Physics-Reconstructed Neural Networks, a case study on evapotranspiration

Anonymous Authors[1]

Abstract

In the field of nature sciences, due to inadequate grasp of existing mechanisms, unexplainable errors are always contained in simulations from both Artificial Intelligence (AI) and physical process-based models. Since AI could quickly get high-precision results, but could hardly illustrate parameters and answer scientific questions as mechanism models, in recent years, it has become a demand and trend to hybridize these two methods to make compensation. Current hybrid methods have made some progresses in improving accuracy, but it is still in an early stage when it comes to improving other shortcomings, for example, little interpretability of AI models, especially from the perspective of model structures. In this paper, by combining spectral clustering with small neural network blocks, a novel model called Physics-Reconstructed Neural Networks (PRNN) that can simulate complex mechanisms, like evapotranspiration, was introduced for the first time. PRNN was validated mainly in terms of enhancing interpretability by reconstructing the calculation of mechanisms, which could further bring prospects and challenges in grasping the known and unknown knowledge from another perspective of AI in terms of nature science.

1. Introduction

Complex mechanisms are restricted with state-of-the-art process-based models. Evapotranspirationan accounts for around 60% of precipitation, making it an indispensable part in water cycle, and an important role in surface energy budget(Katul et al., 2012), which means accurate evaluation of evapotranspiration is a key point in related research in nature science. Via studying its physical process, many models have already been established to quantitatively describe evapotranspiration, such as Penman-Monteith Equation(Penman & Keen, 1948; Monteith, 1965; Sinclair, 2019), surface energy balance models(Bastiaanssen et al., 1998) and so forth, which were mostly built via empirically simplifying unknown processes and carefully structuring equations for known processes. For example, Penman(Penman & Keen, 1948) combined two theoretical approaches, aerodynamic and energy basis, to describe evaporation, and tested the equation on open water, bare soil and grass. Based on that, Monteith(Monteith, 1965) added the process of evaporation from leaves to fulfill the Penman-Monteith equation. These equations or models have been demonstrated through measurements, and became cornerstones for follow-up studies. However, they also contain certain insufficiency, like some errors brought by simplification of unknown mechanical processes and the necessity of being fixed in different areas(Nian-xiu, 2011). More precisely, the accuracy of estimating evapotranspiration by mechanism models is restricted mainly by uncertainties of parameters and structures, due to inadequate knowledge of mechanisms, which is one of the reasons that Artificial Intelligence(AI) is so popular in natural science.

Hybridization is of highly demand in developing AI and mechanism models. The core concept of Artificial Intelligence is to find the underlying relationship between input and output data, with rare consideration on physical processes, which has shown advantages on both accuracy and efficiency, whereas performs worse than physical process-based models in solving scientific problems, especially in terms of interpretability. Those features between mechanism models and AI are obviously contradictory and in other words, complementary, making researchers highly devoted to coupling or hybridizing them to take advantages over both of them. In previous studies, the mainstream of coupling is to set AI and mechanism models in series, mostly achieving in enhancing the final precision. And gradually, demands of improving other shortages developed more methods of deeper hybridization, which could be classified into two categories(Hu et al., 2023; Shen & Zhang, 2023). One is merging physical constraints into AI models, to improve the performance of AI, by adding constraints into input data(Yang et al., 2019), structures(Hoedt et al.,

[1]Anonymous Institution, Anonymous City, Anonymous Region, Anonymous Country. Correspondence to: Anonymous Author <anon.email@domain.com>.

Preliminary work. Under review by the International Conference on Machine Learning (ICML). Do not distribute.

2021), and loss functions(Chen et al., 2022), to force AI in accord with physical laws, with successfully enhanced accuracy and slightly strengthened interpretability obtained. The other is to use AI to promote the development of physical process-based models, such as taking place of empirical parameters(Zhao et al., 2019), solving mathematical equations(Raissi et al., 2017), as well as being used for data assimilation(Cintra et al., 2016). In conclusion, according to studies on hybridization of AI and mechanism models, it has been proved that AI has the ability to promote the development of mechanisms, but it is still in an early stage with the shortage of a little interpretability.

