Development of a Modelling System for Refinement of Groundwater Scenarios in France: The FROGS (French Refinement Of Groundwater Scenarios) Shell

UIPP Environmental Methodology Working Group

presented by Klaus Hammel, Bayer CropScience

French Refinement Of Groundwater Scenarios
Workgroup

Workgroup Members, September 2010

- Claude Beigel (BASF)
- Michael Berardozzi (Dow)
- Marie Cecchi (Syngenta)
- Christian Guyot (Bayer CropScience)
- Klaus Hammel (Bayer CropScience)
- Stefan Huber (BASF)
- Gunnar Kahl (Dr. Knoell Consult)
- Steve Knowles (Dow)
- Ludovic Loiseau (Syngenta)

History

ComTox Methodology Groundwater Workgroup: Regulators, scientific institutes (INRA, INA-PG), technical institutes (Arvalis) and industry (UIPP)

- **André-Bernard Delmas (INRA – SSM – Versailles)**
- **Brigitte Rémy (INRA – SSM – Versailles)**
- **Laure Mamy (INRA – SSM – Versailles)**
- **Paul Gaillardon (expert ComTox),**
- **Christine Lebas (INRA – Infosol – Orléans)**
- **Xavier Morvan (INRA – Infosol – Orléans)**
- **Ary Bruand (Université d'Orléans)**
- **Benoît Réal (Arvalis – Institut du Végétal)**
- **Igor Dubus (BRGM), Yves Coquet (INRA – INA PG)**
- **Enrique Barriuso (INRA – EGC – Grignon)**
- **Guy Soulas (Université Bordeaux II)**

History

ComTox Methodology Groundwater Workgroup

- **Substantial progress 2004-2006**

Common effort stopped in Sep. 2006 with establishment of AFSSA

- **No more collaboration possible with industry on methodology**
- **AFSSA expressed wish to continue work**

UIPP progresses on its own since 2007 (BASF + BCS + Dow + Syngenta)

French Refinement Of Groundwater Scenarios
Zonation and Agronomic Units

Climate regions

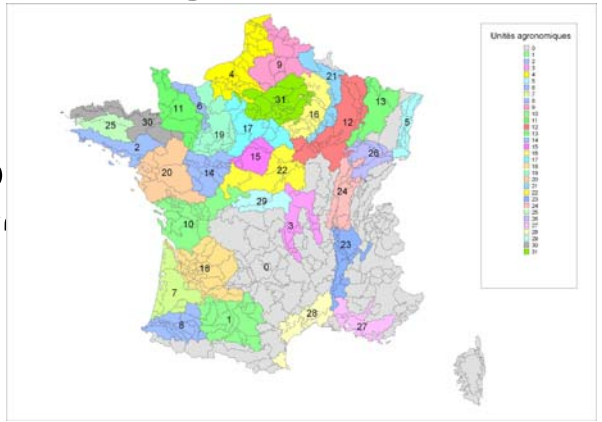
Hydro-eco regions

Geomorphology, topography, soil coverage

Climate

Land use by crop

31 Agronomic Units

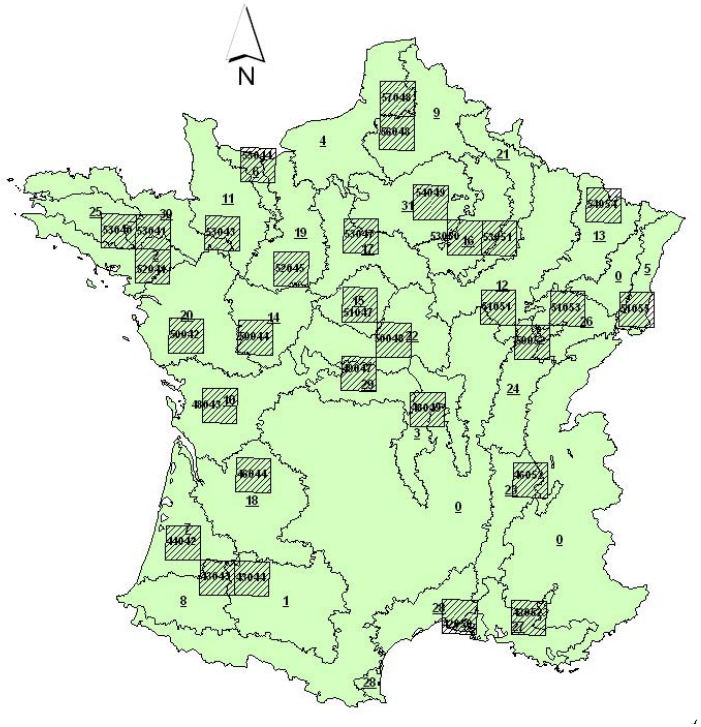


Sufficiently homogeneous „eco pedo-agro-climatic“ zones

Small agronomic regions, aggregated to cropping basins

MARS EU weather database

- One data set per AU (representing max of target area)
- Selection of MARS grid was checked to sufficiently represent the weather conditions in the AU



