Supplementary Materials

Table S1. Data sources of the potential spatial predictors for water quality (i.e. catchment characteristics). See Lintern et al. (2018) for details.

	Catchment characteristic	Data Source
Climate	Average annual radiation (MJ $m^{-2}day^{-1}$)	(Geoscience Australia, 2011)
	Average temperature (°C)	(Geoscience Australia, 2011)
	Average temperature of warmest quarter (°C)	(Geoscience Australia, 2011)
	Average temperature of coldest quarter (°C)	(Geoscience Australia, 2011)
	Maximum temperature of hottest month (°C)	(Geoscience Australia, 2011)
	Minimum temperature of coldest month (°C)	(Geoscience Australia, 2011)
	Annual average rainfall (mm)	(Geoscience Australia, 2011)
	Average rainfall of the wettest quarter (mm)	(Geoscience Australia, 2011)
	Average rainfall of the driest quarter (mm)	(Geoscience Australia, 2011)
	Average rainfall of the coldest quarter (mm)	(Geoscience Australia, 2011)
	Average rainfall of the warmest quarter (mm)	(Geoscience Australia, 2011)
	Annual average catchment rainfall erosivity (MJ $mm^{-1}ha^{-1}hr^{-1}yr^{-1}$)	(Geoscience Australia, 2011)
Hydrology	Average annual runoff (mm)	(Geoscience Australia, 2011)
	Average of average daily flow (ML d^{-1})	Calculated using instantaneous flows from DELWP (2016)
	Standard deviation of average daily flow (ML d^{-1})	Calculated using instantaneous flows from DELWP (2016)
	Pereniality of runoff (%) (proportion of "contribution to mean annual discharge by the driest six months of the year" (Geoscience Australia, 2011))	(Geoscience Australia, 2011)
	Mean number of days where there is no flow annually (days $year^{-1}$)	Calculated using daily flows from DELWP (2016)
	Mean 7-day low flow (ML d^{-1})	Calculated using instantaneous flows from DELWP (2016)
	Mean Base Flow Index	Calculated using method outlined in Grayson et al. (1996)
	Maximum distance upstream to dam wall or reservoir (km)	(Geoscience Australia, 2011)
	Area of catchment comprised of farm dams (%)	(Department of Environment Land Water and Planning Victoria, 2016)
	Total storage capacity of dams in catchment normalized to average daily flow (ML $ML^{-1}d^{-1}$)	(Geoscience Australia, 2004)
Land use	Area of catchment urbanized (%)	(Bureau of Rural Sciences, 2010)
	Area of catchment made up of roads (%)	(Bureau of Rural Sciences, 2010)
	Area of catchment used for horticulture (%)	(Bureau of Rural Sciences, 2010)
	Area of catchment used for agriculture (%)[1]	(Bureau of Rural Sciences, 2010)
	Area of catchment used for pastures (grazing) (%)	(Bureau of Rural Sciences, 2010)
	Area of catchment used for cropping (%)[2]	(Bureau of Rural Sciences, 2010)
Land cover	Mean width of vegetated riparian zone (m)	(Department of Environment Land Water and Planning, 2014)
	Average fragmentation of riparian zone (%)	(Department of Environment Land Water and Planning, 2014)
	Area of catchment covered with grass (%)[3]	(Geoscience Australia, 2011)
	Area of catchment covered with forest (%)[4]	(Geoscience Australia, 2011)
	Area of catchment covered with shrubs (%)[5]	(Geoscience Australia, 2011)
	Area of catchment covered with woodland (%)[6]	(Geoscience Australia, 2011)
	Area of catchment bare (%)	(Geoscience Australia, 2011)

Soil type and geology	Area of catchment underlain by unconsolidated bedrock (%)	(Geoscience Australia, 2011)
	Area of catchment underlain by igneous bedrock (%)	(Geoscience Australia, 2011)
	Area of catchment underlain by sedimentary bedrock (%)	(Geoscience Australia, 2011)
	Area of catchment underlain by mixed igneous and sedimentary bedrock (%)	(Geoscience Australia, 2011)
	Average soil TP content (mg kg^{-1})	(Terrestrial Ecosystem Research Network, 2016)
	Average soil TN content (mg kg^{-1})	(Terrestrial Ecosystem Research Network, 2016)
	Average soil clay content (%)	(Terrestrial Ecosystem Research Network, 2016)
	Area of catchment with saline aquifers (%)	(Department of Agriculture and Water Resources, 2013)
Topography	Catchment area ($km^{2)}$	(Geoscience Australia, 2011)
	Mean catchment elevation (m)	(Geoscience Australia, 2011)
	Maximum catchment elevation (m)	(Geoscience Australia, 2011)
	Area of catchment made up of valley bottoms (%)	(Geoscience Australia, 2011)
	Total catchment length (km)	(Geoscience Australia, 2011)
	Mean catchment slope (%)	(Geoscience Australia, 2011)
	Mean channel slope (%)	Calculated using BOM (2012)

1. Agricultural activities include all primary production activities including plantation forests, grazing pastures, cropping and horticulture. This includes both dryland and irrigation agricultural activities.

2. Cropping refers to the production of commodities such as cereals, beverage and spice crops, hay, oilseeds, sugar, cotton, alkaloid poppies and pulses.

3. Grass refers to grasslands with tussock, hummock, reeds/rushes.

4. Forest refers to rainforests, Eucalypt forests, mangroves and low closed forests (e.g., Acacia, Melaleuca or Banksia species). Areas with high density of vegetation (>30% cover) and tall trees (>10 m).

5. Shrubs refers to open and dry woodlands and shrublands with hummock or tussock grass, Melaleuca shrublands, lignum shrublands, saltbush and chenopods. Areas with vegetation <2 m tall.

6. Woodlands refer to areas with medium trees (<10 m) at medium density (<30% cover).

Table S2. Data sources of the potential temporal predictors for water quality. See Guo et al. (2019) for details.

Data		**Source**
Daily rainfall (mm)		Australian Water Availability Project (AWAP) (Raupach et al., 2009, 2012) Available from: http://www.csiro.au/awap; http://www.bom.gov.au/jsp/awap/index.jsp
Daily average temperature (°C)		
Daily actual ET (mm)		Australian Water Resources Assessment (Frost et al., 2016) Available from: http://www.bom.gov.au/water/landscape
Daily average root zone soil moisture		
Daily average deep soil moisture		
Monthly NDVI	January 1994 – December 1999	Advanced Very High Resolution Radiometer product (AVHRR) (Eidenshink, 1992) Available from: https://earthdata.nasa.gov/
	January 2000 – December 2013	Moderate Resolution Imaging Spectroradiometer (MODIS); MOD13A3 (NASA LP DAAC, 2017) Available from: https://earthdata.nasa.gov/

Table S3. Log-Sinh transformation parameter (a and b) values for 50 potential spatial predictors for stream water quality (i.e. catchment characteristics).

Catchment characteristics	***a***	***b***
Annual radiation (MJ $m^{-2}day^{-1}$)	3.458	2.052
Annual temperature (°C)	2.425	3.133
Annual rainfall (mm)	0.008	0.001
Erosivity (MJ $mm^{-1}ha^{-1}hr^{-1}yr^{-1}$)	0.030	0.000
Driest quarter rain (mm)	0.099	0.003
Wettest quarter rain (mm)	0.002	0.003
Warmest quarter rainfall (mm)	0.039	0.005
Coldest quarter rainfall (mm)	0.001	0.001
Coldest month minimum temperature (°C)	4.999	0.000
Hottest month maximum temperature (°C)	0.000	0.002
Coldest quarter mean temperature (°C)	4.986	4.996
Warmest quarter mean temperature (°C)	3.805	2.193
Average of average daily flow (ML d^{-1})	0.002	0.001
Average of average daily flow (ML d^{-1})	0.034	0.002
Standard deviation of average daily flow (ML d^{-1})	0.012	0.430
Pereniality of runoff (%) (proportion of 'contribution to mean annual discharge by the driest six months of the year'	0.106	0.152
Mean number of days where there is no flow annually (days $year^{-1}$)	0.000	0.066
Mean 7-day low flow (ML d^{-1})	0.045	3.319
Mean Base Flow Index	4.896	0.000
Maximum distance upstream to dam wall or reservoir (km)	0.034	0.006
Area of catchment comprised of farm dams (%)	0.000	5.000
Total storage capacity of dams in catchment normalized to average daily flow (ML $ML^{-1}d^{-1}$)	0.003	0.002
Area of catchment urbanized (%)	0.000	0.135
Area of catchment made up of roads (%)	0.055	0.729
Area of catchment used for agriculture (%)	4.998	4.995
Area of catchment used for pastures (grazing) (%)	0.174	0.114
Area of catchment used for cropping (%)	0.000	0.079
Area of catchment used for horticulture (%)	0.000	0.373
Mean width of vegetated riparian zone (m)	0.293	0.013
Average fragmentation of riparian zone (%)	0.174	0.132
Area of catchment covered with grass (%)	0.000	0.158
Area of catchment covered with forest (%)	0.238	0.020
Area of catchment covered with shrubs (%)	0.000	0.403
Area of catchment covered with woodland (%)	0.002	0.108
Area of catchment bare (%)	0.000	5.000
Area of catchment underlain by unconsolidated bedrock (%)	0.024	0.050
Area of catchment underlain by igneous bedrock (%)	0.034	0.068
Area of catchment underlain by sedimentary bedrock (%)	4.998	4.995
Area of catchment underlain by mixed igneous and sedimentary bedrock (%)	0.000	0.032
Average soil TP content (mg kg^{-1})	0.044	4.744