Physics-reconstructed neural networks. Recently, it was noted that the capability of AI could also be enlarged to construct mechanical processes, for example, SciNet, built to discover simple physical concepts between distances and angles while earth-moon system is moving in its orbit(Iten et al., 2020), which just gave an inspiration of solving problems above. So, to construct more sophisticated physical relationships, like evapotranspiration, a method, using clustering and neural networks, named Physics-Reconstructed Neural Networks (PRNN) was introduced in this paper. PRNN consisted of two parts, clustering and fitting. Grouped by relevance, highly correlated input variables were put into one group, and input variables with a little correlation were divided into different groups. Small blocks of neural networks were then assigned to each group to output intermediate variables collecting information of each group. By doing so, each intermediate variable was generated with actual meanings, like what was done in the calculation of physical process-based models, and was then passed to the final block of neural networks to simulate the target variable.

Contributions. With a case study of evapotranspiration, PRNN was demonstrated that it could make neural networks more interpretable, with some parameters entitled actual meanings, and is feasible in reconstructing mechanical processes, with calculation similar to physical processed-based models, which would to some extent benefit our understandings of known and unknown physical processes in other areas.

2. Data and methods

2.1. Data

Daily samples are provided by the FLUXNET 2015 Tier1 dataset(Pastorello et al., 2020), which was calculated on average of original data sampled half an hour to avoid interference from diurnal variations and weather conditions that greatly affects evapotranspiration. Arrangements on data were as follows. Firstly, since some variables, such as: P(Precipitation), PPFD(Photosynthetic photon flux density), TS(Soil Temperature) and SWC(Soil water content) lacked daily data on many stations, so although these data also play important roles in evapotranspiration equation, it would not be considered in this paper. Next, since latent heat flux (LE) can reflect the actual evapotranspiration when energy is mainly considered(Wang & Dickinson, 2012), LE is thus used to describe the evapotranspiration process as the output. Finally, 13 input variables, including VPD (Vapor Pressure Deficit, hPa), PA (atmospheric pressure, °C), WS (wind speed, m/s), USTAR (friction velocity, m/s), LW (long-wave radiant energy, long radiation, W/m^2),CO_2 (CO_2 mole fraction, mol/mol), SW (Short Radiation, W/m^2), NETRAD (Net Radiation, W/m^2), TA (Air temperature, °C), G (Soil heat flux, W/m^2), H (sensible heat flux, W/m^2), RECO (Ecosystem respiration in daytime, gC/(m^2.d)), NEE (Net ecosystem exchange, gC/(m^2.d))) were selected according to three categories, measurement, energy and ecosystem that were provided in the dataset.

Although there existed some variables not taken into account as mentioned above, the data collected have covered variables from both aerodynamics and energy balance that were recognized as the main processes of evapotranspiration(Penman & Keen, 1948), which may not be comprehensive, but already representative. In addition, we shuffled the chronological order of data on each site and divided them into a training set and a validation set in a ratio of 8:2. The reason of no testset was that some sites left a small amount of data after removing missing values, and the purpose of this article is to prove the feasibility instead of giving an optimal accuracy of the method, so no testset was prepared here.

2.2. Spectral clustering

Since the evapotranspiration involves many physical factors, in order to find the connection between each other, we first calculated the Pearson correlation coefficient among them, marked variables as point set V, and connected them with weighted undirected edges (set E) to form an undirected graph $G(V, E)$. Therefore, to cluster these variables via weighted edges, the spectral clustering algorithm evolved from graph theory was chosen appropriately(Von Luxburg, 2007).

W$_{ij}$was defined as the weight between point V$_i$ and V$_j$, which means for points connected with a weighted edge, W$_{ij} > 0$, whereas for points without edge connection, W$_{ij} = 0$. And thus formed the adjacency matrix W$n \times n$, where W$_{ij}$ is the value of column j in row i. For diagonal matrix D, the diagonal value, d$_i$, equals to the absolute row sums of W$n \times n$. The equation is defined as Eq. (1), where non-diagonal elements are 0. Laplacian matrix (L) was the difference between diagonal matrix and adjacency

matrix($L = D - W$).