Soils and Soil Coverage

INRA INFOSOL Orléans

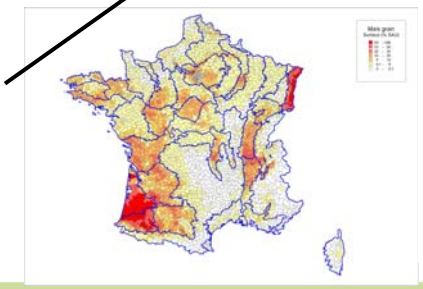
BDGSF soil database (1:1000000)

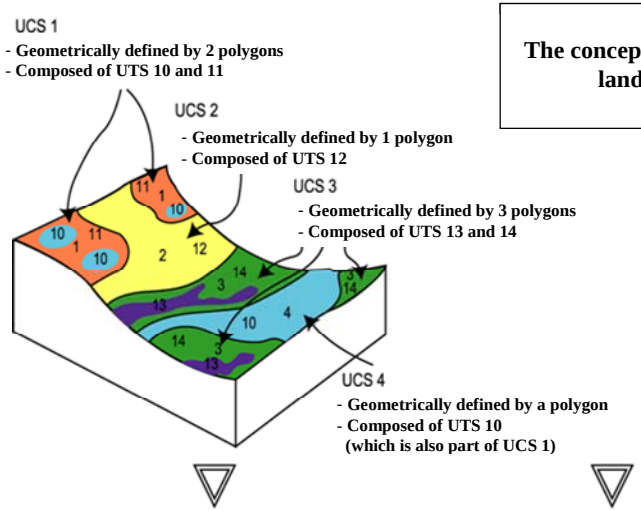
DONESOL 2

Limited number of representative
- **soil types**
- **soil properites**

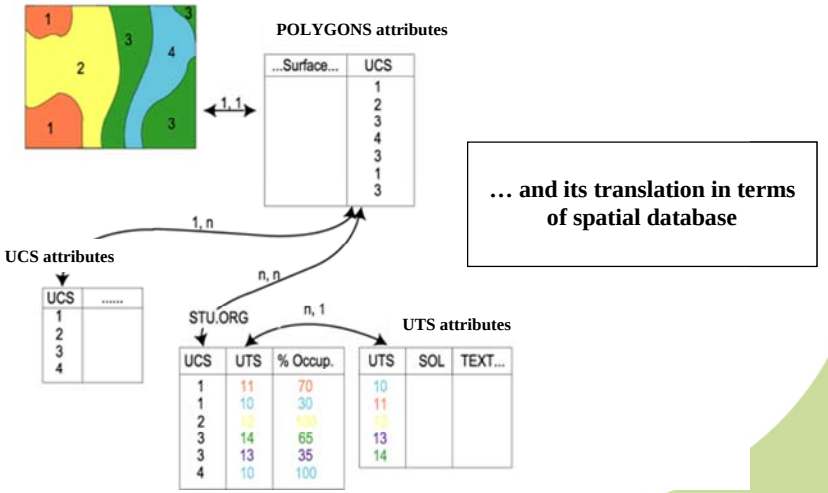
for arable land

CORINE land cover & 2000 Agricultural census





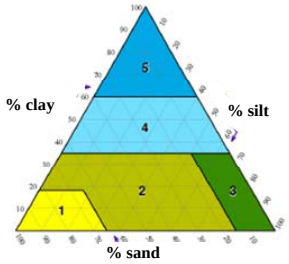
The concept of pedological landscape…



… and its translation in terms of spatial database

Set of 19 dominant soils

n° soil-type	FAO denomination	Texture class	Depth of profile
1	Luvisol	3	>80 cm
2	Cambisol	4	>80 cm
3	Rendzine	2	>80 cm
4	Luvisol	2	>80 cm
5	Cambisol	3	60 cm
6	Rendzine	2	60 cm
7	Rendzine	4	40 cm
8	Fluvisol	2	>80 cm
9	Fluvisol	1	>80 cm
10	Gleysol	4	>80 cm
11	Cambisol	2	60 cm
12	Podzoluvisol	3	>80 cm
13	Cambisol	3	>80 cm
14	Podzoluvisol	2	>80 cm
15	Cambisol	2	>80 cm
16	Rendzine	3	60 cm
17	Rendzine	3	>80 cm
18	Solonchak	4	>80 cm
19	Arenosol	1	>80 cm