Average soil TN content (mg kg^{-1})	0.213	1.733
Average soil clay content (%)	0.000	0.021
Area of catchment with saline aquifers (%)	0.001	0.000
Catchment area (km^2)	0.177	0.001
Mean catchment elevation (m)	0.044	0.001
Area of catchment made up of valley bottoms (%)	0.002	0.074
Total catchment length (km)	0.003	0.001
Mean catchment slope (%)	0.078	0.068
Mean channel slope (%)	0.029	4.899
Average soil clay content (%)	0.103	0.040

Table S4. Box-Cox transformation parameter (lambda) values for the six water quality constituents and the potential temporal predictors.

Water Quality Constituent	***lambda***
TSS	-0.249
TP	-0.058
FRP	-0.836
TKN	0.141
NO_x	0.107
EC	-0.024
Temporal predictors	***lambda***
Rainfall (mm)	-0.243
Rainfall on previous day (mm)	0.107
Averaged rainfall over previous 3 days (mm)	0.108
Averaged rainfall over previous 7 days (mm)	0.157
Averaged rainfall over previous 14 days (mm)	0.220
Averaged rainfall over previous 30 days (mm)	0.193
Streamflow (mm d^{-1})	0.115
Streamflow on previous day (mm d^{-1})	-0.014
Averaged Streamflow over previous 3 days (mm d^{-1})	-0.028
Averaged Streamflow over previous 7 days (mm d^{-1})	-0.033
Averaged Streamflow over previous 14 days (mm d^{-1})	-0.032
Averaged Streamflow over previous 30 days (mm d^{-1})	-0.023
Dry spell length in the past 14 days (days)	-0.005
NDVI for the month	0.258
Water temperature (°C)	3.712
Air temperature (°C)	0.234
Evaporation (mm)	0.021
Root zone soil moisture (%)	0.094
Deep soil moisture (%)	0.910

Table S5. Key factors affecting the spatial variability for each of six constituents (see Section 2.3 in the main text, and also Lintern et al. (2018)).

Constituent	**Key factors that affect spatial variability**
TSS	Hottest month maximum temperature Percentage area covered by grass Percentage area covered by shrub Percentage cropping area Maximum elevation Dam storage Percentage clay area
TP	Erosivity

	Percentage area covered by grass Percentage area covered by shrub Percentage area made up of roads Percentage cropping area Average soil TP content
FRP	Percentage area covered by shrub Percentage cropping area Catchment area Average soil TP content Mean channel slope
TKN	Percentage clay area Warmest quarter mean temperature Coldest quarter rainfall Percentage cropping area Percentage pasture area Average soil TP content
NO_x	Annual radiation Warm quarter rainfall Hottest month maximum temperature Average soil TP content Mean channel slope
EC	Annual radiation Annual rainfall Wettest quarter rain Hottest month maximum temperature Percentage agriculture area Percentage cropping area Percentage area covered by shrub Average soil TN content

Table S6. Key factors affecting the temporal variability for each of six constituents (see Section 2.3 in the main text, and also Guo et al. (2019)). The third column shows the two key catchment characteristics that affect the spatial variability in each temporal factor, which were selected by correlation analyses between the coefficient values of the temporal effects and the catchment characteristics.

Constituent	**Key factors that affect temporal variability**	**Key factors that affect spatial variability in temporal effects**
TSS	Same-day streamflow	Annual rainfall, Hottest month maximum temperature
	7-day antecedent streamflow	Annual runoff, Mean elevation
	Water temperature	Daily flow standard deviation, Total catchment length
	Soil moisture root	Percentage area with saline aquifers, Hottest month maximum temperature
	Soil moisture deep	Maximum distance upstream to dam wall or reservoir, Percentage area covered by grassland
TP	Same-day streamflow	Annual rainfall, Hottest month maximum temperature
	30-day antecedent streamflow	Erosivity Percentage cropping area
	NDVI	Mean 7-day low flow, Maximum distance upstream to dam wall or reservoir
	Water temperature	Coldest quarter rainfall, Maximum distance upstream to dam wall or reservoir
	Soil moisture root	Warmest quarter average temperature, Percentage pasture area
	Soil moisture deep	Hottest month maximum temperature, Warmest quarter average temperature
FRP	Same-day streamflow	Percentage agriculture area,

		Coldest quarter mean temperature
	Water temperature	Total catchment length, Coldest quarter mean temperature
	Soil moisture deep	Percentage area used for roads, Percentage aea covered by woodland
TKN	Same-day streamflow	Annual rainfall, Hottet month maximum temperature
	30-day antecedent streamflow	Erosivity, Percentage cropping area
	NDVI	Mean 7-day low flow, Maximum distance upstream to dam wall or reservoir
	Water temperature	Coldest quarter rainfall, Maximum distance upstream to dam wall or reservoir
	Soil moisture root	Warmest quarter mean temperature, Percentage pasture area
	Soil moisture deep	Hottest month maximum temperature, Warmest quarter mean temperature
NOx	Same-day streamflow	Total storage capacity of dams in catchment, Mean soil TN content
	30-day antecedent streamflow	Coldest quarter rainfall, Hottest month maximum temperature
	Water temperature	Percentage area covered by woodland, Maximum elevation
	NDVI	Percentage area underlain by mixed igneous bedrock, Percentage urbanized area
	Soil moisture root	Annual rainfall, Warmest quarter average temperature
	Soil moisture deep	Percentage horticulture area, Wettest quarter rainfall
EC	Same-day streamflow	Percentage area covered by grassland, Percentage area covered by woodland
	14-day antecedent streamflow	Mean 7-day low flow, Percentage area covered by forest
	Water temperature	Coldest month minimum temperature, Mean catchment slope
	Soil moisture root	Mean 7-day low flow, Average soil TN content
	Soil moisture deep	Maximum elevation, Percentage area covered by woodland

