Heterogeneous Land-Surface Effects on TKE and Cloud Formation: Statistical Insights from LES Cases

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Abstract

To aid development of sub-grid scale (SGS) parameterizations for Earth system models which consider heterogeneity in landsurface fields and land-atmosphere coupling, results from large-eddy simulations of 92 shallow convection cases over the Southern Great Plains are presented and analyzed. Each case is simulated with heterogeneous surface fields obtained from an offline fieldscale land-surface model, and with spatially homogeneous surface fields with the same domain-wide mean value. By comparing corresponding heterogeneous and homogeneous cases, it is found that turbulent kinetic energy and liquid water path has a high correlation with the spatial variance of the surface heat flux fields. By further comparing the source of this correlation over the range of wavelengths in the surface fields, it is found that the majority of the heterogeneous land-atmosphere coupling is contained in wavelengths of order 10 km and larger, suggesting an encouraging degree of feasibility of including land-surface heterogeneity in global-scale SGS parameterizations.

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Key Points:

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7	• Analysis of 92 LES cases shows strong statistical correlations between land-surface	
8	heterogeneity and mesoscale atmospheric development	
9	• Correlation between surface heterogeneity and circulation/cloud production is dom	1-
10	inated by the largest wavelengths in the land-surface field	

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11 Abstract

To aid development of sub-grid scale (SGS) parameterizations for Earth system mod-12 els which consider heterogeneity in land-surface fields and land-atmosphere coupling, re-13 sults from large-eddy simulations of 92 shallow convection cases over the Southern Great 14 Plains are presented and analyzed. Each case is simulated with heterogeneous surface 15 fields obtained from an offline field-scale land-surface model, and with spatially homo-16 geneous surface fields with the same domain-wide mean value. By comparing correspond-17 ing heterogeneous and homogeneous cases, it is found that turbulent kinetic energy and 18 liquid water path has a high correlation with the spatial variance of the surface heat flux 19 fields. By further comparing the source of this correlation over the range of wavelengths 20 in the surface fields, it is found that the majority of the heterogeneous land-atmosphere 21 coupling is contained in wavelengths of order 10 km and larger, suggesting an encour-22 aging degree of feasibility of including land-surface heterogeneity in global-scale SGS pa-23 rameterizations. 24

²⁵ Plain Language Summary

To help efforts to alleviate some of the issues associated with the relatively low-26 resolution grids used by modern global weather and climate models, we first created a 27 dataset of 92 high-resolution simulations over the Southern Great Plains region of Ok-28 lahoma. All of the cases in the dataset are based on days which where observed to pro-29 duce shallow clouds, which can have a significant impact on the incoming solar radia-30 tion. The high-resolution simulations were designed to cover a region large enough to 31 contain relevant cloud production which is also too small to be represented on a mod-32 ern global model. The dataset of high-resolution simulations is analyzed to compare the 33 strength of the patterns in the land surface to the associated increase in cloud produc-34 tion. It is hoped that this and similar future studies will provide insights which increase 35 the fidelity of cloud production models which intend to capture effects which are smaller 36 than the grid used for global models. 37

38 1 Introduction

Modern coupled Earth system models (ESMs) are run at horizontal resolutions 39 that are $\mathcal{O}(10-100 \text{ km})$, which is decided by the balance between computational re-40 sources and the demands of the atmospheric component of the coupled model, while 41 the land-surface model (LSM) component could conceivably have an effective hori-42 zontal spatial resolution around $\mathcal{O}(10-100 \text{ m})$ (e.g., Chaney et al., 2018). This loss 43 of land-surface information is made more significant by the fact that it spans the 44 relevant length scales for many important coupled processes, namely those related to 45 boundary-layer growth and cloud production (Bertoldi et al., 2013; Kang & Bryan, 46 2011; Ntelekos et al., 2008; Weaver, 2004). 47

The parameterization associated with sub-grid scale (SGS) cumulus production is very important in contemporary ESMs, by virtue of the importance of cloud production to the Earth system in general. Many modeling and observational studies find that secondary circulations induced by thermal surface heterogeneity can act as sources of convection and significantly alter local cloud production rates and distribution (e.g., Albertson et al., 2001; Dixon et al., 2013; Kang, 2020; Marsham et al., 2008; Mendes & Prevedello, 2020; Taylor et al., 2011; Phillips & Klein, 2014).

While the aforementioned land-surface patterns are SGS on grids used for most modern global models, there is a large amount of information available regarding the characteristics of the land-surface which could potentially be utilized by SGS parameterizations. Towards this effort, we present a large-eddy simulation (LES) study of 92 shallow convection cases over the Southern Great Plains (SGP) site, based on cases developed by the LES ARM Symbiotic Simulation and Observation
Workflow (LASSO) campaign (W. Gustafson et al., 2019; W. I. Gustafson et al.,
2020). The cases are run using high-resolution spatially-heterogeneous land-surface
fields and also using spatially-homogeneous land-surface fields, which match the heterogeneous cases' domain-wide mean values through time but contain none of the
spatial structure.