$$d_i = \sum_{j=1}^{n} W_{ij}, (i = 1, 2, ..., n, j = 1, 2, ..., n) \quad (1)$$

In general, $W_{n\times n}$ is unknown, which needs to be calculated via different methods like K_nearest neighbor method, Gaussian kernel function. But in this research, weights were correlation coefficient between variables, and we defined the weight to be 0, if its absolute value is less than 0.5. The core component of spectral clustering is to divide the graph $G(V, E)$ into k connected components, which is also called k categories, by removing some edges. $NCut$ and $RatioCut$ were widely used in cutting graph, with the help of W, D, L. Considering $RatioCut$ not only minimizing sums of weights among different categories, but also maximizing sizes of each category to avoid the extreme case that one category contains only one variable. So $RatioCut$(Hagen & Kahng, 1992) was used to cut graphs, and the equation was shown in Eq. (2). By introducing extra vector $\vec{h}$, Eq. (2) equals to $\vec{h_i^T} L \vec{h_i}$, which turns the target of minimizing $RatioCut$ into minimizing $tr(H_T LH)$, under the circumstances of $H^T H = I$. After getting the first k_1 corresponding eigenvectors by ascending eigenvalues after the calculation of $D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$, normalizing them to form the matrix $F_{n\times k_1}$, and then classifying the matrix to k_2 categories, we could finally cut the original graph into k_2 components. And in this paper, to reduce the complexity of $k_1$and k_2, they were entitled them with the same value.

$$RatioCut(V_1, V_2, ..., V_n) = \frac{1}{2} \sum_{i=1}^{k} \frac{W(V_i, \bar{V_i})}{||V_i||} \quad (2)$$

where for $A \in V$, $A + \bar{A} = V$, $||V_i||$ is the number of points in set V_i, and when set $A \in V$ and $B \in V$, $W(A, B) = \sum_{V_i \in A, V_j \in B} W_{ij}$.

2.3. Physics-reconstructed neural networks

Since the model proposed aimed to simulate the operation of mechanism models, to simulate the whole process, small fully connected neural networks blocks were thus used as the basic unit of computation, after spectral clustering. The whole model contained two layers in sequence. Each block in the first layer learned the features of variables from each group, which made each intermediate output theoretically learn features from its input data, thus named *feature learning*. Later on, all the outputs were collected to build connections with the target via the last block, hence was named *feature collection*. The structure was shown in Fig. 1

2.4. Model Evaluation

For evaluating accuracy of clustering, the confusion matrix for multiple categories was used to show how many variables were assigned as our expectation (Tab. 1). The *Accuracy* was calculated as $\frac{A_1+B_2+C_3}{T}$ or $\frac{A_1+B_2}{T}$, where A_1,B_2 and C_3 were the number of variables that were matched as experiences, and T represented the total amount of all variables, with a better clustering, if $Accuracy$ is closer to 1.

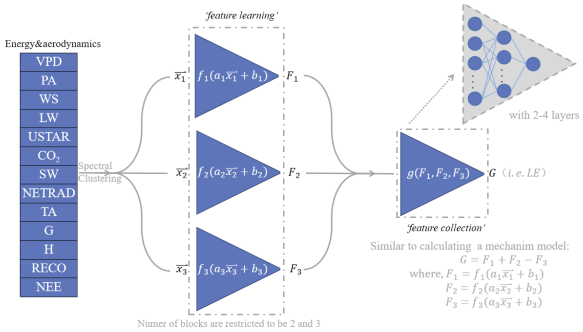

Figure 1. Comparison of processes between the proposed model and a mechanism model

Table 1. The confusion matrix for two and three groups

EMPIRICAL \ PRACTICAL	GROUPA	GROUPB	GROUPC
GROUPA	A_1	B_1	C_1
GROUPB	A_2	B_2	C_2
GROUPC	A_3	B_3	C_3

For evaluating accuracy of the whole model, statistical parameters, root mean square error (Eq. 3) and coefficients of determination (Eq. 4) were set to indicate the performance,where y_i is the measurement at time i, y_i^{hat} is the simulation at time i, and $\bar{y}$ is the average of measurements. N is the number of all samples. . The closer R^2 to 1, or the smaller $RMSE$ is, the better performance of the model is. Equations are as follows:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_i^{hat} - y_i)^2}{N}} \quad (3)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i^{hat} - y_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2} \quad (4)$$

3. Results and Discussions

3.1. Performances on reconstructing mechanisms

While operating a mechanism model, advanced rules like multiplication, division, and power, etc. always preferentially participate in the calculation over the low-level rules

like addition and subtraction. Since it is important to know which variables would be firstly calculated together in mechanism models, it is equally essential to figure out which variables would be in the same state in PRNN, because the corresponding block of neural networks would thus represent a physical process like what was done in mechanism models. So the result of spectral clustering determined the quality of reconstructing mechanisms.