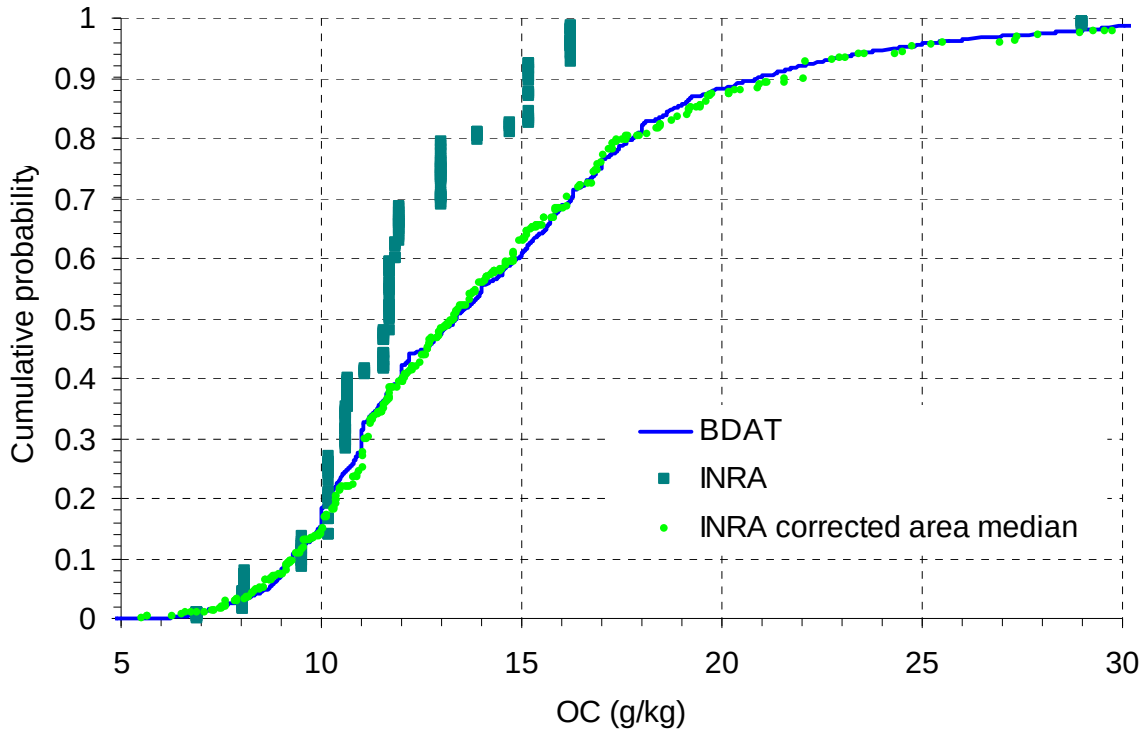
Hydraulic properties: HYPRES PTF
Bulk density: PEARL PTF
Dispersivity: FOCUS default
Biodeg. factors: FOCUS default

Evaluation depth: Depth of profile !

Adjustment of OC

OC is key soil factor for leaching

- **OC from soil data set are relatively scarce and potentially biased**
- **Comparison with BDAT comprehensive topsoil data (2000-2004)**
- **Introduction of AU specific correction factor**



AU Soil Crop Relations

AU x Soil (SID) Surface
(AU 3: Limagnes - Plaine du Forez)

AUID	SID	Area (kha)
3	2	89
3	5	7
3	6	21
3	8	71
3	9	25
3	11	35
3	14	215
3	15	30
3	19	4

Crop (CID) x Soil (SID)
(CID 1: sugar beets)

CID	SID
1	1
1	2
1	3
1	6
1	8
1	9
1	13
1	19

AU x Soil x Crop

AUID	SID	CID	MeteoStation
3	2	1	48049
3	6	1	48049
3	8	1	48049
3	9	1	48049
3	19	1	48049

Crop Rotations

UA code	UA Name	Primary crop	Crop rotation	Rotation length (years)
1	Collines molassiques - Lauragais	Winter Wheat	Winter Wheat-Sunflower	2
		Oil seed rape	Oil seed rape-Winter Wheat-Sunflower	3
		Maize fodder	Maize fodder	1
		Maize grain	Maize grain-Winter Wheat	2
		Barley	Barley-Winter Wheat-Sunflower	3
		Sunflower	Sunflower-Winter Wheat	2
2	Bretagne sud	Winter Wheat	Winter Wheat-Maize fodder-Barley	3
		Oil seed rape	Oil seed rape-Winter Wheat-Maize fodder	3
		Maize fodder	Maize fodder-Winter Wheat-Barley	3
		Maize grain	Maize grain-Winter Wheat	2
		Barley	Barley-Maize fodder-Winter Wheat	3
		Sunflower	Sunflower-Winter Wheat	2
3	Limagnes - Plaine du Forez	Sugar beet	Sugar beet-Winter Wheat-Winter Wheat	3
		Winter Wheat	Winter Wheat-Maize fodder	2
		Oil seed rape	Oil seed rape-Winter Wheat-Barley	3
		Maize fodder	Maize fodder-Winter Wheat	2
		Maize grain	Maize grain-Barley-Winter Wheat	3
		Barley	Barley-Winter Wheat-Sugar beet	3
		Sunflower	Sunflower-Winter Wheat	2
4	Bordure Nord - Picardie - Normandie	Sugar beet	Sugar beet-Winter Wheat-Winter Wheat	3
		Winter Wheat	Winter Wheat-Barley-Maize fodder	3
		Oil seed rape	Oil seed rape-Winter Wheat-Barley	3
		Maize fodder	Maize fodder-Winter Wheat-Barley	3
		Maize grain	Maize grain-Winter Wheat	2
		Barley	Barley-Winter Wheat-Sugar beet	3
		Potatoe	Potatoe-Winter Wheat-Barley	3

