UNIVERSITEIT GENT

FACULTY OF BIOSCIENCE ENGINEERING

Nitrate source identification in various water bodies via isotopic fingerprinting

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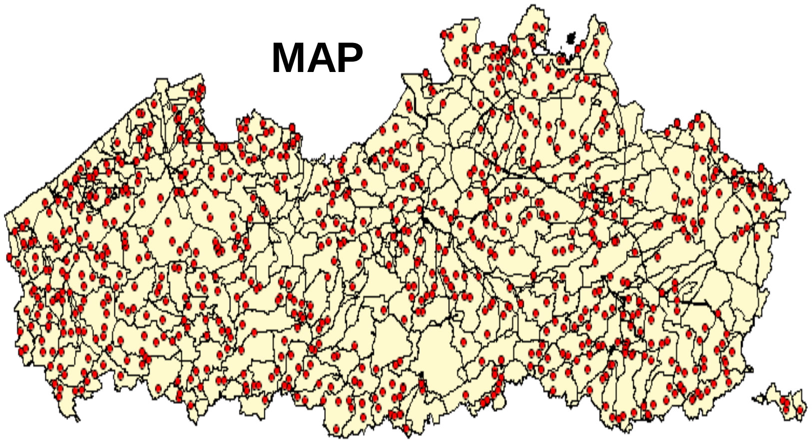
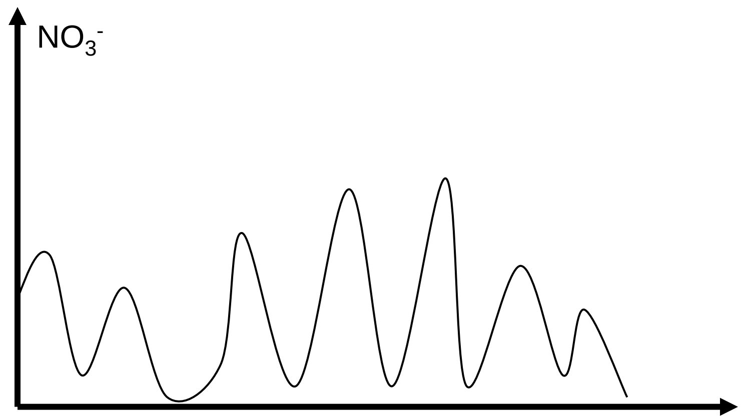
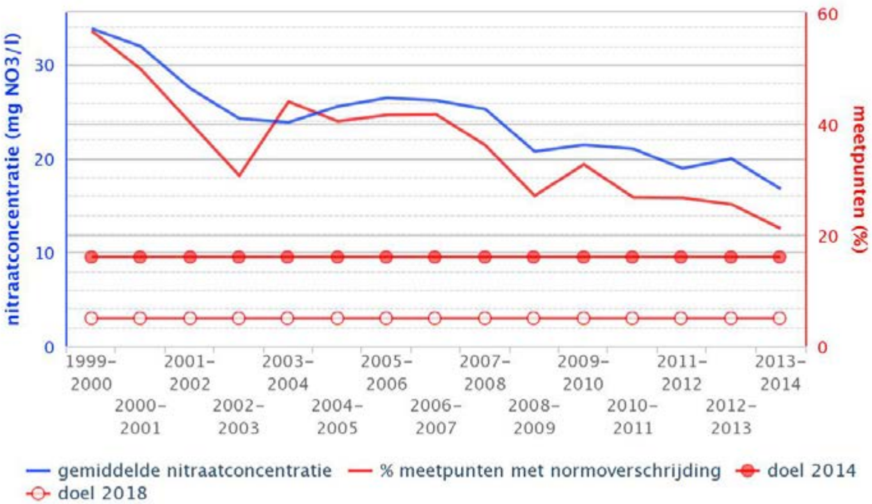
15 years NO_3^- management in Flanders: 1999-2014



Surface water, #800



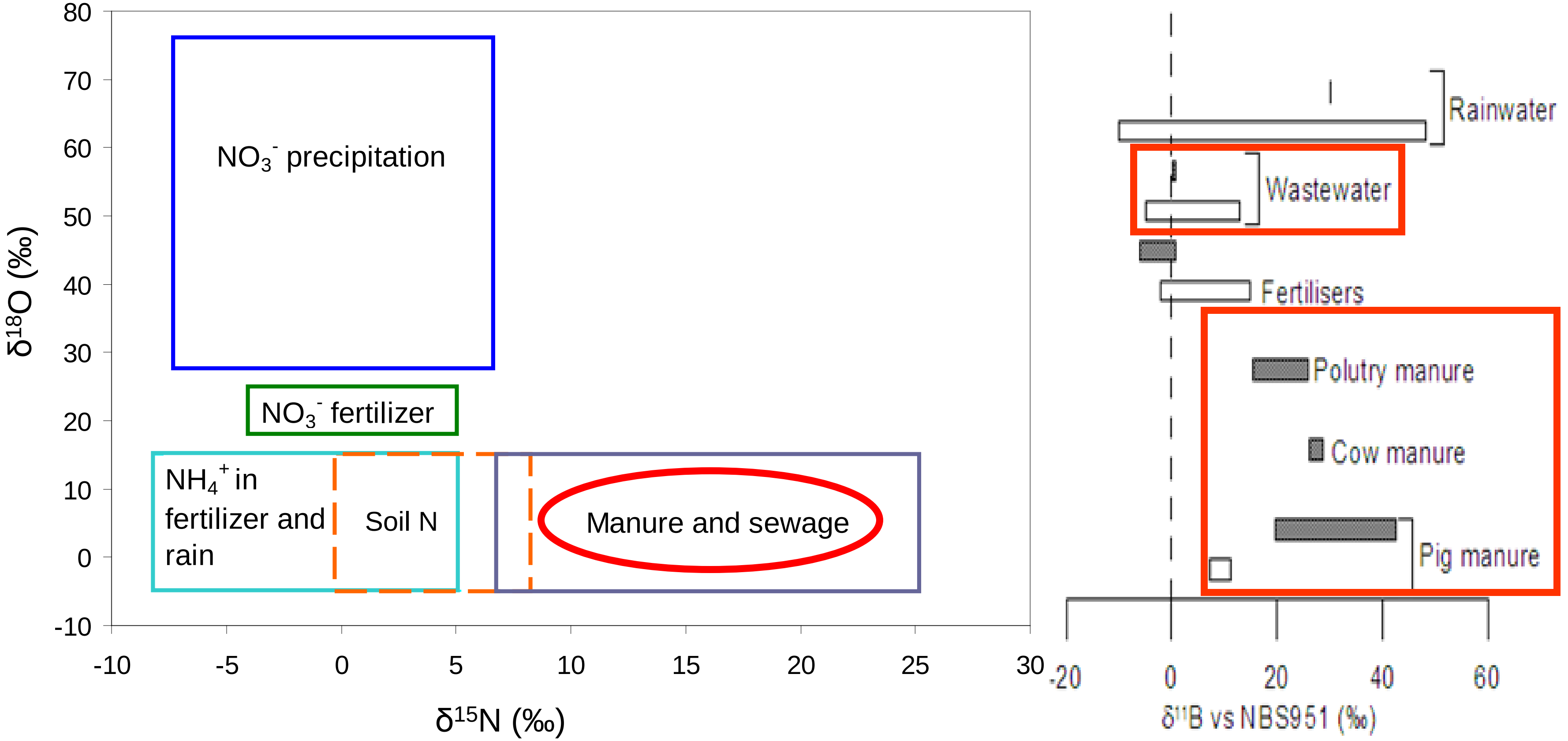
Nitrate in surface water and % sample points above 50 ppm thresholds



Sources?