According to previous research, evapotranspiration was related to aerodynamics and energy balance(Penman & Keen, 1948), which would thus restrict the number of clustering to be 2 or 3(3 for variables that might be related to both of the two processes). But when the number was adjusted to 4, results showed that it failed to make successful clustering and remained two or three groups, adhering to what was known and expected, which indicated that, spectral clustering, this method was effective and reliable for grouping input data. Based on that, results of clustering exhibited the interpretability of PRNN. Firstly, taking AT_Neu station as an example, it got three groups, which entitled three intermediate outputs in the original black-box model with features of PA, CO_2 respectively, and features mainly related to energy. Although there existed some variables empirically related to ecosystems or aerodynamics, like NEE and WS in the third group, the result that many variables clustered in one group that mainly related to energy also showed a consistency with previous research that energy balance is quite useful in estimating evaporation(Penman & Keen, 1948).

But it needed to be noticed that clustering result at AT_Neu station, the understanding from the perspective of AI, was not identical to our recognition. For further evaluation of differences between AI and human knowledge, empirical groups were set based on our experiences. Similarities were shown via Accuracy. At 42 stations, Tab. 5 showed Accuracy ranged from 0.23 to 0.85, with an average of 0.57, which suggested a varying difference on the understandings of mechanisms of evapotranspiration between PRNN and our knowledge.

Table 2. Empirical groups

NUMBER OF GROUPS.	AERODYNAMICS	ENERGY	BOTH
3	VPD,PA WS,USTAR	LW,SW,NETRAD TA,G,H	RECO,NEE
2	VPD,PA WS,USTAR RECO,NEE	LW,SW,RECO NETRAD,TA,G CO_2,H,NEE	

3.2. Performances on simulation

Apart from interpretability, the quality of reconstructing mechanisms actually depends on the precision. Due to different conditions on each station, the size of groups would vary in a wide range, which could result in overfitting, if the structure of the model on each station was fixed. So, hyperparameters of each model on each station, like the layers of each block of neural netorks should dynamically vary with the size of each group(Tab. 3). And since we viewed *feature learning* firstly doing calculation as advanced rules, and *feature collection* calculating as low-level rules just as what was done in mechanism models, we assumed that *feature learning* did the main learning process, more complex than what *feature collection* would do, so searching ranges of units thus were different between the two processes (Tab. 4). To find a good combination all hyperparameters, we introduced RandomizedSearchCV(Pedregosa et al., 2011; Buitinck et al., 2013) to resample 30 times to give an appropriate solution.

Table 3. The relationship between layers and input variables for each neural network

NUMBER OF VARIABLES	[1,3)	[3,6)	[6,12)
TOTAL LAYERS	2	3	4

Table 4. Searching ranges of hyper-parameters

UNITS OF *feature learning*	$k_1(k_2)$	UNITS OF *feature collection*
2,6,10,14,18,22,26	2,3	1,2,4,8

Also taking station AT_Neu as an example, the performance in validation set was depicted in Fig. 2. It could be seen that the fitting line is really close to the real line, which showed the good performance of the proposed model. Further, Among 42 sites, statistical evaluation was displayed in Tab. 5. Compared with pure artificial neural networks(ANN) and physics-constrained neural networks(Zhao et al., 2019), under the circumstances of a huge difference, 1-2 orders of magnitude smaller in samples' size, R^2 in this paper was just slightly worse than ANN, but almost equal to that of the method that used neural networks to take place of an empirical parameter, with $RMSE$ considerably dropping by 72.82% at least. But it should be noticed that the high precision gained at AT_Neu station accompanying the lowest similarity(0.23) between PRNN and human experience, which indicated that a different understanding of mechanism from AI could also make a precise simulation. Besides, the varying precision on different stations also proved the feasibility and robustness of the PRNN.