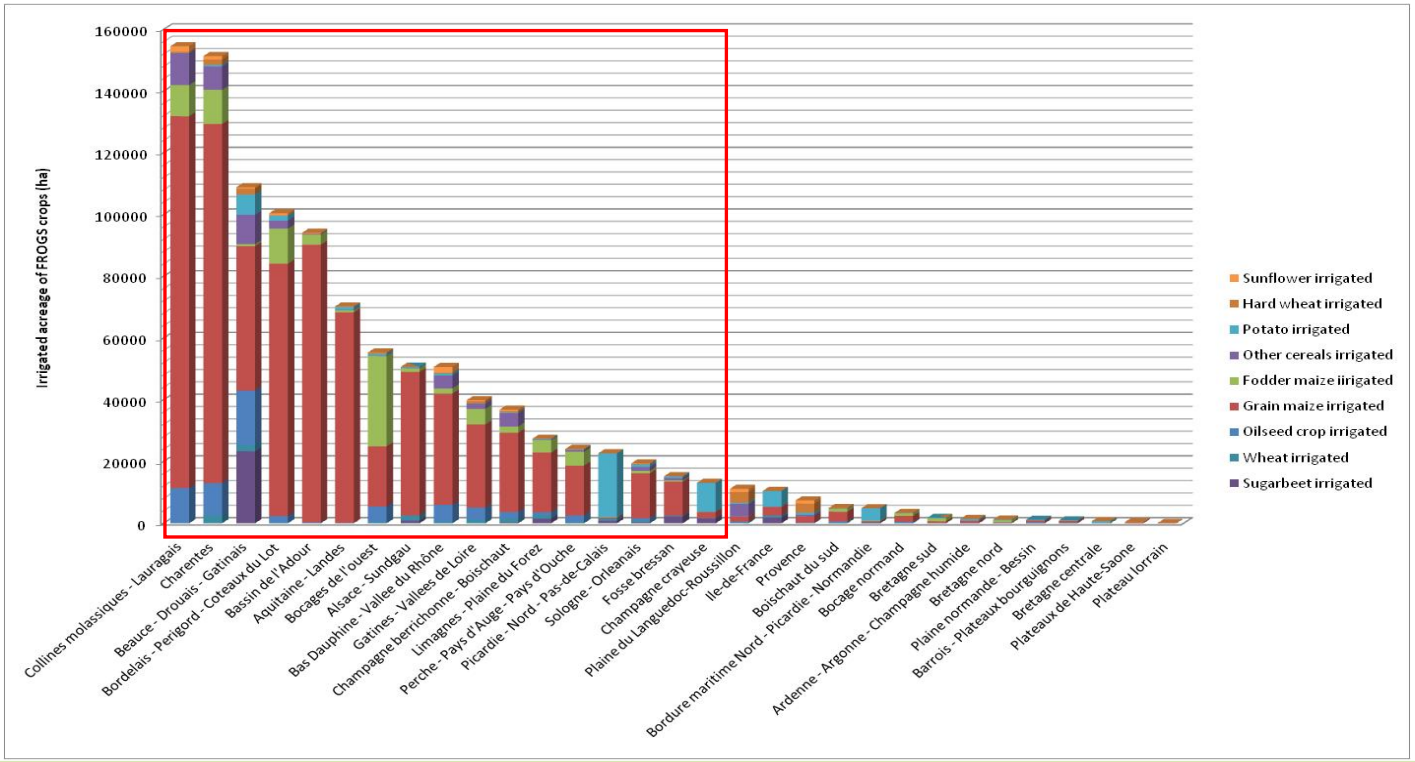
Crop parameters

- **FOCUS values from Châteaudun (Piacenza) scenario**

- **Arvalis – Institut du Végétal and UIPP expert knowledge aligned with Agreste data**

Irrigation

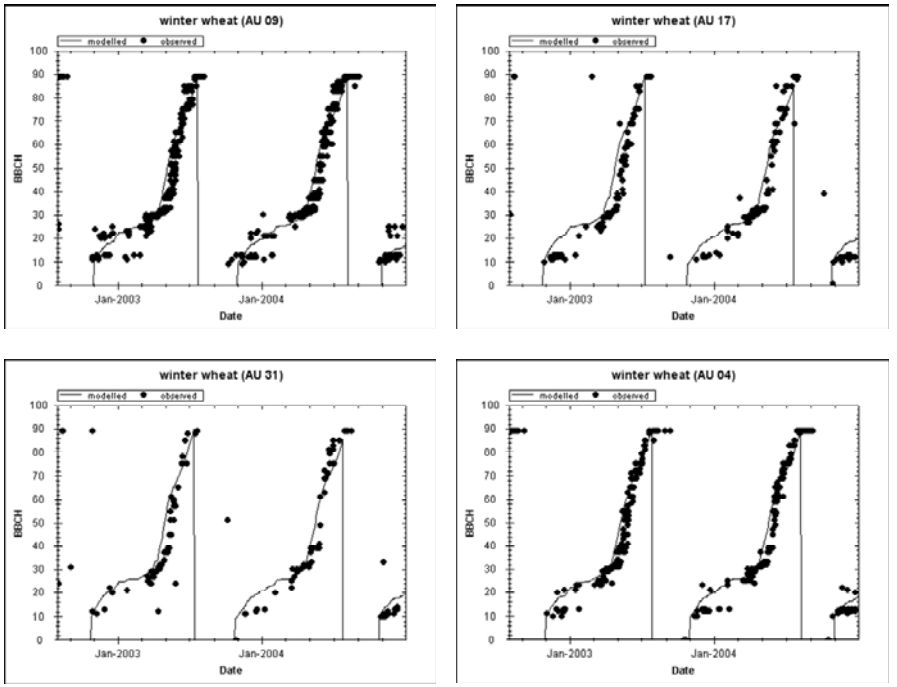
- considered for grain maize, fodder maize, sugar beet and potato (represent 85 % of irrigated crops)
- realistic irrigation practice
- derived from French agricultural census (Agreste)