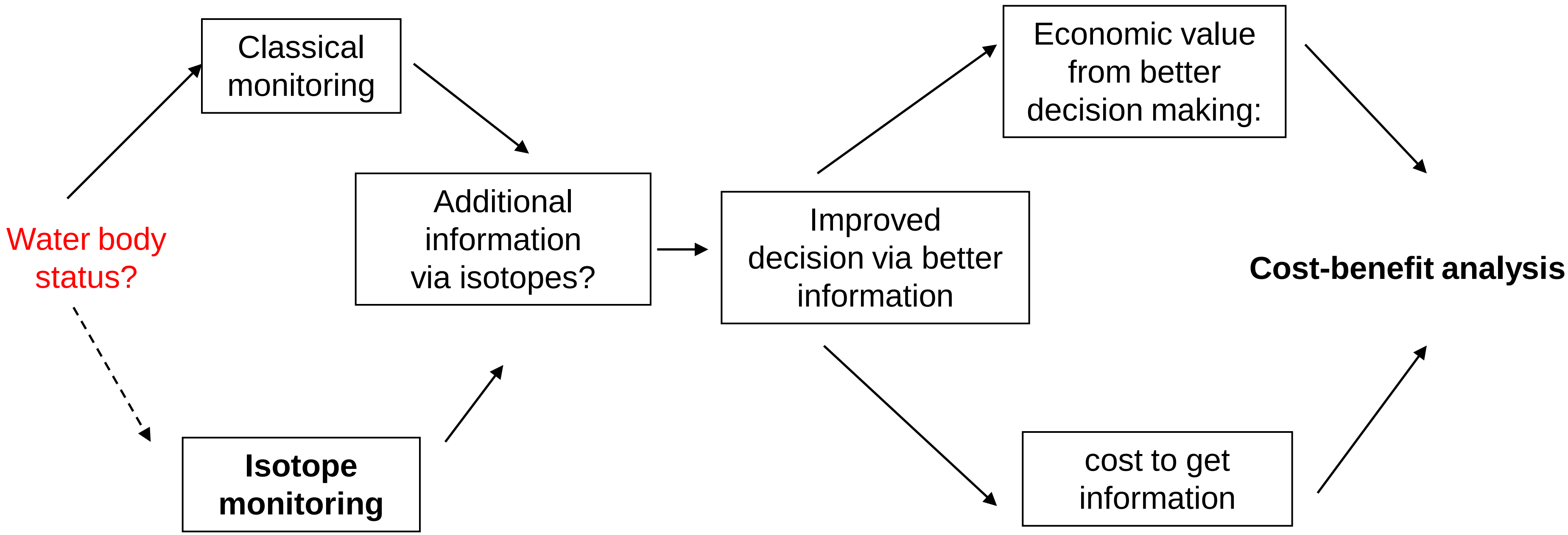
*"If you are uncertain about a status you will search for **additional information** before taking action"*

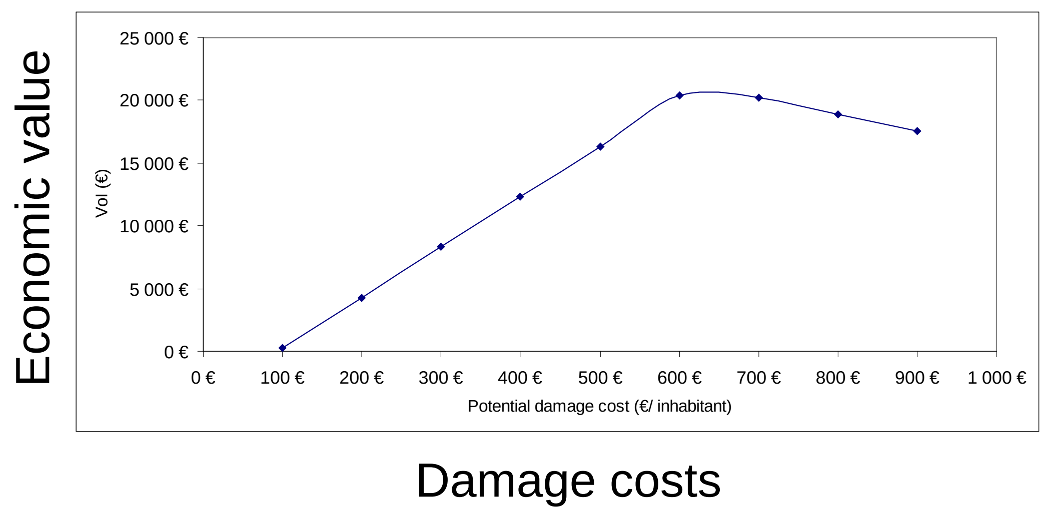
NO_3^- source aportionment



Xue et al. 2009

Economic value of including isotopes increases with potential damage costs





Objectives

To **quantify NO_3^- sources** in surface water

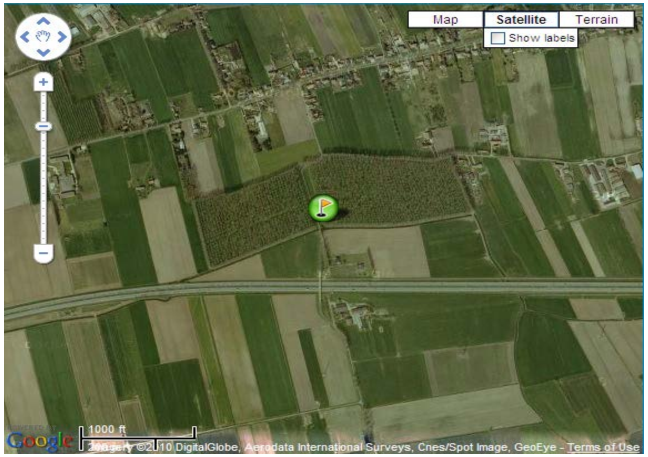
To **classify** surface waters in **NO_3^- pollution classes** via stable isotopes in NO_3^-

