterization of both model and observation errors (R. H. Reichle,
 261 2008; Kumar, Dong, et al., 2016). An ensemble of perturbations is generally applied to
 262 the forcing variables (e.g., precipitation) as a low-rank approximation of the true sys-
 263 tem errors. The ensemble mean of the model states is typically used as the expected model
 264 estimate and the ensemble spread is used as a proxy for the model error variance (Houtekamer
 265 & Mitchell, 1998; Burgers et al., 1998). In line with previous work (Xue et al., 2018),
 266 the perturbation settings used in this study are summarized in Table 2.

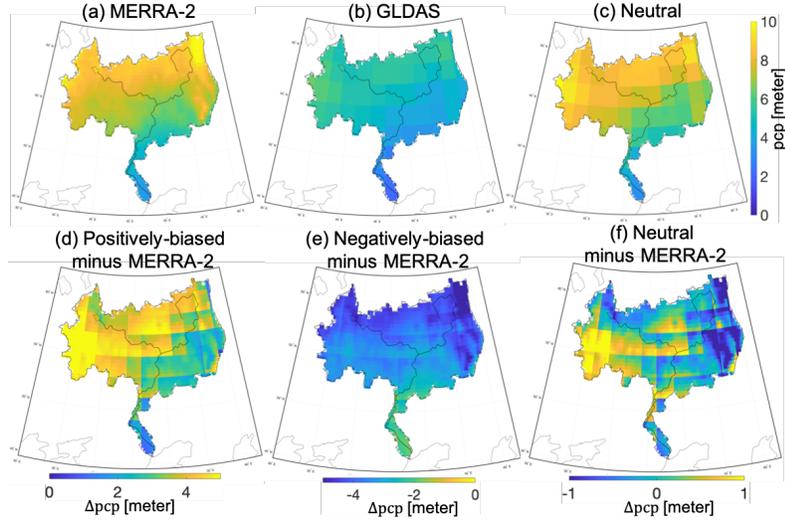


Figure 3. Cumulative precipitation (pcp [m]; from years 2002 to 2011): (a) MERRA-2 precipitation, (b) GLDAS precipitation, (c) neutral precipitation, (d) positively-biased minus MERRA-2 precipitation, (e) negatively-biased minus MERRA-2 precipitation, and (f) neutral minus MERRA-2 precipitation.

Table 2. Parameters for meteorological forcings perturbation in the assimilation experiments

Model Variables	Type	Standard Deviation	x, y_{corr}	t_{corr} (day)	Cross-correlation		
					pcp	sw	lw
pcp	M ^a	0.5	2°	3	NA	-0.8	0.5
sw	M	0.3	2°	3	-0.8	NA	-0.5
w	A ^b	20 W m ⁻²	2°	3	0.5	-0.5	NA

^aMultiplicative (M) or ^bAdditive (A) perturbations are applied to precipitation (pcp), downwelling shortwave radiation (sw), downwelling longwave radiation (lw). Spatial correlations are indicated as x, y_{corr} and temporal correlations as t_{corr} .

4.3.1 Ensemble Size

With a small ensemble size, only a small subset of the error space is sampled, and thus, the statistical (or sampling) error is non-negligible (Keppenne, 2002; R. Reichle et al., 2002; Evensen, 2003). The ensemble size, in part, dictates whether or not the relevant part of the error structure (e.g., error variance) can be captured by the finite ensemble size of model trajectories. In this study, a range of ensemble sizes from $N = 14$ to $N = 74$ was tested. An ensemble size of $N = 24$ is ultimately chosen because $N > 24$ show no significant change in the ensemble spread (i.e., the ensemble SWE standard deviation over the study domain) compared to $N = 24$. Therefore, it is assumed an ensemble size of 24 replicates could reasonably represent the low-rank approximation of the true error probability distribution.

4.4 Data Assimilation

An existing, one-dimensional (1-D) ensemble Kalman filter (EnKF) framework (R. H. Reichle & Koster, 2003; R. H. Reichle et al., 2010) is employed for daily, synthetic AMSR-E ΔT_b assimilation in this study. In a 1-D EnKF, the computational units are processed independently from one another, which suggests that spatial error correlations between different catchments within the study domain are negligible (R. H. Reichle & Koster, 2003). Only the essential details of the EnKF are discussed here. Further information regarding the EnKF equations can be found in R. H. Reichle et al. (2002).

The EnKF alternates between an ensemble forecast step and an update step. During the forecast step, an ensemble of model state vectors containing the relevant model prognostic variables (e.g., SWE) are propagated forward in time by Catchment. Using the available synthetic ΔT_b observations y_t at time t , the prior state vector, x_t^{i-} , is updated to a new value, x_t^{i+} , based on the relative uncertainties between the state vector (SWE in this particular study) and the predicted observation using appropriate weights expressed in the Kalman gain K_t (R. H. Reichle et al., 2001; Zaitchik et al., 2008; Kumar, Zaitchik, et al., 2016) via:

$$x_t^{i+} = x_t^{i-} + K_t(y_t + v^i - \phi_t(x_t^{i-})), v \sim \mathcal{N}(0, 3^2) \quad (3)$$

where v^i represents the representativeness errors that are assumed here to be Gaussian with zero mean and a spatially- and temporally-uncorrelated covariance of $3^2 K^2$; $\phi_t(\cdot)$ is the SVM-based observation operator that maps the model states (e.g, SWE, SLWC) into ΔT_b observation space (see Appendix A); and i represents a single replicate drawn from the ensemble of size $N = 24$. The superscripts $-$ and $+$ refer to the *a priori* state vector and *a posteriori* state vector, respectively. K_t is the Kalman gain matrix and can be computed as:

$$K_t = C_{x_t y_t}^- [C_{y_t y_t}^- + R]^{-1} \quad (4)$$

where $C_{x_t y_t}^-$ is the error cross-covariance between the modeled SWE estimates and the SVM-based ΔT_b prediction prior to the update; $C_{y_t y_t}^-$ is the error covariance (a.k.a., sample covariance) of the SVM-based ΔT_b prediction prior to the update; and R is the observation error variance.

4.4.1 Observation Operator and SVM Controllability

It is important to highlight the issue of controllability with the SVM-based observation operator (see Appendix A) (Kwon et al., 2019). As an important factor in optimal control theory, controllability demonstrates the skill of a linear or nonlinear model to guide the model output from any physical plausible initial state towards any physically plausible final state over a finite time period (Ogata & Yang, 2002). That is, the system output for a controllable system can be changed by changing the system input (Gelb, 1974). In the context of data assimilation, controllability of the SVM-based observation operator is critical during the analysis update. The reason is that one of the

Table 3. Descriptions of different ΔT_b data assimilation strategies

Name	Description
baseline DA	Simultaneous assimilation of six ΔT_b channels including: $\Delta T_{b10H-18H}$, $\Delta T_{b10V-18V}$, $\Delta T_{b10H-36H}$, $\Delta T_{b10V-36V}$, $\Delta T_{b18H-36H}$, and $\Delta T_{b18V-36V}$
physically-constrained DA	Update SWE based on prior SWE ensemble mean : If $SWE \leq 120$ [mm], use $\Delta T_{b10H-36H}$, $\Delta T_{b10V-36V}$, $\Delta T_{b18H-36H}$, and $\Delta T_{b18V-36V}$ If $SWE > 120$ [mm], use $\Delta T_{b10H-36H}$, $\Delta T_{b10V-36V}$, $\Delta T_{b10H-18H}$, and $\Delta T_{b10V-18V}$
3-day thinning DA	Simultaneous assimilation of six ΔT_b channels every 3 days including: $\Delta T_{b10H-18H}$, $\Delta T_{b10V-18V}$, $\Delta T_{b10H-36H}$, $\Delta T_{b10V-36V}$, $\Delta T_{b18H-36H}$, and $\Delta T_{b18V-36V}$