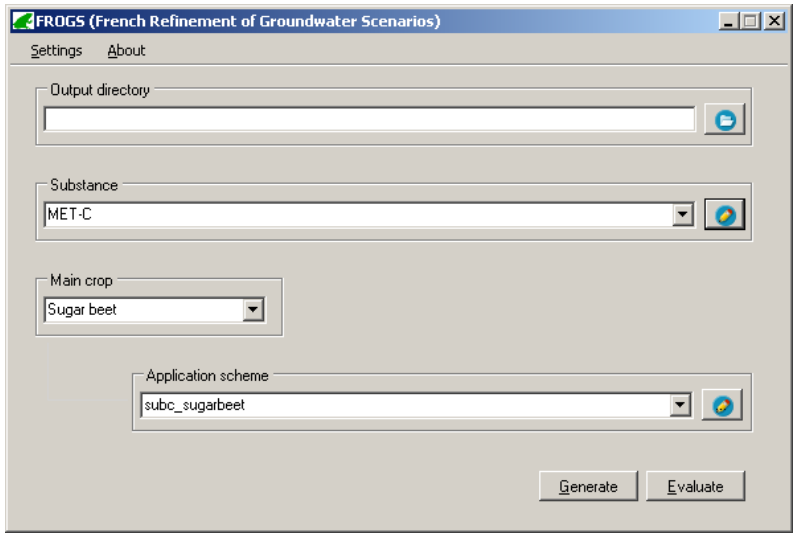
Application Timing

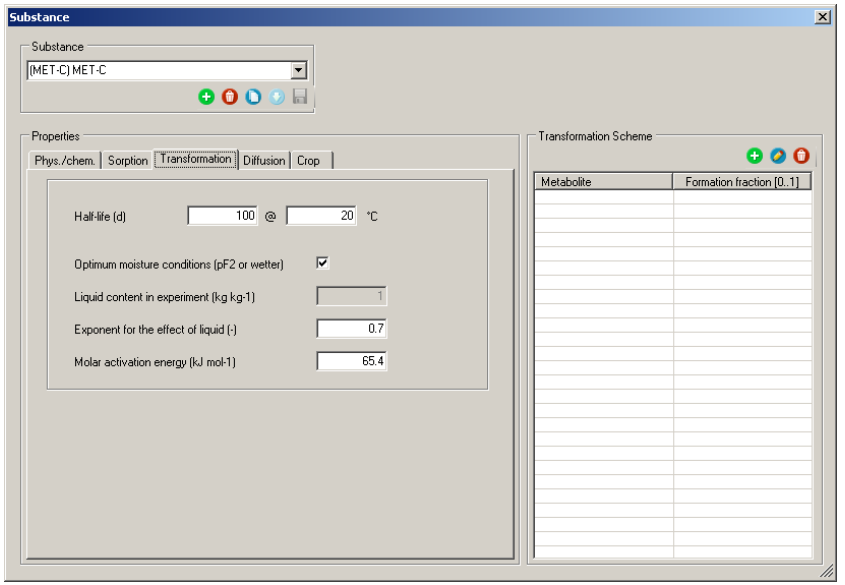
Application timing based on BBCH growth stages utilising a phenolgical model

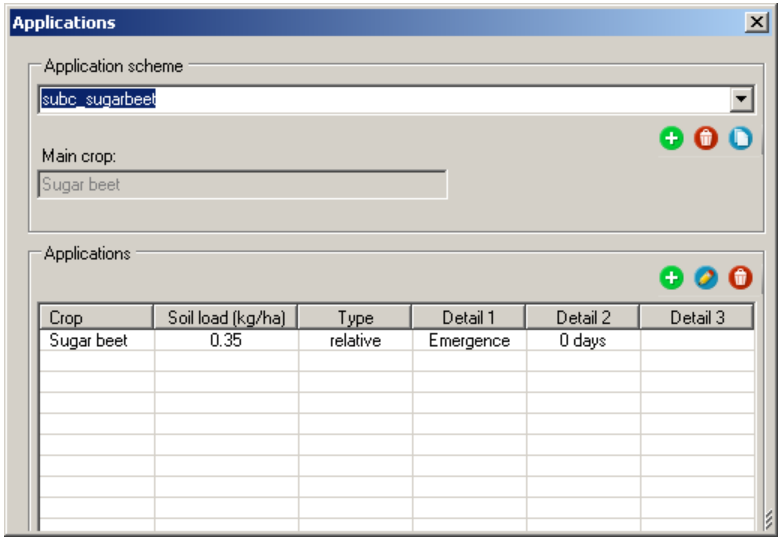
- **equivalent to crop sub-model (SWAP) of FOCUS Pearl 3.3.3 and WOFOST**
- **validation demonstrated formidable performance**
- **reducing ambiguity**
- **user-friendly**