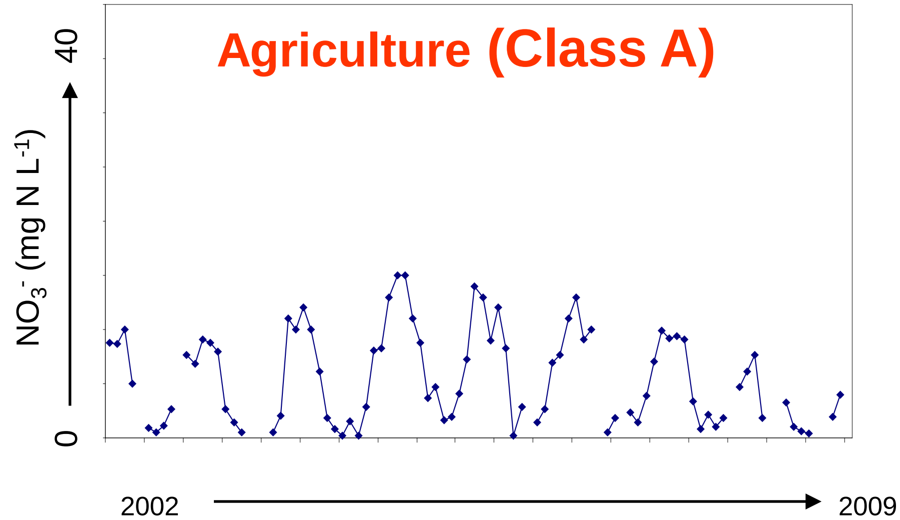
To assess if **physicochemical data** sets can be used to retrieve **NO_3^- pollution** classification

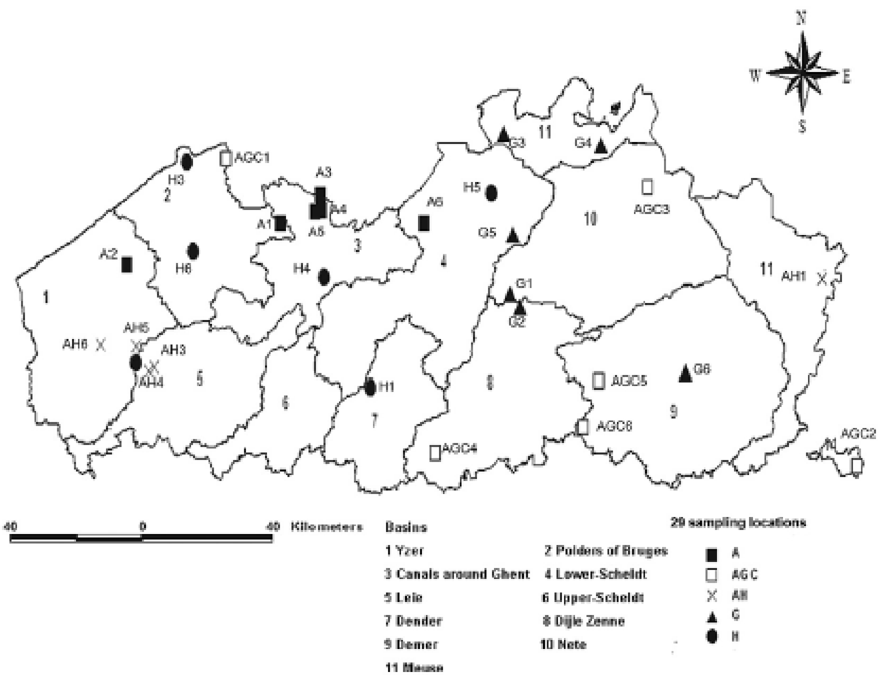
Methodology

- Select representative sampling points (30) for 5 different NO_3^- pollution classes (= based on expert judgment)
- Estimate proportional NO_3^- source contribution per NO_3^- pollution class using a Bayesian isotopic mixing model (SIAR) (monthly sampling during 2 years)
- Re-classify the 30 sampling points in NO_3^- pollution classes via a k-means clustering approach using the SIAR fingerprint as input data
- Build a decision tree model including physicochemical data (10 parameters, monthly sampling during 2 years) to retrieve the classification via expert and k-means clustering