316 assumptions behind the SVM-based DA framework is that model errors predominately
317 correlate back to errors in the SVM-based ΔT_b predictions (Kwon et al., 2019). An “un-
318 controllable” SVM is insensitive to changes in the inputs, and thus, leads to the collapse
319 of the ensemble of SVM-based ΔT_b predictions (Kwon et al., 2019). Controllability is
320 related to the set of training data and the inability of the SVM to accurately predict snow
321 ΔT_b when the given inputs that are outside of the prediction space implicit in the train-
322 ing data (Ahmad et al., 2019). As a result, the model error would no longer correlate
323 back to the corresponding error in the SVM-based observation operator, which can lead
324 to spurious error correlations that ultimately degrade the model estimate (Kwon et al.,
325 2019). To avoid this, prior SWE is updated only when the standard deviation of the prior
326 SVM-predicted ΔT_b is greater than 0.05 K based on heuristics outlined in Kwon et al.
327 (2019).

328 It is worth noting that there is no DA performed around water bodies. This is due
329 to that fact that grid cells with more than 5% coverage by water (ocean or inland wa-
330 ter bodies) are excluded from the data assimilation analysis because surface water im-
331 poundments are not explicitly accounted for in the Catchment model. Therefore, grid
332 cells containing surface impoundments are not included in the EnKF update.

333 4.4.2 *Shallow-to-Medium versus Medium-to-Deep Snow Algorithm*

334 Following the methods of Xue et al. (2018) and Kwon et al. (2019), the DA exper-
335 iments start with simultaneous assimilation of six different ΔT_b s, including $\Delta T_{b10H-18H}$,
336 $\Delta T_{b10V-18V}$, $\Delta T_{b10H-36H}$, $\Delta T_{b10V-36V}$, $\Delta T_{b18H-36H}$, and $\Delta T_{b18V-36V}$ (baseline DA;
337 Table 3) in this study. However, these studies demonstrated that DA, at times, could
338 degrade the snow estimation (also see section 7.1). To prevent DA degradation, a physically-
339 constrained DA approach (section 4.4.2) and a data thinning DA approach (section 4.4.3)
340 are introduced.

341 An important assumption behind spectral difference assimilation is that ΔT_b is posi-
342 tively correlated with SWE and that the T_b at the highest frequency (i.e., 36.5 GHz)
343 decreases as SWE increases while the lower frequency (i.e., 10.65 GHz or 18.7 GHz) T_b
344 is relatively insensitive to increasing snow mass (Kim & England, 2003; Derksen et al.,
345 2010). However, the correlation between SWE and T_b at 36.5 GHz can reverse once SWE
346 is greater than 100 to 200 mm (Schanda et al., 1983; Seve et al., 1986; Mätzler, 1994;
347 Derksen, 2008; Derksen et al., 2010; Kwon et al., 2019). This occurrence is often referred
348 to as signal saturation. Furthermore, ΔT_{b10-18} may introduce errors during shallow snow
349 conditions because the signal is more representative of the soil moisture rather than the
350 snow mass (Roy et al., 2013). In other words, the observation error covariance of ΔT_{b18-36}
351 during deep snow conditions or ΔT_{b10-18} during shallow snow conditions may not be ad-
352 equately represented by the prescribed error parameters, and hence, may introduce spu-

353 rious errors during the EnKF update. If an observational data set contains data whose
 354 errors are not well represented by the prescribed error parameters, the EnKF will not
 355 be able to accurately estimate the true fields (R. H. Reichle, 2008). Therefore, one hy-
 356 pothesis for DA degradation in the snow estimates is due to the simultaneous assimila-
 357 tion of all six ΔT_b when many of the ΔT_b s are not truly representative of snow mass.
 358 Further, the presence of signal saturation during deep snow conditions also result in a
 359 degraded estimate when the general assumption that ΔT_b is positively correlated with
 360 SWE is no longer the case.

361 Instead of simultaneously assimilating all available multifrequency and polariza-
 362 tion spectral differences into a land surface model as done in the works of Xue et al. (2018)
 363 and Kwon et al. (2019), a new assimilation strategy based on prior SWE information is
 364 explored here such that ΔT_b is assimilated more selectively. In this new approach, the
 365 ensemble mean of the prior SWE is used as an indicator to determine which ΔT_b should
 366 be assimilated. That is, shallow-to-medium snow conditions now only utilize $\Delta T_{b18H-36H}$,
 367 $\Delta T_{b18V-36V}$, $\Delta T_{b10H-36H}$, and $\Delta T_{b10V-36V}$ whereas medium-to-deep snow conditions
 368 now only simultaneously utilize $\Delta T_{b10H-18H}$, $\Delta T_{b10V-18V}$, $\Delta T_{b10H-36H}$, and $\Delta T_{b10V-36V}$
 369 (physically-constrained DA; Table 3). The SWE threshold used to differentiate between
 370 the shallow-to-medium and medium-to-deep snow is somewhat subjective. In this study,
 371 the shallow-to-medium snow refers to $SWE \leq 120$ [mm] while $SWE > 120$ [mm] is consid-
 372 ered as the medium-to-deep snow based on peer-reviewed literature (Matzler et al., 1982;
 373 Mätzler, 1994; De Sève et al., 1997).

374 4.4.3 Data Thinning

375 Another common issue with snow ΔT_b assimilation is ensemble collapse (i.e., lit-
 376 tle or no ensemble spread) (Figure 4). Ensemble collapse results in an under-representation
 377 of the true model uncertainty. Given the fact the optimal combination of the observa-
 378 tions with the model is predicated on the consideration of the respective uncertainties
 379 of each (R. H. Reichle et al., 2008), a poor representation of model uncertainty will of-
 380 ten lead to degraded snow estimation.

381 Ensemble collapse, in part, is exacerbated by the multi-observation nature of the
 382 assimilation approach (i.e., multiple observations assimilated daily). In addition, the high-
 383 frequency errors embedded in the AMSR-E observations (Figure 1) often overwhelm the
 384 snow-related information, and thus, can further degrade DA performance. In an attempt
 385 to mitigate such high-frequency noise, the synthetic ΔT_b observations (all six channels)
 386 are assimilated every 3-, 5-, 7-, 10-, and 15-day intervals rather than daily in order to
 387 explore the impact of using fewer observations on DA performance (Table 3).

388 5 Normalized Innovation and Filter Optimality Assessments

389 The optimal operation of the Kalman filter is closely related to the statistical prop-
 390 erties of the innovation sequence, which is the difference between the observation and
 391 model forecast (R. H. Reichle & Koster, 2002). In theory, the information exchange dur-
 392 ing the filter update is optimal when the normalized innovation sequence appears as white
 393 noise (i.e., mean zero with unit variance and temporally uncorrelated). If the models are
 394 unbiased and linear (both the land surface model and the observation operator) and all
 395 errors are uncorrelated and Gaussian (and correctly specified), then the normalized in-
 396 novation sequence, NI , should appear similar in form to a standard normal distribution
 397 $\mathcal{N}(0, 1)$ (R. H. Reichle & Koster, 2002). Although both the land surface model and ob-
 398 servation operator used here are nonlinear, the investigation of the normalized innova-
 399 tion sequence can still provide useful information as to the performance of the DA pro-
 400 cedure.

