Using Multi-Criterea Calibration Methods to Estimate Nitrate Pollution in a Large Basin with Limited Data

Daniel Hawtree

Stefan Julich, Karl-Heinz Feger

SWAT Conference

Warsaw | Poland | 28-30 June 2017

TECHNISCHE UNIVERSITÄT DRESDEN

Technische Universität Dresden,
Institute of Soil Science & Site Ecology

Education and Culture
Erasmus Mundus

Forest and Nature for Society (FONASO)
Joint Doctoral Program

universidade de aveiro

University of Aveiro, CESAM &
Department of Environment and Planning

Presentation Overview

- Study Site, Objectives, & Calibration Approach

- Parameter Set Selection

  1. Kling-Gupta Efficiency → rescaling of components

  2. Kolmogorov–Smirnov (KS) Test → utility for nutrient calibration

  3. Pareto Selection Method

- Preliminary Conclusions: Pros / Cons

Vouga River Basin

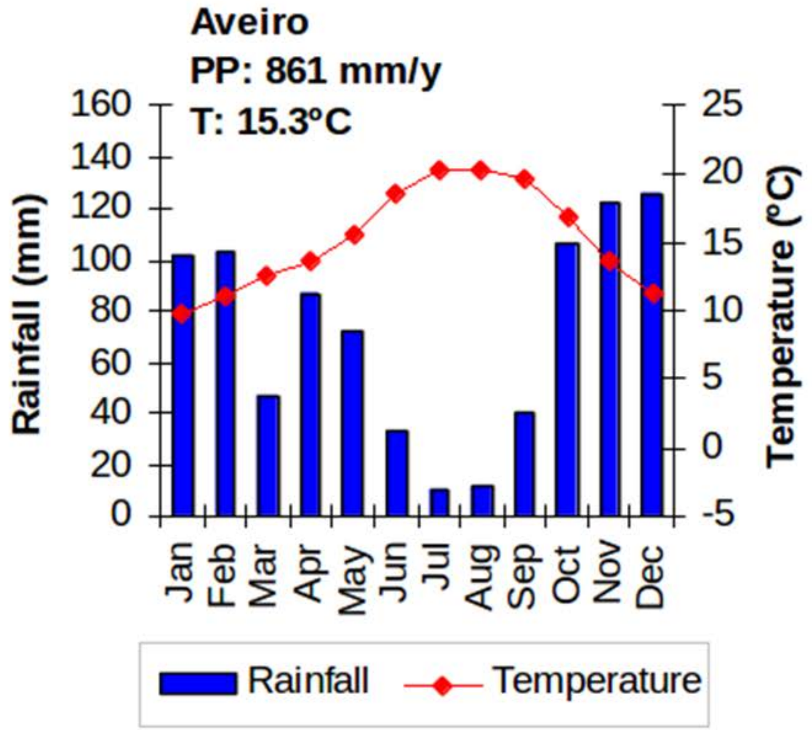
2,298 km^2

Aridity index - Rainfall / PET

Dry climates

Hyper-arid	🟥	< 0.05	🟩	0.65 - 0.8
Arid	🟧	0.05 - 0.2	🟩	0.8 - 1
Semi-arid	🟨	0.2 - 0.5	🟦	1 - 1.5
Dry/sub-humid	🟨	0.5 - 0.65	🟦	>1.5