Expert classification of 30 sampling points

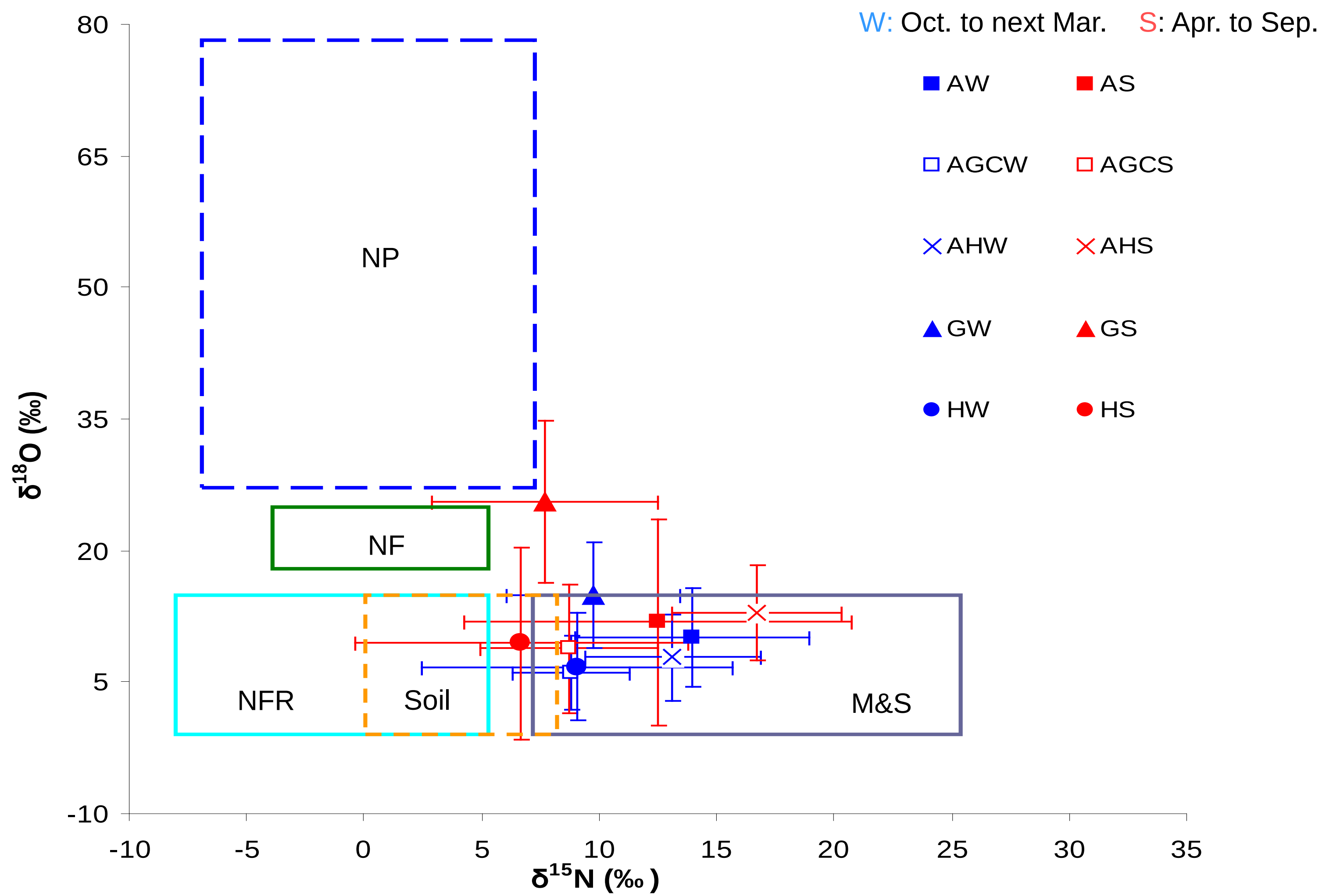




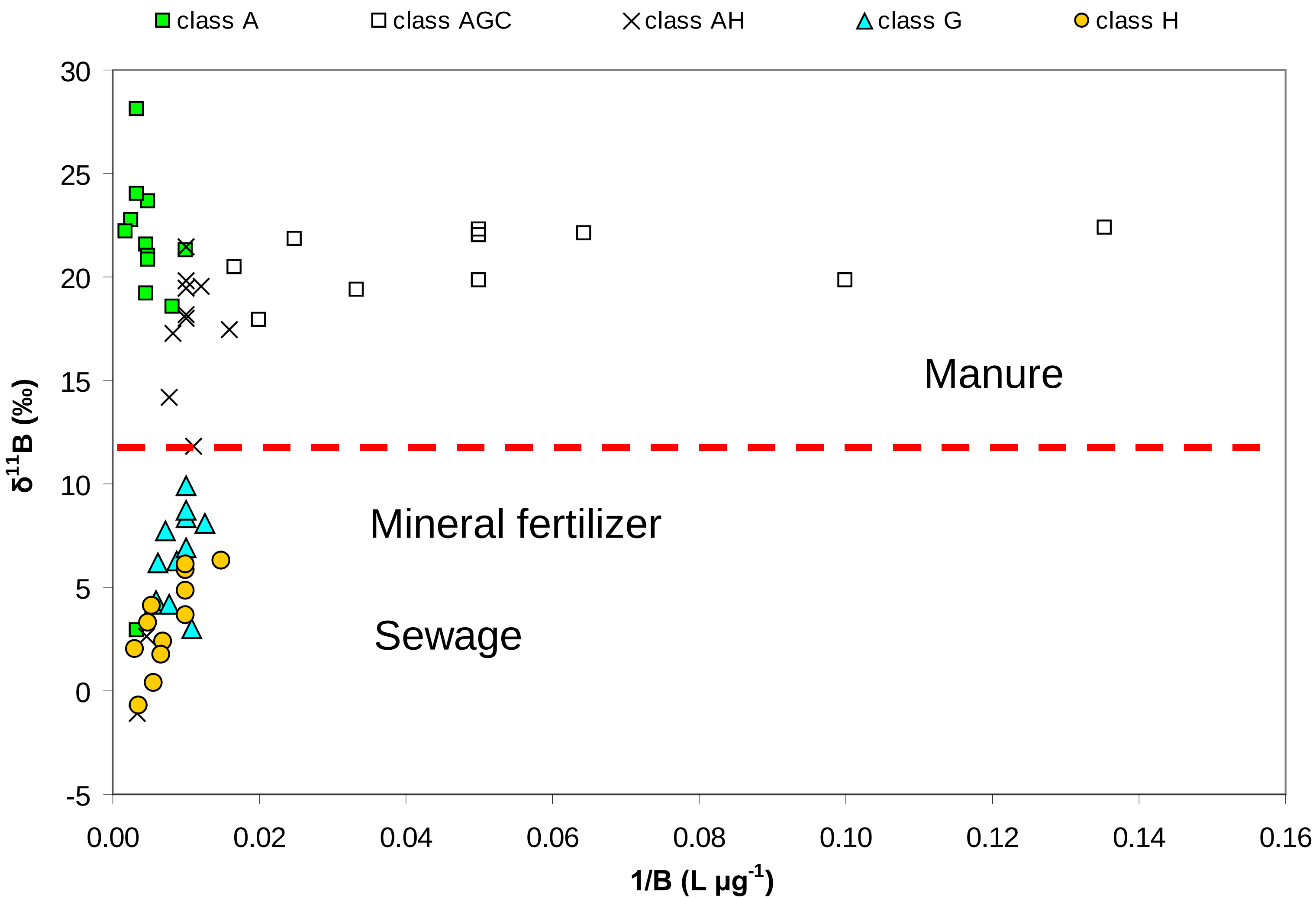


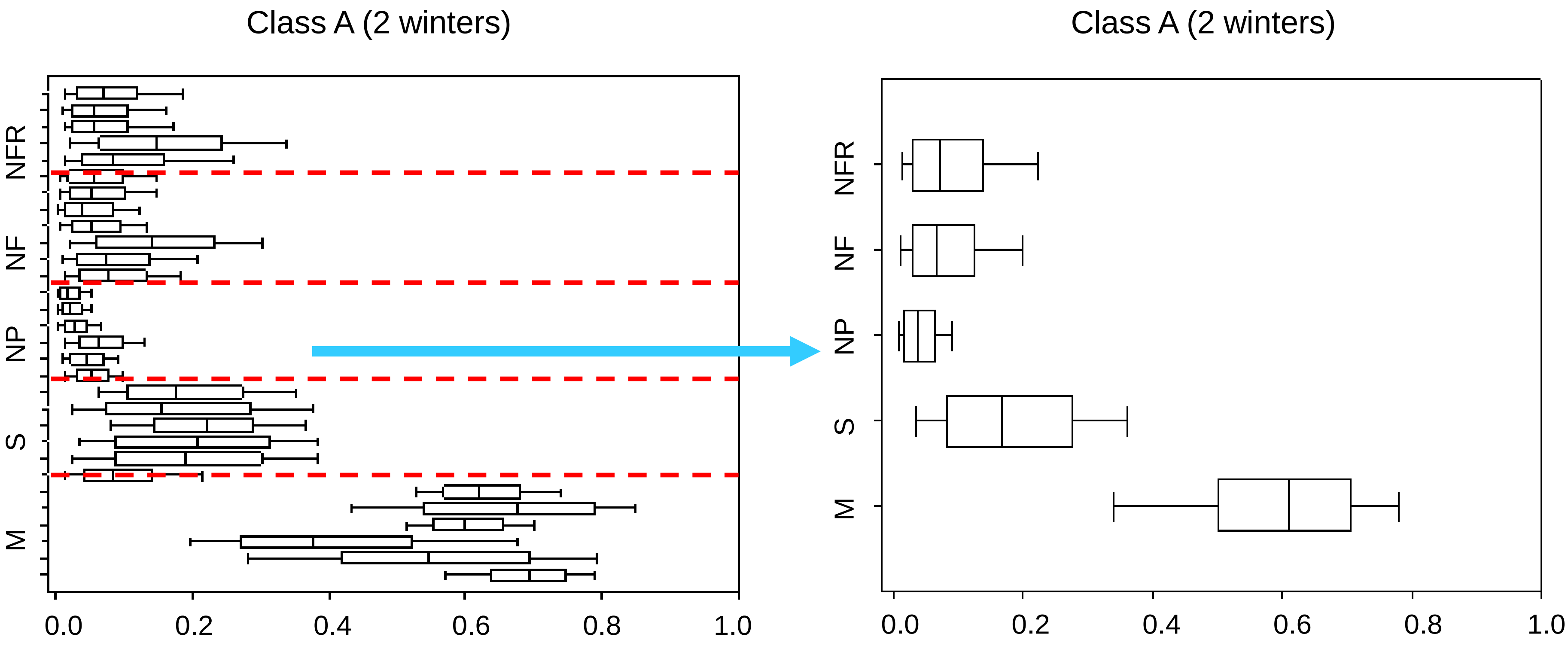
A: Agriculture
AGC: Agr. with ground water compensation
AH: Agriculture + Horticulture
G: Greenhouses
H: Households

