

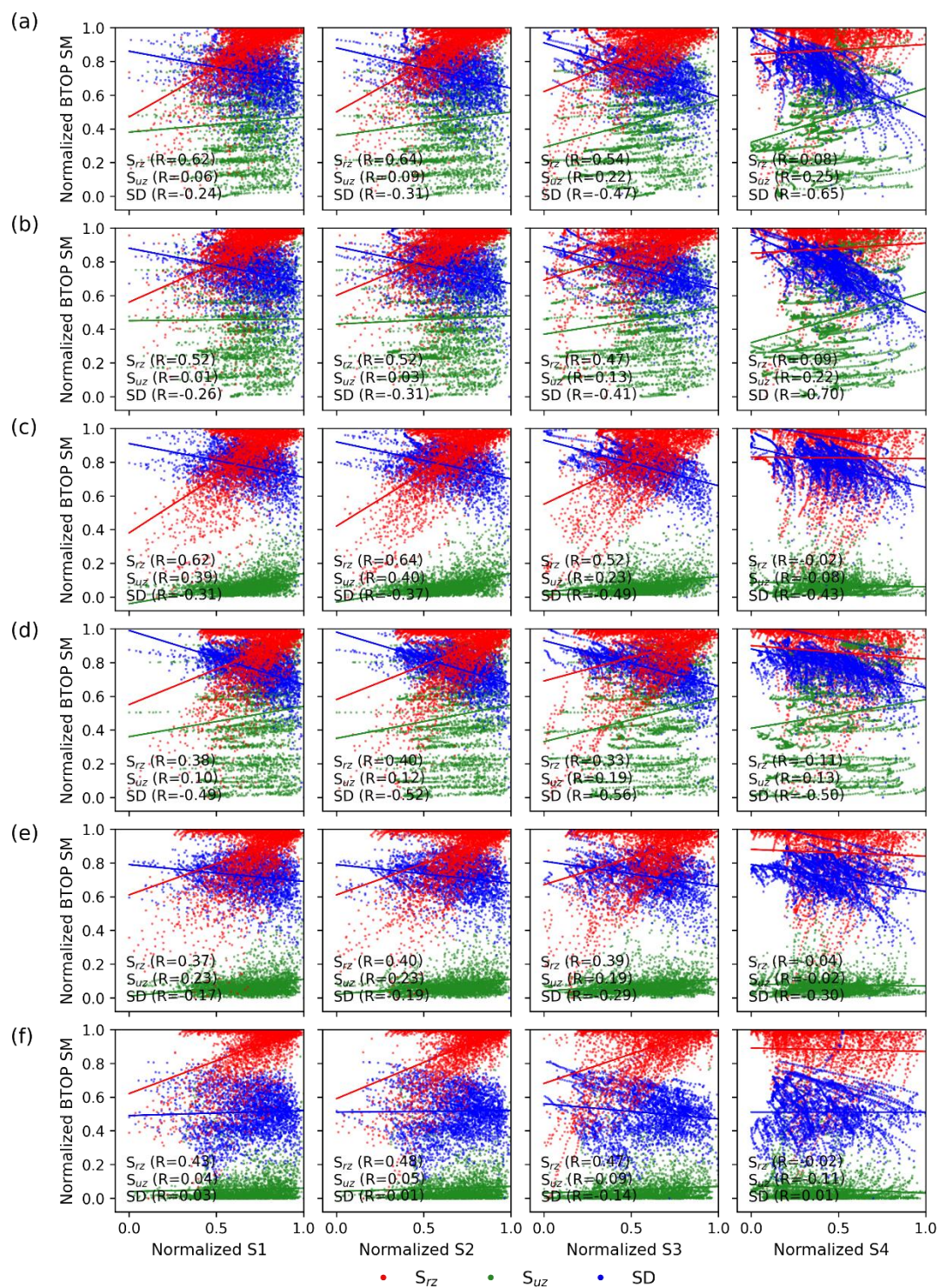


Figure S1 Daily scale scatterplots of the various normalized SM variable between BTOP and ERA5-Land in each sub-basin. (a) FRB-1; (b) FRB-2; (c) SRB-1; (d) SRB-2; (e) SRB-3; (f) SRB-4.