Humid climates

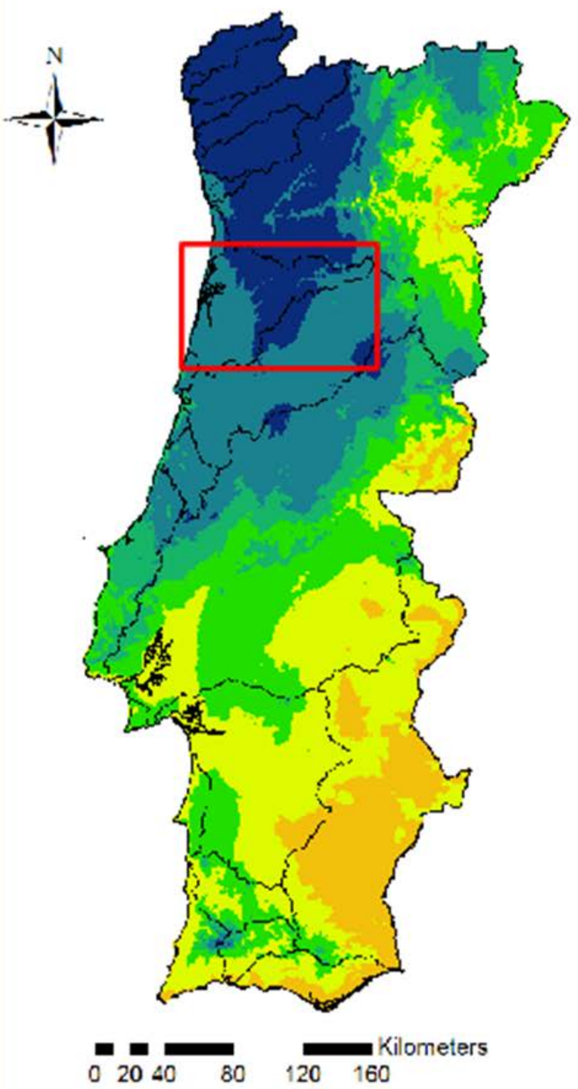


Aveiro

PP: 861 mm/y

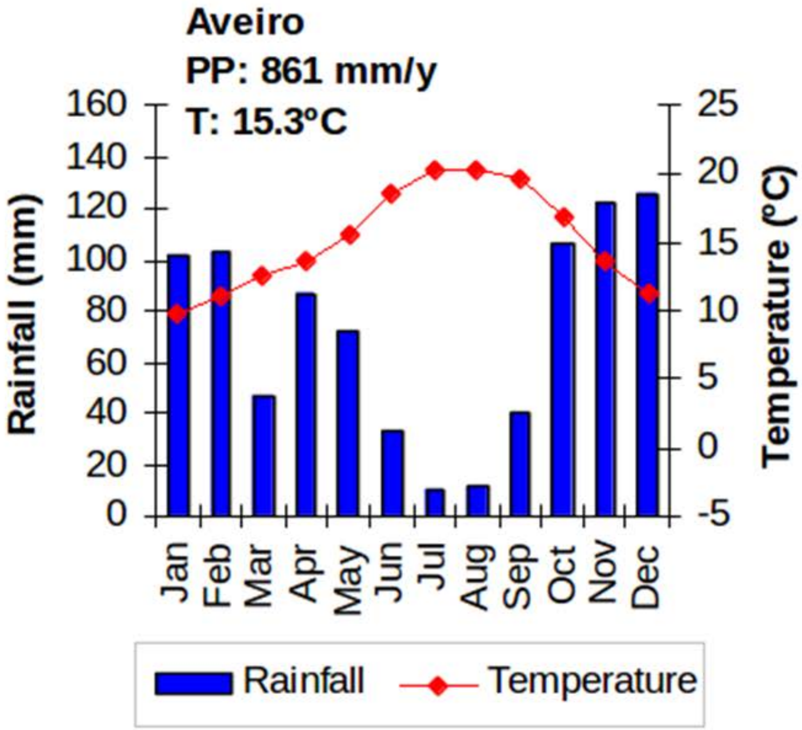
T: 15.3°C

Precipitation in Study Area: 1,000-2,500 mm/y

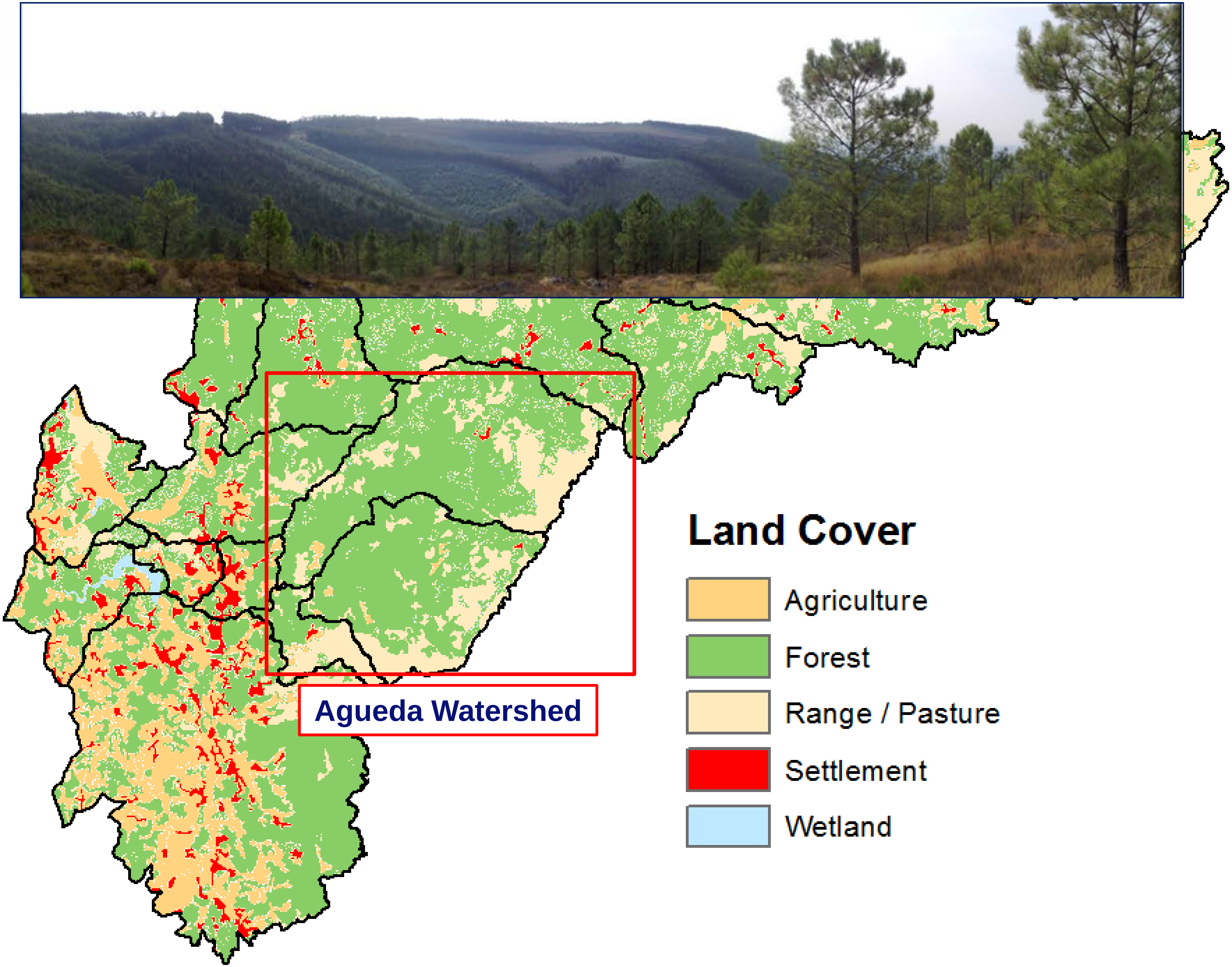


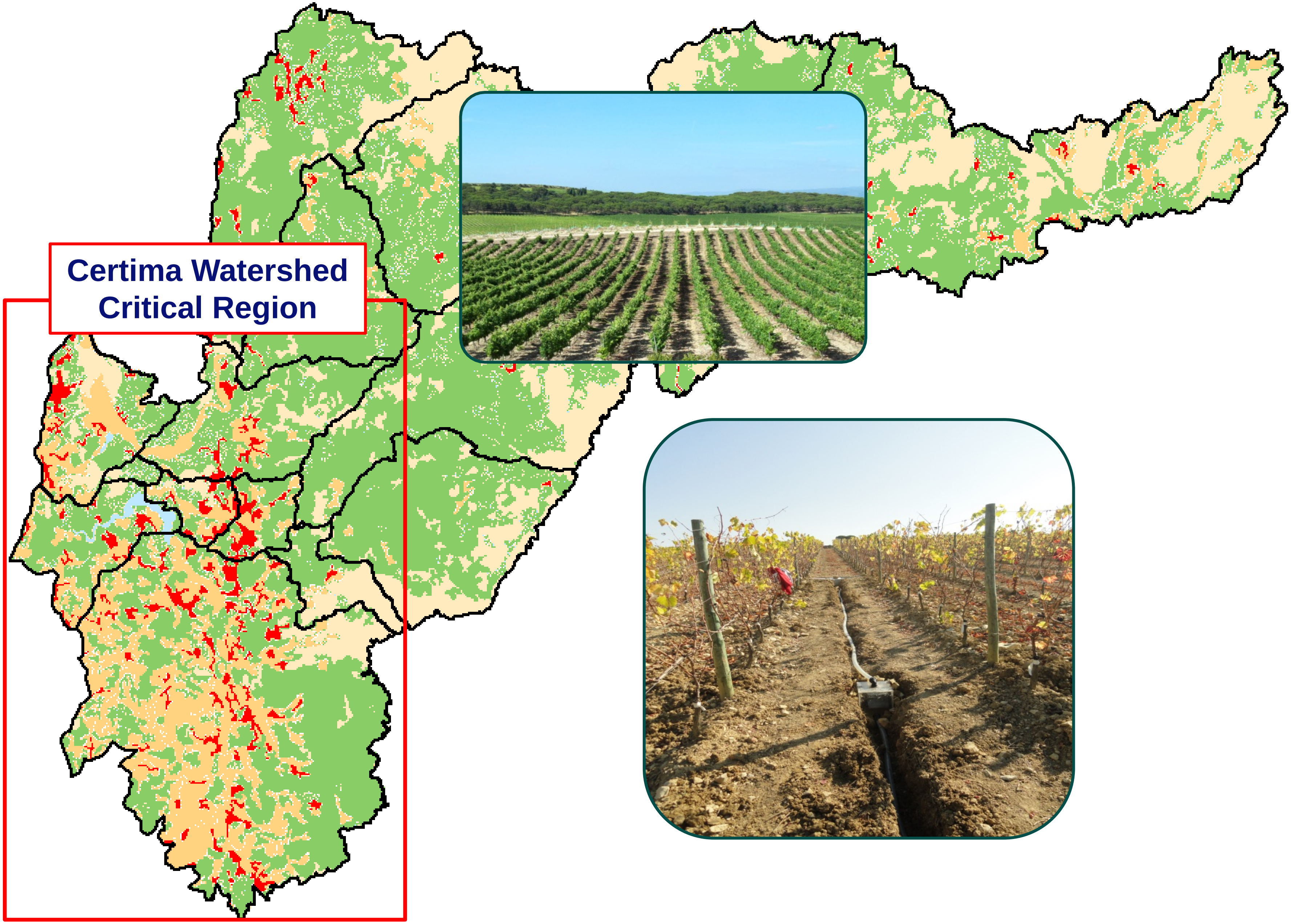
Aridity index - Rainfall / PET

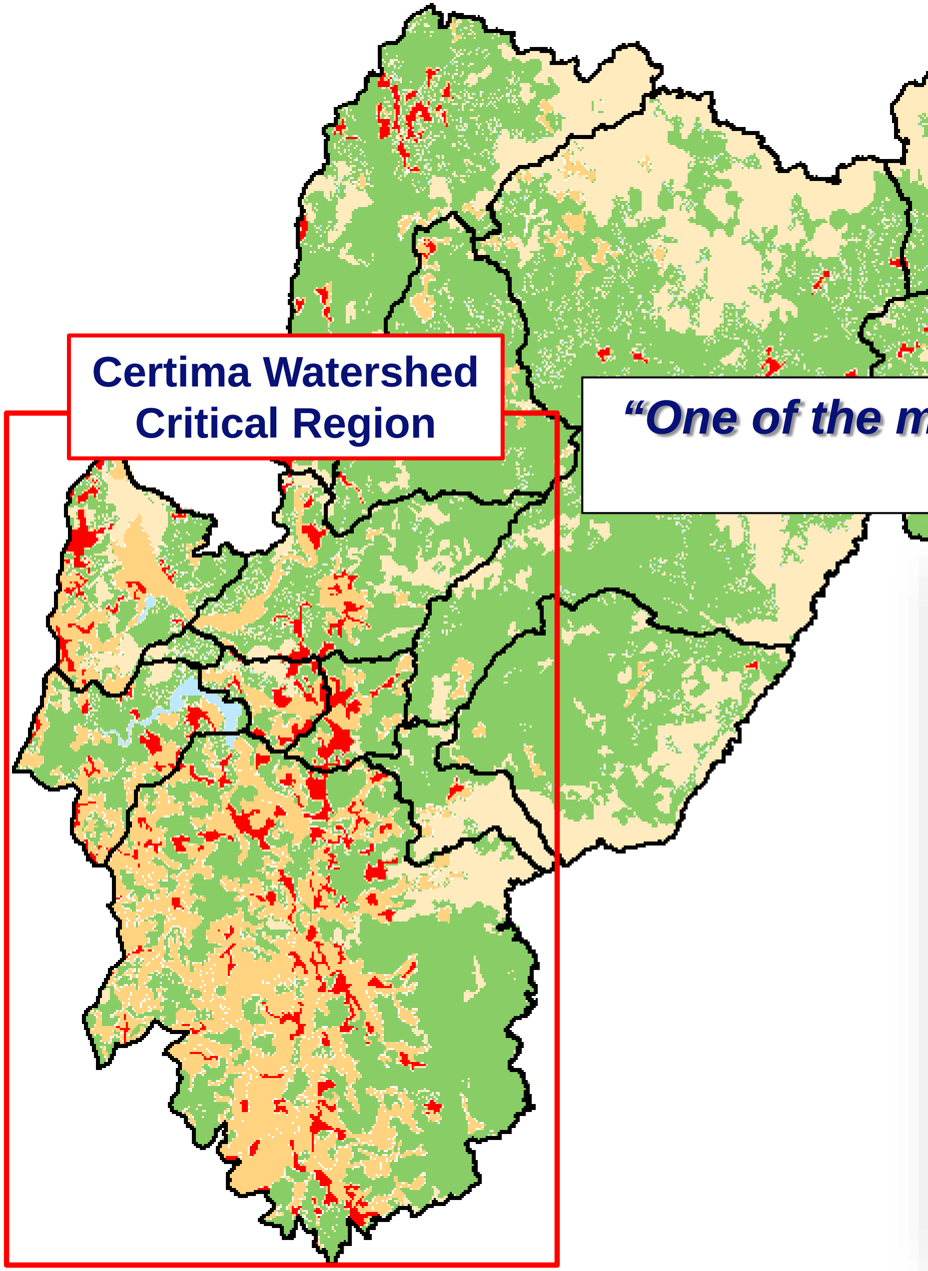
Dry climates					Humid climates
Hyper-arid	🟥	< 0.05	🟩	0.65 - 0.8	
Arid	🟧	0.05 - 0.2	🟩	0.8 - 1	
Semi-arid	🟨	0.2 - 0.5	🟦	1 - 1.5	
Dry/sub-humid	🟨	0.5 - 0.65	🟦	>1.5	


Aveiro
PP: 861 mm/y
T: 15.3°C

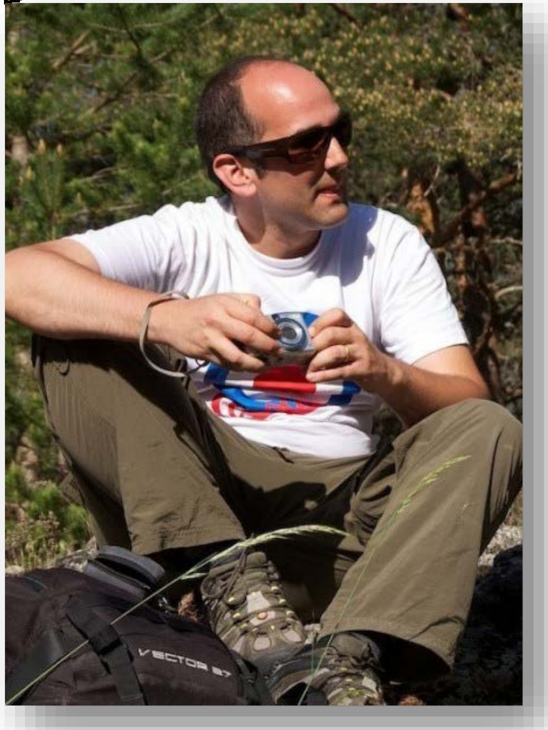
Precipitation in Study Area: 1,000-2,500 mm/y


Agueda Watershed
Land Cover
Agriculture
Forest
Range / Pasture
Settlement
Wetland


Certima Watershed
Critical Region

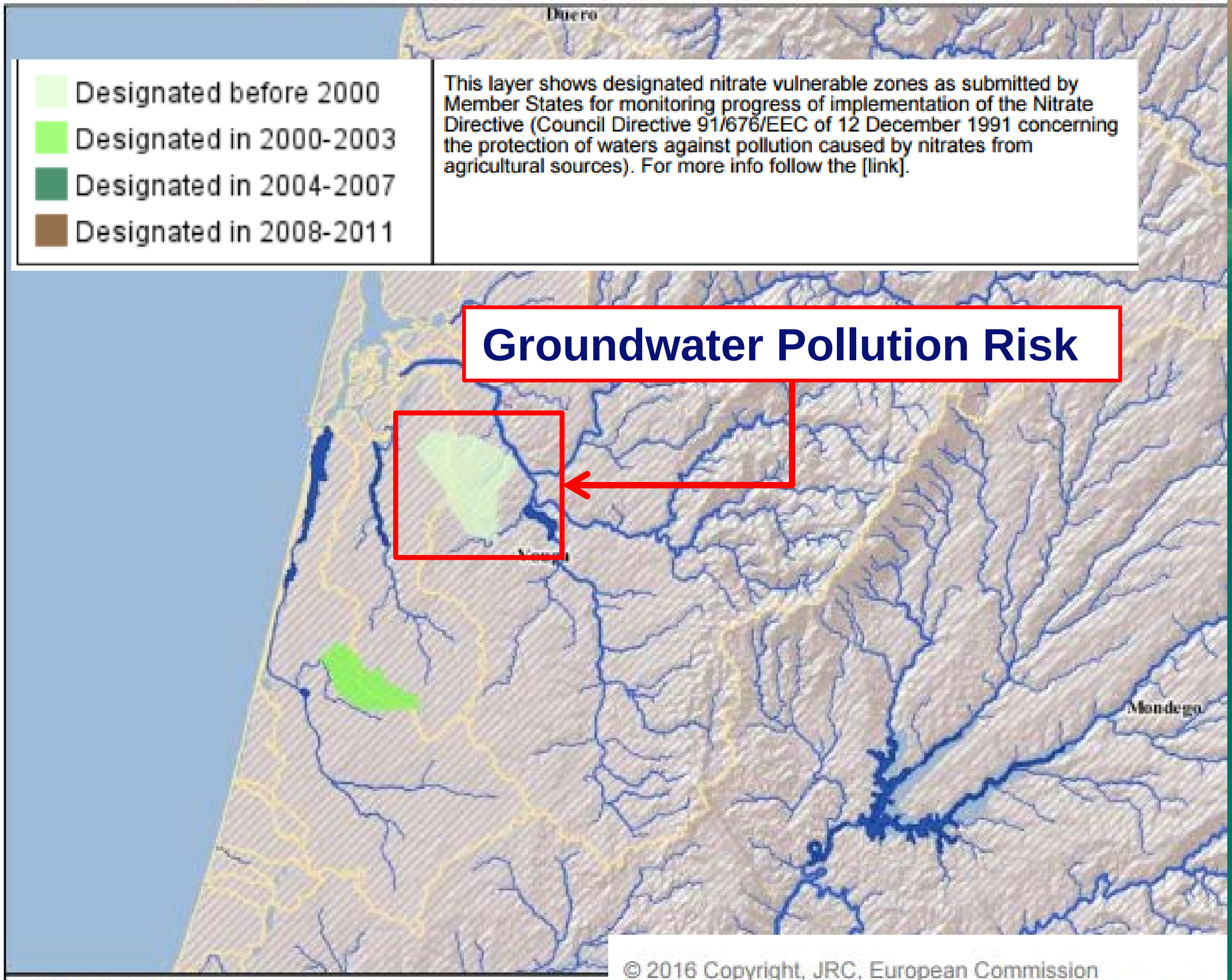


"One of the most polluted water bodies in the EU."
(Rocha, Wednesday)



EUROPEAN COMMISSION
JOINT RESEARCH CENTRE
Institute for Environment & Sustainability
Rural, Water and Ecosystem Resources Unit

Nitrates Directive EU27, Nitrate Vulnerable Zones (NVZs) Map



- ▢ Designated before 2000
- 🟩 Designated in 2000-2003
- 🟩 Designated in 2004-2007
- 🟫 Designated in 2008-2011

This layer shows designated nitrate vulnerable zones as submitted by Member States for monitoring progress of implementation of the Nitrate Directive (Council Directive 91/676/EEC of 12 December 1991 concerning the protection of waters against pollution caused by nitrates from agricultural sources). For more info follow the [link].

Groundwater Pollution Risk

Scale 1:433344

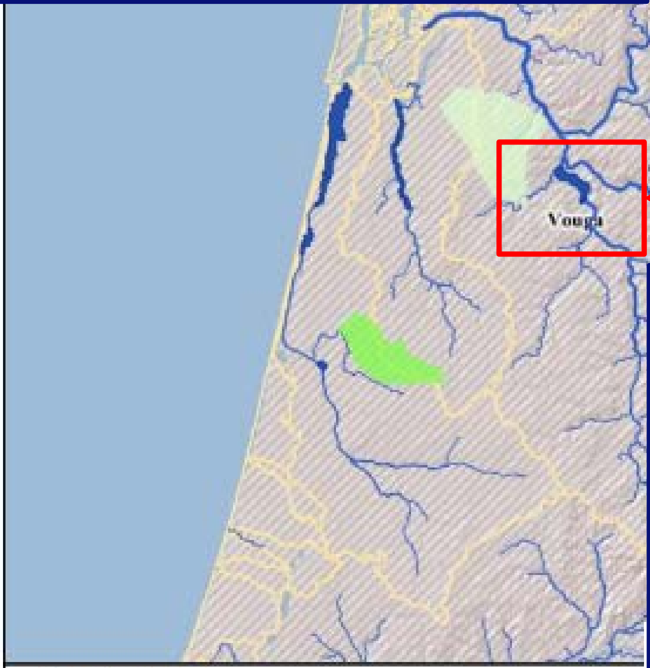
For further details please contact : fate@jrc.ec.europa.eu

EUROPEAN COMMISSION
JOINT RESEARCH CENTRE
Institute for Environment & Sustainability
Rural, Water and Ecosystem Resources Unit

Nitrates Directive EU27 Nitrate Vulnerable Zones (NVZs) Map

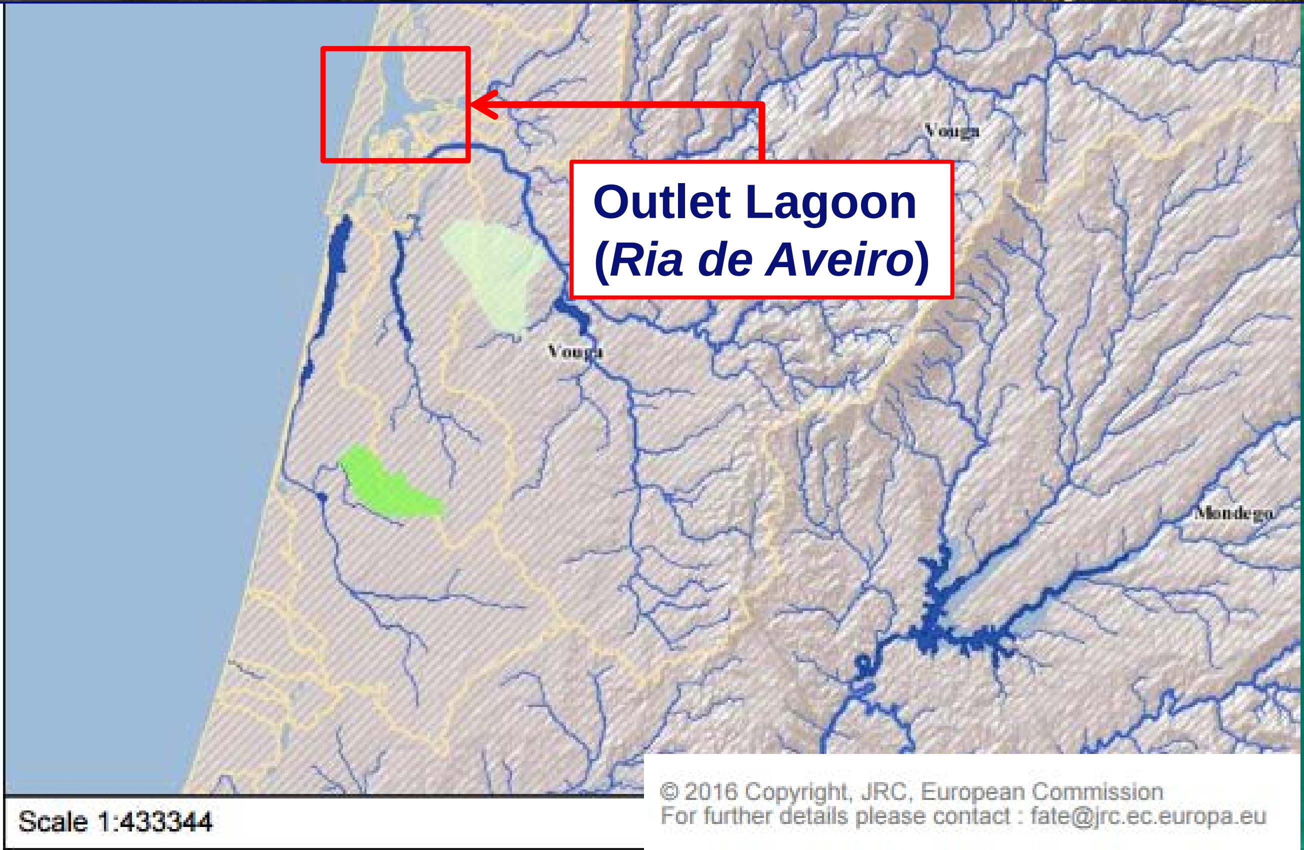
esignated nitrate vulnerable zones as submitted by
monitoring progress of implementation of the Nitrate
Directive 91/676/EEC of 12 December 1991 concerning
aters against pollution caused by nitrates from
s). For more info follow the [link].