Seasonal NO_3^- source identification (2 year data)



One year ^{11}B data





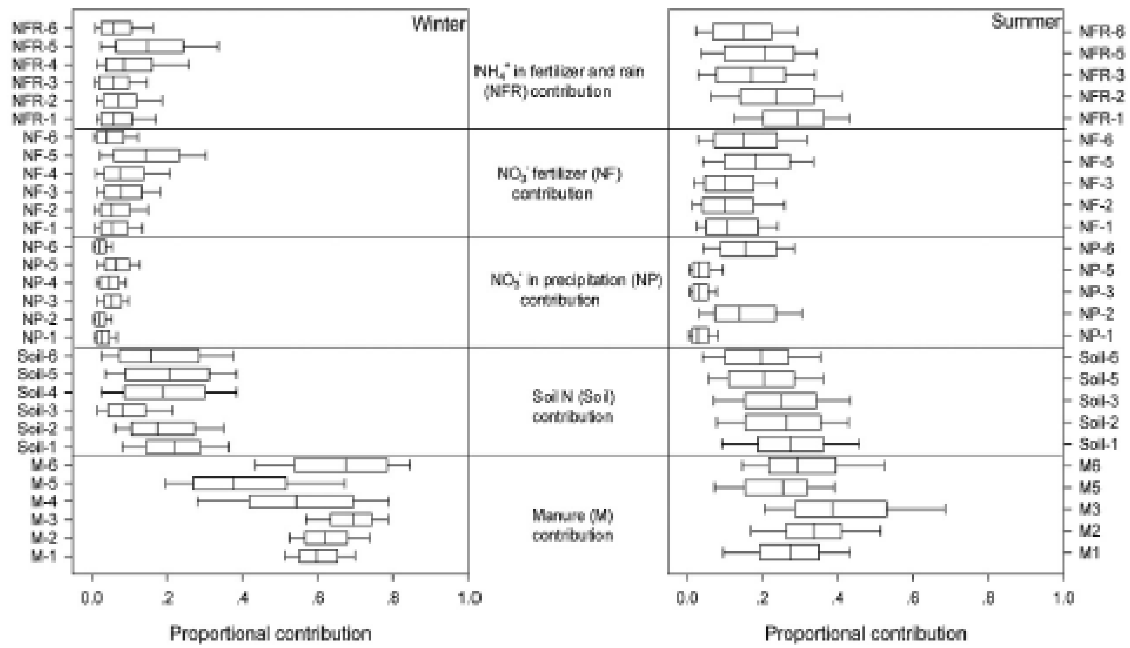
Journal of Environmental Quality TECHNICAL REPORTS

SURFACE WATER QUALITY

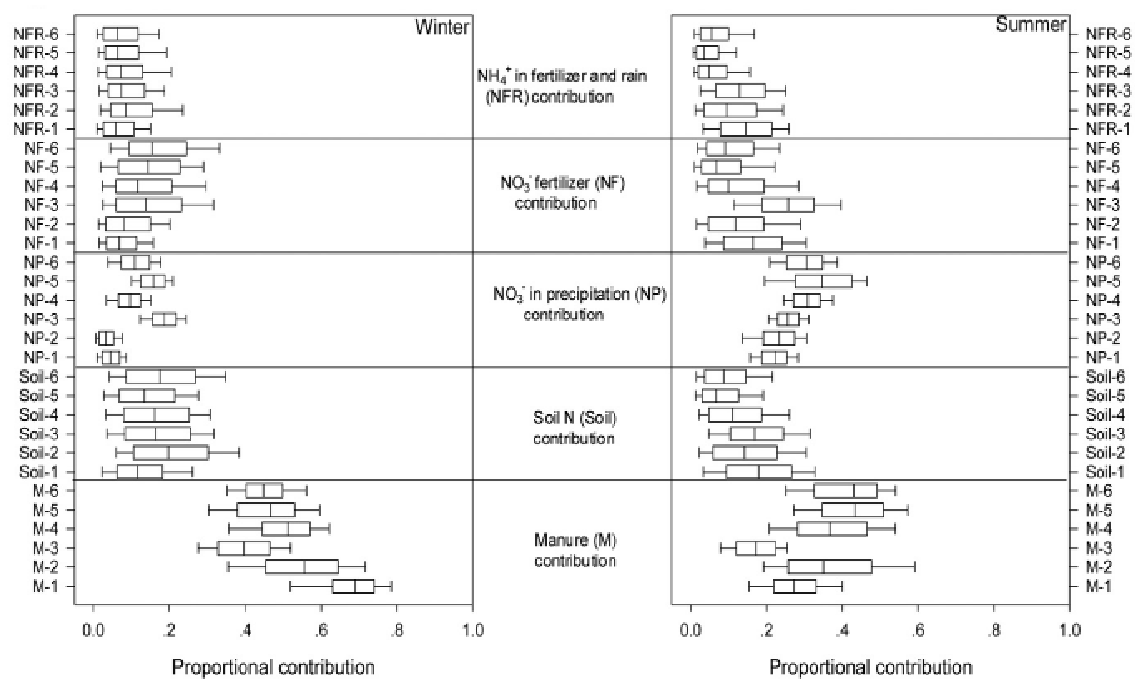
Classification of Nitrate Polluting Activities through Clustering of Isotope Mixing Model Outputs

Dongmei Xue,* Bernard De Baets, Oswald Van Cleemput, Carmel Hennessy, Michael Berglund, and Pascal Boeckx

Class A
Agriculture



Class G
Greenhouses



K-means clustering results for winter (SIAR)

Expert classification†	Sampling location	Three clusters via k-means	Four clusters via k-means
A	A1	**cluster 3‡**	cluster 2
	A2	cluster 2	**cluster 4**
	A3	cluster 2	cluster 2
	A4	cluster 2	cluster 2
	A5	cluster 2	**cluster 4**
	A6	**cluster 1**	**cluster 1**
AGC	AGC1	cluster 3	**cluster 2**
	AGC2	cluster 3	cluster 3
	AGC3	**cluster 2**	**cluster 4**
	AGC4	cluster 3	**cluster 2**
	AGC5	cluster 3	cluster 3
	AGC6	cluster 3	cluster 3
AH	AH1	**cluster 3**	**cluster 2**
	AH2	**cluster 2**	cluster 4
	AH3	**cluster 2**	cluster 4
	AH4	**cluster 3**	**cluster 2**
	AH5	**cluster 2**	cluster 4
G	G1	cluster 1	cluster 1
	G2	cluster 1	cluster 1
	G3	**cluster 2**	**cluster 4**
	G4	**cluster 3**	**cluster 2**
	G5	cluster 1	cluster 1
	G6	cluster 1	cluster 1
Silhouette		0.6	0.6