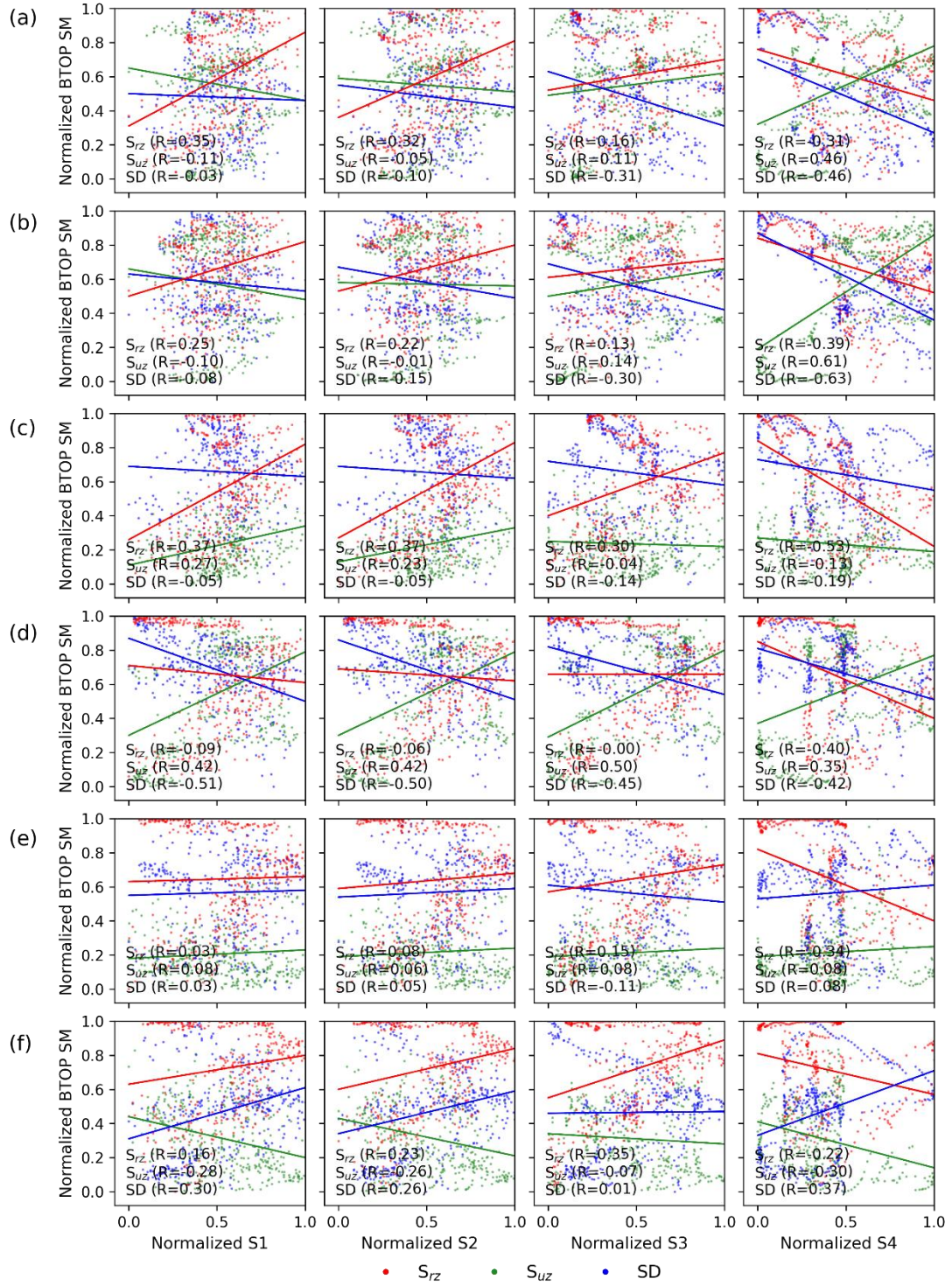


Figure S2 Annual average daily scale scatterplots of the various normalized SM variable between BTOP and ERA5-Land in each sub-basln. (a) FRB-1; (b) FRB-2; (c) SRB-1; (d) SRB-2; (e) SRB-3; (f) SRB-4.