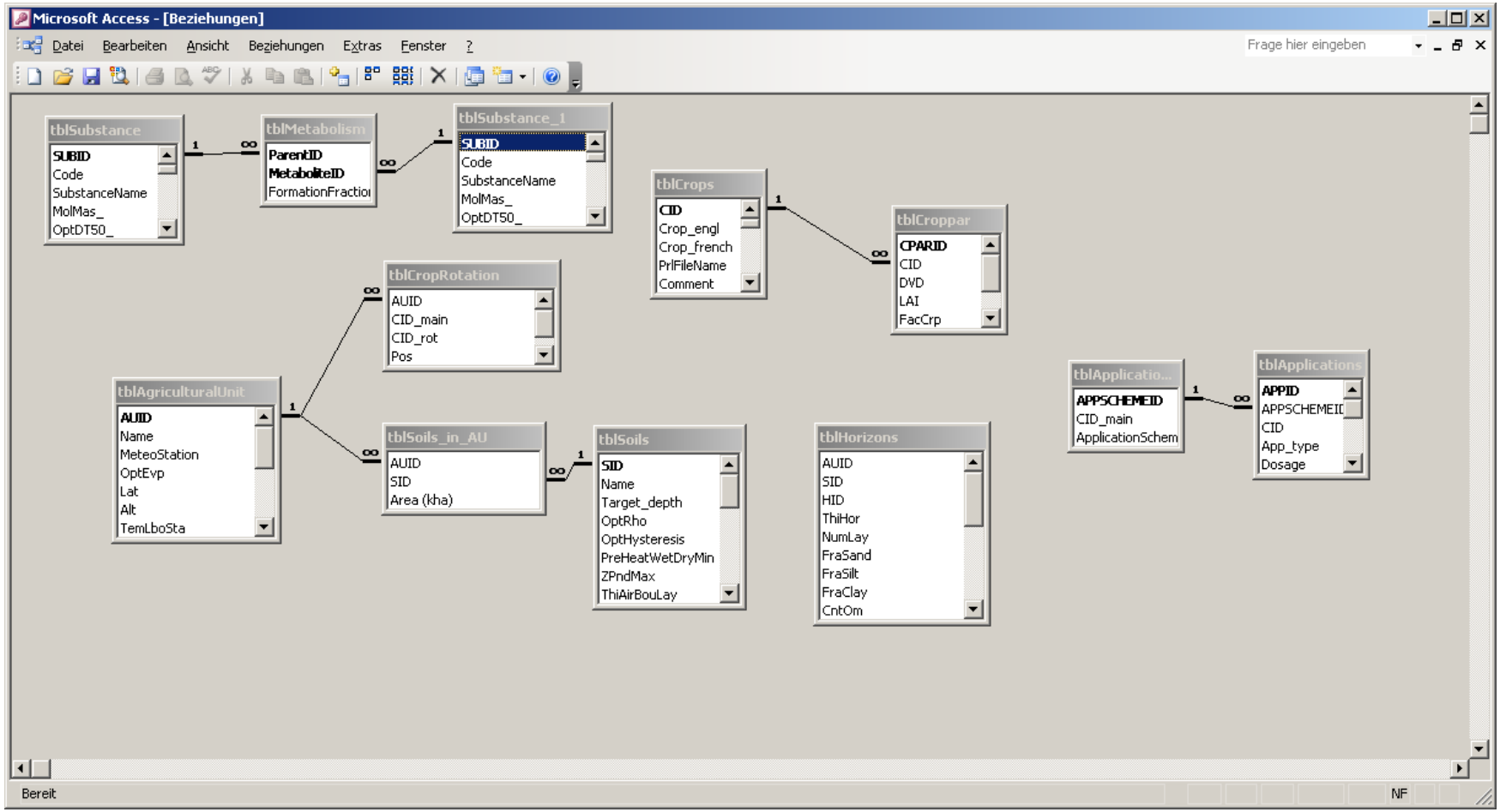
French Refinement Of Groundwater Scenarios
The Shell







French Refinement Of Groundwater Scenarios
The Database



Output summary (*.txt)