The normalized innovation (NI) at time t can be written as:

$$NI_t = \frac{y_t - \phi_t(x_t^-)}{\sqrt{C_{y_t y_t} + R}} \quad (5)$$

where the numerator is the difference (or innovation) between the synthetic ΔT_b observation (y_t) and SVM-based predicted (prior) ΔT_b observation ($\phi_t(x_t^-)$), and the denominator is the square root of the sum of the background error covariances ($C_{y_t y_t}$) and the observation error covariance (R). The normalized innovation sequence is merely the vector concatenation of all NI_t across the duration of the assimilation experiment that is explored for mean zero, unit variance, temporally-uncorrelated Gaussian-like features that can be used as a proxy for filter optimality.

6 Validation Approach

A synthetic, identical twin experiment is designed such that the “true” values of hydrologic states and fluxes are known. Therefore, the validation is performed against the true states (e.g., SWE) derived from the synthetic truth run. Several goodness-of-fit statistics are used for the validation activities: (1) bias, (2) root mean squared error (RMSE), (3) unbiased root mean squared error (ubRMSE), (4) correlation coefficient (R), (5) Nash-Sutcliffe efficiency (NSE), and (6) containing ratio ($CR_{2\sigma}$). In addition, normalized information contribution (NIC) is used to quantify the DA improvement (or degradation) relative to the OL (Kumar et al., 2009, 2014). Details about all of these calculations can be found in Appendix B.

7 Results and Discussion

7.1 SWE Estimates

The DA experiments started with simultaneous assimilation of six different ΔT_b s, including $\Delta T_{b10H-18H}$, $\Delta T_{b10V-18V}$, $\Delta T_{b10H-36H}$, $\Delta T_{b10V-36V}$, $\Delta T_{b18H-36H}$, and $\Delta T_{b18V-36V}$. For illustrative purposes, two relatively ideal locations, Grid #1 and Grid #2, (i.e., long snow season; relatively dry snow conditions; no forest cover; and relatively shallow snow such that $SWE_{max} < 200$ mm) are selected. Given the fundamental physics of PMW T_b remote sensing of snow, if assimilation does not work at these idealized locations (assuming appropriate specification of input error parameters), then assimilation will likely not work at other locations in the Volga basin. Therefore, we chose to present these locations prior to discussing results across the remainder of the basin.

Figure 4 highlights the performance of DA (denoted as baseline DA as shown in blue) at these idealized locations under the neutral forcing conditions. As shown in Figure 4a) and 4b), simultaneous assimilation of all six ΔT_b channels actually degraded model SWE estimates. Starting in late-January 2010 (Figure 4a), the DA SWE estimates diverged from the OL (gray color) and the synthetic truth (black dots). This divergence resulted in degraded SWE estimates with approximately 82%, 80%, and 85% increases in RMSE, bias, and ubRMSE, respectively, relative to the OL. Similarly, the baseline DA SWE estimates at Grid #2 also diverged from the synthetic truth early in the snow season (Figure 4b) such that the DA routine was unable to recover.

The following sections will discuss whether the physically-constrained DA or the data thinning strategy could serve as a feasible solution in preventing filter divergence, and hence, DA degradation while assimilating PMW ΔT_b s.

7.1.1 *Shallow-to-Medium versus Medium-to-Deep Snow Algorithm*

As shown in Figure 4a), the new assimilation strategy (denoted as physically-constrained DA, red color) improved the Grid #1 SWE estimates with a 58%, 80%, and 41% reduc-

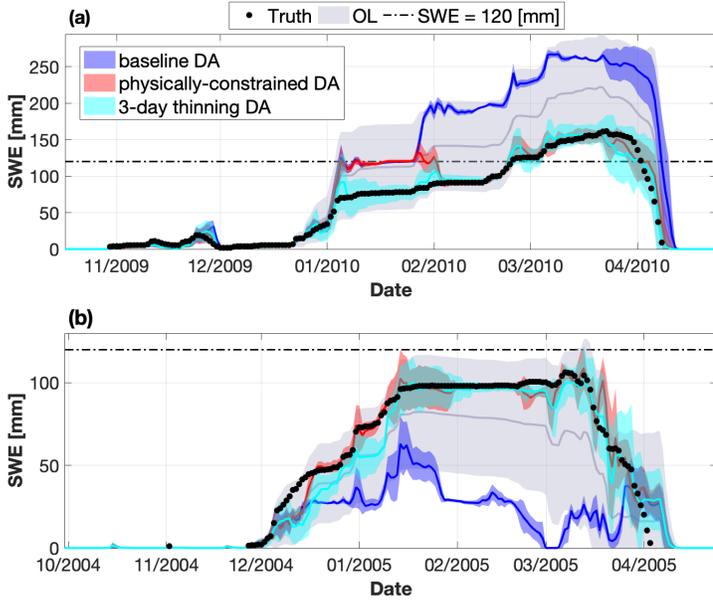


Figure 4. Example time series of snow water equivalent (SWE) for (a) Grid #1 (54.1685° N, 47.3343° E) from October 2009 to May 2010 and (b) Grid #2 (49.1489° N, 54.0778° E) from October 2004 to May 2005. Physically-constrained DA and data thinning (3-day) improve model results whereas baseline DA (no physical constraint) actually degrades model results relative to the open loop.

446 tion in RMSE, bias, and ubRMSE, respectively, relative to the OL. Starting in late-January
 447 2010 (SWE \approx 120 mm), the physically-constrained DA converged toward the synthetic
 448 truth (black dots) and was able to encapsulate more of the synthetic truth resulting in
 449 a larger containing ratio, $CR_{2\sigma}$ (0.26) than the baseline DA ($CR_{2\sigma} = 0.10$) (see Ap-
 450 pendix B). These results suggest that the physically-based shallow-to-medium versus medium-
 451 to-deep snow algorithm effectively mitigated much of the negative influence of spurious
 452 correlations between SWE and ΔT_{b18-36} during deep snow conditions. Figure 4b) fur-
 453 ther illustrates the benefits of the physically-constrained shallow-to-medium versus medium-
 454 to-deep snow algorithm during the shallow snow conditions.

455 As shown in Figure 5a) and 5b), the correlation coefficient (R) between the syn-
 456 thetic truth SWE and SVM-based synthetic ΔT_{b10-18} observations for Grid #2 was 0,
 457 whereas the correlation coefficients between the synthetic truth SWE and SVM-based
 458 synthetic ΔT_{b10-36} (Figure 5c, 5d) and ΔT_{b18-36} (Figure 5e, 5f) observations were greater
 459 than 0. This implies that ΔT_{b10-18} contained little or no information about shallow snow
 460 conditions (i.e., SWE \leq 120 mm) given the fact that both 10 GHz and 18 GHz undergo
 461 little or no scattering across such a shallow snow pack (Durand & Margulis, 2006). That
 462 is, these T_b frequencies (and ΔT_b by construct) are effectively transparent through such
 463 shallow snow. After removing ΔT_{b10-18} from the observation vector, the physically-constrained
 464 DA (red color) was able to correct the model SWE estimates towards the synthetic truth
 465 (black dots) during the middle of December 2004, which resulted in a 24%, 92%, and 24%
 466 reduction in RMSE, bias, and ubRMSE, respectively, relative to the OL. Further, the
 467 $CR_{2\sigma}$ was increased from 0.04 (baseline DA) to 0.29 (physically-constrained DA), which
 468 suggested the physically-constrained DA was superior to the more uniformed, baseline
 469 approach.