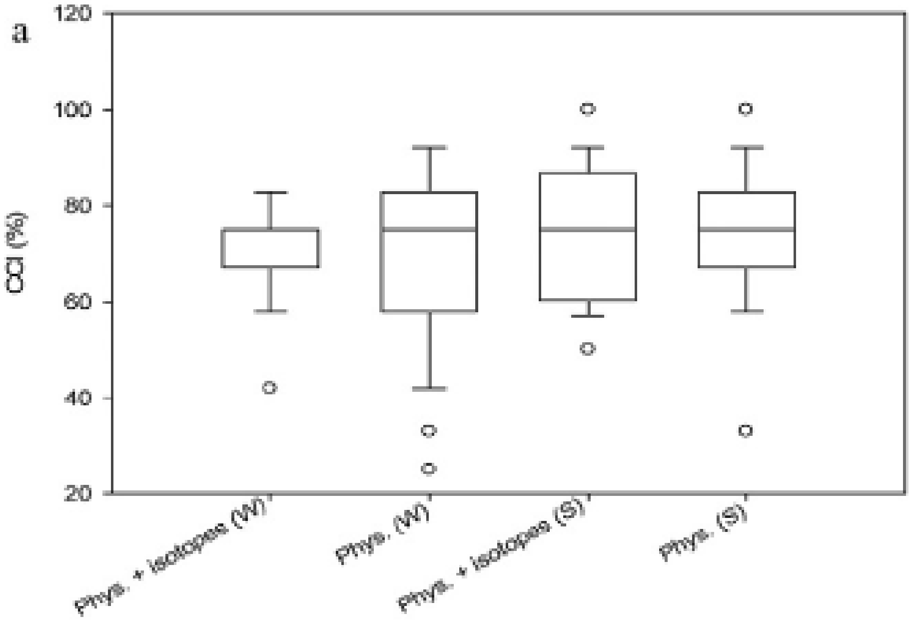
4 classes: A, AGC, G and H based on ^{11}B + 3-means clustering

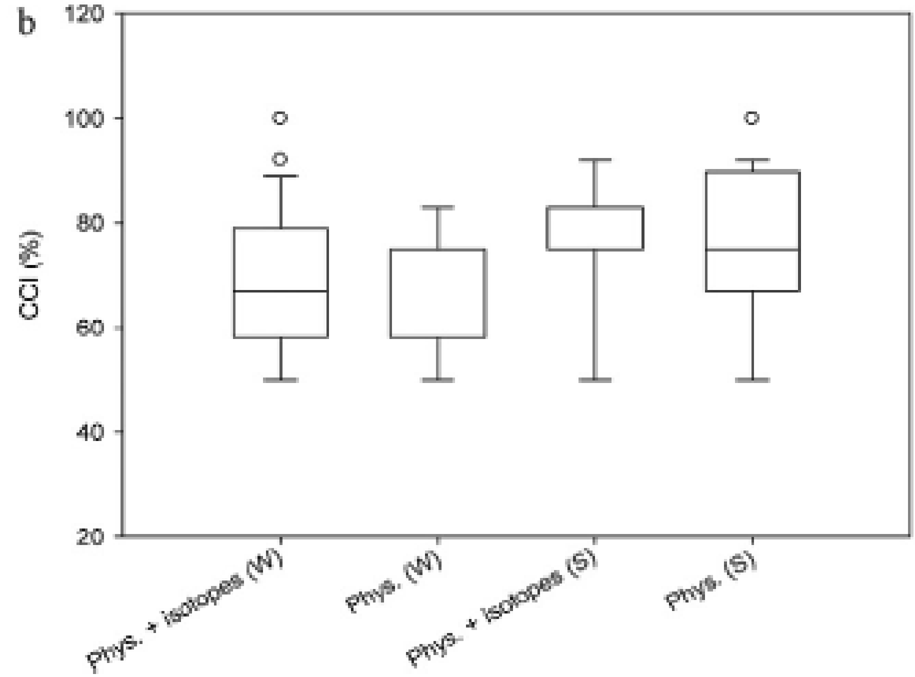
Comparison of expert classification and k-means clustering

Season	Cluster comparison	Rand index
Winter	expert classification vs. 3 clusters	0.7
	expert classification vs. 4 clusters	0.7
Summer	expert classification vs. 3 clusters	0.7
	expert classification vs. 4 clusters	0.7

K-means clustering using SIAR output retrieves 70% of expert classification!

Retrieve expert (a) and 3-means clustering (b) classification via decision tree models





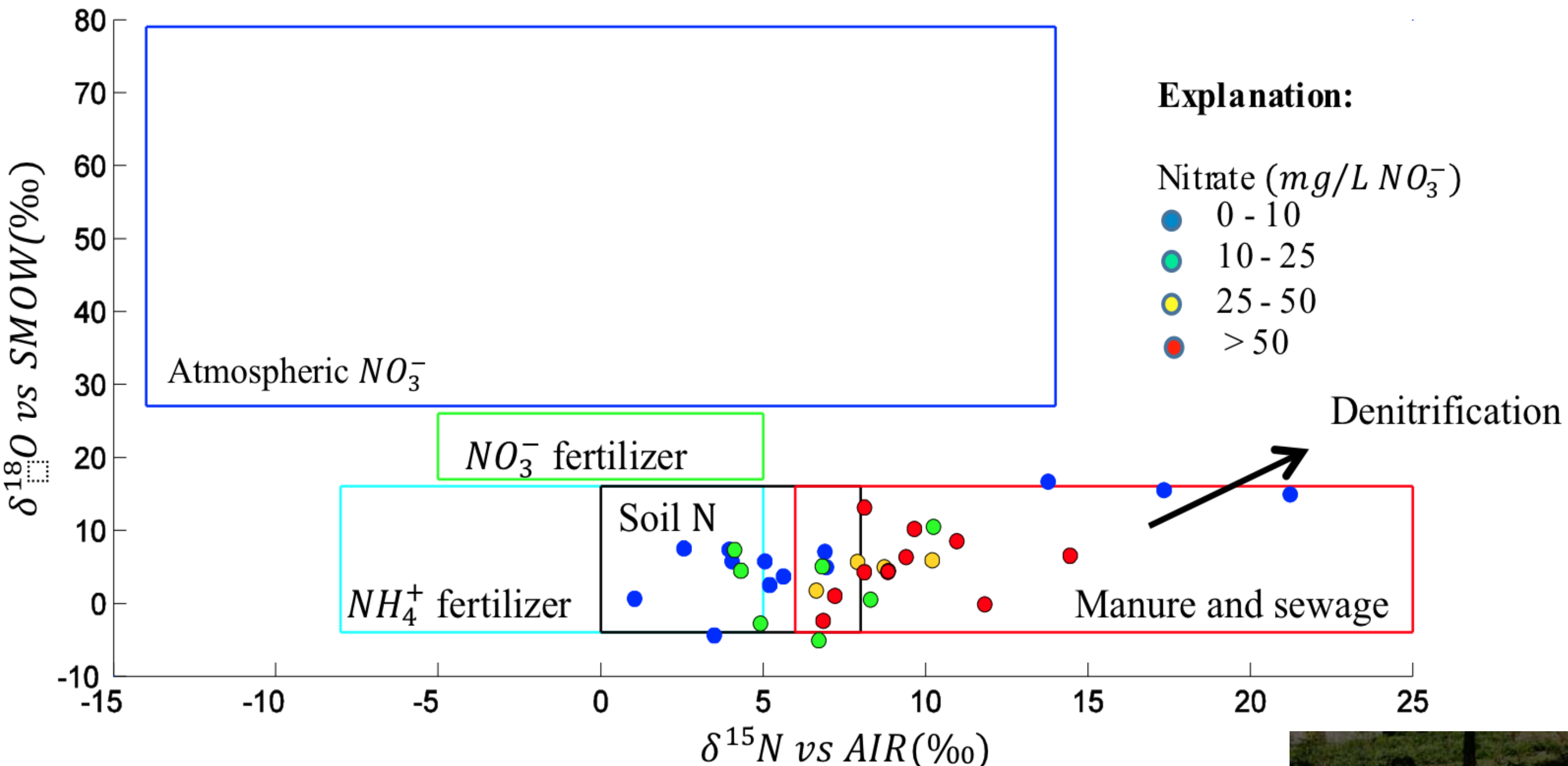
Conclusions and future application

- Coupled “SIAR” – “k-means clustering” approach is a promising tool to determine the number of NO_3^- pollution classes when expert knowledge for a basin is absent