4. Uncertainties

Previous research of hybridization noticed shortcomings, such as little interpretability, vulnerable generalization from

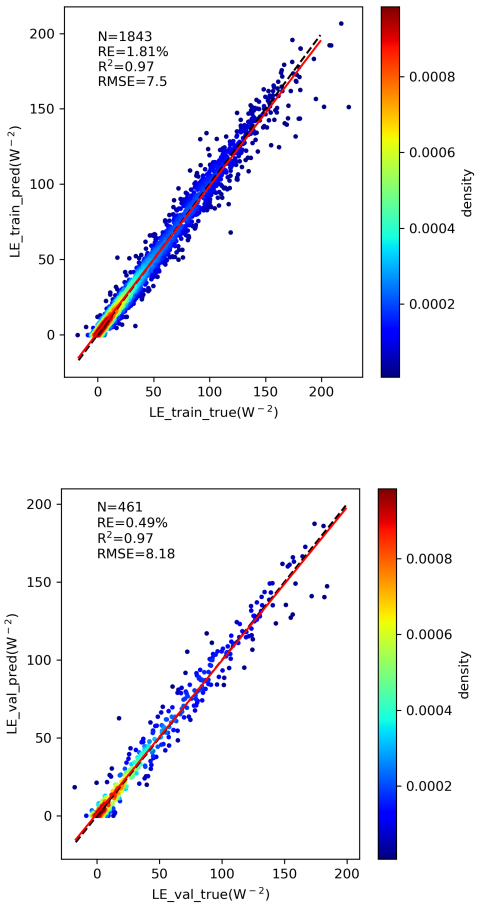

Figure 2. The performance of proposed model on train set(up) and validation set(down) at AT_Neu station (The black dashed line depicts the 1:1 line, and the red solid line depicts non-biased linear regression line)

Table 5. The statistical value of the evaluation indicators among 42 stations

STATISTICAL VALUE	*Accuracy*	$RMSE(Wm^{-2})$	R^2
MAXIMUM	0.85	34.67	0.97
MINIMUM	0.23	4.52	0.18
AVERAGE	0.57	13.98	0.77

Table 6. Comparison of results on validation set among different research

MODEL	R^2	$RMSE(Wm^{-2})$
ANN	0.81	46.26
PHYSICS-CONSTRAINED NEURAL NETWORKS	0.78	51.45
PRNN	0.77	13.98

AI and uncertainties of structures and parameters from mechanism models. Although we entitled meanings to some parameters in neural networks, breaking the black box, enhanced interpretability and validated feasibility in reconstructing mechanisms through AI, there are more uncertainties to be added. Firstly, the uncertainty of searching ranges, restricted by our assumptions, there were some sites in original data set with inappropriate model structures finally obtained after searching, which could not learn physical processes, resulting only less than 50% stations being effective. Besides, The input data was manually selected and it would be possible to get different clustering result with multiple input data.

5. Conclusion

Taking evapotranspiration as an example, this paper proved the feasibility of the proposed method, by comparing with the measurement and previous research. With analyses on clustering and proof on precision, we illustrated the possibility on entitling physical meanings on some parameters to improve interpretability and demonstrated even though the understanding of physical relationships were different from human knowledge, AI can still finish reconstructing mechanical processes with a high precision and less data demand through PRNN, which provided a new idea of hybridizing Artificial Intelligence and mechanism models for future work, which could be utilized in exploring the known and even in pre-simulating of the unknown knowledge.

References

Bastiaanssen, W., Menenti, M., Feddes, R., and Holtslag, A. A remote sensing surface energy balance algorithm for land (sebal). 1. formulation. *Journal of Hydrology*, 212-213:198–212, 1998. ISSN 0022-1694. doi: https://doi.org/10.1016/S0022-1694(98)00253-4.