Freshwater Habitat
(*Pateira de Fermentelos*)



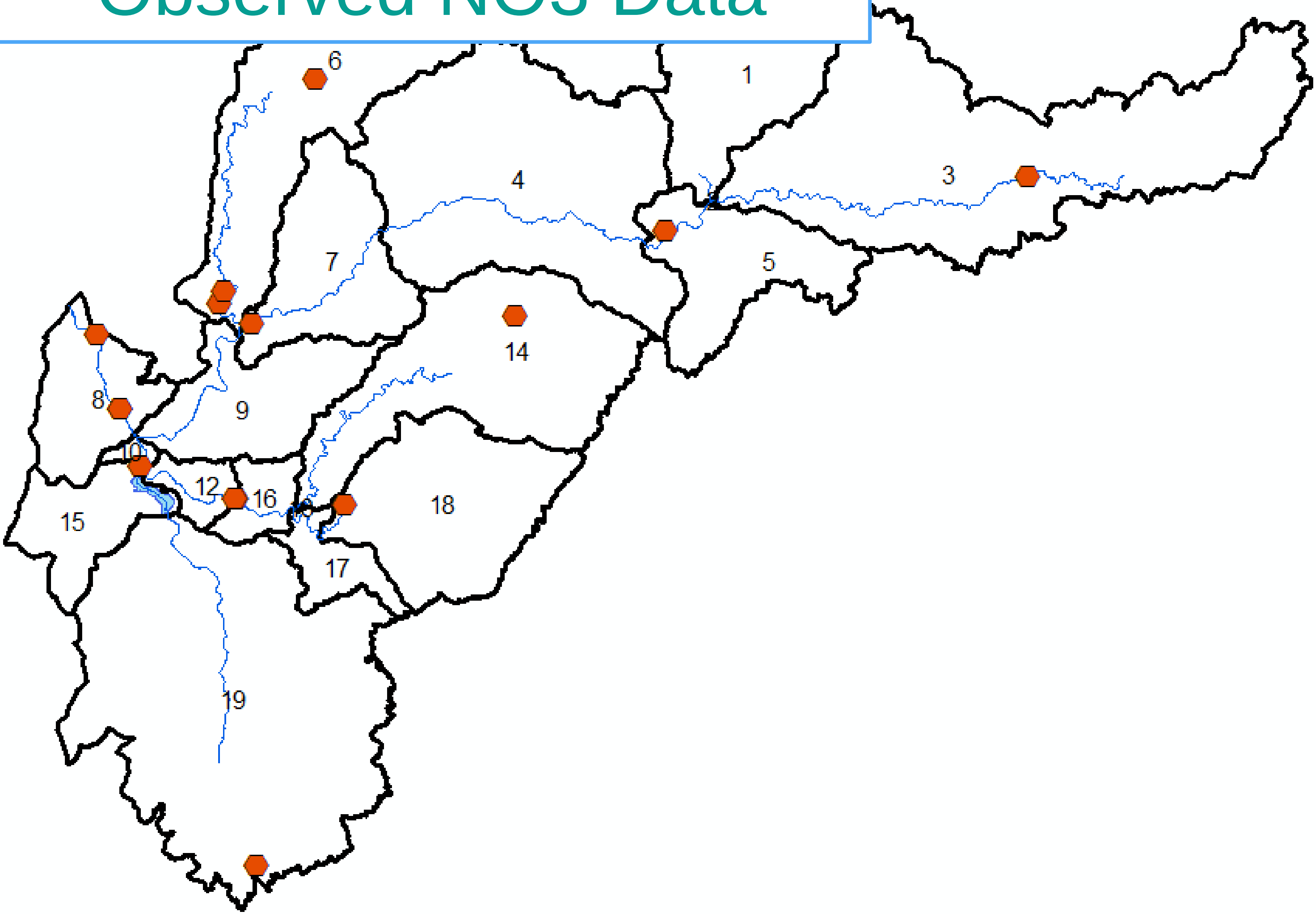
Scale 1:433344

For further details please contact : fate@jrc.ec.europa.eu

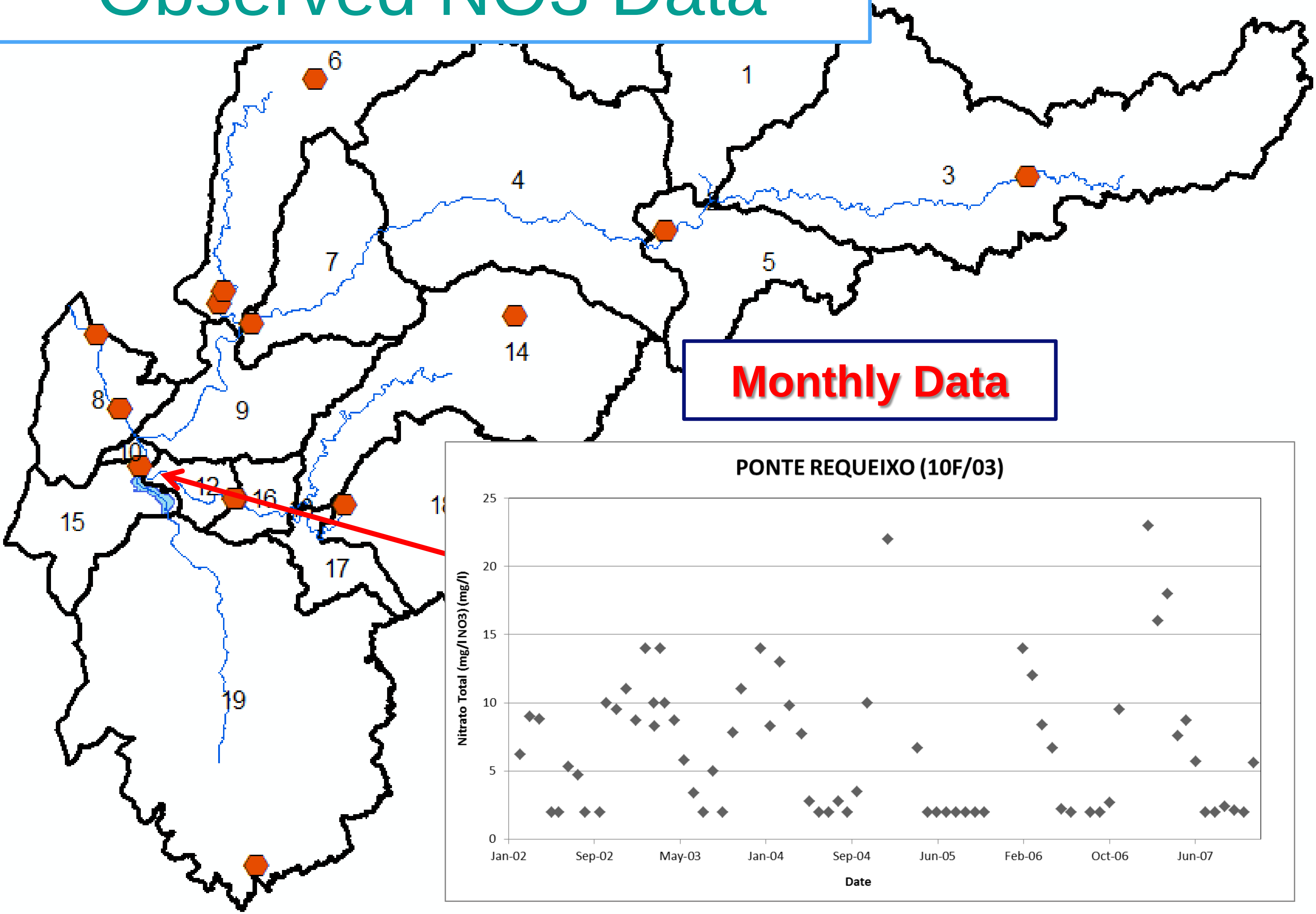


Outlet Lagoon
(*Ria de Aveiro*)

Observed NO3 Data



Observed NO3 Data



Monthly Data

Calibration Approach

- Divided basin into three distinct regions:
  - geology, topography, land-cover/use

- Calibrate each independently at a site with „acceptable“ observed N & Q data

- Parameter Set Selection Using

1. Kling-Gupta Efficiency (KGE): Streamflow
2. Kolmogorov–Smirnov (KS) Test: Nitrogen
3. Select Pareto Optimal Parameter Sets

Kling – Gupta Efficiency (KGE)

$$KGE' = 1 - \sqrt{(r-1)^2 + (\beta - 1)^2 + (\gamma - 1)^2}$$

Timing **Magnitude** **Variability**

$$\beta = \frac{\mu_s}{\mu_0}$$

$$\gamma = \frac{CV_s}{CV_o} = \frac{\sigma_s / \mu_s}{\sigma_o / \mu_o}$$

Kling – Gupta Efficiency (KGE)

$$KGE' = 1 - \sqrt{(r-1)^2 + (\beta - 1)^2 + (\gamma - 1)^2}$$

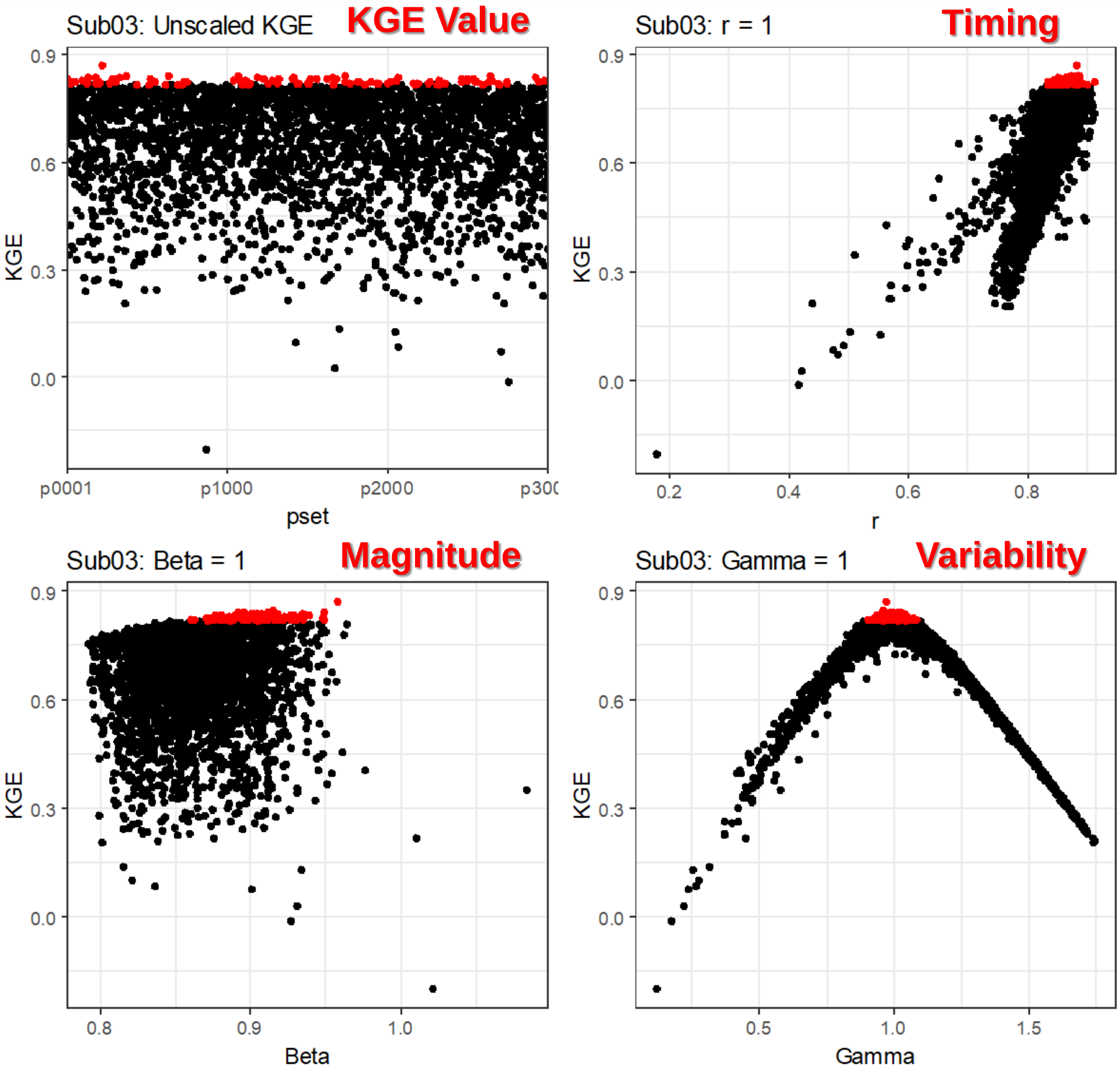
Timing **Magnitude** **Variability**

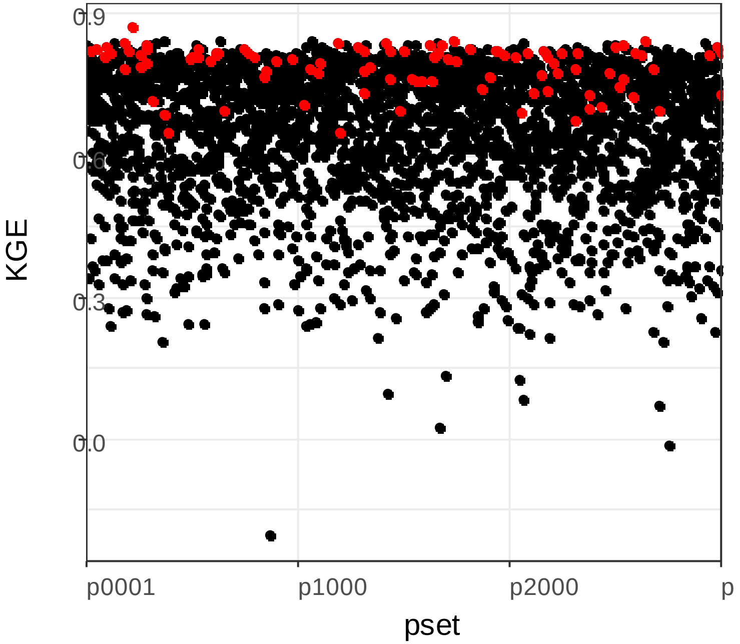
$$\beta = \frac{\mu_s}{\mu_0}$$

$$\gamma = \frac{CV_s}{CV_o} = \frac{\sigma_s/\mu_s}{\sigma_o/\mu_o}$$

Can be re-scaled to put more / less emphasis on different components

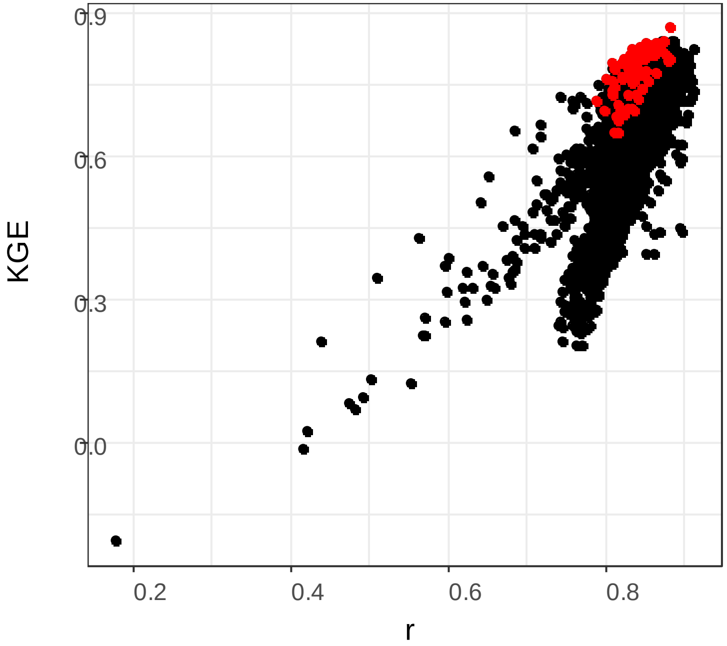
('hydroGOF' - R)


Sub03: Unscaled KGE
KGE Value
0.9
0.6
0.3
0.0
KGE
p0001
p1000
p2000
p30
pset
Sub03: r = 1
Timing
0.9
0.6
0.3
0.0
KGE
0.2
0.4
0.6
0.8
r
Sub03: Beta = 1
Magnitude
0.9
0.6
0.3
0.0
KGE
0.8
0.9
1.0
Beta
Sub03: Gamma = 1
Variability
0.9
0.6
0.3
0.0
KGE
0.5
1.0
1.5
Gamma