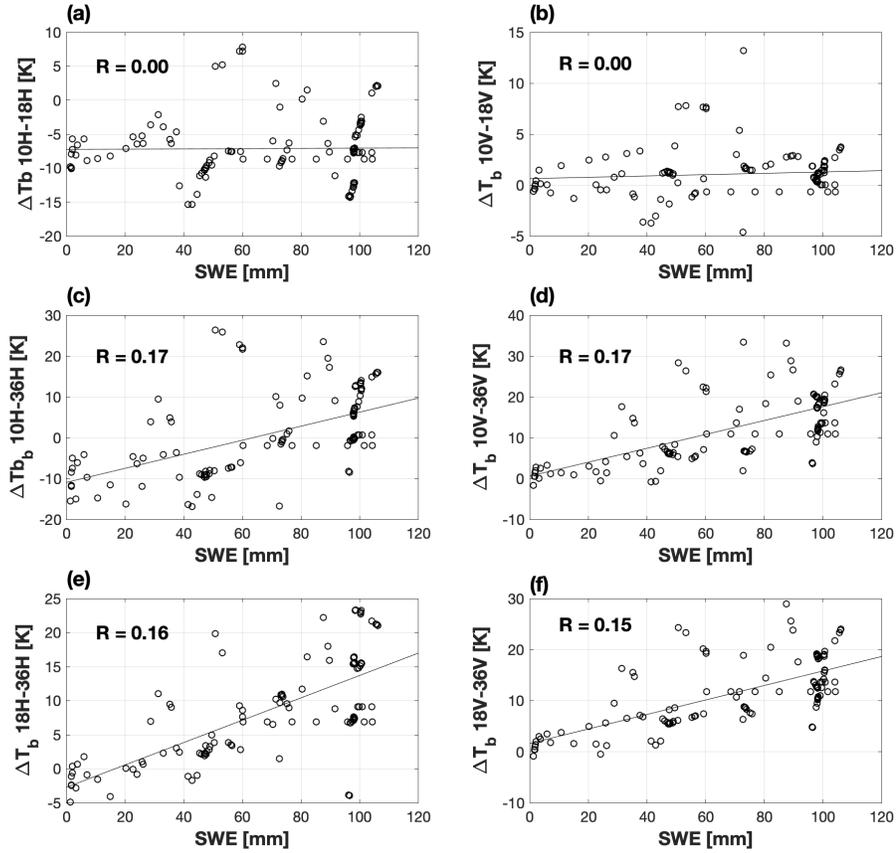


Figure 5. Scatter plots (with correlation in upper-left corner) between the synthetic truth SWE and the SVM-based brightness temperature spectral difference (ΔT_b) for (a) 10H – 18H, (b) 10V – 18V, (c) 10H – 36H, (d) 10V – 36V, (e) 18H – 36H, and (f) 18V – 36V estimates for Grid #2 (49.1489° N, 54.0778° E) from 1 September 2002 to 1 September 2011.

470 However, such a strategy is far from a panacea and is only effective at some loca-
 471 tions. One possible reason is that if the prior SWE estimate is incorrect, it is possible
 472 the spectral differences used in the update are not the most appropriate. As an alter-
 473 native, information from the observations can be used directly to help guide which of the
 474 ΔT_b s to assimilate into model at a given point in time and space. For example, if ΔT_{b18-36}
 475 observation suggests the spectral difference is nearing saturation, then one can assim-
 476 ilate the longer wavelengths as ΔT_{b10-18} . This approach will be explored in a future study
 477 and is considered beyond the current project scope.

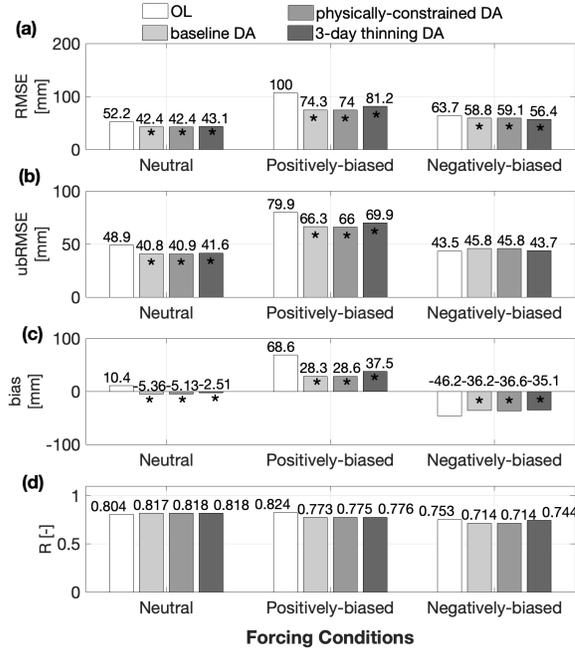


Figure 6. Histograms of Volga basin-averaged SWE statistics showing (a) RMSE, (b) ubRMSE, (c) bias, and (d) R under the neutral (first set), positively-biased (second set), and negatively-biased (third set) forcing conditions. The white bar is for the Open Loop (OL). The light gray bar is for baseline DA. The medium gray bar is for physically-constrained DA and the dark gray bar is for DA 3-day thinning as listed in Table 3. Bars marked with * indicate DA yields statistically significant statistics with a level of significance of 5%.

478 As shown in Figure 6, the Volga basin-averaged results suggested the physically-
 479 constrained DA (bias = -5.1 mm; R = 0.818) showed limited improvements in SWE es-
 480 timation over the baseline DA (bias = -5.4 mm; R = 0.817) under the neutral forcing
 481 conditions. Similarly, the $CR_{2\sigma}$ increased from 0.24 (baseline DA) to 0.25 (physically-
 482 constrained DA). Over 57% of the basin grids had improved $CR_{2\sigma}$. The SWE ensemble
 483 spread (σ), which was defined as the long-term time-average of the instantaneous en-
 484 semble standard deviation, was also changed from 3.33 mm (baseline DA) to 3.56 mm
 485 (physically-constrained DA), which suggested the physically-constrained DA effectively
 486 inflated the ensemble spread, and had better ability to capture more of the synthetic truth.
 487 All these results suggest that the physically-constrained DA marginally improved the ac-
 488 curacy of SWE estimation relative to the baseline DA under the neutral forcing condi-
 489 tions.

Table 4. Domain-averaged SWE Statistics for DA thinning experiments from 1 September 2002 to 1 September 2011 under the neutral forcing conditions

Statistics	OL	DA baseline	DA thinning 3-day	DA thinning 5-day	DA thinning 7-day	DA thinning 10-day	DA thinning 15-day
RMSE [mm]	52	42	43	44	45	46	47
ubRMSE [mm]	49	41	42	43	43	44	45
bias [mm]	10	-5.4	-2.5^a	-0.73	0.16	1.3	3.6
CR _{2σ}	0.30	0.25	0.26	0.27	0.28	0.28	0.28

Bold^a number indicates which experiment yields statistically significant statistics with a level of significance of 5%.