Buitinck, L., Louppe, G., Blondel, M., Pedregosa, F., Mueller, A., Grisel, O., Niculae, V., Prettenhofer, P., Gramfort, A., Grobler, J., Layton, R., VanderPlas, J., Joly, A., Holt, B., and Varoquaux, G. API design for machine learning software: experiences from the scikit-learn project. In *ECML PKDD Workshop: Languages for Data Mining and Machine Learning*, pp. 108–122, 2013.

Chen, H., Huang, J. J., Dash, S. S., Wei, Y., and Li, H. A hybrid deep learning framework with physical process description for simulation of evapotranspiration. *Journal of Hydrology*, 606:127422, 2022.

Cintra, R., de Campos Velho, H., and Cocke, S. Tracking the model: Data assimilation by artificial neural network. In *2016 International Joint Conference on Neural Networks (IJCNN)*, pp. 403–410. IEEE, 2016.

Hagen, L. and Kahng, A. B. New spectral methods for ratio cut partitioning and clustering. *IEEE transactions on computer-aided design of integrated circuits and systems*, 11(9):1074–1085, 1992.

Hoedt, P.-J., Kratzert, F., Klotz, D., Halmich, C., Holzleitner, M., Nearing, G. S., Hochreiter, S., and Klambauer, G. Mc-lstm: Mass-conserving lstm. In *International Conference on Machine Learning*, pp. 4275–4286. PMLR, 2021.

Hu, Y.-C., Li, N., Jiang, Y., Bao, X., and Li, X.-Y. Research progress on coupling artificial intelligence and eco-environmental models. *Ying yong sheng tai xue bao = The journal of applied ecology*, 34 1:257–263, 2023.

Iten, R., Metger, T., Wilming, H., Del Rio, L., and Renner, R. Discovering physical concepts with neural networks. *Physical review letters*, 124(1):010508, 2020.

Katul, G. G., Oren, R., Manzoni, S., Higgins, C., and Parlange, M. B. Evapotranspiration: A process driving mass transport and energy exchange in the soil-plant-atmosphere-climate system. *Reviews of Geophysics*, 50, 2012.

Monteith, J. L. Evaporation and environment. *Symposia of the Society for Experimental Biology*, 19:205–34, 1965.

Nian-xiu, Q. Improved priestley-taylor method and its application in complementary relationship evapotranspiration model. 2011.

Pastorello, G., Trotta, C., Canfora, E., Chu, H., Christianson, D., Cheah, Y.-W., Poindexter, C., Chen, J., Elbashandy, A., Humphrey, M., et al. The fluxnet2015 dataset and the oneflux processing pipeline for eddy covariance data. *Scientific data*, 7(1):1–27, 2020.

Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., and Duchesnay, E. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.

Penman, H. L. and Keen, B. A. Natural evaporation from open water, bare soil and grass. *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences*, 193(1032):120–145, 1948. doi: 10.1098/rspa.1948.0037.

Raissi, M., Perdikaris, P., and Karniadakis, G. E. Physics informed deep learning (part i): Data-driven solutions of nonlinear partial differential equations. *arXiv preprint arXiv:1711.10561*, 2017.

Shen, H. and Zhang, L. Mechanism-learning coupling paradigms for parameter inversion and simulation in earth surface systems. *Science China Earth Sciences*, 66(3):568–582, 2023.

Sinclair, T. "natural evaporation from open water, bare soil and grass" by harold l. penman, (1948) a193:120–146. *Crop Science*, 59, 11 2019. doi: 10.2135/cropsci2019.05.0292.

Von Luxburg, U. A tutorial on spectral clustering. *Statistics and computing*, 17:395–416, 2007.

Wang, K. and Dickinson, R. E. A review of global terrestrial evapotranspiration: Observation, modeling, climatology, and climatic variability. *Reviews of Geophysics*, 50(2), 2012.

Yang, T., Sun, F., Gentine, P., Liu, W., Wang, H., Yin, J., Du, M., and Liu, C. Evaluation and machine learning improvement of global hydrological model-based flood simulations. *Environmental Research Letters*, 14(11):114027, 2019.

Zhao, W. L., Gentine, P., Reichstein, M., Zhang, Y., Zhou, S., Wen, Y., Lin, C., Li, X., and Qiu, G. Y. Physics-constrained machine learning of evapotranspiration. *Geophysical Research Letters*, 46(24):14496–14507, 2019.