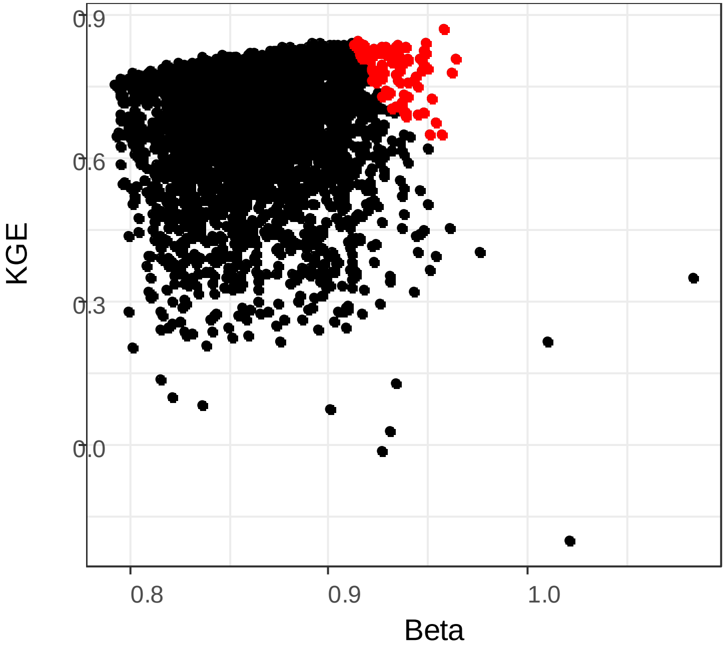
Sub03: Scaled KGE

KGE Value



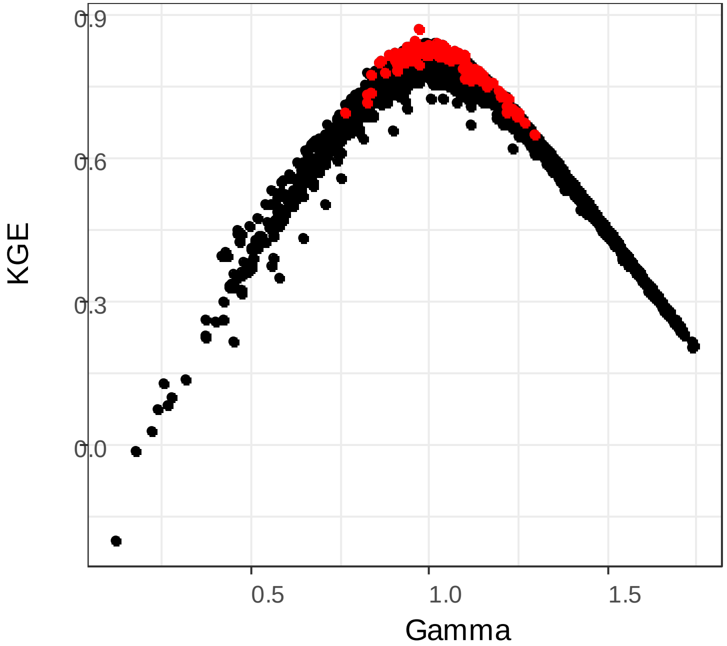
Sub03: r = 0.15

Timing



Sub03: Beta = 0.70

Magnitude

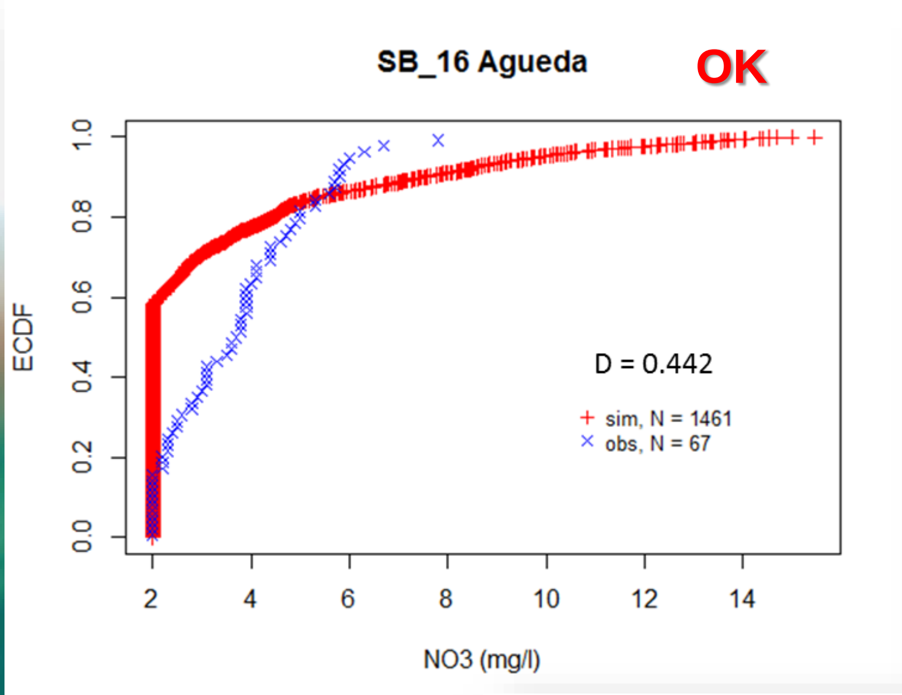


Sub03: Gamma = 0.15

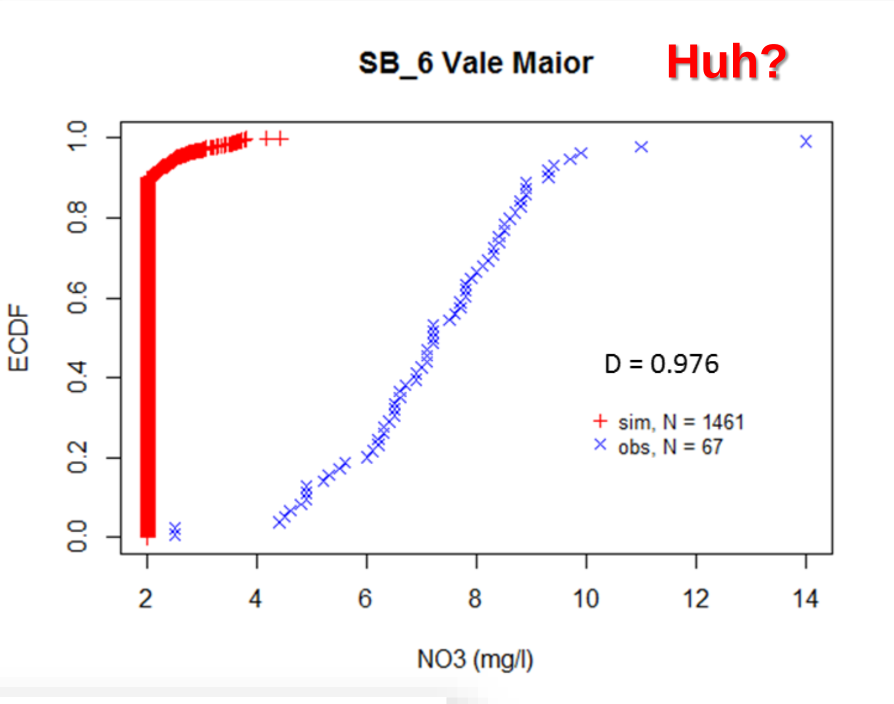
Variability

Kolmogorov–Smirnov (KS) Test

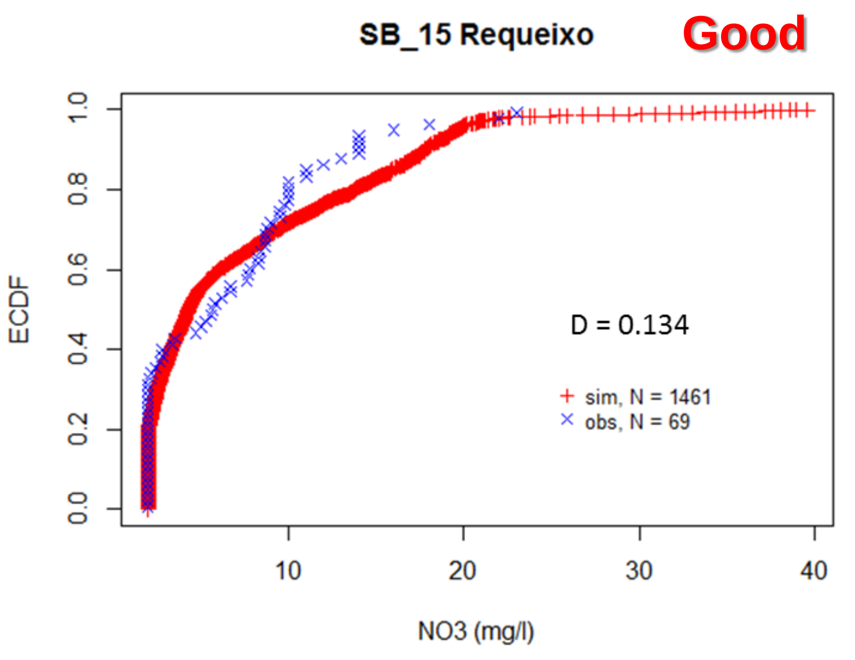
- Non-Parametric Statistical Test – compare a sample of data against a known set (or distribution).
- Generates a similarity measure – which can serve as a goodness-of-fit measure
- Removes the time component, only compares distribution (% exceedence) - model vs observed


SB_16 Agueda

OK

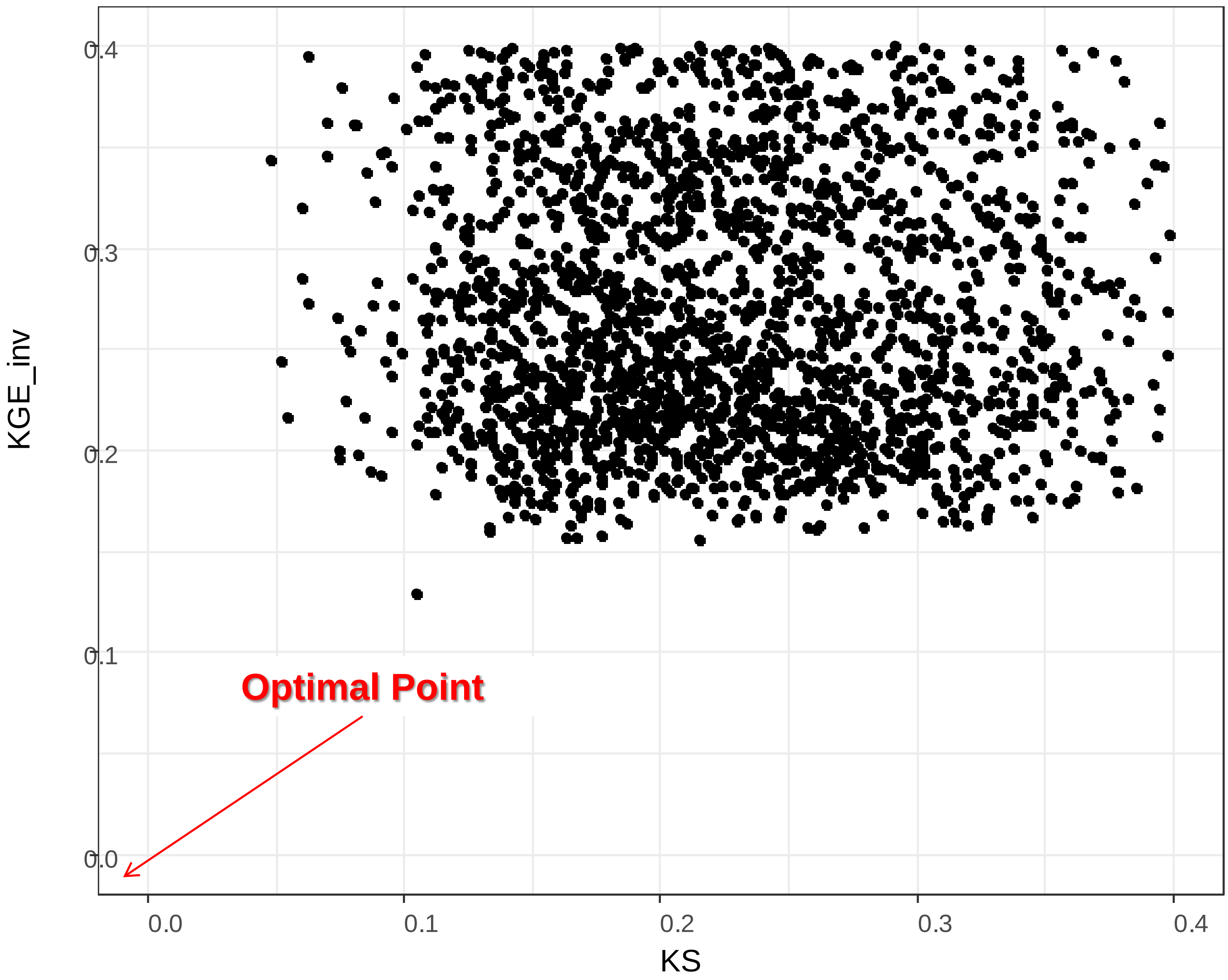

SB_6 Vale Maior

Huh?