7.1.2 Data Thinning

An example of data thinning to once every three days (cyan color) for Grid #1 under the neutral forcing conditions is shown in Figure 4a). SWE estimates were improved with a 80%, 98%, and 70% reduction in RMSE, bias, and ubRMSE, respectively, relative to the OL. CR_{2 σ} increased from 0.055 (OL) to 0.25 implying that using fewer observations in time during the DA update can help better capture the synthetic truth. In addition, the SWE ensemble spread increased from 1.86 mm (baseline DA) to 3.02 mm (3-day thinning DA), but was significantly less than the OL (9.79 mm). The bigger SWE ensemble spread indicated the 3-day thinning DA effectively prevented ensemble collapse from January to February. The 3-day thinning strategy also significantly improved SWE estimates for Grid #2 as shown in Figure 4b). The 3-day thinning strategy helped prevent SWE divergence in December 2004, and as a result, yielded a 50%, 72%, and 25% reduction in RMSE, bias, and ubRMSE, respectively, relative to the OL. As a measure of the standard deviation of the errors, the decrease in ubRMSE suggested that the data thinning strategy effectively mitigated some of the introduction of high-frequency noise (random error) at both locations.

The Volga basin-averaged results under the neutral forcings are summarized in Table 4. SWE RMSE increased from 43 mm to 47 mm as fewer observations were assimilated into the model from once a day to every 15 days. This corroborated the earlier results that synthetic assimilation indeed added utility to the model; in the absence of assimilation (i.e., if data thinning approached an infinite amount of time) the results would revert back to the original OL results. Further, there was no statistically significant difference between the baseline DA RMSE and 3-day thinning DA RMSE. In aggregate, these results suggest assimilating the synthetic ΔT_b every 3 days yielded the same amount of SWE errors with daily assimilation.

As fewer observations were assimilated beyond every 3 days, ubRMSE increased from 41 mm (baseline DA) to 45 mm (15-day thinning DA) indicating that assimilating the noisy observations every few days did not help mitigate the random noise embedded in the synthetic ΔT_b observations. The bias, however, were statistically significant (at a level of significance of 5%) and decreased from 10 mm (OL) to -2.5 mm and -0.73 mm when the model simultaneously assimilated with all six channels every three and five days, respectively, rather than once a day. These results imply that daily assimilation using all six channels tended to underestimate SWE (in part due to filter divergence) and may have overconstrained the model, and hence, often resulted in degraded SWE estimation in terms of bias.

Compared to the baseline DA, all DA thinning strategies enhanced the ability to better capture the synthetic truth (i.e., larger CR_{2 σ}) in part by preventing ensemble col-

lapse, which was also proven by the bigger SWE ensemble spread of 4.6 mm (3-day thinning DA) relative to 3.3 mm (baseline DA). It can be reasonably argued that the 3-day thinning data assimilation strategy was better for SWE estimation under the neutral forcing conditions given the statistical results along with the benefit of a reduction in computational demand.

7.1.3 Effects of Precipitation Bias

Figure 6 shows the spatially-averaged statistics for the Volga river basin using three different sets of boundary (forcing) conditions. All the DA strategies (including the baseline DA, physically-constrained DA, and 3-day thinning DA) had the best performance in terms of SWE estimation under the positively-biased forcing conditions. Compared to the OL, the RMSE was reduced by approximately 30%, 31%, and 24% with the baseline DA, physically-constrained DA, and 3-day thinning DA, respectively. On the contrary, DA with the negatively-biased forcing conditions had relatively smaller improvements with approximately 7.6% (baseline DA), 7.2% (physically-constrained DA), and 11% (3-day thinning DA) reduction in RMSE relative to the OL. Under the negatively-biased forcing conditions, all the DA strategies even degraded the SWE estimation in terms of more ubRMSE relative to the OL. The same results were found for bias and ubRMSE.

These results highlights a unique facet of snow assimilation – it is easier for the DA system to remove excess mass than to add missing mass. That is, in part, because the SVM can only make a prediction when snow exists, and hence, can only update the land surface model when snow is present in the model. This behavior is not unique to the SVM, but could also be said when a radiative transfer model is used as the observation operator as part of an ensemble-based DA approach for snow.

7.2 Filter Diagnostics

Figure 7 shows the temporal mean (\overline{NI}) and standard deviation (σ_{NI}) of the normalized innovation sequence (NI) over the study domain under the neutral forcing conditions. In general, the negative \overline{NI} s computed at $\Delta T_{b10H-18H}$ and $\Delta T_{b10V-18V}$ suggest the SVM-based ΔT_b forecasts had a small negative bias relative to the synthetic ΔT_b observations. On the contrary, SVM-based $\Delta T_{b10H-36H}$, $T_{b10V-36V}$, $\Delta T_{b18H-36H}$ and $\Delta T_{b18V-36V}$ forecasts had positive biases relative to the synthetic ΔT_b observations.

The σ_{NI} (i.e., the standard deviation of the NI) values computed from horizontally polarized spectral differences were greater than for the vertically polarized spectral differences. In addition, the spatially-averaged σ_{NI} were greater than 1, implying that all DA strategies underestimated the observation and/or forecast errors for each frequency and polarization combination under the neutral forcing conditions. Such underestimation could be corrected using a fraternal twin experiment (rather than an identical twin experiment), but is considered well beyond the scope of this study. The σ_{NI} computed at $\Delta T_{b10H-36H}$ and $T_{b10V-36V}$ were the smallest, which can be explained by the fact $\Delta T_{b10H-18H}$, $T_{b10V-18V}$ are not as sensitive to shallow snow conditions, and hence, typically exhibit smaller variability during the entire study period.

Compared to the baseline DA (blue color), the physically-constrained DA (red color) and 3-day thinning DA (black color) had a smaller σ_{NI} for each frequency and polarization combination. It suggested that the prescribed observation error characteristics are more optimal for the physically-constrained DA and 3-day thinning DA compared to the baseline DA. However, the SVM-based $\Delta T_{b10H-36H}$, $T_{b10V-36V}$, $\Delta T_{b18H-36H}$ and $\Delta T_{b18V-36V}$ forecasts within the physically-constrained DA and 3-day thinning DA had a relatively larger bias relative to the synthetic ΔT_b observations. The \overline{NI} and σ_{NI} computed at $\Delta T_{b10H-18H}$ and $\Delta T_{b10V-18V}$ for the 3-day thinning DA were the closest to 0 and 1, respectively, relative to baseline DA and physically-constrained DA. These results

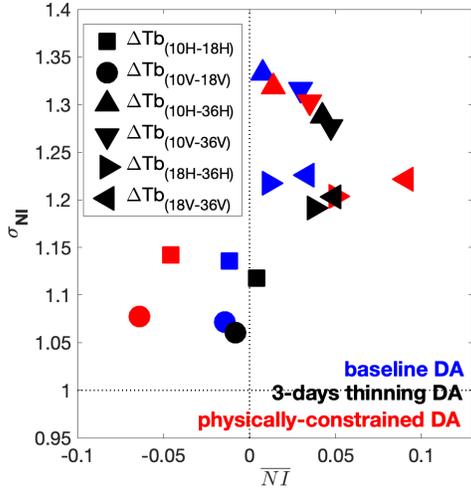


Figure 7. Innovation statistics for $\Delta T_{b10H-18H}$, $\Delta T_{b10V-18V}$, $\Delta T_{b10H-36H}$, $\Delta T_{b10V-36V}$, $\Delta T_{b18H-36H}$, and $\Delta T_{b18V-36V}$ shown as different marker shapes. The different marker colors represent different DA strategies as listed in Table 3.

576 suggest that the observation error characteristics for ΔT_b assimilation in this study may
 577 be too simplistic. Observation error standard deviations as a function of frequency, po-
 578 larization, and land cover type (i.e., forested versus non-forested) should be explored
 579 in the future.