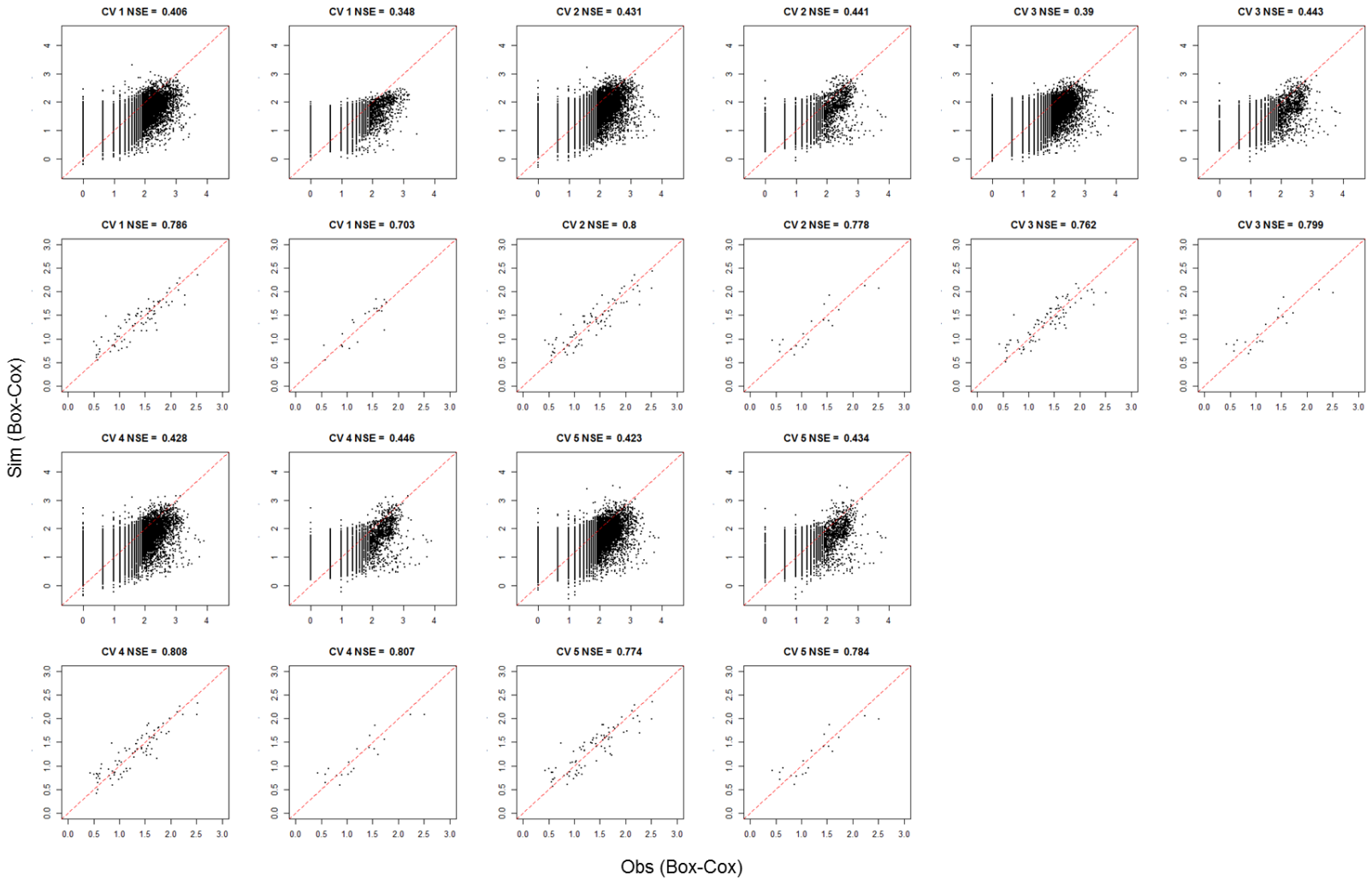


Figure S1. Fittings of the five partial models for TSS (see Section 2.4 in text for calibration/validation approaches), each within a 2x2 panel and showing the calibration and validation fittings in the left and right columns, respectively. Within each partial model, top row shows the fitting to all data whereas bottom row shows fitting to site-level mean concentrations. All values are presented in Box-Cox transformed space and the dashed red lines indicate 1:1 (perfect fit).

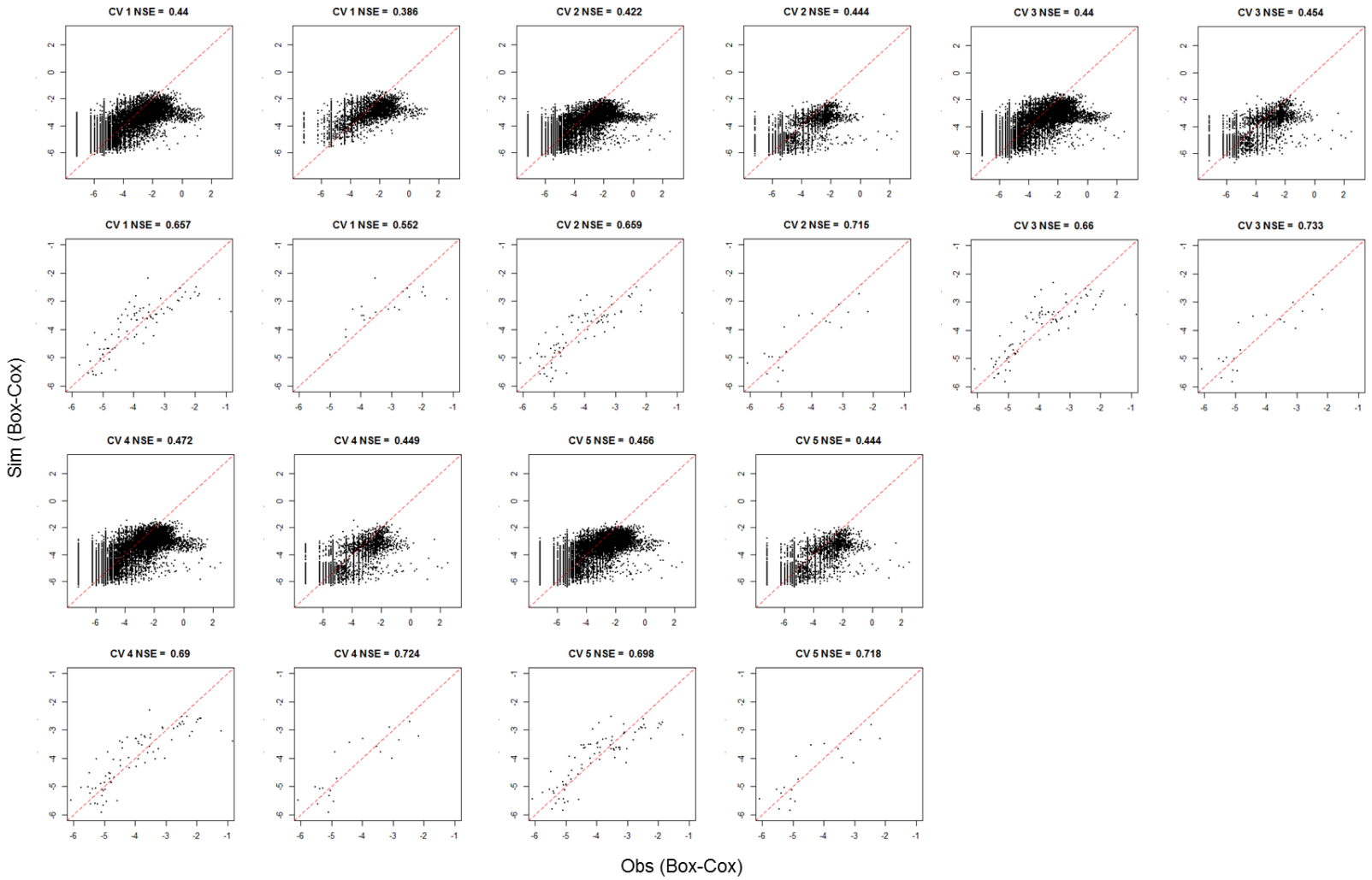


Figure S2. Fittings of the five partial models for TP (see Section 2.4 in text for calibration/validation approaches), each within a 2x2 panel and showing the calibration and validation fittings in the left and right columns, respectively. Within each partial model, top row shows the fitting to all data whereas bottom row shows fitting to site-level mean concentrations. All values are presented in Box-Cox transformed space and the dashed red lines indicate 1:1 (perfect fit).