We find that there is a strong correlation between basic metrics of heterogeneity in the surface heat flux fields and the resultant additional production of liquid water path (LWP) and circulating kinetic energy. We also find that, for the cases considered here, the majority of the relevant information about the heterogeneity of the land-surface is contained in the few Fourier modes of the fields with the largest wavelengths, which is encouraging from the perspective of computational resources potentially required to consider SGS land-surface features.

73 2 Model description

Large-eddy simulations are conducted using version 3.8.1 of the WRF 74 model (Skamarock et al., 2008) with modifications as described by J. S. Simon 75 et al. (2021). Cases here use a horizontal resolution of 250 m and a domain of 76 $130 \times 130 \text{ km}^2$ laterally. The land-surface fields in the outer 15 km of the domain 77 are tapered to linearly approach their domain-wide mean on each boundary to elim-78 inate discontinuities in the land-surface that may otherwise be introduced by the 79 periodic boundary conditions. Each domain is also rotated to closer align the bulk 80 liquid-water flux normally to the boundaries, based on results from an initial simu-81 lation using the unrotated land-surface, to limit artificial spreading of liquid water 82 caused by the fluxes through the boundaries not aligning with the periodicity of 83 the domain. The model configuration is otherwise the same as in J. S. Simon et al. 84 (2021).85

Each case is run with heterogeneous and homogeneous land-surface fields (sen-86 sible heat flux, latent heat flux, skin temperature, albedo, and momentum drag co-87 efficient), where homogeneous cases specify a uniform (in space) surface of each field 88 to match the time-evolving domain-wide mean of the corresponding heterogeneous 89 case. There is no feedback from the atmosphere to the land surface in the LES; the 90 HydroBlocks LSM is run offline and the output surface fields are specified as the 91 bottom boundary in the WRF model. Further details of the HydroBlocks LSM and 92 its coupling to the WRF model can be found in the Supporting Information. 93



Figure 1. Example maps of sensible (H) and latent (Q) heat flux fields.

94 **3 Results**

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3.1 Evaluation Metrics

The domain-wide measure of vertically-integrated, mass-coupled turbulent kinetic energy (TKE) is compared between cases, serving as a metric for general activity in ABL development. For brevity, "TKE" will refer to the vertically-integrated, mass-coupled form unless otherwise stated. On the discretized WRF grid, the TKE is found as

$$\text{TKE} = \sum_{z} \rho_a \left[\frac{1}{2} \left(u'^2 + v'^2 + w'^2 \right) \right] \Delta_z, \tag{1}$$

where ρ_a is air density, (u, v, w) are the velocity components in the (x, y, z) directions, Δ_z is the grid spacing in the vertical direction, and a primed variable indicates deviation from the mean value in the (x, y) plane. For illustration, a time series of TKE for heterogeneous and homogeneous simulations of an example case is shown in Fig. 2a. Cases are also compared by their domain-wide LWP signal, which serves as a proxy for overall cloud production. On the discretized WRF grid, our measure of LWP is found as

$$LWP = \sum_{z} \rho_a q_l \Delta_z, \tag{2}$$

where q_l is liquid water mixing ratio.

Part of the LASSO modification to the WRF code is the addition of output solution fields as average values over a given interval of time, in addition to the standard instantaneous output fields. Here, time-averaged fields are found over 10 min intervals from samples taken internally every 30 s. Notationally, we will use $\mu(\phi)$ and $\sigma(\phi)$ to indicate the spatial mean and standard deviation, respectively, of a field $\phi = \phi(x, y)$ at a point in time. For temporal averages, we will use the notation mean $[\vartheta]$, found as

$$\operatorname{mean}[\vartheta] = \frac{\sum_{t} g_s \vartheta}{\sum_{t} g_s},\tag{3}$$

where $\vartheta = \vartheta(t)$ is a domain-wide scalar, with $g_s = g_s(t)$ defined as

$$g_s(t) = \begin{cases} 1 & : \quad s(t) > 0.05 \max(s), \\ 0 & : \quad s(t) \le 0.05 \max(s), \end{cases}$$
(4)

where s(t) is the surface downward clear-sky shortwave radiation at time t, and

 $\max(s)$ is the maximum value of s over the given simulation. The averaging pro-

cedure in (3) is used for both the atmospheric fields (Fig. 2c) and the land-surface

statistics (Fig. 2e).