**** Main crop
Winter Wheat (WWHEAT)

**** Compounds

	XYZ	XYZ-I	XYZ-A	XYZ-D	XYZ-C	XYZ-G	XYZ-B		
MolMas_*	369.4	355	155.2	355.4	389.8	273.3	274.3	(g.mol-1)	Molar mass [10|10000]
OptDT50_*	Input	Input	Input	Input	Input	Input	Input		Option for DT50: Input or Calculate
DT50Ref_*	17.2	4.4	19	11	42	1000	25.5	(d)	Half-life time [1|1e6]
TemRefTra_*	20	20	20	20	20	20	20	(C)	Temperature at which DT50 is measured [5|30]
ExpLiqTra_*	0.7	0.7	0.7	0.7	0.7	0.7	0.7	(-)	Exponent for the effect of liquid [0|5]
OptCntLiqTraRef_*	non-opt	non-opt	non-opt	non-opt	non-opt	non-opt	non-opt	non-opt	OptimumConditions (opt.) or NonOptimumConditions (non-opt.)
CntLiqTraRef_*	1	1	1	1	1	1	1	(kg.kg-1)	Liq. content at which DT50 is measured [0|1]
MolEntTra_*	65.4	65.4	65.4	65.4	65.4	65.4	65.4	(kJ.mol-1)	Molar activation energy [0|200]
OptCofFre_*	pH-independent	pH-independent	pH-independent	pH-independent	pH-independent	pH-independent	pH-independent		pH-dependent, pH-independent, CofFre
ConLiqRef_*	1	1	1	1	1	1	1	(mg.L-1)	Reference conc. in liquid phase [0.1]-]
ExpFre_*	0.98	1	0.89	0.93	0.914	0.905	1	(-)	Freundlich sorption exponent [0.1|1.3]
KomEql_*	11.4	0	229	11.3	15.7	7.54	0	(L.kg-1)	Coef. eql. sorption on org. matter [0|1e9]
KomEqlAcid_*	375	375	375	375	375	375	375	(L.kg-1)	Coef. for eql. sorption on om - acid [0|1e9]
KomEqlBase_*	8	8	8	8	8	8	8	(L.kg-1)	Coef. for eql. sorption on om - base [0|1e9]
pKa_*	4.6	4.6	4.6	4.6	4.6	4.6	4.6	(-)	Coef. for influence of pH on sorption [0|14]
pHCorrection	0	0	0	0	0	0	0	(-)	pH correction [-2|1]
KSorEql_*	1	1	1	1	1	1	1	(L.kg-1)	Coef. for equilibrium sorption [0|1e9]
MolEntSor_*	0	0	0	0	0	0	0	(kJ.mol-1)	
TemRefSor_*	20	20	20	20	20	20	20	(C)	
PreVapRef_*	1.3E-05	5.6E-08	0.0372	5.6E-08	1.9E-08	5.2E-08	8.6E-09	(Pa)	Saturated vapour pressure [0|2e5]
TemRefVap_*	20	20	20	20	20	20	25	(C)	measured at [0|40]
MolEntVap_*	95	95	95	95	95	95	95	(kJ.mol-1)	Molar enthalpy of vaporisation [-200|200]
SlbWatRef_*	3070	30200	5484	30200	15700	2100	13882	(mg.L-1)	Solubility in water [1e-9|1e6]
TemRefSlb_*	20	20	20	20	20	20	20	(C)	measured at [0|40]
MolEntSlb_*	27	27	27	27	27	27	27	(kJ.mol-1)	Molar enthalpy of dissolution [-200|200]
CofDesRat_*	0	0	0	0	0	0	0	(d-1)	Desorption rate coefficient [0|0.5]
FacSorNeqEql_*	0	0	0	0	0	0	0	(-)	CofFreNeq/CofFreEql [0|-]
FacUpt_*	0.5	0.5	0.5	0.5	0.5	0.5	0.5	(-)	Coefficient for uptake by plant [0|10]
OptDspCrp_*	Lumped	Lumped	Lumped	Lumped	Lumped	Lumped	Lumped		Lumped or Specified
DT50DspCrp_*	1000000	1000000	1000000	1000000	1000000	1000000	1000000	(d)	Half-life at crop surface [1|1e6]
DT50PenCrp_*	-	-	-	-	-	-	-	(d)	Half-life due to penetration [1|1e6]
DT50VolCrp_*	-	-	-	-	-	-	-	(d)	Half-life due to volatilization [1|1e6]
DT50TraCrp_*	-	-	-	-	-	-	-	(d)	Half-life due to transformation [1|1e6]
FacWasCrp_*	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	(m-1)	Wash-off factor [1e-6|0.1]
CofDiffWatRef_*	4.3E-05	4.3E-05	4.3E-05	4.3E-05	4.3E-05	4.3E-05	4.3E-05	(m2.d-1)	Reference diff. coeff. in water [10e-5|3e-4]
CofDiffAirRef_*	0.43	0.43	0.43	0.43	0.43	0.43	0.43	(m2.d-1)	Reference diff. coeff. in air [0.1|3]
TemRefDif_*	20	20	20	20	20	20	20	(C)	Diff. coeff measured at temperature [10|30]

**** Transformation scheme
0.37 XYZ -> XYZ-I
0.161 XYZ -> XYZ-A
0.469 XYZ -> XYZ-D
0.842 XYZ-D -> XYZ-C
0.527 XYZ-I -> XYZ-G
0.195 XYZ-I -> XYZ-B

**** Application scheme "wwheat autumn Em+7"

Crop	Soil load (kg/ha)	Type		
WWHEAT	0.0225	relative	Emergence	7 days
BARLEY	0.0225	relative	Emergence	7 days