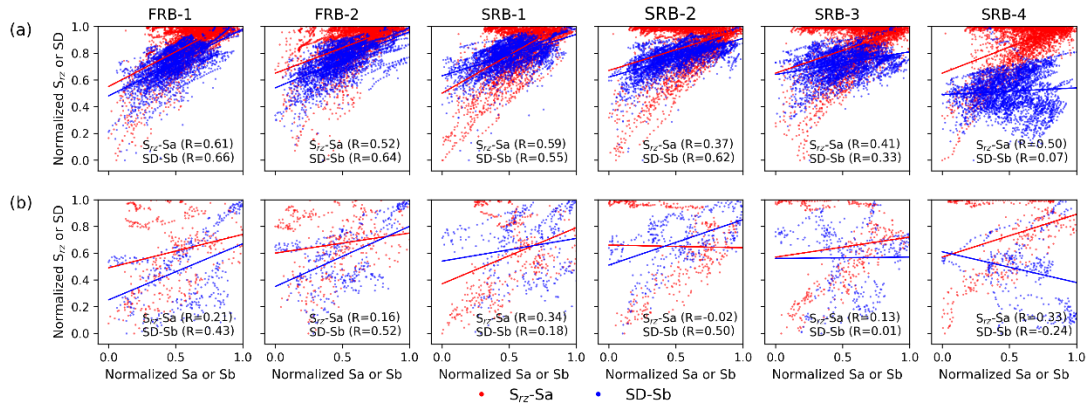


Figure S3 Scatterplots of S_{rz} - Sa and SD - Sb at the sub-basins in FRB and SRB. (a)

Daily scale. (b) Annual average daily scale.

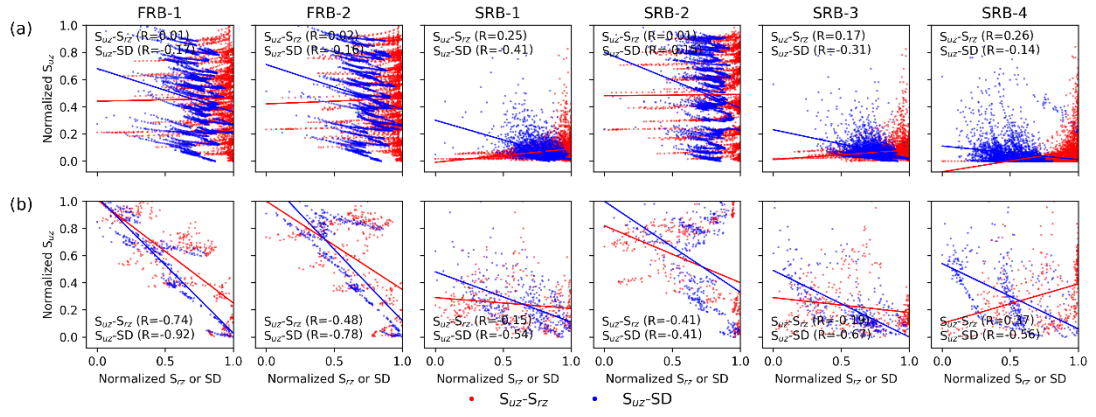


Figure S4 Scatterplots of $S_{uz}-S_{rz}$ and $S_{uz}-SD$ in the sub-basins of FRB and SRB. (a)

Daily scale. (b) Annual average daily scale.