The heterogeneous vs. homogeneous statistics for TKE and LWP are compared using the metric $\gamma(\vartheta)$, defined as

$$\gamma(\vartheta) = \operatorname{mean}\left[\log\gamma_t(\vartheta)\right],\tag{5}$$

where

$$\gamma_t(\vartheta) = \frac{g_s \vartheta_{\text{heterogeneous}} + 1}{g_s \vartheta_{\text{homogeneous}} + 1}.$$
(6)

Equations (6) and (5) are demonstrated visually in Fig. 2c and d, respectively. The

form of (6) is motivated as a ratio of ϑ between heterogeneous and homogeneous

 $_{103}$ cases, which is weighted by g_s to isolate daytime values. The addition of 1 to both

terms is included to limit the influence of very small values which are effectively negligible, as well as to avoid the edge cases of $\gamma_t = 0$ or $\gamma_t = \infty$ when $\vartheta_{\text{heterogeneous}} = 0$ or $\vartheta_{\text{homogeneous}} = 0$, respectively. When $\vartheta \approx 0$ for both the heterogeneous and homogeneous cases, $\gamma_t \approx 1$, indicating the two cases have approximately equal measures of ϑ , as intended. In (6), TKE is given in units of kg s⁻² and LWP in units of g m⁻².

In addition to $\gamma(\text{TKE})$ and $\gamma(\text{LWP})$, we also compare corresponding heterogeneous and homogeneous cases by only the circulating portion of kinetic energy. This is found from the turbulence spectra of 10-minute averaged u and v fields, where only the energy from modes that are in the lowest 5 km of the atmosphere and longer than 10 km laterally are included. The ratio of circulating energy between the heterogeneous and homogeneous cases, which we denote χ , is found as similarly to the TKE and LWP fields, as

$$\chi = \text{mean}\left[\log\sqrt{\gamma_t(E_u)\gamma_t(E_v)}\right],\tag{7}$$

where

$$E_{\varphi} = E_{\varphi}\left(t\right) = \sum_{z < 5 \text{ km}} \left[\sum_{\ell > 10 \text{ km}} |\widehat{f}(\varphi')|^2\right],\tag{8}$$

and $|\hat{f}(\varphi')|$ is absolute value of the normalized two-dimensional discrete Fourier transform of φ' , ℓ is the component of the Fourier mode's wavelength, λ , in the direction aligned with φ (e.g., $\ell = \lambda_x$ for $\varphi = u$).

Two length-scale metrics, L_{Δ} and L_2 , are presented for the land-surface fields, based on their Fourier spectra (the relaxation to the mean value on the outer 15 km of the land-surface fields render their boundaries as effectively periodic). The L_{Δ} length scale gives the approximate scale of the largest coherent structures in the field, and is found as

$$L_{\Delta}(\phi) = \frac{\sum_{\lambda} \lambda \Delta_{\lambda} \sqrt{|\hat{f}(\phi)|}}{\sum_{\lambda} \Delta_{\lambda} \sqrt{|\hat{f}(\phi)|}},\tag{9}$$

where $\phi = \phi(x, y)$ is a heterogeneous surface field, and Δ_{λ} is the difference between λ and the next (smaller) wavelength in the discrete spectrum. The L_2 length scale gives the approximate scale of the smallest coherent structures in the field, and is found as

$$[L_2(\phi)]^2 = \frac{\sum_{\lambda} \lambda^2 \sqrt{|\hat{f}(\phi)|}}{\sum_{\lambda} \sqrt{|\hat{f}(\phi)|}}.$$
(10)

Correlations between atmosphere and land-surface fields are evaluated by the Pearson (ρ_p) and Spearman (ρ_s) correlation coefficients, as implemented by Virtanen et al. (2020) (e.g., Fig. 2f).



Figure 2. Demonstration of the comparison process for heterogeneous and homogeneous cases: (a) the domain-wide time series of TKE for the two simulations of 2017/08/30; (b) the time filter, g_s , used by the mean[ϑ] function as described by (4); (c) the calculation of γ_t , as described by (6); (d) the calculation of γ as described by (5); (e) the application of the time filter, g_s , and the mean[ϑ] function to the $\sigma(H)$ time series; (f) an example scatter plot of mean[$\sigma(H)$] vs. γ (TKE) for all 92 days with the datapoint for 2017/08/30 shown in red.

3.2 Land-Atmosphere Correlation

The emergent secondary circulations driven by land-surface heterogeneity are 117 analyzed by the correlation between χ and each of $\mu(H)$, $\sigma(H)$, $L_{\Delta}(H)$, and $L_{2}(H)$ 118 (Figs. 3a–d, respectively). There is a strong positive relationship between χ and all 119 of $\sigma(H)$, $L_{\Delta}(H)$, and $L_2(H)$, but only a trivial correlation with $\mu(H)$. The same 120 presentation is repeated for $\gamma(LWP)$ in Fig. 3e–h. The $\gamma(LWP)$ data is very similar 121 to that of the χ metric, but with ~ 20% smaller magnitudes. Of the 92 cases, 4 have 122 more liquid water production in the homogeneous simulation, indicated by a nega-123 tive value of $\gamma(LWP)$; these datapoints are not shown in Fig. 3 but are included in 124 the calculation of the correlation coefficients. 125