580 7.3 Seasonality

581 To further investigate DA performance over the Volga Basin, the basin-averaged
 582 bias and RMSE as a function of season for positively-biased, negatively-biased, and neu-
 583 tral forcing conditions are presented in Figure 8. Similar patterns were found for ubRMSE
 584 (not shown). As expected, the baseline DA performance showed a strong seasonal com-
 585 ponent under all three forcing conditions. During the snow accumulation period, gener-
 586 ally from September to March, DA SWE estimates outperformed OL in terms of smaller
 587 bias and RMSE.

588 Starting in April, DA performance waned in terms of SWE estimation due to deep
 589 snow conditions and/or wet snow conditions given the limited skill of PMW remote sens-
 590 ing of snow (Clifford, 2010). As a measure of the presence of random error, ubRMSE had
 591 the largest value during April for DA SWE (not shown). The increase in ubRMSE can
 592 be explained, in large part, by the introduction of high-frequency errors originating from
 593 the synthetic ΔT_b observations along with the fact that PMW remote sensing skill is least
 594 when the snow is deep and/or wet (Clifford, 2010). One main reason for the degrada-
 595 tion via DA during April was that snow liquid water (i.e., liquid water coating the snow
 596 grains) was commonplace during the snow ablation period.

597 It has been shown that wet snow introduces additional uncertainties in the esti-
 598 mation of SWE (Walker & Goodison, 1993; Clifford, 2010). The presence of liquid wa-
 599 ter within the snowpack alters the electromagnetic response from a dry microwave scat-
 600 ter to a wet microwave emitter (Walker & Goodison, 1993; R. L. A. Brodzik & J., 2001).
 601 When the snow is wet, the general assumptions implicit in ΔT_b -based remote sensing of
 602 snow are violated (Walker & Goodison, 1993), and hence, the information content in the
 603 ΔT_b observations need not be related to snow mass. As an example shown in Figure 9,

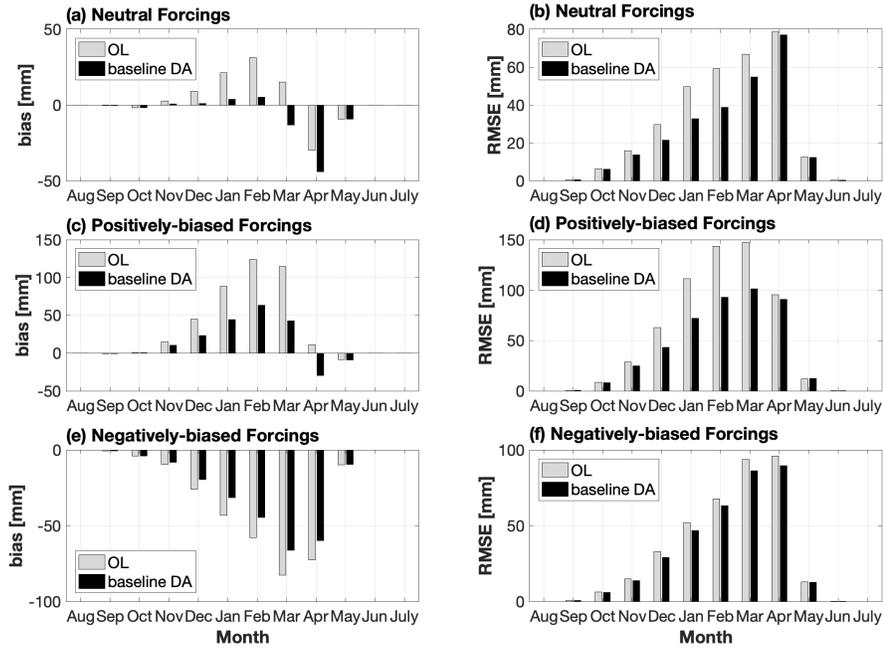


Figure 8. Histograms of monthly Volga basin-averaged SWE bias (first column) and RMSE (second column) under the neutral (first row), positively-biased (second row), and negatively-biased (third row) forcing conditions. Bias and root mean squared error (RMSE) were computed by comparing OL or DA SWE ensemble mean against the synthetic truth. The light gray bar is for the Open Loop (OL) and the black bar is for the baseline DA as listed in Table 3.

604 the correlations between dry (gray plus signs) or wet snow (black dots) and the SVM-
 605 based $\Delta T_{b18V-36V}$ synthetic observations changed dramatically. Namely, $\Delta T_{b18V-36V}$
 606 increased as SWE increased for dry snow. Alternatively, $\Delta T_{b18V-36V}$ transitioned to a
 607 zero (Figure 9a) or negative (Figure 9b) correlation with SWE when the snow pack ripens.

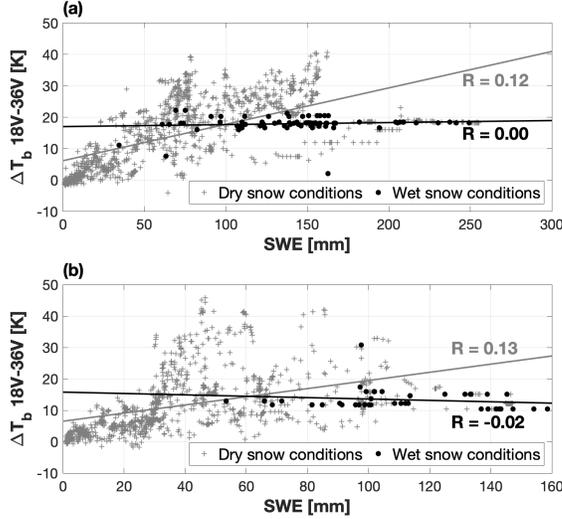


Figure 9. Scatter plots (with correlations) between the model dry snow (gray plus signs) and wet snow (black dots) along with SVM-based brightness temperature spectral difference $\Delta T_{b18V-36V}$ estimates for (a) Grid #1 (54.1685° N, 47.3343° E) and (b) Grid #2 (49.1489° N, 54.0778° E) from 1 September 2002 to 1 September 2011.

608 It is worth noting that DA had the worst performance in terms of SWE estima-
 609 tion under the negatively-biased forcing conditions. The relatively small change in RMSE
 610 between the OL and DA suggested that DA could not significantly improve SWE esti-
 611 mates. In addition, DA had a larger ubRMSE than OL across the entire snow season.
 612 It suggested that ΔT_b assimilation under the negatively-biased forcing conditions was
 613 suboptimal. This latter point highlights the fact that assimilation works better at ame-
 614 liorating a positive bias (positively-biased forcings) more so than a negative bias.

615 7.4 Effects of Forest Attenuation

616 The performance of the snow DA framework in forested regions is explored here
 617 in more detail because the presence of forest canopy can significantly alter the PMW ΔT_b
 618 signal as measured at the top of the atmosphere. More specifically, a low sensitivity of
 619 PMW ΔT_b from terrestrial snow is often observed in densely-forested areas. Overlying
 620 vegetation attenuates the PMW radiation emitted from the underlying snowpack while
 621 simultaneously adding its own contribution to the signal that is measured by the radiome-
 622 ter (Derksen et al., 2005). Among all these three frequency channels (i.e., 10.65 GHz,
 623 18.6 GHz, and 36.5 GHz), microwave emission at 36.5 GHz is most strongly absorbed
 624 by standing vegetation (Derksen, 2008). Consequently, the scattering signal from the un-
 625 derlying snowpack can be overwhelmed by upwelling microwave radiation from the canopy
 626 (Derksen, 2008).