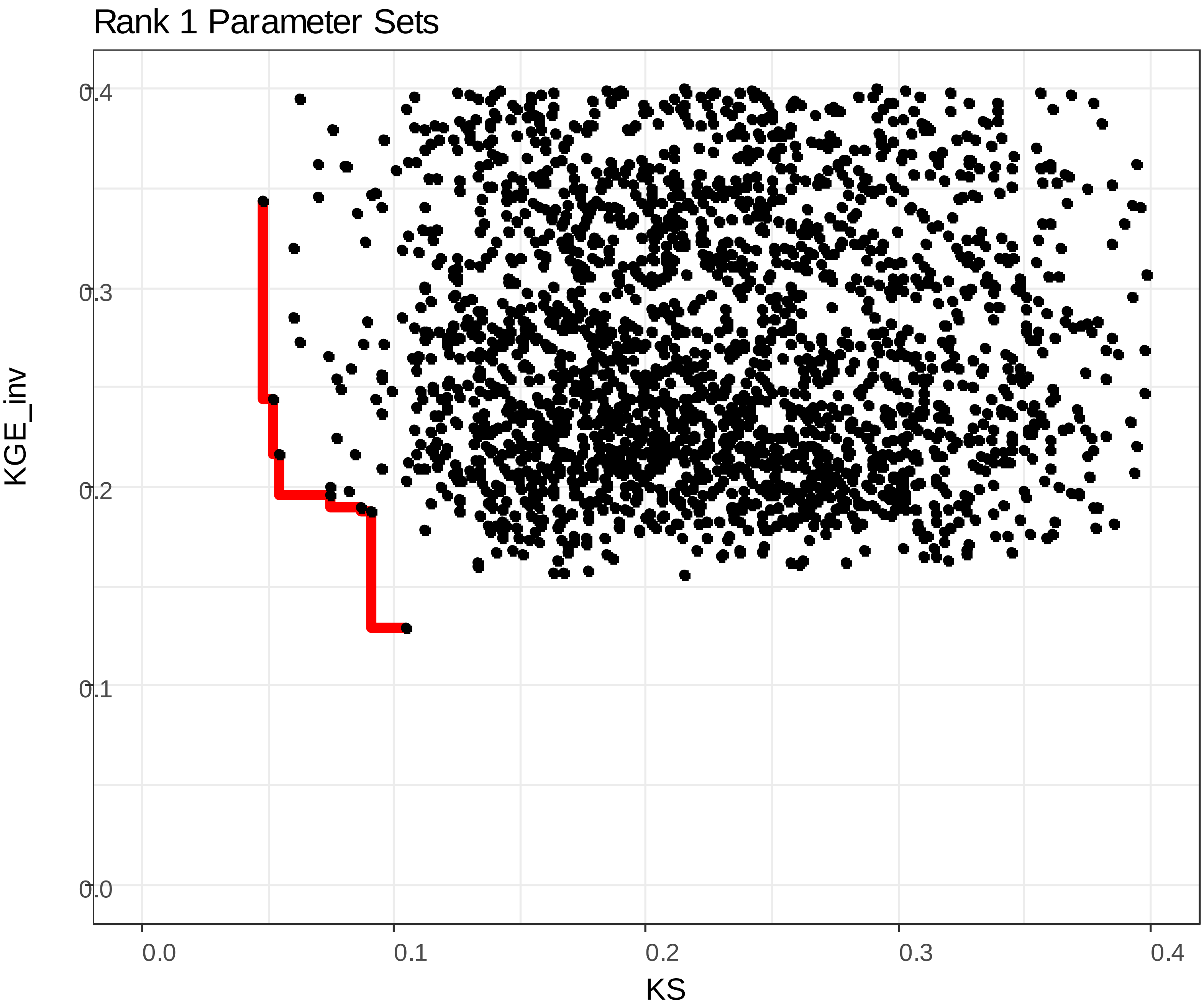

SB_15 Requeixo

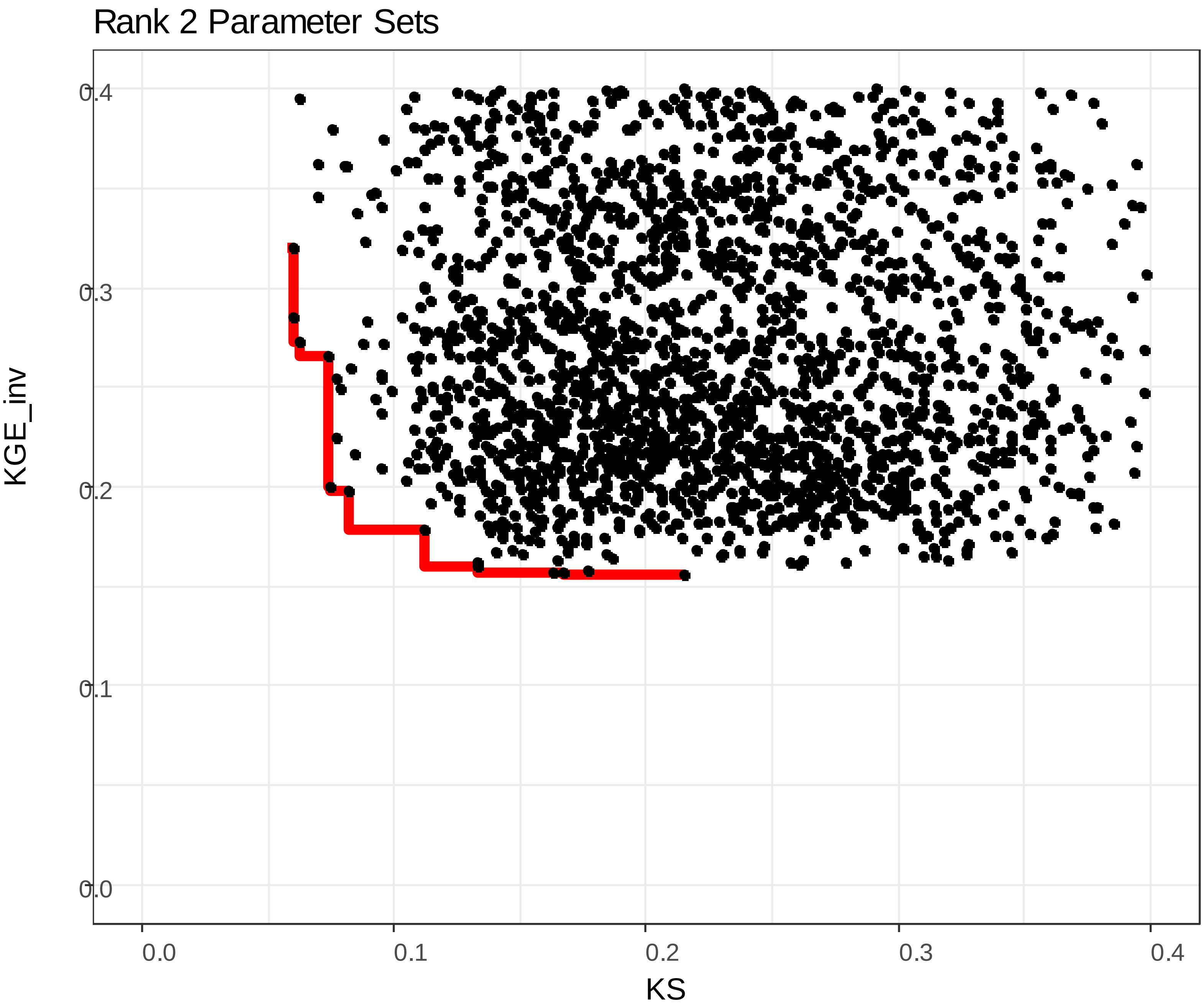
Good

Pareto Parameter Set Selection

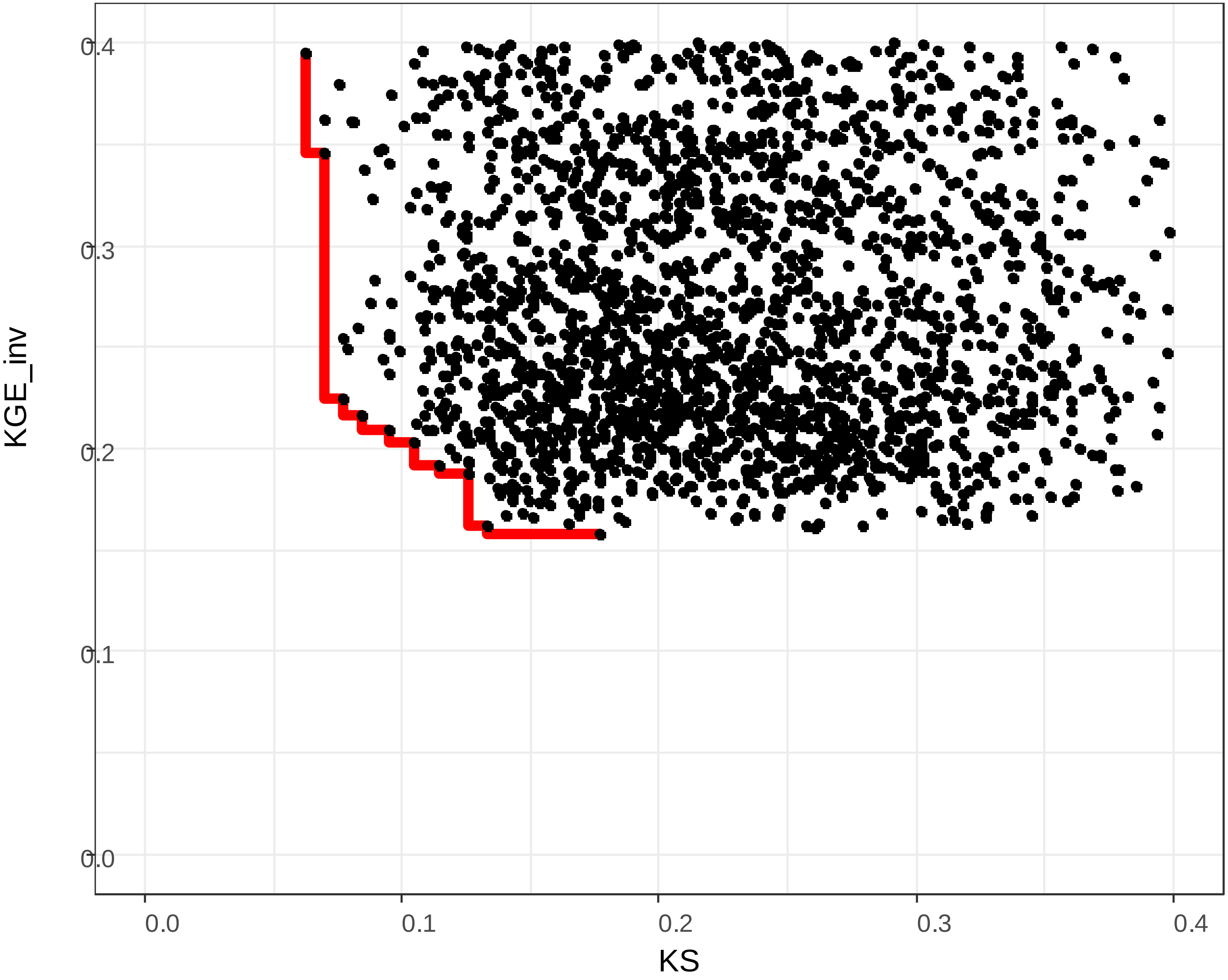


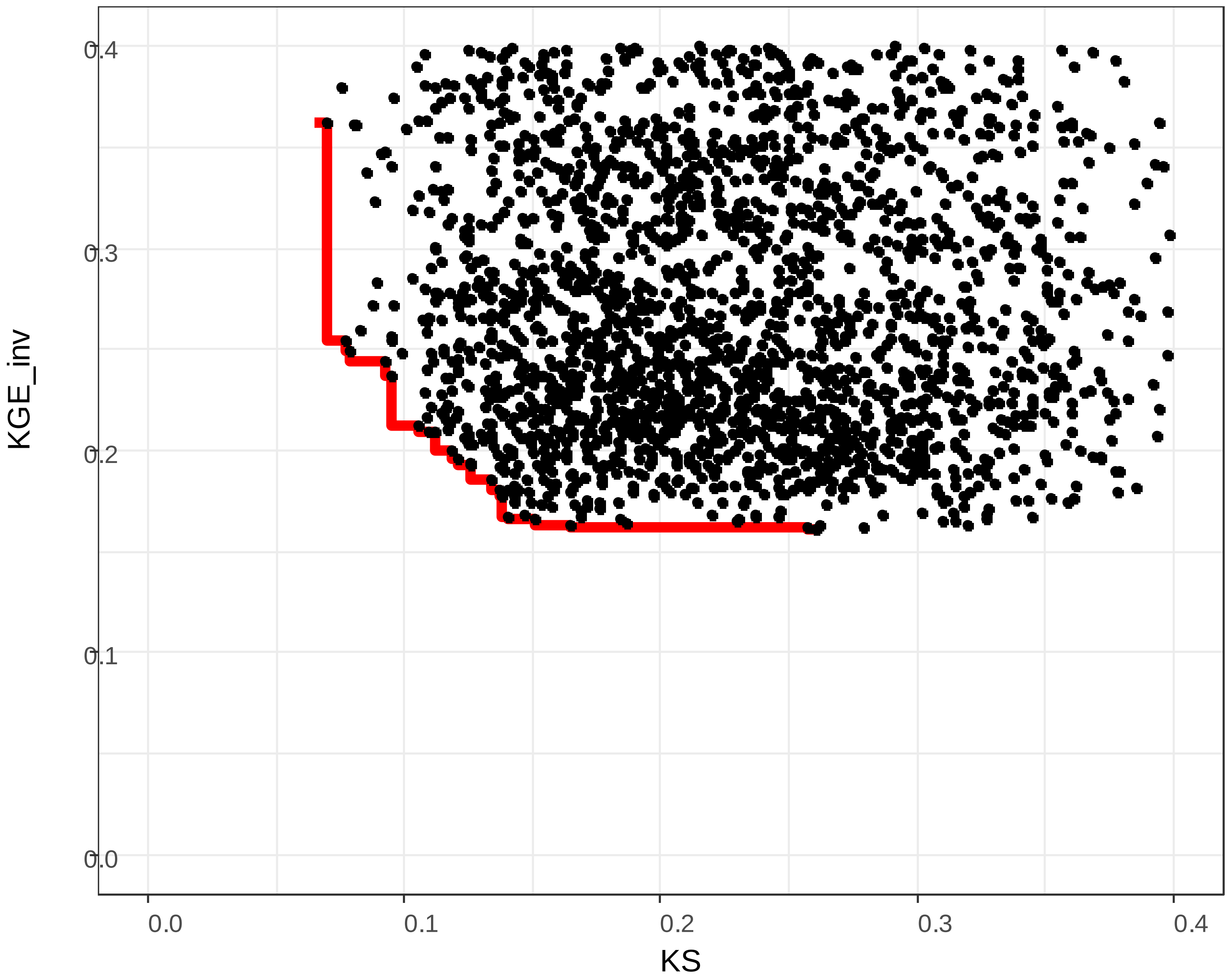
Optimal Point


Rank 1 Parameter Sets
KGE_inv
0.4
0.3
0.2
0.1
0.0
0.0
0.1
0.2
0.3
0.4
KS

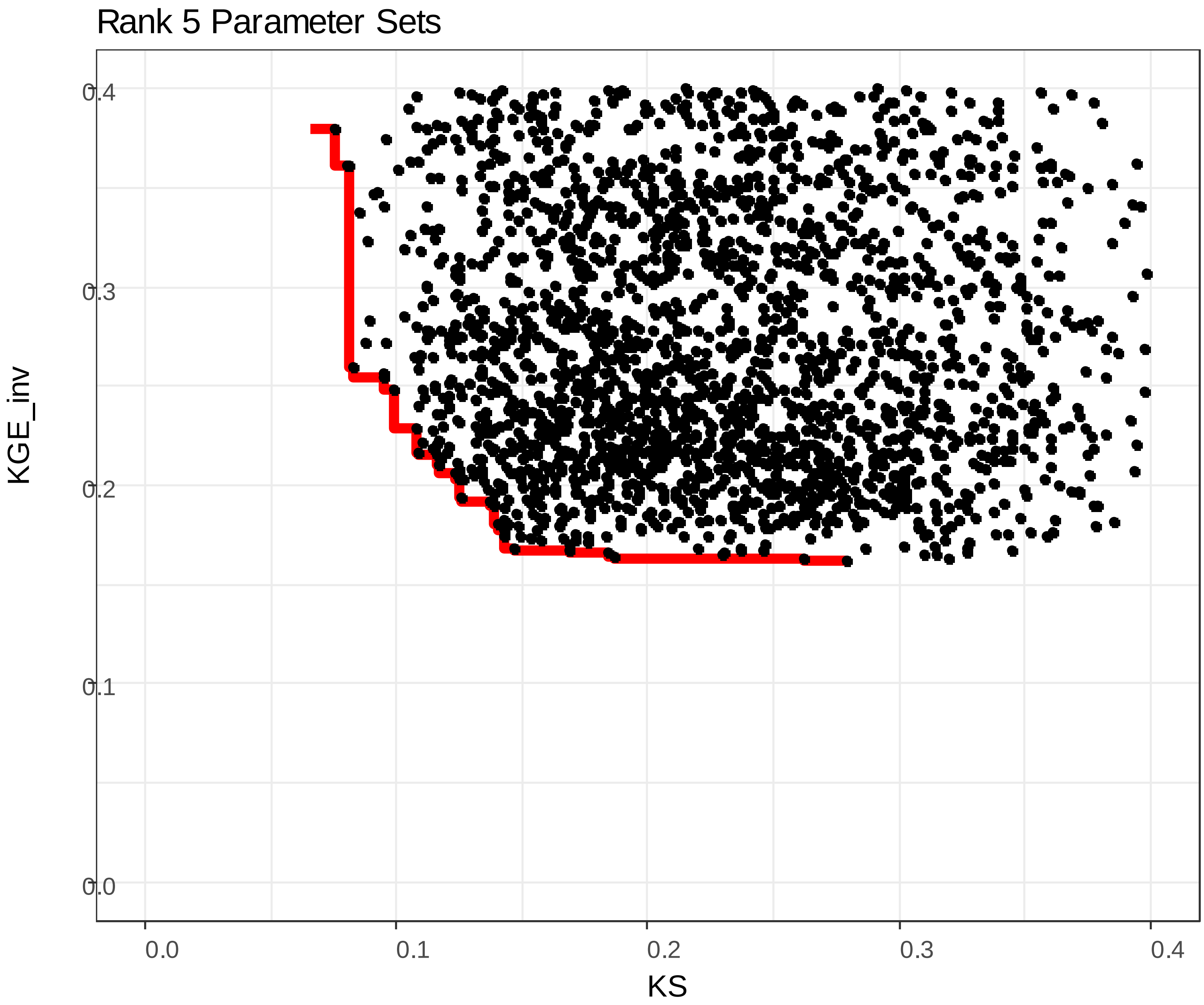

Rank 2 Parameter Sets
KGE_inv
0.4
0.3
0.2
0.1
0.0
KS
0.0
0.1
0.2
0.3
0.4

Rank 3 Parameter Sets

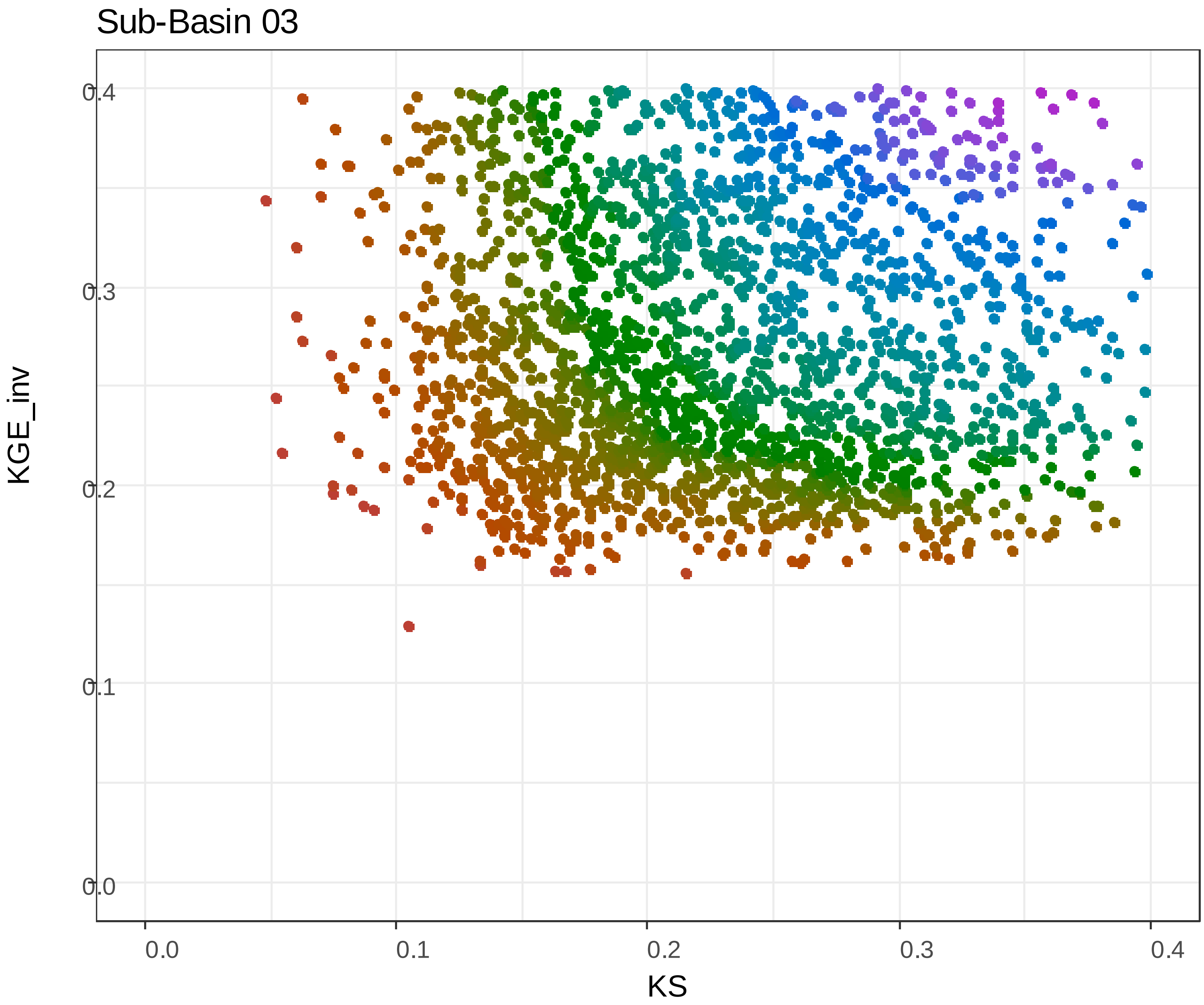


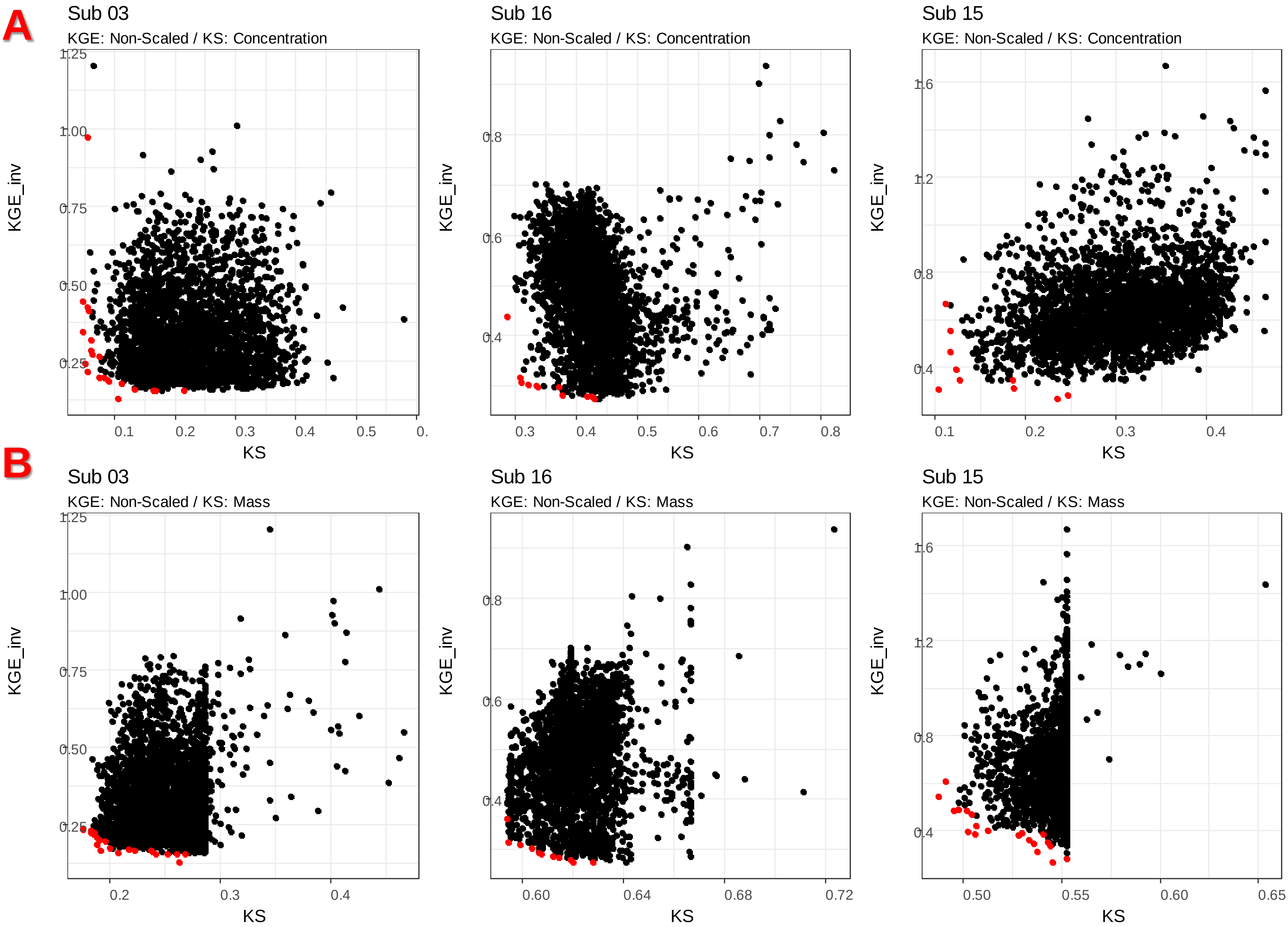


Rank 4 Parameter Sets

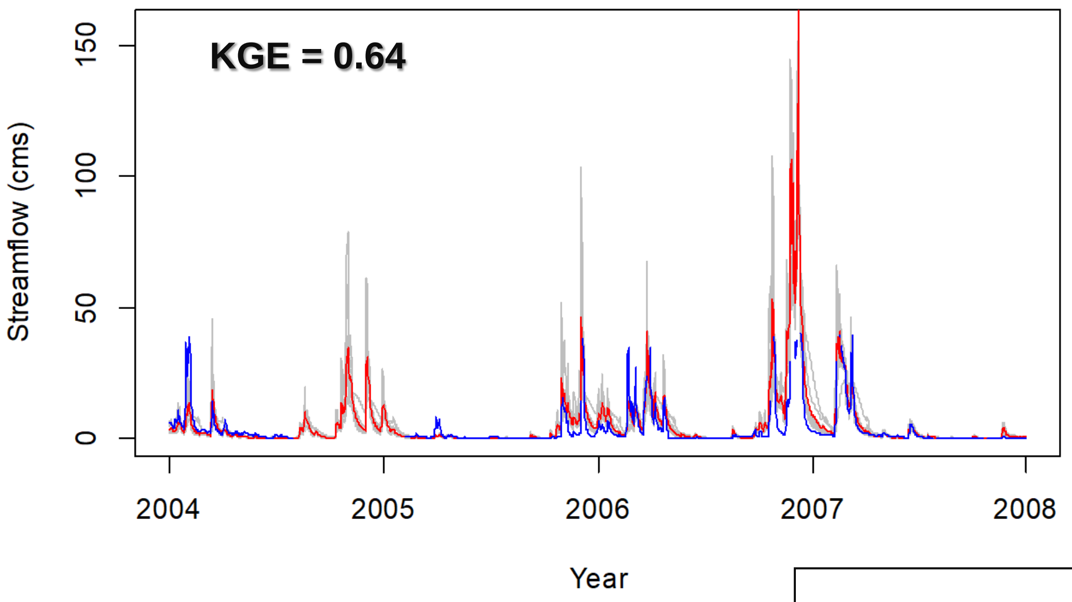


Rank 5 Parameter Sets


Sub-Basin 03
KGE_inv
0.4
0.3
0.2
0.1
0.0