Visually, the data for $\gamma(\text{LWP})$ compared to $\sigma(H)$, $L_{\Delta}(H)$, and $L_{2}(H)$ show a 126 very similar pattern as χ but with a broader spread, suggesting from that LWP pro-127 duction is statistically driven similarly to circulation production but with additional 128 considerations which are not captured by the land-surface heterogeneity, which is 129 certainly in agreement with the physical perspective of ABL development. The same 130 analysis considering γ (TKE), or using statistics from the latent heat flux or skin 131 temperature fields gives very similar results, which is presented in the Supporting 132 Information. 133



Figure 3. The χ (a – d) and γ (LWP) (e – h) metrics as functions of statistics of the surface sensible heat flux field, H. Four negative-valued data points for γ (LWP) with magnitudes $\mathcal{O}(10^{-4})$ are not shown, but are included in the calculation of ρ_p and ρ_s .

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3.3 Dominant Length Scales

The results presented in Sec. 3.2 bolster the motivation to include information about the underlying land-surface heterogeneity in global SGS boundary-layer parameterizations. The best methodology to make such considerations in either existing or new parameterization models is not immediately obvious, and potential solutions must add value on a level that is commensurate with their computational and implementation costs. To evaluate the relevance of the different ranges of length scales present in the land surface on the present dataset, the land surface fields are filtered over a range of length scales and compared. The filter, F, is applied in Fourier space as

$$F = 1 - \exp\left[-2\pi^2 \left(\frac{\Delta_{\text{filter}}}{\lambda}\right)^2\right],\tag{11}$$

where Δ_{filter} is the nominal filter length. To avoid ambiguity in the discussion, the operation of F is referred to as passing $\lambda < \Delta_{\text{filter}}$. An example of a mid-day sensible heat flux field from the dataset for different filter lengths is shown in the Supporting Information.

For each filter length, the heterogeneous land-atmosphere coupling is reevaluated following the same procedure as in Sec. 3.2. The average value over the dataset of mean[$\sigma(H)$] as a function of filter length is shown in Fig. 4a. Correlation coefficients for mean[$\sigma(H)$] of the filtered dataset with $\gamma(\text{TKE})$, $\gamma(\text{LWP})$, and χ are shown as a function of filter length in Fig. 4b, c, and d, respectively.



Figure 4. Average value of mean[$\sigma(H)$] over the 92 days after filtering (a) and correlation coefficients of mean[$\sigma(H)$] after filtering with $\gamma(\text{TKE})$ (b), $\gamma(\text{LWP})$ (c), and χ (d).

Figure 4a demonstrates that the majority of the standard deviation in the sensible heat flux field over the dataset is contained in length scales 10 km and larger. Figures 4b – d show the same concentration at length scales larger than 10 km for the Pearson and Spearman correlation coefficients between $\sigma(H)$ and $\gamma(\text{TKE})$, $\gamma(\text{LWP})$, χ . Because the wavelengths of Fourier modes grow geometrically, the results seen in Fig. 4 suggest that the bulk of the correlation between $\sigma(H)$ and the atmospheric metrics is contained in the longest few modes.

¹⁵¹ 4 Discussion and Conclusions

We have presented a statistical analysis of the TKE and cloud production 152 caused by land-surface heterogeneity for 92 LES cases representing different summer 153 days from 2015 – 2019 over the SGP site by comparing simulations using heteroge-154 neous and homogeneous land-surface fields. In Sec. 3.2 it is found that, despite all 92 155 days having unique initial profiles and large-scale tendencies, there is a strong corre-156 lation between the production of circulating TKE (measured as the metric χ) over a 157 diurnal cycle and land-surface heterogeneity. The correlation between cloud produc-158 tion, as measured by LWP, is $\sim 20\%$ smaller but is also significant. It is also seen in 159 Sec. 3.3 that a large portion of the correlation between the atmosphere and hetero-160 geneous land-surfaces is concentrated in a relatively small number of the largest (by 161 wavelength) modes in the land-surface fields. 162

The results in Sec. 3.2 demonstrate a strong, but incomplete, correlation between heterogeneous land surface fluxes and secondary circulations. The land-surface heterogeneity is more strongly related to χ than LWP, which was expected: while TKE production does depend on the temperature and stability of the initial atmospheric profile, liquid water production is additionally constrained by condensation conditions. Still, the correlation coefficient values seen between $\gamma(LWP)$ and $\sigma(H)$,

even without considerations for the state of the atmosphere, are quite strong with 169 $\rho_p = 0.70$ (Fig. 3f). The concentration of relevant land-surface heterogeneity in 170 structures with length scales of $\mathcal{O}(10 \text{ km})$ and larger seen in Sec. 3.3 is easily un-171 derstood in the context of heterogeneous land-atmosphere coupling being largely 172 driven by emergent mesoscale circulations. That there is such a sharp increase in 173 correlation contained in the longest few modes of the land surface does have the 174 encouraging implication that the level of detail necessary for the successful devel-175 opment of global-scale SGS parameterizations of heterogeneous land-atmosphere 176 coupling may not be overwhelming. 177