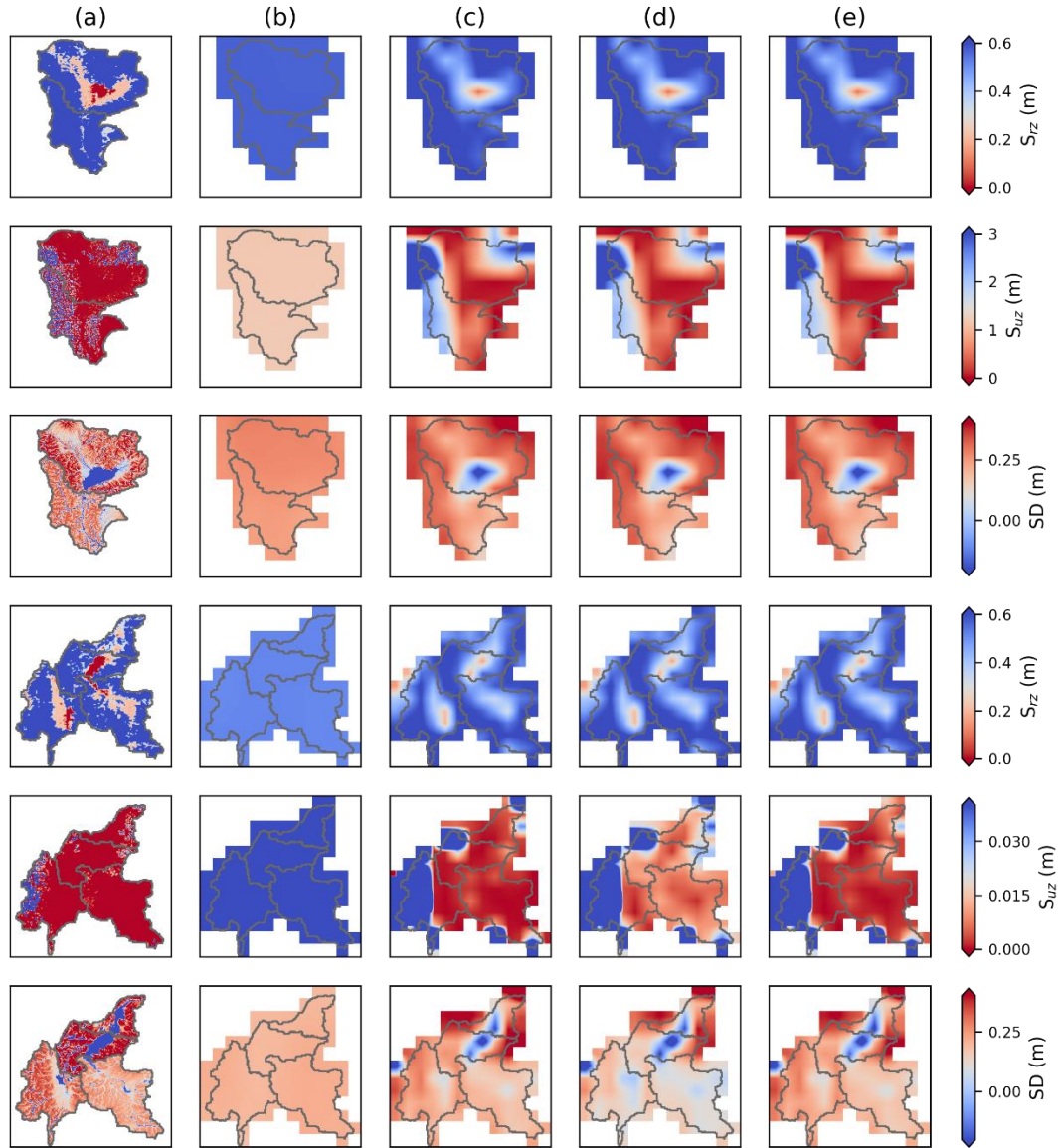


Figure S5 Spatial performance of the predicted SM using the developed relationships with the corresponding optimal curve fitting functions and LSTM at grid scales on December 31st, 2008. (a) Referee data (BTOP model output); (b) Optimal curve fitting with basin-scale relationship; (c) Optimal curve fitting with grid-scale relationship; (d) LSTM with basin-scale relationship; (e) LSTM with grid-scale relationship.

Note: This date represents general evaluation as it is in the test and validation period, and the hydrological simulation generally starts the first day of a year. Moreover, the results of other days (e.g., January 1st 2009, June 31st 2009) are similar.

Table S1 Performance of the ‘optimal’ Case1 during the calibration and validation period.

Sub-basins	Calibration			Validation		
	NSE	KGE'	R	NSE	KGE'	R
FRB-1	0.724	0.754	0.883	0.576	0.787	0.853
FRB-2	0.533	0.340	0.753	0.598	0.336	0.835
SRB-1	0.802	0.784	0.913	0.624	0.743	0.831
SRB-2	0.577	0.589	0.818	0.674	0.757	0.862
SRB-3	0.742	0.633	0.899	0.659	0.751	0.890
SRB-4	0.686	0.392	0.858	0.508	0.240	0.806
SRB-5	0.172	0.494	0.566	0.122	0.367	0.513
SRB-6	-0.341	0.075	0.157	-0.055	0.337	0.405
SRB-7	0.201	0.495	0.561	0.130	0.397	0.508

Note: The subbasins in grey color are discarded due to poor performance. The possible reasons for the poor simulated results may be the flat area and division projects, etc.