0.0
0.1
0.2
0.3
0.4
KS

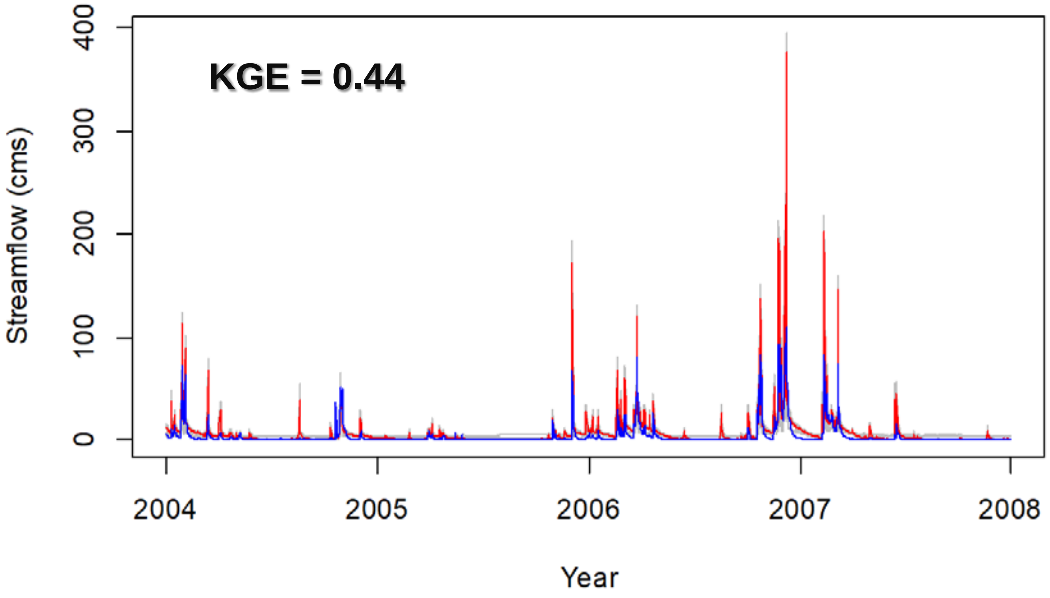
A
Sub 03
KGE: Non-Scaled / KS: Concentration
KGE_inv
1.25
1.00
0.75
0.50
0.25
0.1
0.2
0.3
0.4
0.5
0.
KS
Sub 16
KGE: Non-Scaled / KS: Concentration
KGE_inv
0.8
0.6
0.4
0.3
0.4
0.5
0.6
0.7
0.8
KS
Sub 15
KGE: Non-Scaled / KS: Concentration
KGE_inv
1.6
1.2
0.8
0.4
0.1
0.2
0.3
0.4
KS
B
Sub 03
KGE: Non-Scaled / KS: Mass
KGE_inv
1.25
1.00
0.75
0.50
0.25
0.2
0.3
0.4
KS
Sub 16
KGE: Non-Scaled / KS: Mass
KGE_inv
0.8
0.6
0.4
0.60
0.64
0.68
0.72
KS
Sub 15
KGE: Non-Scaled / KS: Mass
KGE_inv
1.6
1.2
0.8
0.4
0.50
0.55
0.60
0.65
KS

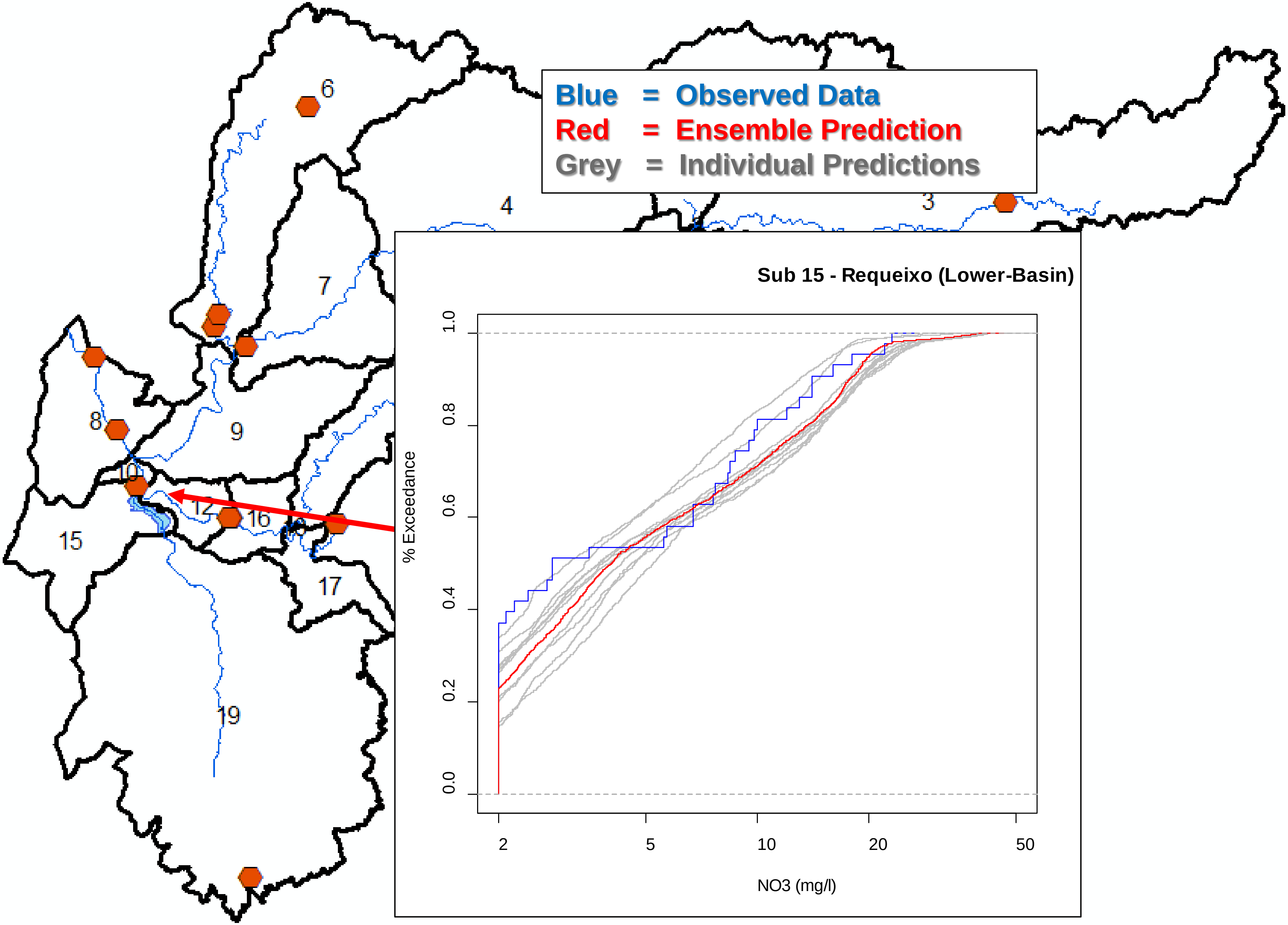
Sub 15 - Requeixo (Lower-Basin)