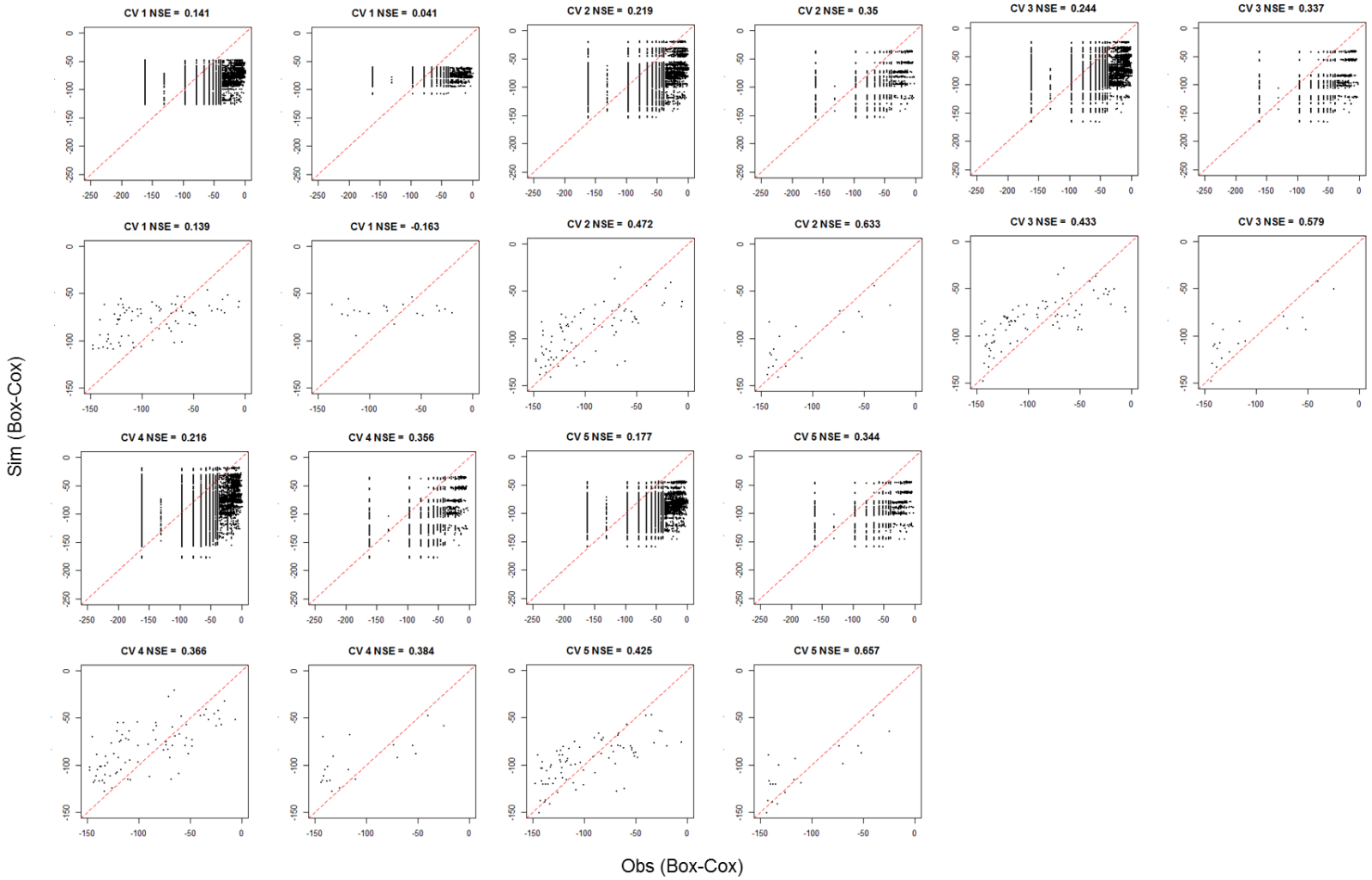


Figure S3. Fittings of the five partial models for FRP (see Section 2.4 in text for calibration/validation approaches), each within a 2x2 panel and showing the calibration and validation fittings in the left and right columns, respectively. Within each partial model, top row shows the fitting to all data whereas bottom row shows fitting to site-level mean concentrations. All values are presented in Box-Cox transformed space and the dashed red lines indicate 1:1 (perfect fit).

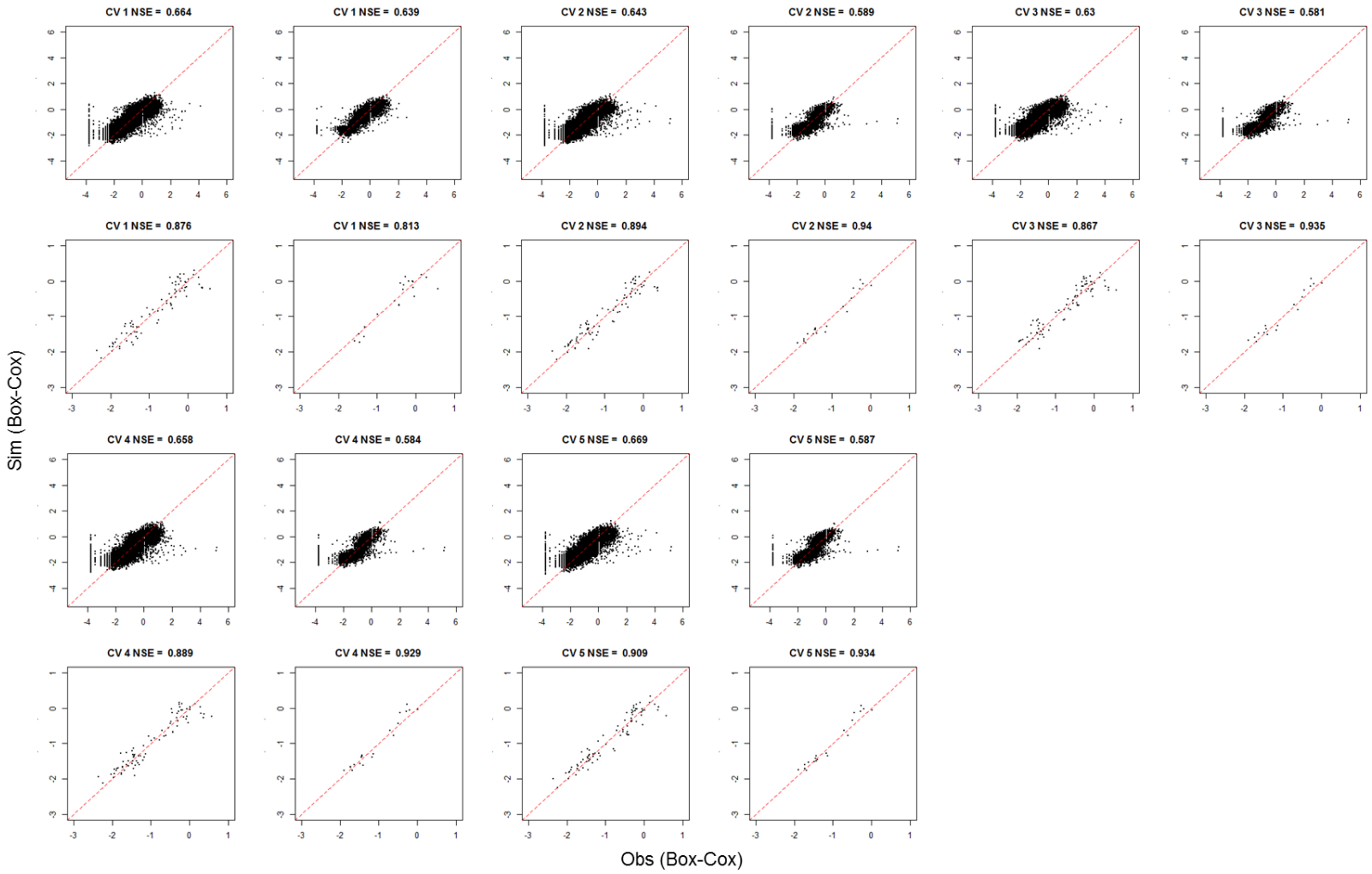


Figure S4. Fittings of the five partial models for TKN (see Section 2.4 in text for calibration/validation approaches), each within a 2x2 panel and showing the calibration and validation fittings in the left and right columns, respectively. Within each partial model, top row shows the fitting to all data whereas bottom row shows fitting to site-level mean concentrations. All values are presented in Box-Cox transformed space and the dashed red lines indicate 1:1 (perfect fit).