- Decision trees using physicochemical data can be applied to classify a larger number of monitoring points of that basin into the established NO_3^- pollution classes

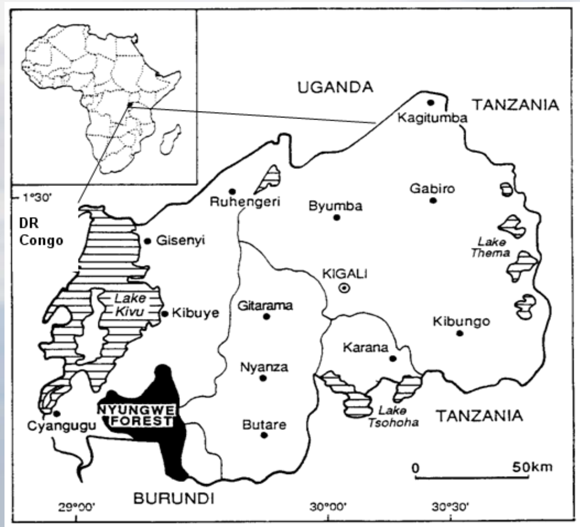
- *Away from Europe,…*

Kinshasa, DR Congo

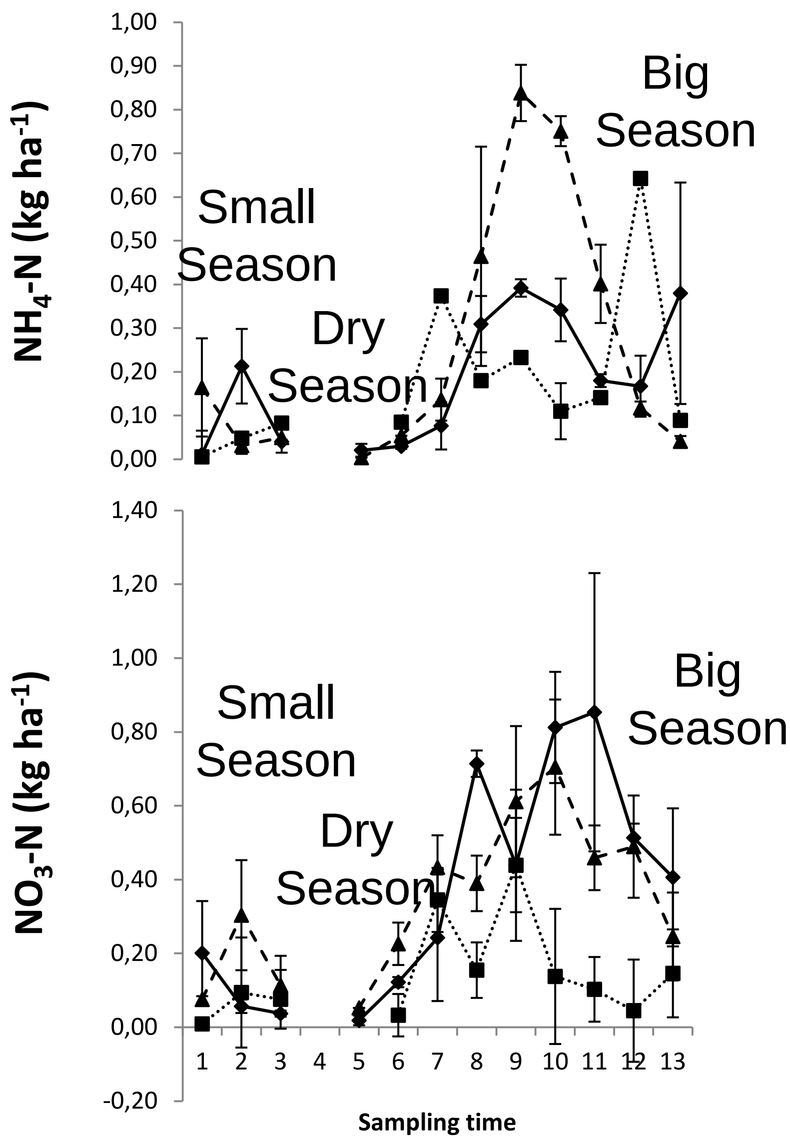


Nitrate concentration in groundwater boreholes
Range: 0.1 - 339.7 mg L^{-1}
Average: 39.2 $\pm$ 56.5 mg L^{-1}

Nyungwe - tropical mountain forest



Atmospheric N deposition



NH_4^+: 2.5 kg N ha^{-1} yr^{-1}
NO_3^-: 5.2 kg N ha^{-1} yr^{-1}

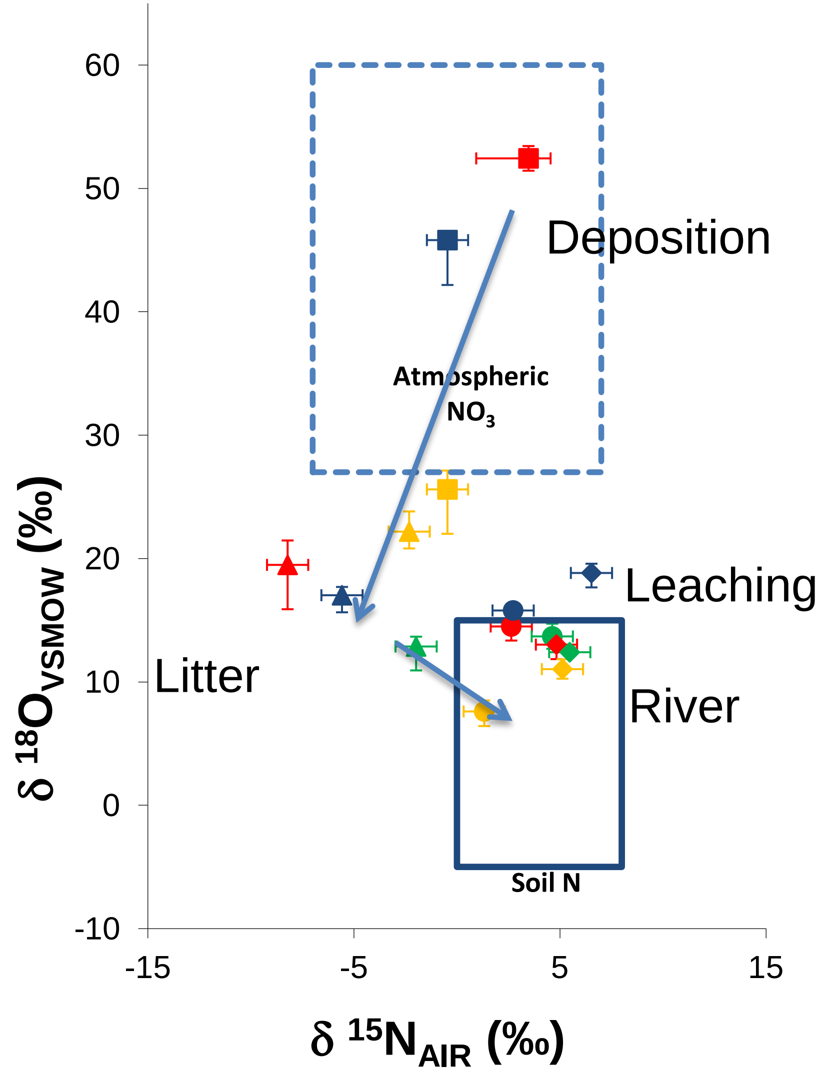
Compare with:

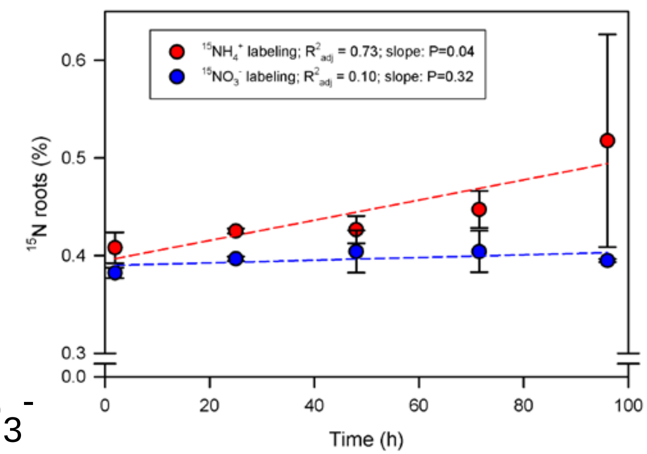
- Temperate forest (Belgium)
≈ 20 - 35 kg N ha^{-1} yr^{-1}

- Temperate forest (south Chile)
≈ 8 kg N ha^{-1} yr^{-1}

Nitrate leaching and source

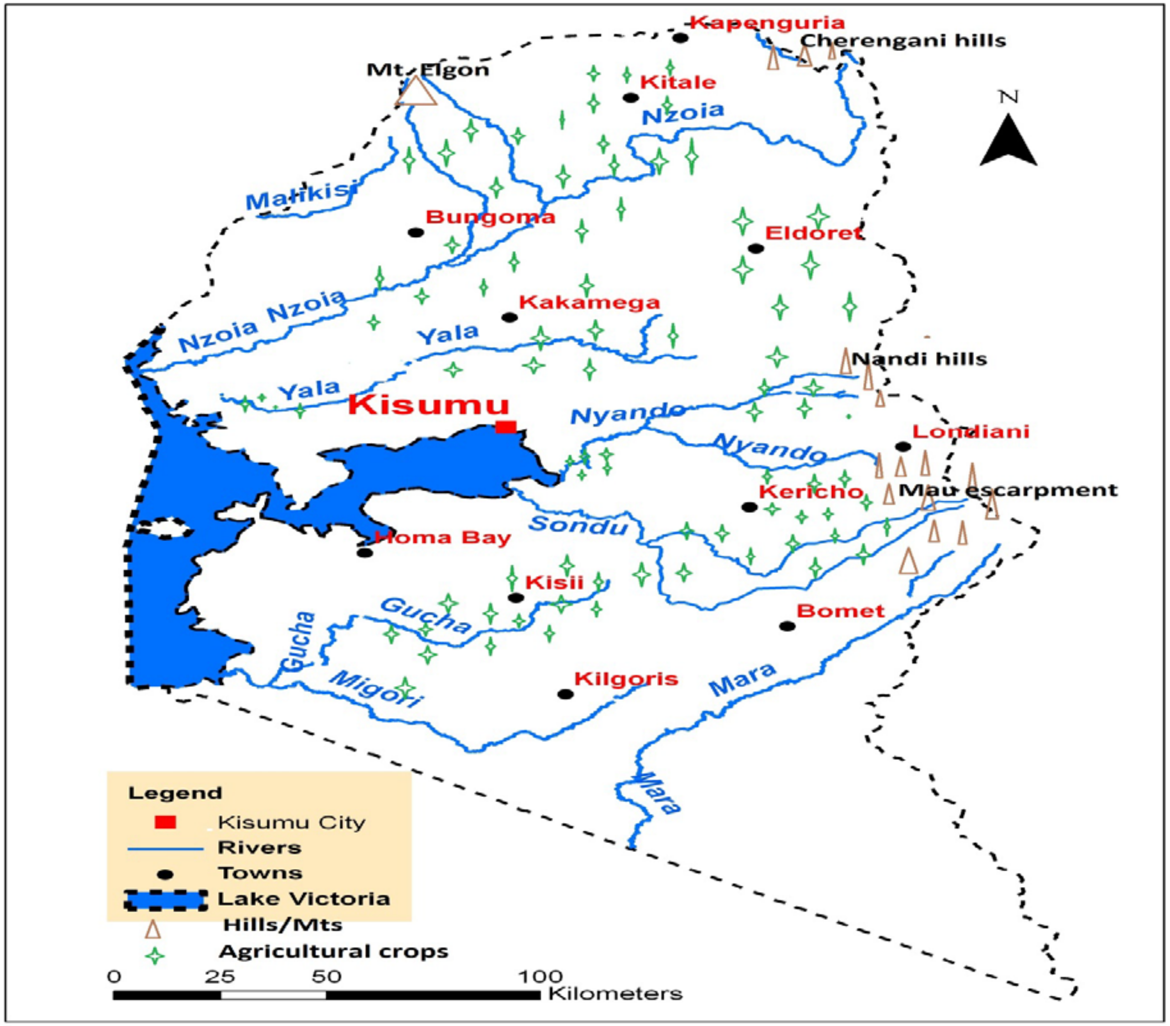
- Loss of **NO_3^- = 19.7** kg N ha^{-1} yr^{-1}
- NO_3^- loss 4-fold higher than deposition





Plants use NH_4^+ and not NO_3^-

Lake Victoria, Kenya catchment



WATER RESEARCH 43 (2009) 1159–1170

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Review

Present limitations and future prospects of stable isotope methods for nitrate source identification in surface- and groundwater

Dongmei Xue[a,b,*], Jorin Botte[a], Bernard De Baets[b], Frederik Accoe[c], Angelika Nestler[c], Philip Taylor[c], Oswald Van Cleemput[a], Michael Berglund[c], Pascal Boeckx[a]

Bayesian mixing models (mixSIAR) account for uncertainty and isotope fractionation, hence a detailed temporal and spatial isotopic characterization of NO_3^-, and correct assessment of enrichment factor for soil and river denitrification is paramount