Blue = **Observed Data**
Red = **Ensemble Prediction**
Grey = **Individual Predictions**

Sub 16 - Agueda (Mid-Basin)



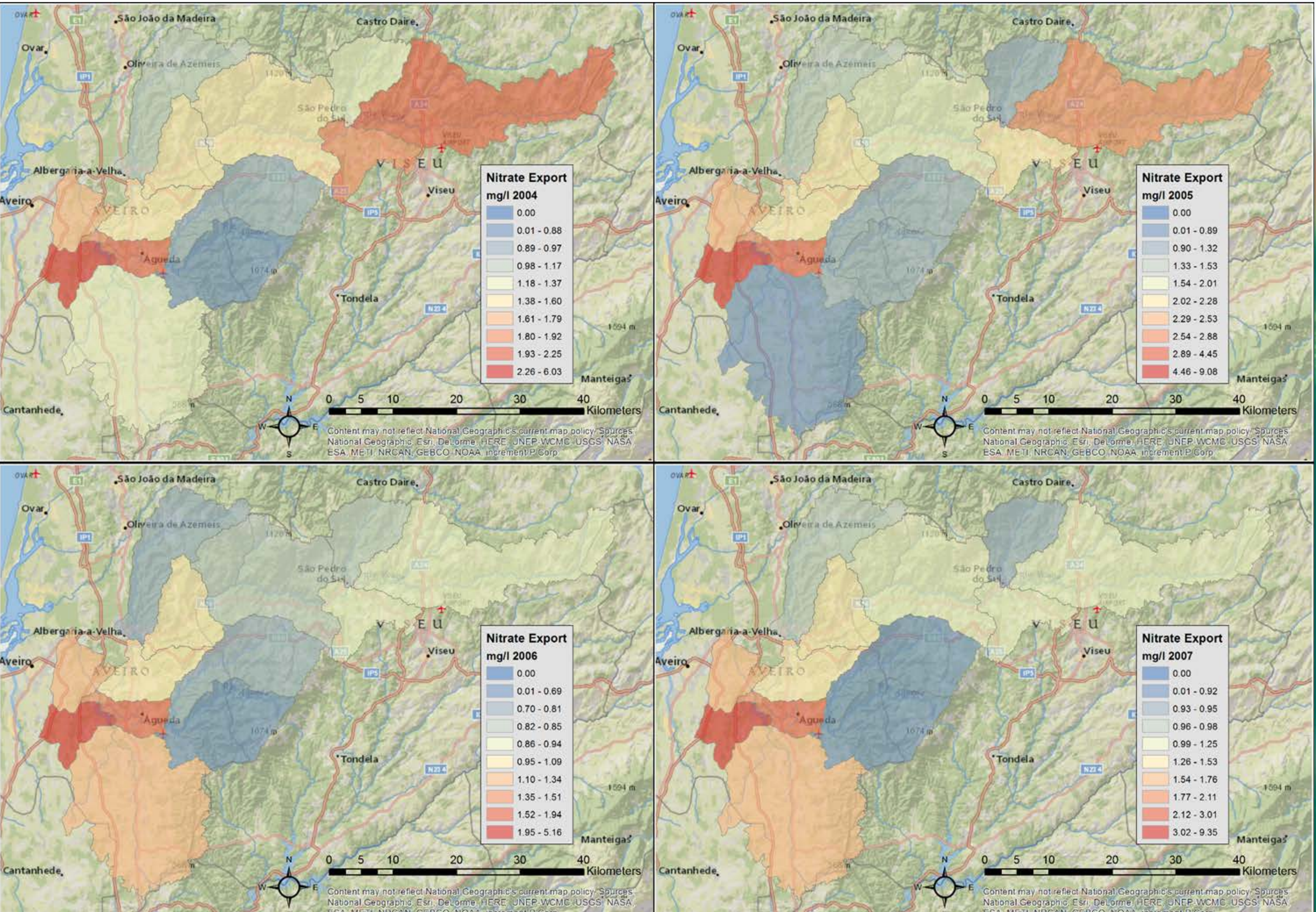


Blue = Observed Data

Red = Ensemble Prediction

Grey = Individual Predictions

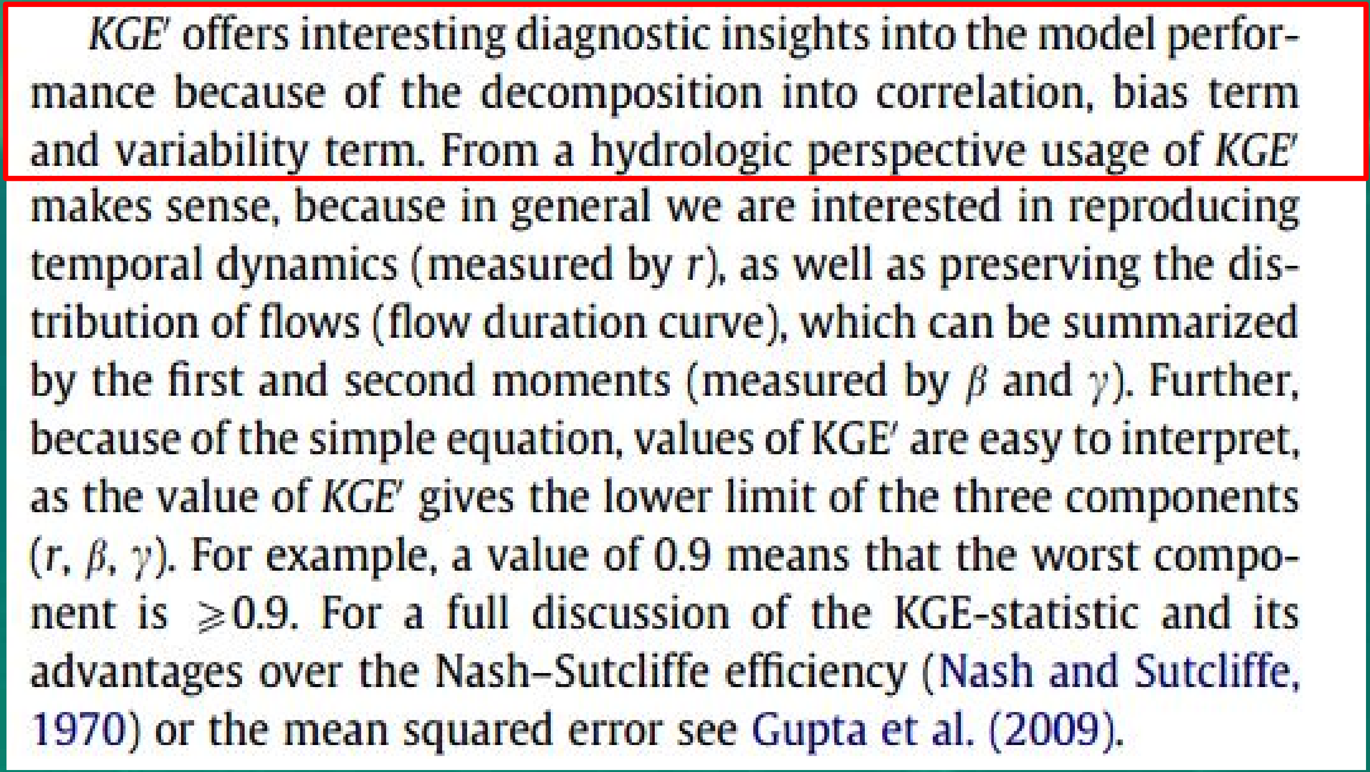
Nitrogen Export – Baseline Predictions



Take-Home Messages

Pros / Cons

1. **Kling-Gupta Efficiency**



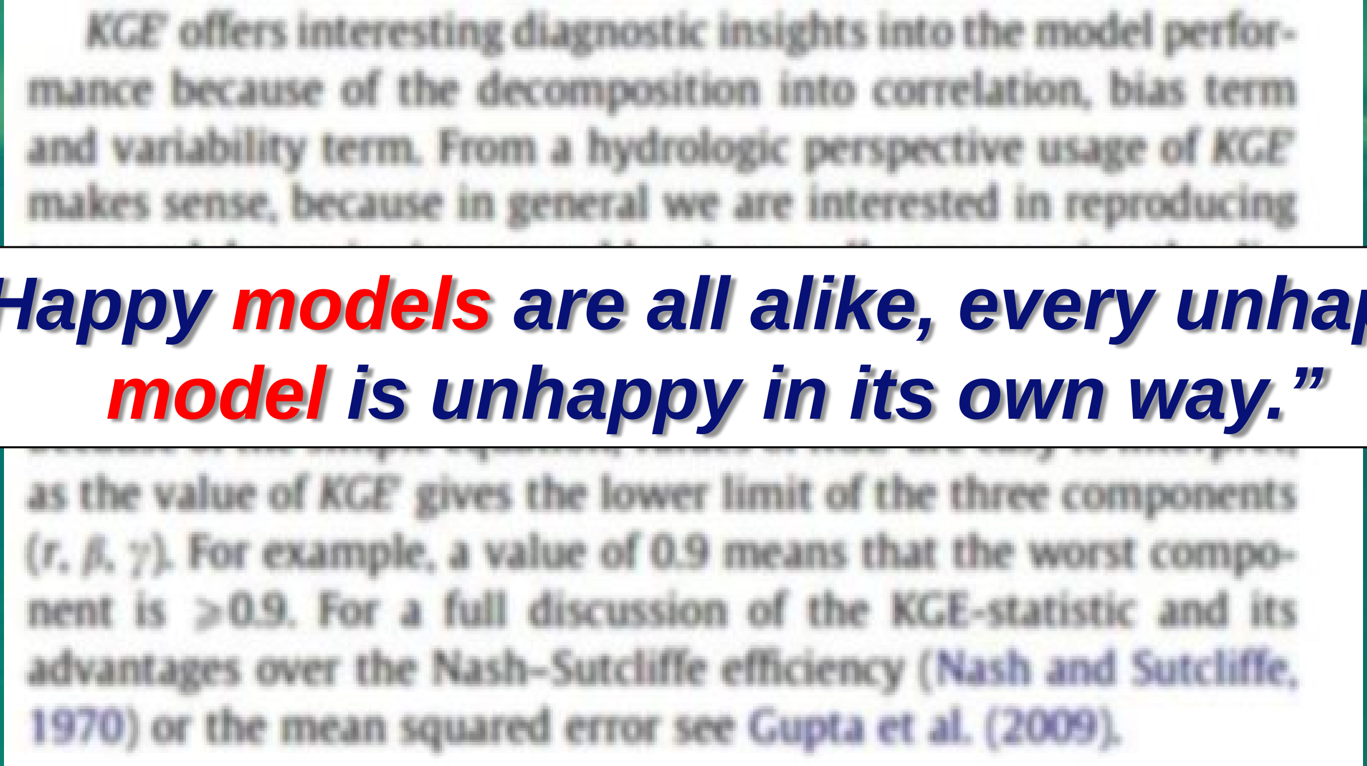
KGE' offers interesting diagnostic insights into the model performance because of the decomposition into correlation, bias term and variability term. From a hydrologic perspective usage of KGE' makes sense, because in general we are interested in reproducing temporal dynamics (measured by r), as well as preserving the distribution of flows (flow duration curve), which can be summarized by the first and second moments (measured by β and γ). Further, because of the simple equation, values of KGE′ are easy to interpret, as the value of KGE' gives the lower limit of the three components (r, β, γ). For example, a value of 0.9 means that the worst component is $\geqslant 0.9$. For a full discussion of the KGE-statistic and its advantages over the Nash–Sutcliffe efficiency (Nash and Sutcliffe, 1970) or the mean squared error see Gupta et al. (2009).

Kling et al. (2012)

Take-Home Messages

Pros / Cons

1. **Kling-Gupta Efficiency**



KGE' offers interesting diagnostic insights into the model performance because of the decomposition into correlation, bias term and variability term. From a hydrologic perspective usage of *KGE'* makes sense, because in general we are interested in reproducing

as the value of *KGE'* gives the lower limit of the three components (r, β, γ). For example, a value of 0.9 means that the worst component is >0.9. For a full discussion of the KGE-statistic and its advantages over the Nash–Sutcliffe efficiency (Nash and Sutcliffe, 1970) or the mean squared error see Gupta et al. (2009).

"Happy models are all alike, every unhappy model is unhappy in its own way."

Take-Home Messages

Pros / Cons

1. Kling-Gupta Efficiency
    - ❖ Pro: Useful Objctive Function & Diagnostic Tool
    - ❖ Con: More Difficult to Interpret
        - Lack of Baseline – What is a „Good / Fair / Poor“ KGE?
        - Effect of Scaling

Take-Home Messages
Pros / Cons

1. Kling-Gupta Efficiency
   - ❖ Pro: Useful Objctive Function & Diagnostic Tool
   - ❖ Con: More Difficult to Interpret
     - Lack of Baseline – What is a „Good / Fair / Poor“ KGE?
     - Effect of Scaling

2. Kolmogorov–Smirnov (KS) Test
   - ❖ Pro: Can help capture the overall picture.
     - *What % of time will WQ standards be exceeded?*
   - ❖ Con: Doesn‘t consider the temporal component
     - *What is the nitrogen load on June 30th?*