While a large amount of additional work is necessary before the realization 178 of an effective parameterization, the results seen here are encouraging. The most 179 immediate future work is a detailed analysis of the relationship between initial and 180 large-scale atmospheric conditions and land-surface heterogeneity on the atmospheric 181 response. The necessary increase in cases to realize such an experiment would also 182 enable the use of more sophisticated methods for analysis, perhaps eventually in-183 cluding machine learning, which itself has the potential to provide a huge value to 184 parameterization development efforts. 185

186 Acknowledgments

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188 Data Availability

Simulations here use a modification of WRF version 3.8.1 developed and maintained by the LASSO team. The base WRF code, initial sounding files, and largescale forcing files are available from W. Gustafson et al. (2019). Additional modifications to the WRF code to specify heterogeneous surfaces, data files for surface fields for each simulation, and model control files for each simulation are available at J. Simon et al. (2023a). Relevant model output and scripts used for analysis and plotting are available J. Simon et al. (2023b).

196 **References**

235

- Albertson, J. D., Kustas, W. P., & Scanlon, T. M. (2001). Large-eddy simulation
 over heterogeneous terrain with remotely sensed land surface conditions. *Water Resources Research*, 37(7), 1939–1953.
- Bertoldi, G., Kustas, W. P., & Albertson, J. D. (2013). Evaluating source area
 contributions from aircraft flux measurements over heterogeneous land using
 large-eddy simulation. Boundary-layer meteorology, 147(2), 261–279.
- Chaney, N. W., Van Huijgevoort, M. H., Shevliakova, E., Malyshev, S., Milly, P. C.,
 Gauthier, P. P., & Sulman, B. N. (2018). Harnessing big data to rethink land
 heterogeneity in Earth system models. *Hydrology and Earth System Sciences*,
 226 226 226(6), 3311–3330.
- Dixon, N., Parker, D., Taylor, C., Garcia-Carreras, L., Harris, P., Marsham, J., ...
 Woolley, A. (2013). The effect of background wind on mesoscale circula tions above variable soil moisture in the sahel. *Quarterly Journal of the Royal Meteorological Society*, 139(673), 1009–1024.
- Gustafson, W., Vogelmann, A., Cheng, X., Dumas, K., Endo, S., Johnson, K., ...
 Xiao, H. (2019). Description of the LASSO data bundles product. DOE Atmospheric Radiation Measurement (ARM) user facility. DOE/SC-ARM-TR-216.
- Gustafson, W. I., Vogelmann, A. M., Li, Z., Cheng, X., Dumas, K. K., Endo, S., ...
 Xiao, H. (2020). The Large-eddy simulation (LES) Atmospheric Radiation
 Measurement (ARM) Symbiotic Simulation and Observation (LASSO) activity
 for continental shallow convection. Bulletin of the American Meteorological
 Society, 101(4), E462–E479.
- Kang, S.-L. (2020). Effects of mesoscale surface heterogeneity on the afternoon and
 early evening transition of the atmospheric boundary layer. Boundary-Layer
 Meteorology, 174(3), 371–391.
- Kang, S.-L., & Bryan, G. H. (2011). A large-eddy simulation study of moist con vection initiation over heterogeneous surface fluxes. *Monthly weather review*,
 139(9), 2901–2917.
- Marsham, J. H., Parker, D. J., Grams, C. M., Johnson, B. T., Grey, W. M., & Ross,
 A. N. (2008). Observations of mesoscale and boundary-layer scale circulations
 affecting dust transport and uplift over the sahara. *Atmospheric Chemistry* and Physics, 8(23), 6979–6993.
- Mendes, C. B., & Prevedello, J. A. (2020). Does habitat fragmentation affect
 landscape-level temperatures? A global analysis. Landscape Ecology, 35(8),
 1743–1756.
- Ntelekos, A. A., Smith, J. A., Baeck, M. L., Krajewski, W. F., Miller, A. J., &
 Goska, R. (2008). Extreme hydrometeorological events and the urban en vironment: Dissecting the 7 july 2004 thunderstorm over the Baltimore MD

Metropolitan Region. Water Resources Research, 44(8).