Table S2 Developed formulas between S_{rz} (denoted as y) and Sa (i.e., $S1+S2+S3$, denoted as x) at basin scale by six curve fitting functions.

Curve types	Case set-up	FRB	SRB
Polynomial	$d = 1$	$y = 0.201x + 0.470$	$y = 0.130x + 0.469$
	$d = 2$	$y = -2.476x^2 + 2.035x + 0.132$	$y = -2.144x^2 + 1.712x + 0.178$
	$d = 3$	$y = 53.65x^3 - 61.81x^2 + 23.82x - 2.52$	$y = 71.96x^3 - 81.62x^2 + 30.85x - 3.368$
	$d = 4$	$y = -1032x^4 + 1574x^3 - 899.1x^2 + 228x - 21.13$	$y = -1591x^4 + 2413x^3 - 1369x^2 + 344.4x - 31.91$
Logarithmic	/	$y = 0.075\ln(0.891x) + 0.628$	$y = 0.049\ln(0.759x) + 0.579$
Natural cubic spline	$k = 3$	$y = 0.145\{[(x-0.33)_+^3 - (x-0.40)_+^3]/0.068\} - 0.143\{[(x-0.37)_+^3 - (x-0.40)_+^3]/0.034\} + 0.116x + 0.404$	$y = 0.134\{[(x-0.34)_+^3 - (x-0.40)_+^3]/0.063\} - 0.134\{[(x-0.37)_+^3 - (x-0.40)_+^3]/0.032\} + 0.118x + 0.385$

Note: $(x-\xi)_+^3 = \begin{cases} (x-\xi)^3 & x > \xi \\ 0 & x \leq \xi \end{cases}$; The formulas in bold are selected for relationship development.

Table S3 Developed formulas between SD (denoted as y) and Sb (i.e., Depth minus Sa , denoted as x) at basin scale by six curve fitting functions

Curve types	Case setup	FRB	SRB
Polynomial	$d = 1$	$y = 0.916x - 1.386$	$y = 0.280x - 0.305$
	$d = 2$	$y = -3.911x^2 + 14.64x - 13.42$	$y = -2.636x^2 + 9.534x - 8.423$
	$d = 3$	$y = 63.46x^3 - 337.7x^2 + 599.7x - 355.1$	$y = 41.95x^3 - 223x^2 + 395.3x - 233.4$
	$d = 4$	$y = 103.4x^4 - 661.1x^3 + 1565x^2 - 1621x + 616.6$	$y = 670.1x^4 - 4648x^3 + 12080x^2 - 13950x + 6037$
Logarithmic	/	$y = 1.611\ln(1.066x) - 0.788$	$y = 0.494\ln(1.779x) - 0.376$
Natural spline	cubic $k = 3$	$y = 0.135\{(x-1.70)_+^3 - (x-1.80)_+^3\}/0.104\} - 0.078\{(x-1.75)_+^3 - (x-1.80)_+^3\}/0.052\} - 0.065x + 0.148$	$y = 0.066\{(x-1.70)_+^3 - (x-1.80)_+^3\}/0.100\} - 0.061\{(x-1.75)_+^3 - (x-1.80)_+^3\}/0.050\} + 0.003x + 0.130$

Note: $(x-\xi)_+^3 = \begin{cases} (x-\xi)^3 & x > \xi \\ 0 & x \leq \xi \end{cases}$; The formulas in bold are selected for relationship development.

Table S4 Developed formulas between S_{uz} (denoted as y) and SD (denoted as x) at basin scale by six traditional curve fitting functions.