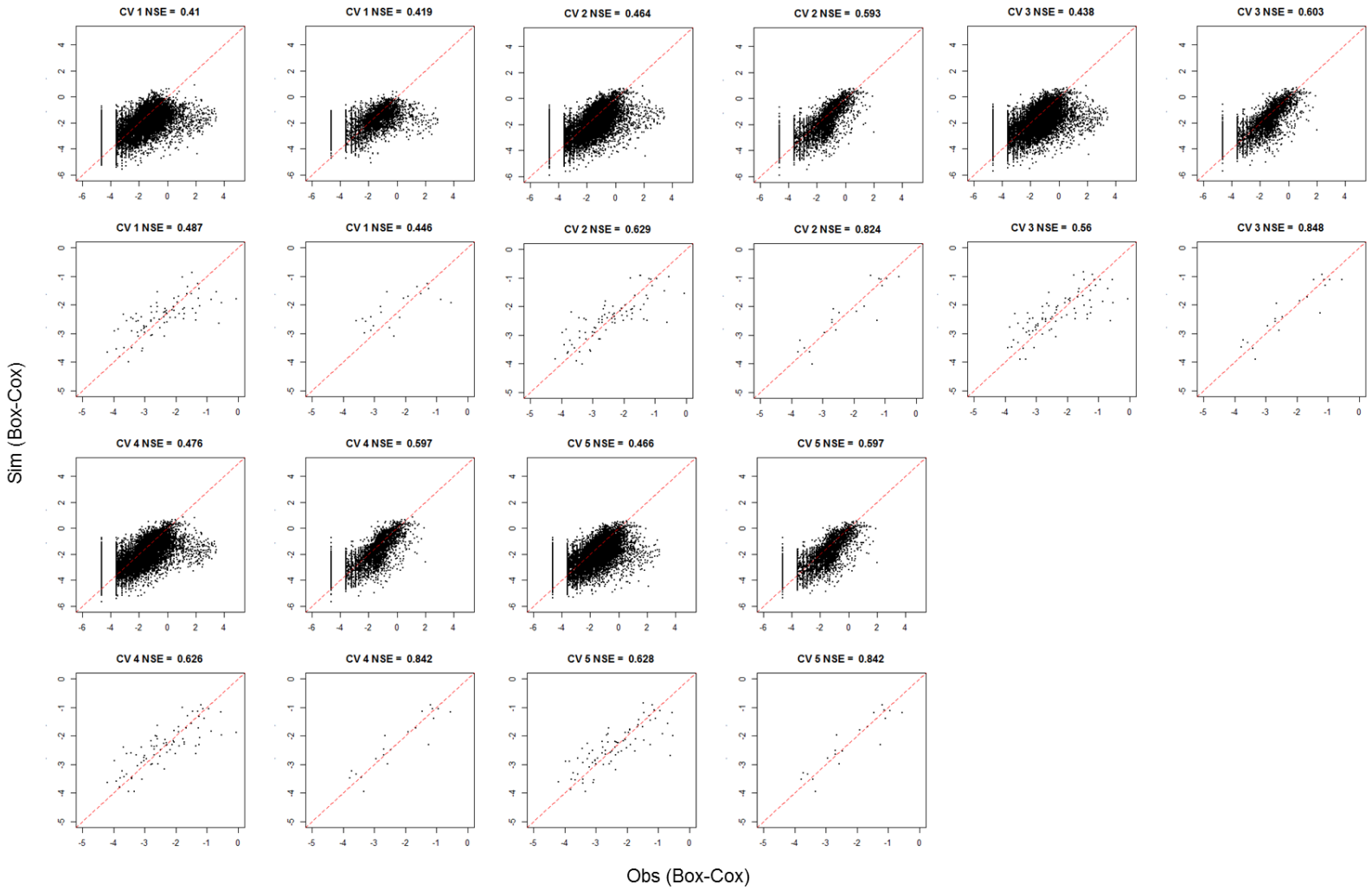


Figure S5. Fittings of the five partial models for NO_x (see Section 2.4 in text for calibration/validation approaches), each within a 2x2 panel and showing the calibration and validation fittings in the left and right columns, respectively. Within each partial model, top row shows the fitting to all data whereas bottom row shows fitting to site-level mean concentrations. All values are presented in Box-Cox transformed space and the dashed red lines indicate 1:1 (perfect fit).

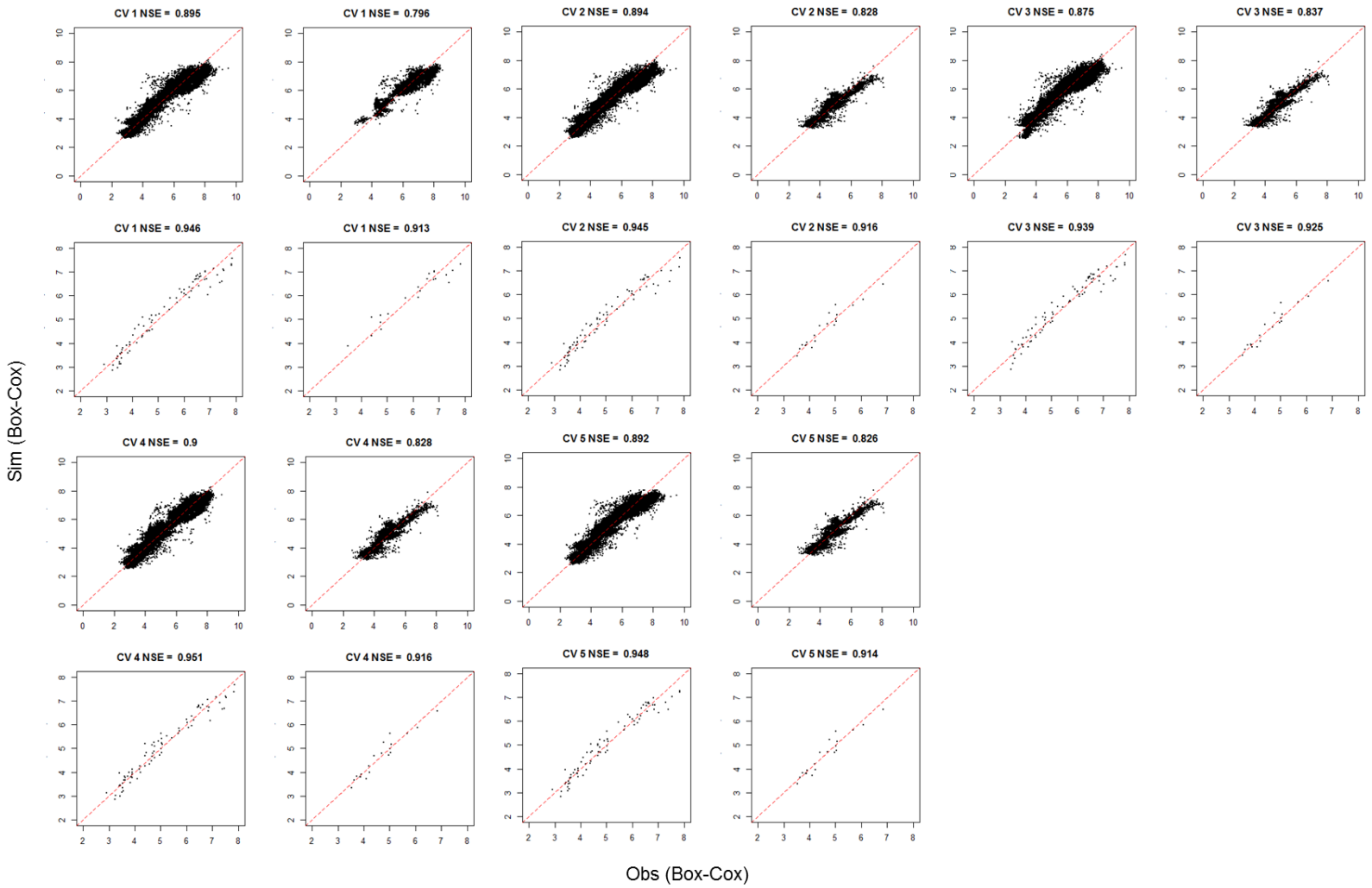


Figure S6. Fittings of the five partial models for EC (see Section 2.4 in text for calibration/validation approaches), each within a 2x2 panel and showing the calibration and validation fittings in the left and right columns, respectively. Within each partial model, top row shows the fitting to all data whereas bottom row shows fitting to site-level mean concentrations. All values are presented in Box-Cox transformed space and the dashed red lines indicate 1:1 (perfect fit).