- Phillips, T. J., & Klein, S. A. (2014). Land-atmosphere coupling manifested in
 warm-season observations on the US southern great plains. Journal of Geo physical Research: Atmospheres, 119(2), 509–528.
- Simon, J., Chaney, N., & Bragg, A. (2023a, August). Data for: Heterogeneous Land-Surface Effects on TKE and Cloud Formation: Statistical
 Insights from LES Cases (model and input). Zenodo. Retrieved from https://doi.org/10.5281/zenodo.8240267 doi: 10.5281/zenodo.8240267
- Simon, J., Chaney, N., & Bragg, A. (2023b, August). Data for: Heterogeneous Land Surface Effects on TKE and Cloud Formation: Statistical Insights from LES
 Cases (model output). Zenodo. Retrieved from https://doi.org/10.5281/
 zenodo.8241941 doi: 10.5281/zenodo.8241941
- Simon, J. S., Bragg, A. D., Dirmeyer, P. A., & Chaney, N. W. (2021). Semi-coupling
 of a field-scale resolving land-surface model and wrf-les to investigate the influ ence of land-surface heterogeneity on cloud development. Journal of Advances
 in Modeling Earth Systems, 13(10), e2021MS002602.

251	Skamarock, W., Klemp, J., Dudhia, J., Gill, D., Barker, D., Duda, M., Powers,
252	J. (2008). A description of the Advanced Research WRF version 3. NCAR
253	Technical Note, NCAR/TN-475+STR.
254	Taylor, C. M., Gounou, A., Guichard, F., Harris, P. P., Ellis, R. J., Couvreux, F., &
255	De Kauwe, M. (2011). Frequency of Sahelian storm initiation enhanced over
256	mesoscale soil-moisture patterns. Nature Geoscience, $4(7)$, $430-433$.
257	Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau,
258	D., SciPy 1.0 Contributors (2020). SciPy 1.0: Fundamental Algorithms for
259	Scientific Computing in Python. Nature Methods, 17, 261–272.
260	Weaver, C. P. (2004). Coupling between large-scale atmospheric processes and
261	mesoscale land–atmosphere interactions in the us southern great plains during
262	summer. Part II: Mean impacts of the mesoscale. Journal of Hydrometeorology,
263	5(6), 1247-1248.

Supporting Information for "Heterogeneous Land-Surface Effects on TKE and Cloud Formation: Statistical Insights from LES Cases"

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Introduction

Information here consists of extended model descriptions, additional results which may be of interest to the reader, and a demonstration of the land-surface filtering method used in the primary document.

WRF Model Description

Large-eddy simulations are conducted using a modification of version 3.8.1 of the WRF model (Skamarock et al., 2008). Changes implemented, maintained, and distributed by the LES ARM Symbiotic Simulation and Observation Workflow (LASSO) campaign (Endo et al., 2015; W. Gustafson et al., 2019; W. I. Gustafson et al., 2020) notably include the addition of specified large-scale tendency terms and enhanced output fields. An additional modification implemented by Simon, Bragg, Dirmeyer, and Chaney (2021) is also used here to specify heterogeneous surface properties from an offline LSM.

Each case is run with heterogeneous and homogeneous land-surface fields. Heterogeneous land-surface cases use solutions from the HydroBlocks LSM to specify twodimensional, time-evolving surface fields for sensible heat flux, latent heat flux, skin temperature (found via specified emissivity and upward longwave radiation fields), albedo, and momentum drag coefficient. The homogeneous cases specify a uniform (in space) surface of each field to match the time-evolving domain-wide mean of the corresponding heterogeneous case (skin temperature is diagnosed from mean values of upward longwave radiation and emissivity, rather than a domain-average of skin temperature directly). There is no feedback from the atmosphere to the land surface in the LES; the HydroBlocks LSM is run offline and the output surface fields are specified as the bottom boundary in the WRF model. Histograms of means and standard deviations of mid-day latent and sensible heat flux fields are shown in Fig. S1.

Following the LASSO configuration, simulations use the Thompson graupel microphysics scheme and the RRTMG radiation scheme (though surfaces are specified offline by HydroBlocks) with the cumulus and PBL schemes turned off. The model timestep is 0.5 s. The domain is approximately 14.5 km tall with 227 vertical levels and a vertical resolution of 30 m in the lower 5 km of the column. Periodic boundary conditions are used in both lateral directions and a *w*-Rayleigh damping layer is applied in the upper 2 km of the column. The LES domain uses a flat bottom boundary, though terrain is considered by the offline HydroBlocks simulation for subsurface and surface routing. Initial profiles for potential temperature, water vapor mixing ratio, and lateral velocity components are obtained from the LASSO database and are applied uniformly to the domain. Large-scale heat and moisture tendency profiles based on the VARANAL dataset, obtained from the LASSO database and configuration, are also included. The model configuration is otherwise the same as in Simon et al. (2021), which is in turn largely based on the LASSO configuration.