Curve types	Case setup	FRB	SRB
Polynomial	$d = 1$	$y = -0.653x + 1.033$	$y = -0.1855x + 0.2134$
	$d = 2$	$y = -5.207x^2 - 1.600x + 0.794$	$y = 2.792x^2 - 1.210x + 0.3068$
	$d = 3$	$y = 16.20x^3 - 15.77x^2 + 3.871x + 0.633$	$y = 143.2x^3 - 75.12x^2 + 12.84x - 0.5328$
	$d = 4$	$y = 953.2x^4 - 797.9x^3 + 242.5x^2 - 32.18x + 2.502$	$y = -2179x^4 + 1709x^3 - 494.7x^2 + 62.56x - 2.73$
Logarithmic	/	$y = -0.137\ln(1.280x) + 0.715$	$y = -0.034\ln(0.543x) + 0.100$
Natural spline	cubic $k = 3$	$y = 0.183\{[(x-0.181)_+^3 - (x-0.240)_+^3]/0.059\} + 0.224\{[(x-0.210)_+^3 - (x-0.240)_+^3]/0.030\} + 0.257x + 0.664$	$y = 0.0397\{[(x-0.160)_+^3 - (x-0.196)_+^3]/0.036\} - 0.0417\{[(x-0.178)_+^3 - (x-0.196)_+^3]/0.018\} + 0.0547x + 0.1362$

Note: $(x-\xi)_+^3 = \begin{cases} (x-\xi)^3 & x > \xi \\ 0 & x \leq \xi \end{cases}$; The formulas in bold are selected for relationship development.

Table S5 Performance of four configured hydrological simulations in the calibration period, the validation period, and 2003.

Sub-basins	Indicators	Calibration				Validation				2003			
		Case1	Case2	Case3	Case4	Case1	Case2	Case3	Case4	Case1	Case2	Case3	Case4
FRB-1	NSE	0.724	0.492	0.689	0.685	0.576	0.449	0.493	0.484	0.599	0.499	0.529	0.528
	KGE'	0.754	0.738	0.811	0.812	0.787	0.674	0.748	0.743	0.733	0.370	0.385	0.374
	R	0.883	0.855	0.866	0.867	0.853	0.907	0.845	0.845	0.856	0.815	0.844	0.848
FRB-2	NSE	0.533	0.178	0.527	0.532	0.598	0.545	0.609	0.610	0.537	0.388	0.516	0.528
	KGE'	0.340	0.425	0.386	0.389	0.336	0.318	0.344	0.343	0.571	0.429	0.612	0.623
	R	0.753	0.631	0.740	0.744	0.835	0.784	0.831	0.831	0.739	0.733	0.730	0.737
SRB-1	NSE	0.802	0.736	0.798	0.806	0.624	0.435	0.478	0.436	0.751	-0.044	0.542	0.596
	KGE'	0.784	0.579	0.734	0.767	0.743	0.244	0.644	0.584	0.824	0.356	0.645	0.745
	R	0.913	0.898	0.911	0.911	0.831	0.875	0.774	0.764	0.874	0.483	0.806	0.812
SRB-2	NSE	0.577	0.422	0.532	0.533	0.674	0.633	0.648	0.665	0.205	-0.469	0.050	0.048
	KGE'	0.589	0.351	0.472	0.476	0.757	0.661	0.712	0.726	0.360	0.055	0.399	0.396
	R	0.818	0.773	0.811	0.810	0.862	0.845	0.865	0.871	0.577	0.199	0.561	0.550
SRB-3	NSE	0.742	0.573	0.735	0.714	0.659	0.582	0.604	0.616	0.256	-1.028	-0.013	-0.121
	KGE'	0.633	0.325	0.626	0.560	0.751	0.431	0.718	0.720	0.574	0.036	0.477	0.420
	R	0.899	0.863	0.898	0.894	0.890	0.886	0.884	0.887	0.656	0.257	0.577	0.578
SRB-4	NSE	0.686	0.638	0.685	0.698	0.508	0.497	0.516	0.529	0.224	-0.100	0.224	0.247
	KGE'	0.392	0.576	0.405	0.438	0.240	0.423	0.272	0.292	0.119	0.081	0.173	0.220
	R	0.858	0.814	0.859	0.859	0.806	0.784	0.804	0.802	0.558	0.179	0.506	0.514
Mean	NSE	0.677	0.506	0.661	0.661	0.606	0.524	0.558	0.557	0.429	-0.126	0.308	0.304
	KGE'	0.582	0.499	0.572	0.574	0.602	0.458	0.573	0.568	0.530	0.221	0.449	0.463
	R	0.854	0.806	0.847	0.848	0.846	0.847	0.834	0.833	0.710	0.444	0.671	0.673