627 Figure 10 shows NIC_{RMSE} as a function of forest fraction under the neutral forc-
 628 ing conditions for baseline DA. Similar results were found for other DA strategies un-
 629 der both the positively-biased and negatively-biased forcing conditions (not shown). Over-

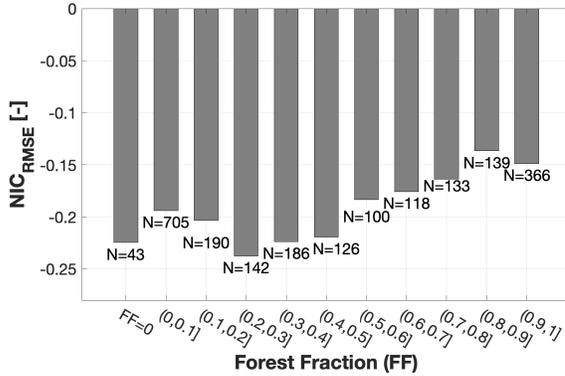


Figure 10. Histograms of the domain-averaged SWE NIC_{RMSE} as a function of forest fraction under the neutral forcing condition across the study domain. N is the number of model grid cells. A negative value of NIC_{RMSE} indicates data assimilation (DA) improves SWE estimates relative to the open loop (OL). Note that the largest improvements occur in the relatively sparsely-forested region where PMW attenuation is less pronounced.

630 all, DA improved the SWE estimates relative to OL in the most sparsely-forested regions
 631 (i.e., forest fraction ≤ 0.4). A hypothesis test at a level of significance of 5% was conducted
 632 to investigate whether the forest cover had a significant effect on the DA performance.
 633 The null hypothesis was that the mean of NIC_{RMSE} for sparsely-forested areas ($FF \leq 0.4$)
 634 was significantly smaller than the mean of NIC_{RMSE} for densely forested areas ($FF > 0.4$)
 635 (i.e., the forest cover has a negative impact on DA performance). The results suggested
 636 the negative effect of forest was statistically significant for the DA algorithm.

637 7.5 Runoff Estimates

638 Monthly domain-averaged runoff estimates from the OL and DA were compared
 639 against true (synthetic) runoff from September 2002 to August 2011. It is encouraging
 640 to see that all basins improved runoff estimation skill with the baseline DA, physically-
 641 constrained DA, and 3-day thinning DA relative to the OL under the neutral, positively-
 642 biased, and negatively-biased forcing conditions.

643 In general, monthly runoff in the Moskva Oka (OL bias = 0.46 mm) and lower Volga
 644 (OL bias = 0.12 mm) basins were overestimated whereas runoff in the upper Volga (OL
 645 bias = -3.8 mm) and Kama basins (OL bias = -5.5 mm) were underestimated under
 646 the neutral forcing conditions. This behavior can be explained by the spatial pattern of
 647 precipitation as shown in Figure 3f). MERRA-2 (synthetic truth) precipitation was greater
 648 than the neutral scenario for the OL run precipitation in the Kama and upper Volga basins,
 649 and hence, the runoff from the synthetic truth run was greater than the OL run in the
 650 Kama and upper Volga basins.

651 As a measure of overall hydrograph fit, Nash-Sutcliffe efficiency (NSE) was calcu-
 652 lated for all monthly instances when either the synthetic truth or OL/DA runoff esti-
 653 mation was nonzero (Nash & Sutcliffe, 1970). All three DA strategies had greater NSE
 654 ($NSE > 0.84$) than the OL ($NSE = 0.82$) for all four sub-basins thereby highlight-
 655 ing the DA skill in runoff estimation beyond simply estimating the mean of the synthetic
 656 truth under the neutral forcing conditions. In addition, DA (baseline) had better per-
 657 formance in the Moskva Oka (RMSE = 8.43 mm) and lower Volga (RMSE = 3.55 mm)
 658 than the upper Volga (RMSE = 15.6 mm) and Kama basins (RMSE = 15.4 mm).

659 For the Volga basin runoff estimation, the physically-constrained DA had the best
 660 performance in terms of the greatest reduction of RMSE (relative to the OL, 30.3%) com-
 661 pared to the baseline DA (30.2%) and 3-day thinning DA (23.7%) under the positively-
 662 biased forcing conditions. This result further illustrated the fact that assimilation worked
 663 better when forced with a positive precipitation bias more so than a negative precipi-
 664 tation bias.

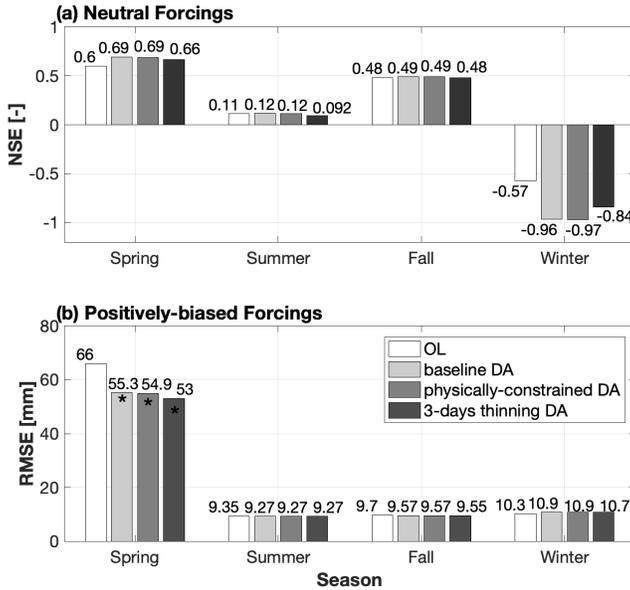


Figure 11. (a) histogram of the Volga basin monthly runoff Nash-Sutcliffe efficiency (NSE) under the neutral forcing conditions and (b) RMSE under the positively-biased forcing conditions. Bars marked with * indicate which experiment yields statistically significant statistics with a level of significance of 5%.

665 It is worth noting that monthly runoff estimation showed a strong seasonality ef-
 666 fect. The spring season had the largest magnitude of runoff among the four different sea-
 667 sons due to the snow melt. All three DA strategies yielded better performance in the runoff
 668 estimation during the spring season compared to the OL in terms of bigger NSE and smaller
 669 RMSE as shown in Figure 11a) and 11b), respectively. Most notably during the positively-
 670 biased forcing conditions, DA strategies showed significant improvement over the OL (Fig-
 671 ure 11b). These results suggest DA effectively improved the model performance in cap-
 672 turing relatively high runoff.

673 8 Conclusions

674 A series of synthetic twin experiments were conducted to explore improvements in
 675 the estimation of SWE in the Volga basin based on prescribed precipitation errors. An
 676 ensemble Kalman filter (EnKF) was used to merge synthetic PMW brightness temper-
 677 ature spectral differences (ΔT_b) into the NASA Catchment land surface model where well-
 678 trained support vector machines served as the observation operator.