HydroBlocks Model Description

HydroBlocks is a field-scale resolving land-surface model (Chaney, Metcalfe, & Wood, 2016) that accounts for the water, energy, and carbon balance to solve land-surface processes at field scales (30 m) over regional to continental extents (Chaney, Metcalfe, & Wood, 2016; Chaney et al., 2020; Vergopolan et al., 2020). The core of HydroBlocks is the Noah-MP vertical land surface scheme (Niu et al., 2011). For this study, HydroBlocks is spun up for two years and uses high-resolution (30 m) soil type and land cover maps from the Probabilistic Remapping of SSURGO (POLARIS) (Chaney, Wood, et al., 2016; Chaney et al., 2019) and National Land Cover Database (NLCD) (Homer et al., 2012) datasets, respectively, and one-eighth degree NLDAS-2 meteorology (Cosgrove

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et al., 2003; Mitchell et al., 2004) with NCEP Stage-IV radar rainfall (~ 4 km) data (Lin & Mitchell, 2005). The hourly state of the land surface produced by HydroBlocks for the period of interest is then used to specify surface values in the WRF model. For consistency, surface-flux fields are adjusted so that the domain-wide averages match the time-evolving scalar surface fluxes specified by the LASSO campaign, which are from the observationally-improved VARANAL dataset.

Additional Fields

The analysis shown in Sec. 3.2 of the primary text for χ and $\gamma(\text{LWP})$ compared to statistics of the surface sensible heat flux field, H, is repeated here for $\gamma(\text{TKE})$ compared to statistics of H in Fig. S2. The correlations between $\gamma(\text{TKE})$ and mean values of $\sigma(H)$, $L_{\Delta}(H)$, $L_2(H)$ are not appreciably different than the correlations between χ and the same statistics of the H field, particularly when considering $\sigma(H)$. There is a small, but nontrivial, negative Pearson correlation between $\gamma(\text{TKE})$ and $\mu(H)$, where $\rho_p = -0.22$ (Fig. S2a), which is understood by recalling that $\gamma(\text{TKE})$ is the ratio of TKE in corresponding heterogeneous and homogeneous cases. Thus, larger mean surface sensible heat flux values reduce the relative significance of TKE generated by any heterogeneous surface patterns, making the total TKE more comparable between heterogeneous and homogeneous cases. Indeed, this negative correlation is virtually eliminated when comparing only the circulating components of TKE (χ) to $\mu(H)$, where $\rho_p = 0.00$ (Fig. 3a in the main text).

The same analysis for χ , $\gamma(\text{LWP})$, and $\gamma(\text{TKE})$ compared to statistics of the surface latent heat flux field, Q, is shown in Fig. S3. The relationships between the χ , $\gamma(\text{LWP})$, and $\gamma(\text{TKE})$ metrics and the surface latent heat flux field are very similar to those seen for the surface sensible heat flux field, both quantitatively and qualitatively. The only notable difference between the two surface fields is that the correlation between $\gamma(\text{TKE})$ and $\mu(Q)$ is positive rather than the negative correlation seen for $\mu(H)$, though the two are similar in magnitude. The small positive correlation between $\gamma(\text{TKE})$ and $\mu(Q)$ (Fig. S3a) appears logical, as a larger mean latent heat flux would not be expected to inherently generate TKE in the atmosphere but may increase cloud production rates and thus exaggerate heterogeneous surface effects.

The relationships between χ , γ (LWP), and γ (TKE) compared to statistics of the surface temperature field, T, do show some distinctive features relative to those with H and Q (Fig. S4). The relationships between the atmospheric metrics and $\sigma(T)$ is very similar to those seen for $\sigma(H)$ and $\sigma(Q)$, but there is a larger correlation between $\mu(T)$ and all three atmospheric metrics, particularly χ (Fig. S4a), than is seen for $\mu(H)$ or $\mu(Q)$. This suggests that while mean energy flux values do not correlate with the development of secondary circulations, larger mean surface temperatures may help in circulation development. As well, both length-scale metrics, $L_{\Delta}(T)$ and $L_2(T)$, show a lower correlation with the atmospheric metrics than the length scales calculated from H or Q, suggesting that the spatial structures of surface heat fluxes are more related to the atmospheric response than the spatial structures of surface temperature. Intuitively, it should be the case that the surface flux fields have a more direct impact on the atmosphere than surface temperature; the surface sensible and latent heat fluxes directly connect the land-surface to the atmosphere whereas the surface temperature is connected to the atmosphere via the surface heat fluxes.

Example Filtered Fields

The filter used in Sec. 3.3 of the primary text, defined as

$$F = 1 - \exp\left[-2\pi^2 \left(\frac{\Delta_{\text{filter}}}{\lambda}\right)^2\right],\tag{1}$$

where Δ_{filter} is the nominal filter length, is shown as applied to a representative mid-day sensible heat flux field at an increasingly fine filter length in Fig. S5.