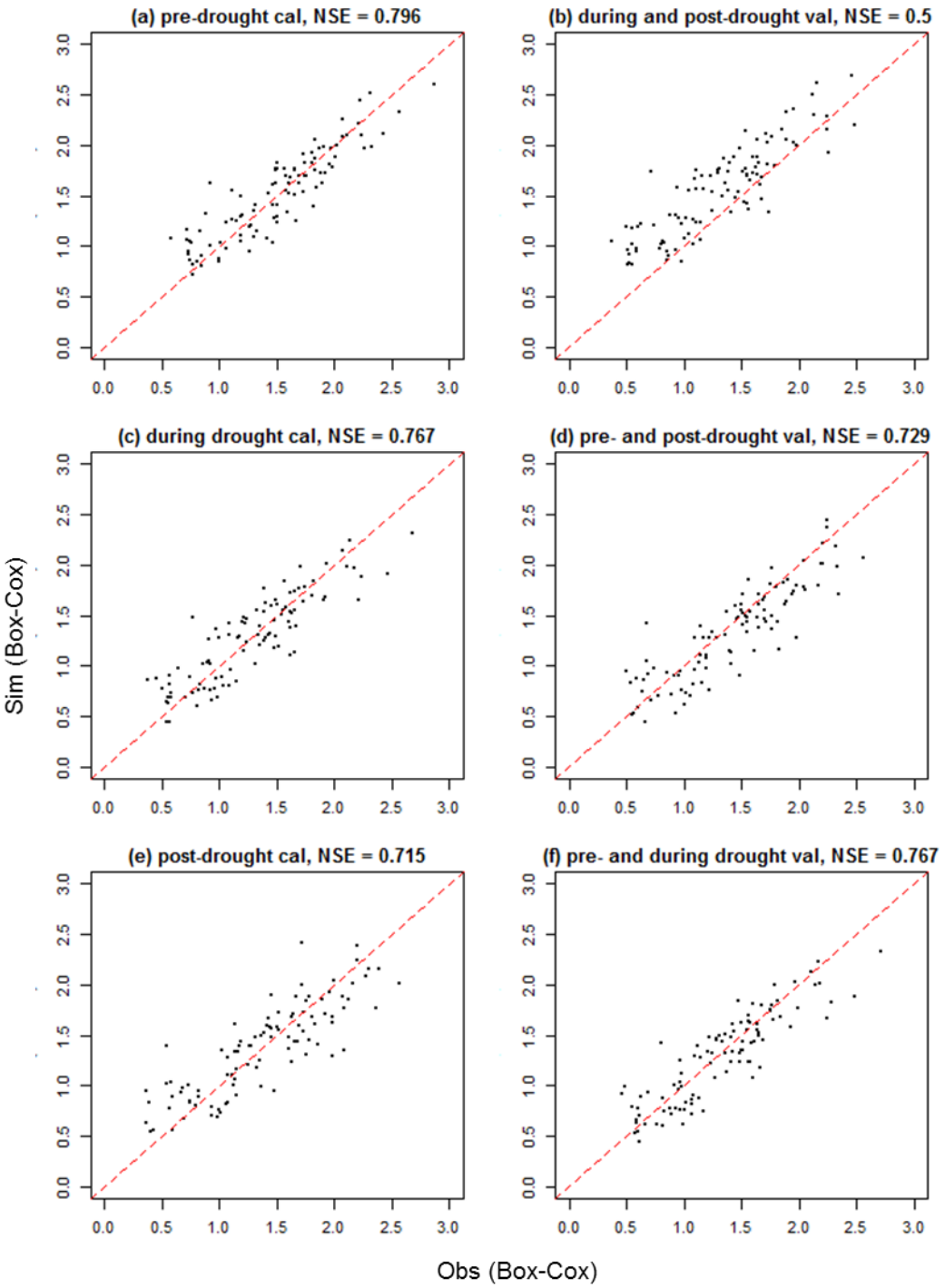


Figure S7. Comparison of the TSS model performance, as the simulated against observed site-level mean concentrations across three different calibration/validation periods for calibrations on the pre-drought (1994-1996), drought (1997-2009) and the post-drought (2010-2014) periods, respectively, see Section 2.4 for details of the calibration and validation approach.

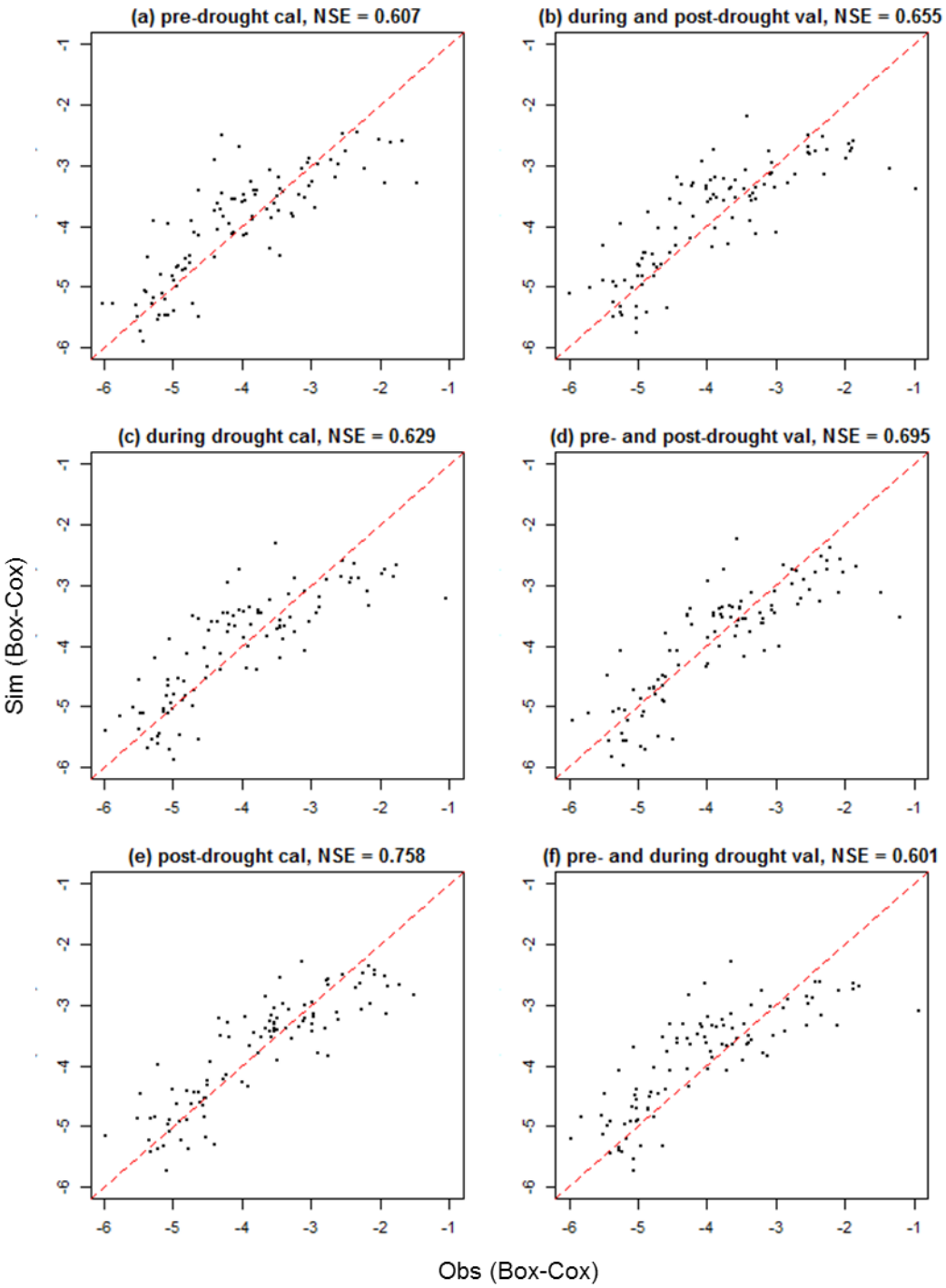


Figure S8. Comparison of the TP model performance, as the simulated against observed site-level mean concentrations across three different calibration/validation periods for calibrations on the pre-drought (1994-1996), drought (1997-2009) and the post-drought (2010-2014) periods, respectively, see Section 2.4 for details of the calibration and validation approach.