Thank You

To FONASO for Funding

To my colleagues in Dresden & Aveiro

To you for your attention

TECHNISCHE UNIVERSITÄT DRESDEN

Technische Universität Dresden,
Institute of Soil Science & Site Ecology

Education and Culture
Erasmus Mundus

Forest and Nature for Society (FONASO)
Joint Doctoral Program

universidade de aveiro

University of Aveiro, CESAM &
Department of Environment and Planning

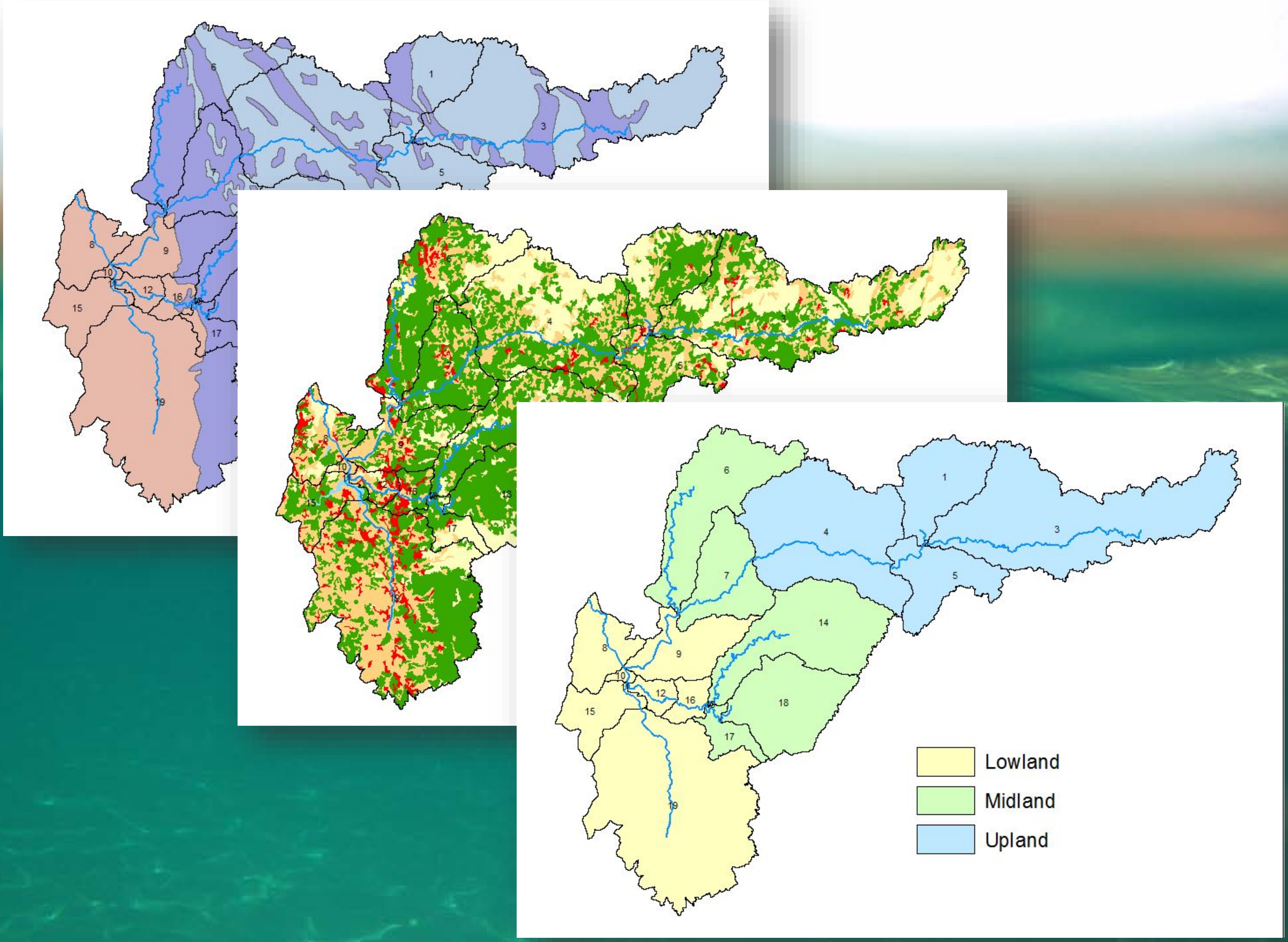
Global Parameters	***Parameter Definition***	***Model Usage***
N_UPDIS	Nitrogen uptake distribution parameter	Plant Nutrient Uptake
CDN	Rate coefficient for denitrification	Denitrification
SDNCO	Threshold value of nutrient cycling water factor for denitrification to occur	
CMN	Rate coefficient for mineralization of the humus active organic nutrients	Mineralization
RSDCO	Rate coefficient for mineralization of the residue fresh organic nutrients	
NPERCO	Nitrate percolation coefficient	Nitrate Transport
SOL_AWC	Available water capacity	Percolation
SOL_K	Saturated hydraulic conductivity of first layer (mm/hr.)	Infiltration / Percolation
SURLAG18	Surface runoff lag coefficient	Surface Runoff & Matter Transport

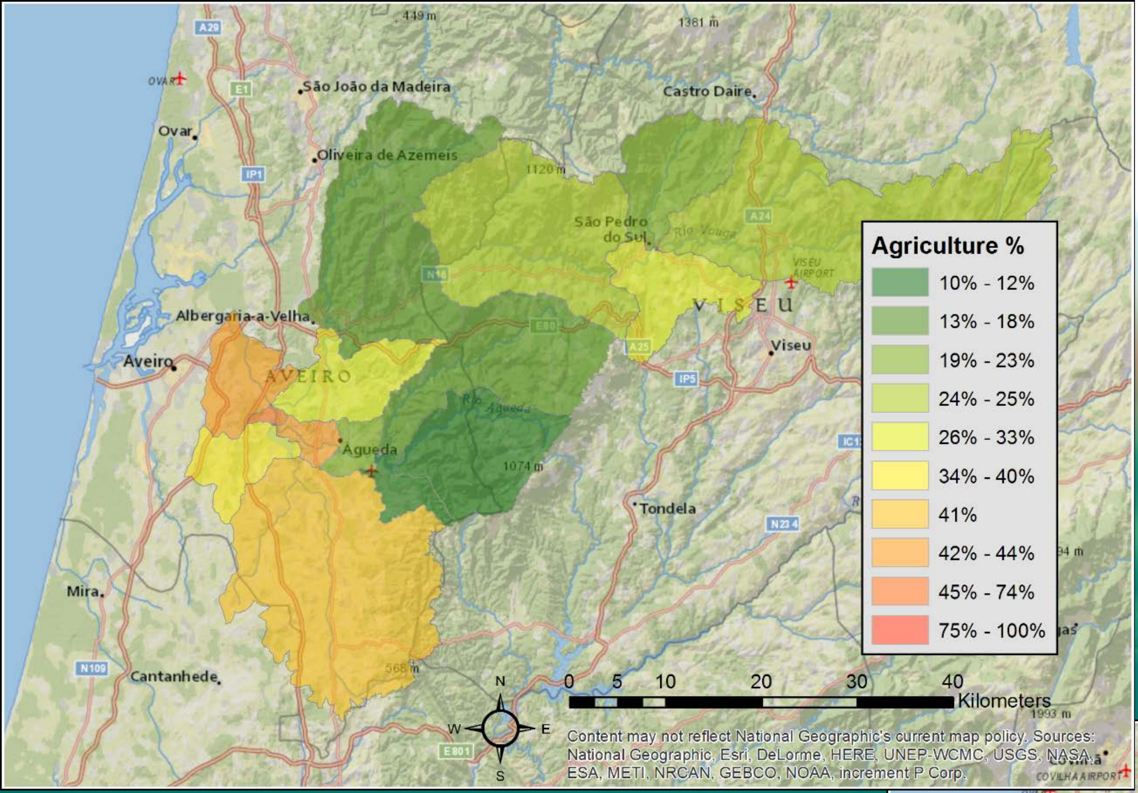
Regional Parameters	***Parameter Definition***	***Model Usage***
ALPHA_BF	Baseflow recession constant	Shallow Aquifer
GW_DELAY	Delay time for aquifer recharge	
GW_QMN	Threshold water level in shallow aquifer for base flow (mm H_2O)	
GW_REVAP	Revap coefficient	
RCHRG_DP	Aquifer percolation coefficient	
CH_K	Effective hydraulic conductivity of channel (mm/hr.)	Transmission Loss
CH_N	Manning's n value for tributary channels	Peak Rate / Channel Flow

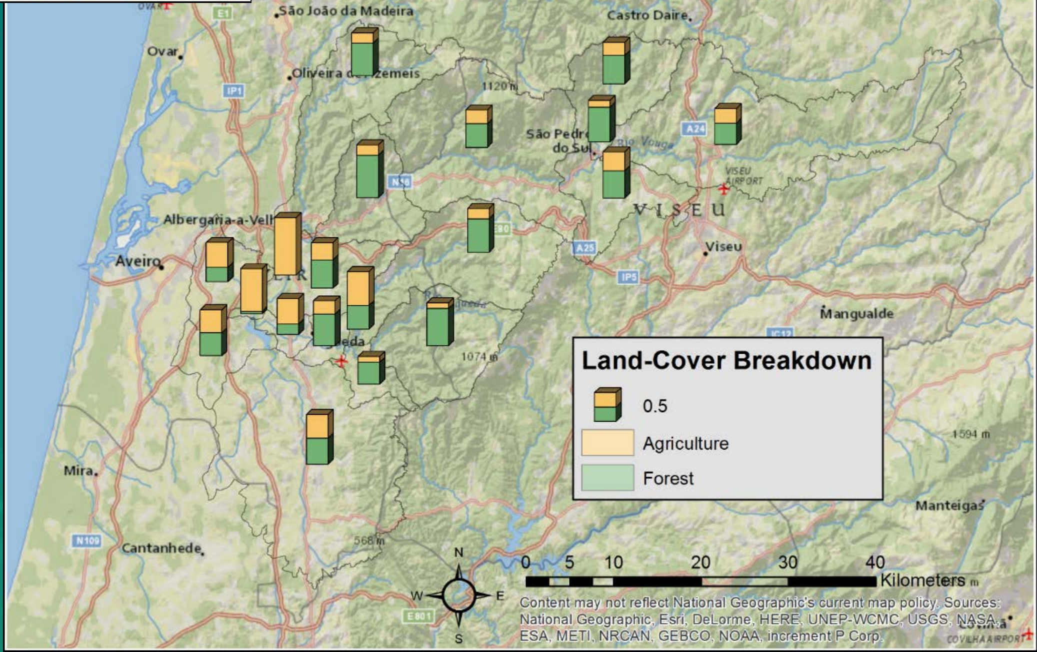
ENSEMBLE COMPARISON

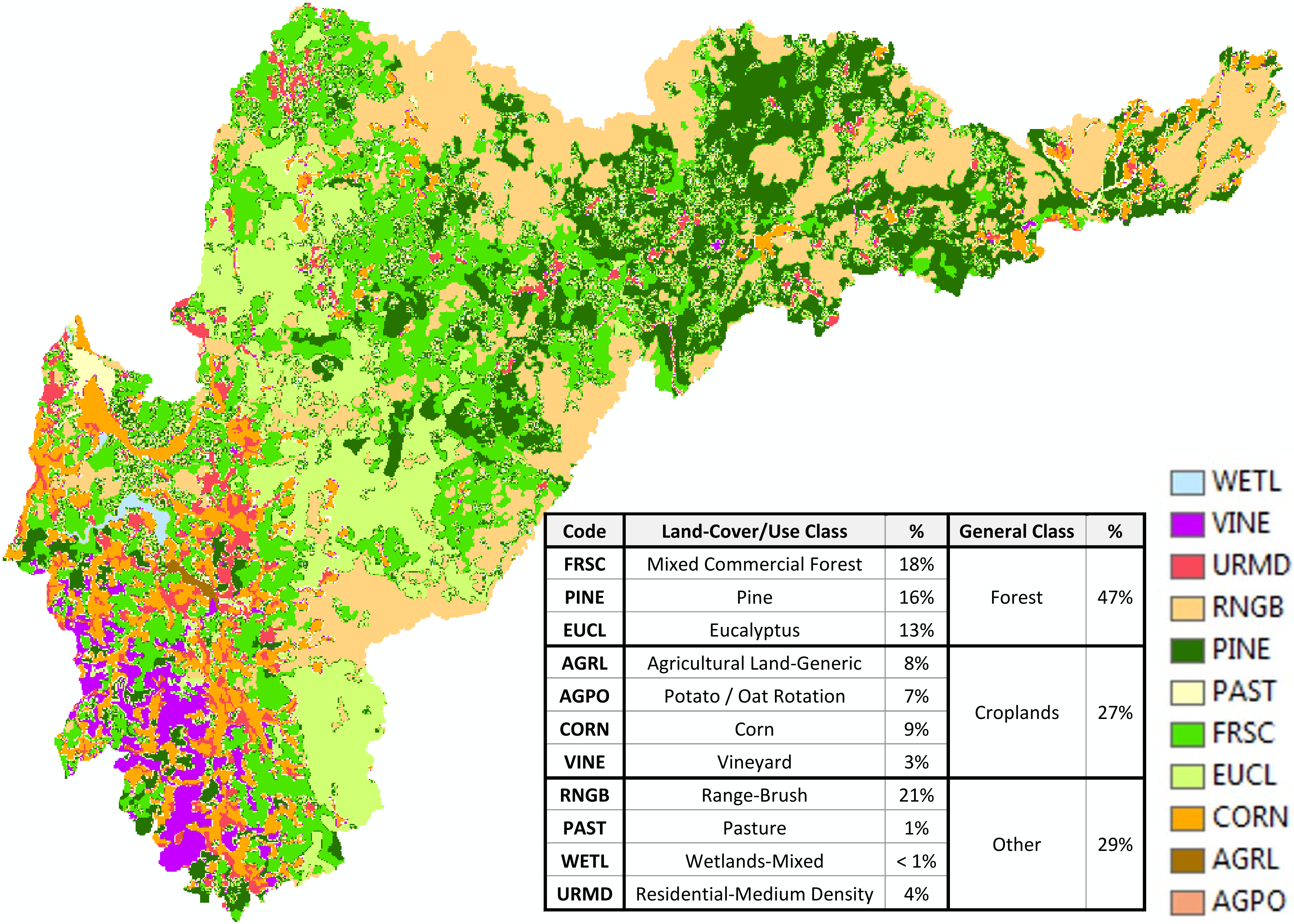
Region	Sub-Basin	Streamflow (KGE = 1.0)				Total Nitrogen (KS = 0.0)				Nitrogen Con. (KS = 0.0)			
		A	B	C	D	A	B	C	D	A	B	C	D
Upper	3 - Cabria	0.77	0.83	0.76	0.82	0.29	0.23	0.29	0.29	0.09	0.16	0.08	0.15
	5 - Vouzela	-0.24	-0.21	-0.25	-0.22	0.38	0.28	0.38	0.38	0.56	0.52	0.58	0.53
	4 - Ribeirada	0.16	-0.26	0.20	-0.37								
Middle	16 - Agueda	0.44	0.54	0.44	0.58	0.66	0.63	0.66	0.66	0.35	0.44	0.35	0.46
	18 - Redonda	-0.77	-0.70	-0.77	-0.67	0.94	0.96	0.94	0.94	0.13	0.15	0.13	0.15
	14 - Ribeiro	0.80	0.83	0.79	0.80								
	6 - Maior									0.97	1.00	0.97	1.00
	7 - Carvoeiro									0.70	0.79	0.70	0.79
Lower	15 - Requeixo	0.64	0.62	0.65	0.61	0.55	0.53	0.55	0.55	0.16	0.25	0.16	0.26
	8 - Frossos									0.75	0.69	0.75	0.67

Ensemble	Kling-Gupta	Kolmogorov–Smirnov
A	Unscaled	Concentration (mg/l)
B	Unscaled	Mass (kg)
C	Scaled	Concentration (mg/l)
D	Scaled	Mass (kg)


6
1
4
3
5
8
9
10
12
16
15
17
19
1
4
3
5
8
9
10
16
15
18
17
6
1
4
3
7
5
14
9
8
10
12
16
15
18
17
19
Lowland
Midland
Upland


Agriculture %
10% - 12%
13% - 18%
19% - 23%
24% - 25%
26% - 33%
34% - 40%
41%
42% - 44%
45% - 74%
75% - 100%
São João da Madeira
Castro Daire
Ovar
Oliveira de Azemeis
São Pedro do Sul
VISEU
Viseu
Albergaria-a-Velha
Aveiro
AVEIRO
Agueda
Tondela
Mira
Cantanhede
0 5 10 20 30 40 Kilometers
N
W
E
S
Content may not reflect National Geographic's current map policy. Sources: National Geographic, Esri, DeLorme, HERE, UNEP-WCMC, USGS, NASA, ESA, METI, NRCAN, GEBCO, NOAA, increment P Corp.


Land-Cover Breakdown
0.5
Agriculture
Forest
São João da Madeira
Castro Daire
Ovar
Oliveira de Azemeis
São Pedro do Sul
VISEU
Viseu
Albergaria-a-Velha
Aveiro
Mangualde
Mira
Cantanhede
Manteigas
0 5 10 20 30 40 Kilometers
N
W
E
S
Content may not reflect National Geographic's current map policy. Sources: National Geographic, Esri, DeLorme, HERE, UNEP-WCMC, USGS, NASA, ESA, METI, NRCAN, GEBCO, NOAA, increment P Corp.



Code	Land-Cover/Use Class	%	General Class	%
FRSC	Mixed Commercial Forest	18%	Forest	47%
PINE	Pine	16%		
EUCL	Eucalyptus	13%		
AGRL	Agricultural Land-Generic	8%	Croplands	27%
AGPO	Potato / Oat Rotation	7%		
CORN	Corn	9%		
VINE	Vineyard	3%		
RNGB	Range-Brush	21%	Other	29%
PAST	Pasture	1%		
WETL	Wetlands-Mixed	< 1%		
URMD	Residential-Medium Density	4%		