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References

- Chaney, N. W., Metcalfe, P., & Wood, E. F. (2016). HydroBlocks: a field-scale resolving land surface model for application over continental extents. *Hydrological Processes*, 30(20), 3543-3559. doi: 10.1002/hyp.10891
- Chaney, N. W., Minasny, B., Herman, J. D., Nauman, T. W., Brungard, C. W., Morgan,
 C. L., ... Yimam, Y. (2019). POLARIS soil properties: 30-m probabilistic maps of soil properties over the contiguous United States. *Water Resources Research*, 55(4), 2916–2938.
- Chaney, N. W., Torres-Rojas, L., Vergopolan, N., & Fisher, C. K. (2020). Twoway coupling between the sub-grid land surface and river networks in Earth system models. *Geoscientific Model Development Discussions*, 2020, 1–31. doi: 10.5194/gmd-2020-291
- Chaney, N. W., Wood, E. F., McBratney, A. B., Hempel, J. W., Nauman, T. W., Brungard, C. W., & Odgers, N. P. (2016). POLARIS: A 30-meter probabilistic soil series map of the contiguous United States. *Geoderma*, 274, 54–67.
- Cosgrove, B. A., Lohmann, D., Mitchell, K. E., Houser, P. R., Wood, E. F., Schaake, J. C., ... others (2003). Real-time and retrospective forcing in the North American Land Data Assimilation System (NLDAS) project. *Journal of Geophysical Research: Atmospheres*, 108(D22).
- Endo, S., Fridlind, A. M., Lin, W., Vogelmann, A. M., Toto, T., Ackerman, A. S., ... Liu, Y. (2015). RACORO continental boundary layer cloud investigations: 2. Largeeddy simulations of cumulus clouds and evaluation with in situ and ground-based

observations. Journal of Geophysical Research: Atmospheres, 120(12), 5993-6014.

- Gustafson, W., Vogelmann, A., Cheng, X., Dumas, K., Endo, S., Johnson, K., ... Xiao,
 H. (2019). Description of the LASSO data bundles product. DOE Atmospheric
 Radiation Measurement (ARM) user facility. DOE/SC-ARM-TR-216.
- Gustafson, W. I., Vogelmann, A. M., Li, Z., Cheng, X., Dumas, K. K., Endo, S., ... Xiao, H. (2020). The Large-eddy simulation (LES) Atmospheric Radiation Measurement (ARM) Symbiotic Simulation and Observation (LASSO) activity for continental shallow convection. Bulletin of the American Meteorological Society, 101(4), E462–E479.
- Homer, C. H., Fry, J. A., & Barnes, C. A. (2012). The national land cover database. US Geological Survey Fact Sheet, 3020(4), 1–4.
- Lin, Y., & Mitchell, K. E. (2005). The NCEP stage II/IV hourly precipitation analyses: Development and applications. In *Proceedings of the 19th conference hydrology*, *american meteorological society, san diego, ca, usa* (Vol. 10).
- Mitchell, K. E., Lohmann, D., Houser, P. R., Wood, E. F., Schaake, J. C., Robock, A., ... others (2004). The multi-institution North American Land Data Assimilation System (NLDAS): Utilizing multiple GCIP products and partners in a continental distributed hydrological modeling system. *Journal of Geophysical Research: Atmospheres*, 109(D7).
- Niu, G.-Y., Yang, Z.-L., Mitchell, K. E., Chen, F., Ek, M. B., Barlage, M., ... others (2011). The community Noah land surface model with multiparameterization options (Noah-MP): 1. model description and evaluation with local-scale measure-

ments. Journal of Geophysical Research: Atmospheres, 116(D12).

- Simon, J. S., Bragg, A. D., Dirmeyer, P. A., & Chaney, N. W. (2021). Semi-coupling of a field-scale resolving land-surface model and wrf-les to investigate the influence of land-surface heterogeneity on cloud development. *Journal of Advances in Modeling Earth Systems*, 13(10), e2021MS002602.
- Skamarock, W., Klemp, J., Dudhia, J., Gill, D., Barker, D., Duda, M., ... Powers, J. (2008). A description of the Advanced Research WRF version 3. NCAR Technical Note, NCAR/TN-475+STR.
- Vergopolan, N., Chaney, N. W., Beck, H. E., Pan, M., Sheffield, J., Chan, S., & Wood, E. F. (2020). Combining hyper-resolution land surface modeling with SMAP brightness temperatures to obtain 30-m soil moisture estimates. *Remote Sensing of Environment*, 242, 111740.



Figure S1. Histogram of mean (μ) and standard deviation (σ) for mid-day sensible (H) and latent (Q) heat flux fields for the 92 cases.



Figure S2. The $\gamma(\text{TKE})$ metric as functions of statistics of the surface sensible heat flux field, *H*. One negative-valued data point for $\gamma(\text{TKE})$ with a magnitudes $\mathcal{O}(10^{-2})$ is not shown, but is included in the calculation of ρ_p and ρ_s .

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statistics of the surface latent heat flux field, Q.



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statistics of the surface temperature field, T.



Figure S5. Comparison of a mid-day sensible heat flux field without filtering (a) and after applying increasingly fine filters (b - f).