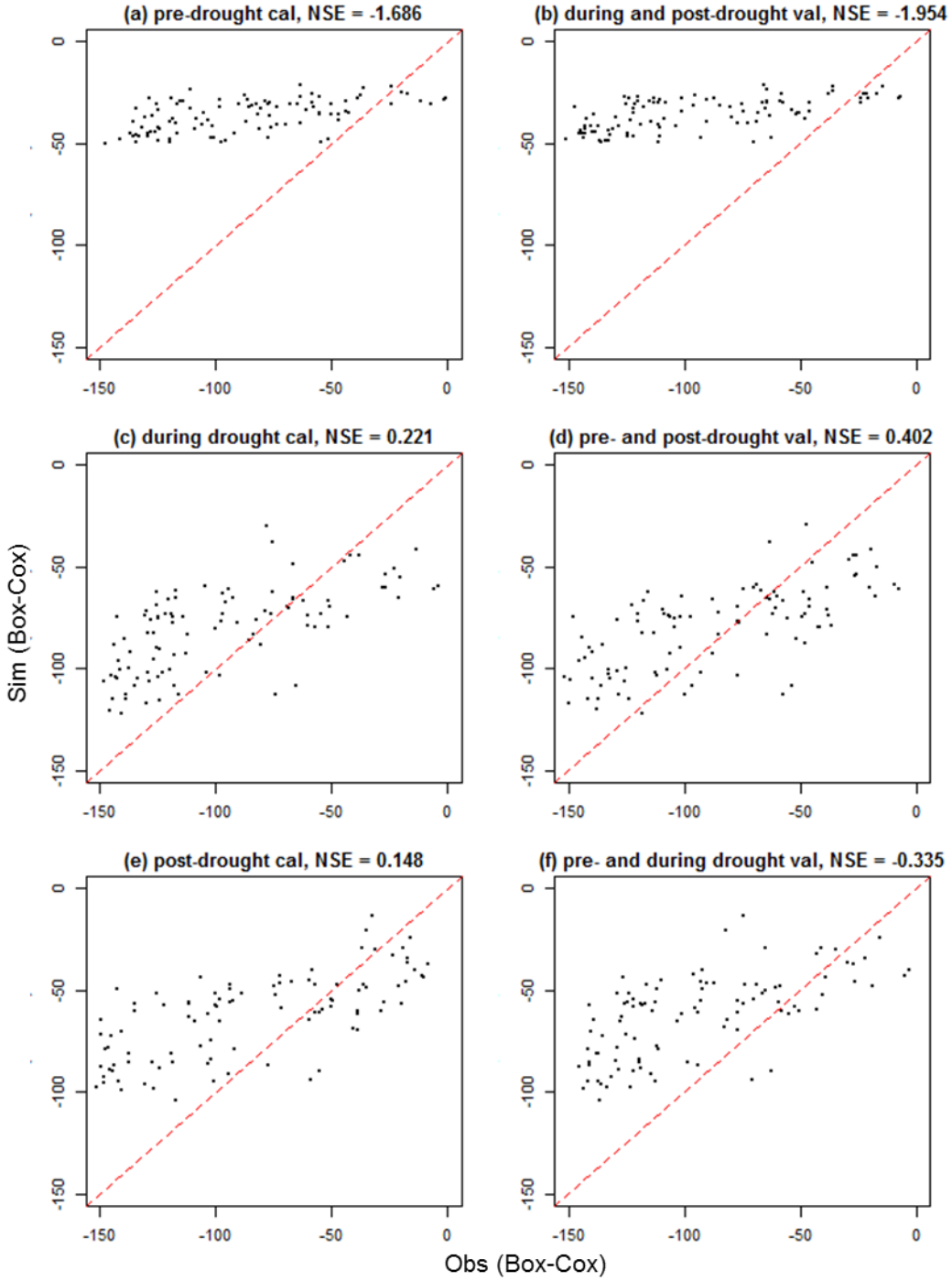


Figure S9. Comparison of the FRP model performance, as the simulated against observed site-level mean concentrations across three different calibration/validation periods for calibrations on the pre-drought (1994-1996), drought (1997-2009) and the post-drought (2010-2014) periods, respectively, see Section 2.4 for details of the calibration and validation approach. Note that the unstable performance can be resulted by the poor performance for the full model, see Section 3.1.

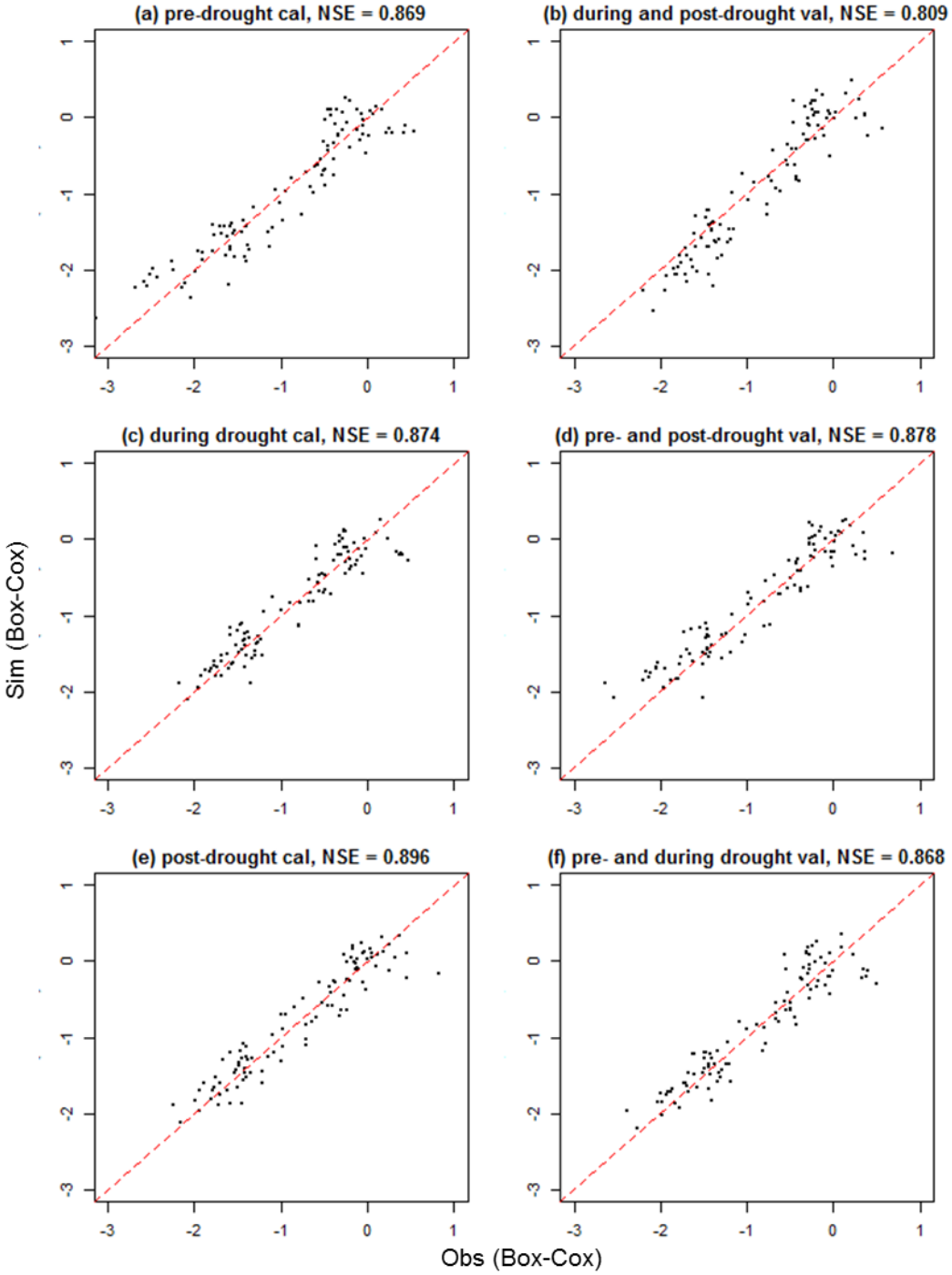


Figure S10. Comparison of the TKN model performance, as the simulated against observed site-level mean concentrations across three different calibration/validation periods for calibrations on the pre-drought (1994-1996), drought (1997-2009) and the post-drought (2010-2014) periods, respectively, see Section 2.4 for details of the calibration and validation approach.

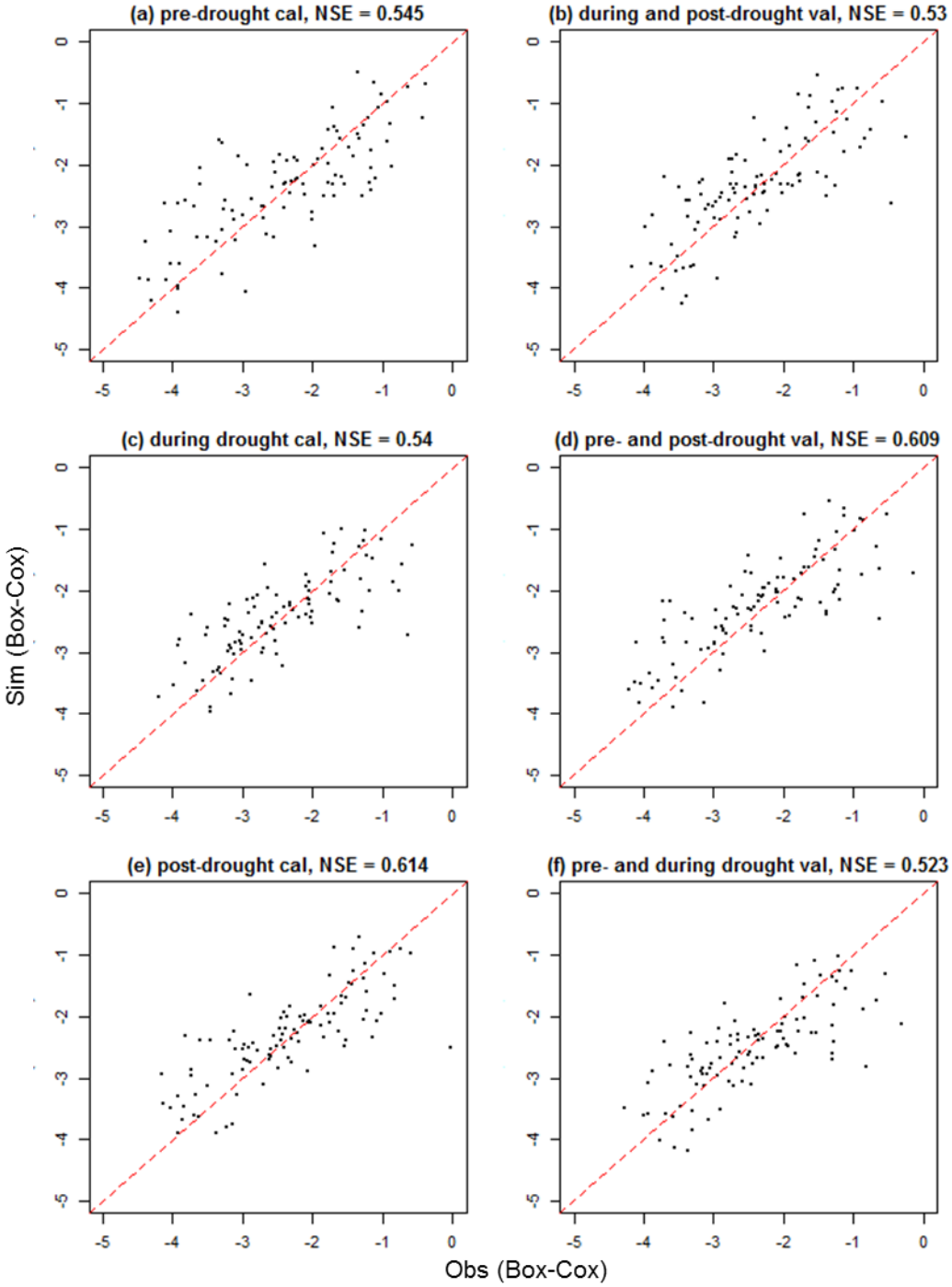


Figure S11. Comparison of the NO_x model performance, as the simulated against observed site-level mean concentrations across three different calibration/validation periods for calibrations on the pre-drought (1994-1996), drought (1997-2009) and the post-drought (2010-2014) periods, respectively, see Section 2.4 for details of the calibration and validation approach.