679 The results suggested that simultaneous assimilation of $\Delta T_{b10H-36H}$, $\Delta T_{b10V-36V}$,
 680 $\Delta T_{b10H-18H}$, $\Delta T_{b10V-18V}$, $\Delta T_{b18H-36H}$, and $\Delta T_{b18V-36V}$ could degrade SWE estima-
 681 tion due to divergence from the synthetic truth at some experimental locations. One rea-

682 son for DA degradation was due to simultaneous assimilation of all six ΔT_b channels and
 683 the presence of signal saturation during deep snow conditions. To help mitigate this degra-
 684 dation, a physically-constrained approach that used the prior SWE ensemble mean as
 685 an indicator was explored. That is, $\Delta T_{b18H-36H}$, $\Delta T_{b18V-36V}$, $\Delta T_{b10H-36H}$, and $\Delta T_{b10V-36V}$
 686 were assimilated during shallow-to-medium snow conditions (i.e., $SWE \leq 120$ mm), while
 687 simultaneously assimilating $\Delta T_{b10H-18H}$, $\Delta T_{b10V-18V}$, $\Delta T_{b10H-36H}$, and $\Delta T_{b10V-36V}$
 688 during medium-to-deep snow conditions (i.e., $SWE > 120$ mm). The physically-constrained
 689 assimilation approach helped improve SWE estimation at some locations but not all.

690 In addition, a simple data thinning assimilation strategy was explored to further
 691 mitigate the high-frequency noise embedded in synthetic AMSR-E ΔT_b observations. That
 692 is, the ΔT_b channels were assimilated every 3-, 5-, 7-, 10-, and 15 days rather than daily.
 693 The results suggested DA with 3-day data thinning modestly reduced Volga basin av-
 694 eraged bias from -5.5 mm to -2.5 mm under the neutral forcing conditions. $CR_{2\sigma}$ was
 695 slightly increased from 0.25 (baseline DA) to 0.26 (3-day thinning DA).

696 DA performance under the neutral, positively-biased, and negatively-biased forc-
 697 ing conditions were investigated. The results suggest AMSR-E ΔT_b DA performed the
 698 best under the positively-biased conditions in terms of SWE estimation. This highlights
 699 a unique facet of snow assimilation that it is easier for the DA system to remove excess
 700 mass than to add missing mass. This is, in part, due to the fact that the snow-centric
 701 DA update can only happen when snow exists in the land surface model.

702 The investigation in forested regions highlighted the significant negative impact of
 703 dense forest on SWE estimation. This is due to the fact the presence of forest canopy
 704 can further alter the PMW ΔT_b signal as measured at the top of the atmosphere. Given
 705 the physical limitations of coarse-scale PMW radiometry of snow in forested areas, such
 706 scenarios should likely be excluded from the snow DA update in densely-forested areas.

707 SWE estimation demonstrated a strong seasonality. That is, DA SWE estimates
 708 outperformed OL in terms of smaller RMSE, bias, and ubRMSE during the snow accu-
 709 mulation period. However, DA SWE estimates were often degraded during the ablation
 710 period due to the presence of liquid water coating the snow grains. The reason for this
 711 is that the presence of liquid water within the snowpack elicits a shift in the electromag-
 712 netic response from a dry microwave scatter to a wet microwave emitter, and hence, the
 713 assumptions implicit in ΔT_b -based remote sensing of snow are regularly violated. The
 714 results of runoff estimation also showed a seasonal pattern. Among all four seasons, DA
 715 runoff estimates had the best performance relative to the OL during the spring season.
 716 This was consistent with the fact that DA SWE estimates were the best during the win-
 717 ter season, and therefore, the runoff derived from snowmelt was vastly improved during
 718 the spring season.

719 Appendix A SVM Training and Prediction

720 SVM regression served as the observation operator for mapping the geophysical states
 721 (e.g., SWE, snow temperature) into observational (i.e., PMW spectral difference) space.
 722 Following Forman et al. (2014) and Forman and Reichle (2015), SVM training used a
 723 split-sample, jackknifing procedure where observations used for validation were excluded
 724 from the training dataset. The training period was from 1 September 2002 to 1 Septem-
 725 ber 2011. A fortnightly (two weeks) training period was selected to best capture seasonal
 726 variability while still providing a sufficiently large enough set for training. The inputs
 727 to SVM training were four Catchment model states relevant to PMW remote sensing of
 728 snow: (1) SWE, (2) snow liquid water content, (3) top-layer soil temperature, and (4)
 729 skin temperature. They were selected based on the results of an extensive sensitivity anal-
 730 ysis (Xue & Forman, 2017b). The SVM outputs were the synthetic ΔT_b truth, includ-
 731 ing $\Delta T_{b10H-36H}$, $\Delta T_{b10V-36V}$, $\Delta T_{b10H-18H}$, $\Delta T_{b10V-18V}$, $\Delta T_{b18H-36H}$, and $\Delta T_{b18V-36V}$.

Appendix B Goodness-of-Fit Statistics

Goodness-of-fit statistics used in this study include bias, root mean squared error (RMSE), unbiased root mean squared error (ubRMSE), correlation coefficient (R), Nash-Sutcliffe efficiency (NSE), normalized information contribution (NIC), and containing ratio ($CR_{2\sigma}$). The symbol x_{est} denotes the OL or DA ensemble mean and the symbol x_{truth} denotes the synthetic truth. The bias was computed as:

$$bias = \frac{1}{N_t} \sum_{i=1}^{N_t} (x_{est,i} - x_{truth,i}), \quad (B1)$$

where x_i is the state variable (e.g., SWE) at time i and N_t is the sample size over the time period t . The RMSE was computed as:

$$RMSE = \sqrt{\frac{1}{N_t} \sum_{i=1}^{N_t} (x_{est,i} - x_{truth,i})^2}, \quad (B2)$$

where x_i is the state variable (e.g., SWE) at time i and N_t is the sample size over the time period t . The ubRMSE was computed as:

$$ubRMSE = \sqrt{\frac{1}{N_t} \sum_{i=1}^{N_t} (x_{est,i} - x_{truth,i})^2 - (\bar{x}_{est} - \bar{x}_{truth})^2}, \quad (B3)$$

where \bar{x}_{est} is the time-averaged estimate of the model state variable (e.g., SWE) and \bar{x}_{truth} is the time-averaged synthetic truth. The R was computed as:

$$R = \frac{\sum_{i=1}^{N_t} (x_{est,i} - \bar{x}_{est})(x_{truth,i} - \bar{x}_{truth})}{\sqrt{\sum_{i=1}^{N_t} (x_{est,i} - \bar{x}_{est})^2} \sqrt{\sum_{i=1}^{N_t} (x_{truth,i} - \bar{x}_{truth})^2}} \quad (B4)$$

The NSE was computed as:

$$NSE = 1 - \frac{\sum_{i=1}^{N_t} (x_{truth,i} - x_{est,i})^2}{\sum_{i=1}^{N_t} (x_{truth,i} - \bar{x}_{est,i})^2} \quad (B5)$$

The NIC for RMSE, NIC_{RMSE} , was computed as

$$NIC_{RMSE} = \frac{RMSE_{OL} - RMSE_{DA}}{RMSE_{OL}} \quad (B6)$$

where the $RMSE_{OL}$ is the OL-based RMSE and $RMSE_{DA}$ is the DA-based RMSE. The containing ratio, $CR_{2\sigma}$, is the number of synthetic truth that fall within the ensemble mean ± 2 times the ensemble standard deviation normalized by the total number of synthetic truth (N_t), and was computed as

$$CR_{2\sigma} = \frac{\sum_{i=1}^{N_t} I[O(x, i)]}{N_t} \quad (B7)$$

where $I[O(x, i)] = 1$ if $x_{min,i} \leq x_{truth,i} \leq x_{max,i}$. In other words, if the synthetic truth at time i , $x_{truth,i}$, is equal to or greater than the minimum of OL or DA ensemble estimates, $x_{min,i}$, and also is less than or equal to the maximum of OL or DA ensemble estimates, $x_{max,i}$, the $I[O(x, i)] = 1$. Otherwise, $I[O(x, i)] = 0$.

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