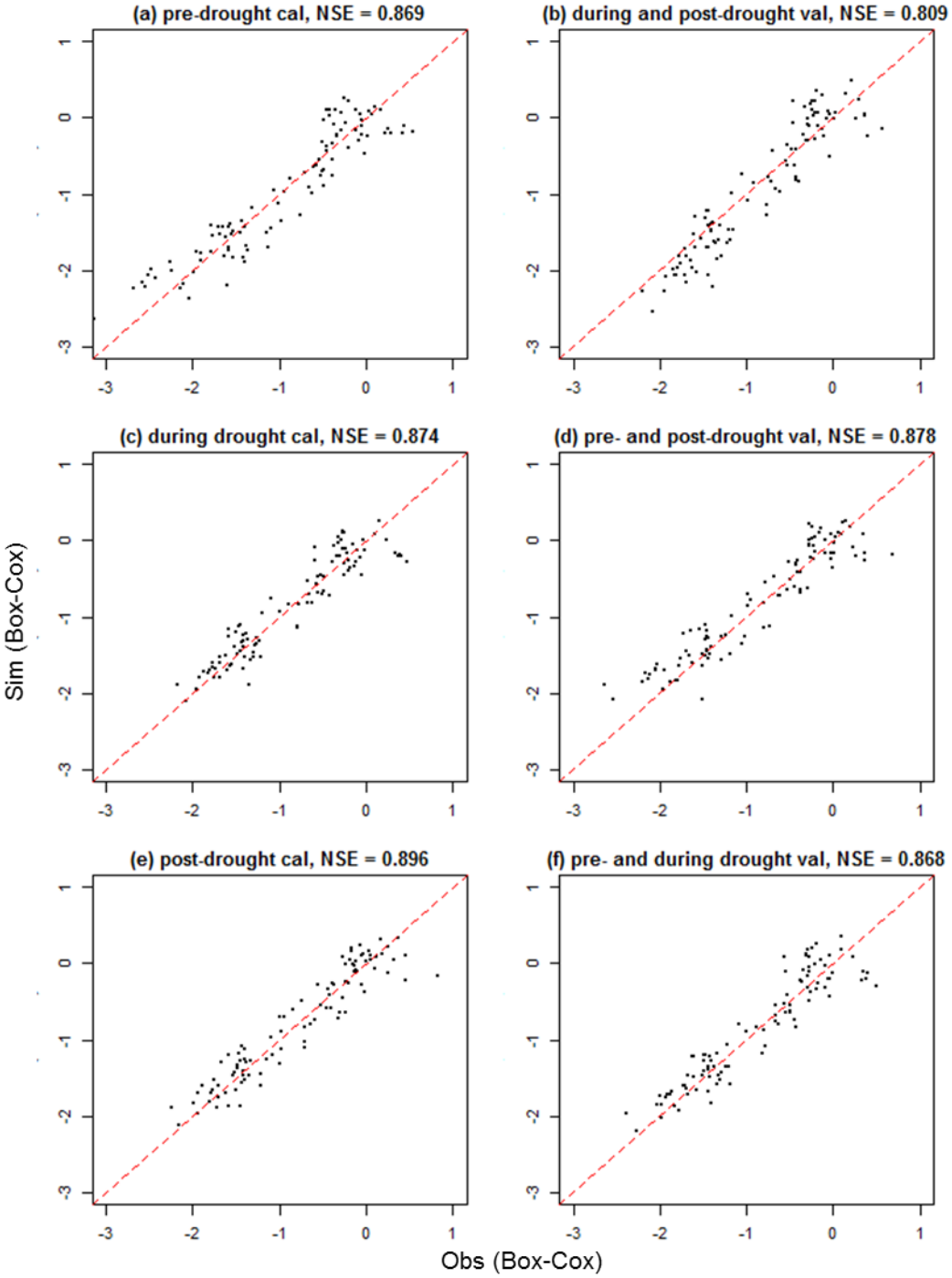
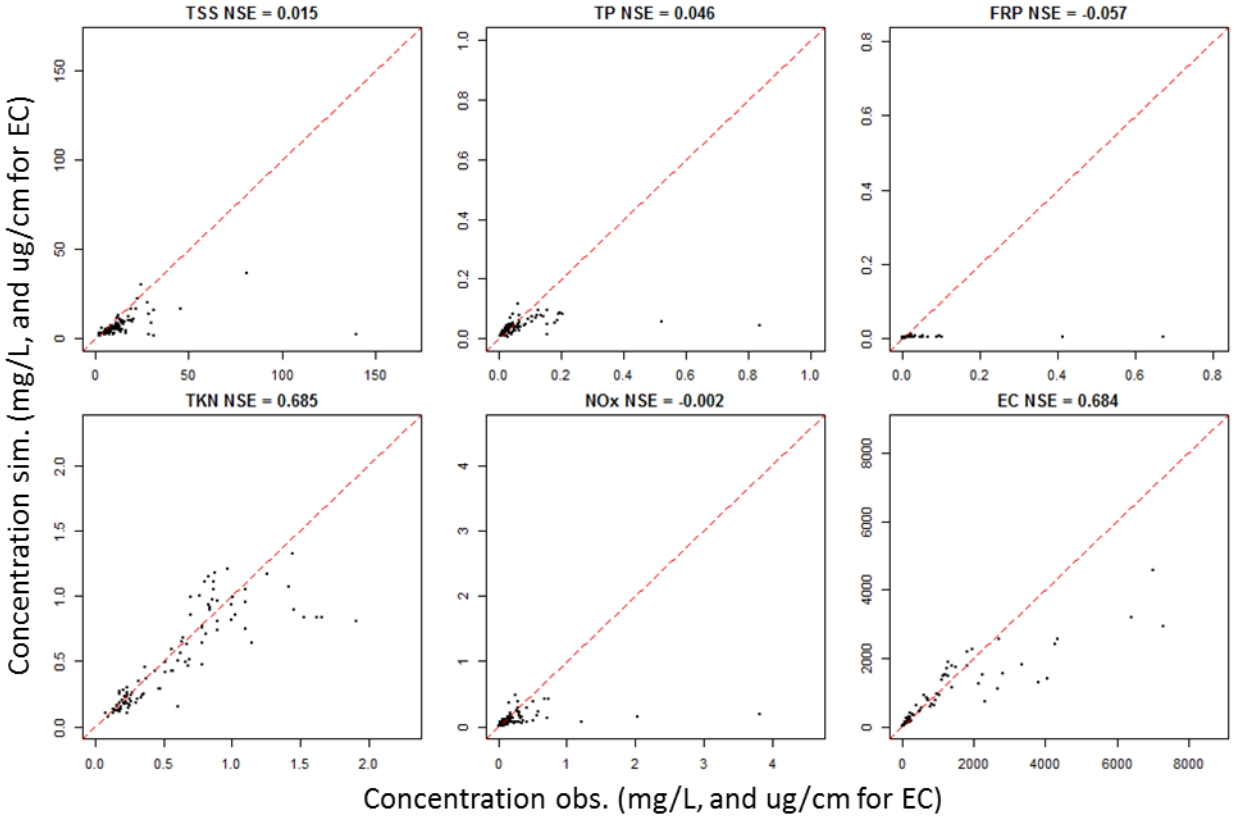


Figure S12. Comparison of the EC model performance, as the simulated against observed site-level mean concentrations across three different calibration/validation periods for calibrations on the pre-drought (1994-1996), drought (1997-2009) and the post-drought (2010-2014) periods, respectively, see Section 2.4 for details of the calibration and validation approach.



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93 **Figure S13. Back-transformation of the model simulations to the measurement scale emphasizes**
94 **influences of unusually high concentrations and thus heavily affects model fitting, illustrated by simulated**
95 **against observed site-level mean concentrations of each constituent in a back-transformed scale.**

96