**** Results

RUNID	AUID	AU	SID	Soil	Area (kha)	Rotation	SUBID	Substance	80th percentile	Year
1	1	1 Collines molassiques - Lauragais	1	Luvisol 3 >80	7	WWHEAT-SUNFL	4	XYZ	0.03091924	1987
1	1	1 Collines molassiques - Lauragais	1	Luvisol 3 >80	7	WWHEAT-SUNFL	5	XYZ-I	0.00561966	1997
1	1	1 Collines molassiques - Lauragais	1	Luvisol 3 >80	7	WWHEAT-SUNFL	8	XYZ-A	2.90E-07	1987
1	1	1 Collines molassiques - Lauragais	1	Luvisol 3 >80	7	WWHEAT-SUNFL	9	XYZ-D	0.00957335	1987
1	1	1 Collines molassiques - Lauragais	1	Luvisol 3 >80	7	WWHEAT-SUNFL	10	XYZ-C	0.09410543	2013
1	1	1 Collines molassiques - Lauragais	1	Luvisol 3 >80	7	WWHEAT-SUNFL	6	XYZ-G	0.5596222	2003
1	1	1 Collines molassiques - Lauragais	1	Luvisol 3 >80	7	WWHEAT-SUNFL	7	XYZ-B	0.02430365	1997
2	2	2 Bretagne sud	1	Luvisol 3 >80	35	WWHEAT-MAIZEF-BARLEY	4	XYZ	0.01329599	2041
2	2	2 Bretagne sud	1	Luvisol 3 >80	35	WWHEAT-MAIZEF-BARLEY	5	XYZ-I	0.00625767	1990
2	2	2 Bretagne sud	1	Luvisol 3 >80	35	WWHEAT-MAIZEF-BARLEY	8	XYZ-A	4.61E-07	2023
2	2	2 Bretagne sud	1	Luvisol 3 >80	35	WWHEAT-MAIZEF-BARLEY	9	XYZ-D	0.00807448	2041
2	2	2 Bretagne sud	1	Luvisol 3 >80	35	WWHEAT-MAIZEF-BARLEY	10	XYZ-C	0.08601183	1999
2	2	2 Bretagne sud	1	Luvisol 3 >80	35	WWHEAT-MAIZEF-BARLEY	6	XYZ-G	0.82261387	2044
2	2	2 Bretagne sud	1	Luvisol 3 >80	35	WWHEAT-MAIZEF-BARLEY	7	XYZ-B	0.02324532	2032
3	4	4 Bordure Nord - Picardie - Normandie	1	Luvisol 3 >80	571	WWHEAT-BARLEY-MAIZEF	4	XYZ	0.10917288	2017
3	4	4 Bordure Nord - Picardie - Normandie	1	Luvisol 3 >80	571	WWHEAT-BARLEY-MAIZEF	5	XYZ-I	0.0341327	2038
3	4	4 Bordure Nord - Picardie - Normandie	1	Luvisol 3 >80	571	WWHEAT-BARLEY-MAIZEF	8	XYZ-A	7.84E-06	1996

Areal PECgw distribution (*.txt)

RUNID	80th percentil	Cumulative A	Cumulative A
3	3.11E-05	61	0.00886113
8	0.0001223	403	0.05854154
15	0.0001358	441	0.06406159
64	0.0001855	444	0.06449739
25	0.0004108	912	0.1324811
11	0.0004226	1243	0.1805636
6	0.0004325	1275	0.1852121
18	0.0004552	1321	0.1918942
69	0.0004634	1325	0.1924753
20	0.0004769	1538	0.2234166
26	0.0005865	1549	0.2250145
41	0.0005894	1552	0.2254503
9	0.0006528	1649	0.239541
7	0.000674	2060	0.2992446
12	0.0006935	2149	0.3121732
2	0.000708	2155	0.3130447
21	0.0007099	2225	0.3232132
5	0.0007505	2231	0.3240848
10	0.0008966	2272	0.3300407
67	0.0008982	2301	0.3342533
72	0.0009347	2317	0.3365776
23	0.001039	2499	0.3630157
4	0.001078	3069	0.4458164
44	0.001132	3099	0.4501743
22	0.001363	3172	0.4607786
66	0.001407	3179	0.4617955
71	0.001414	3184	0.4625218
27	0.00142	3202	0.4651366
17	0.001455	3528	0.5124927
70	0.001473	3536	0.5136548
38	0.001597	3607	0.5239686
63	0.001619	3610	0.5244044
14	0.001629	3797	0.5515689
46	0.001672	3826	0.5557815
68	0.001825	3843	0.558251
1	0.001868	4414	0.641197
65	0.001911	4519	0.6564497
19	0.001922	4638	0.6737362
47	0.001954	4648	0.6751888
49	0.002119	4743	0.688989
16	0.002352	4756	0.6908774
13	0.002654	4859	0.7058396
40	0.003375	4946	0.7184776
43	0.003732	5001	0.7264672
48	0.004209	5051	0.7337304
56	0.004242	5123	0.7441894
53	0.005249	5127	0.7447705
45	0.005674	5174	0.7515979
42	0.005838	5234	0.7603137
61	0.005914	5242	0.7614759
62	0.006353	5360	0.7786171
24	0.006812	5378	0.7812318
58	0.007463	5390	0.782975
39	0.008198	5540	0.8047647
57	0.0115	5545	0.805491
59	0.01156	5605	0.8142068
30	0.01516	5607	0.8144974
55	0.01644	5669	0.8235038
60	0.01893	5675	0.8243754
54	0.01988	5707	0.8290238
52	0.01993	5721	0.8310575
50	0.02274	5746	0.8346891
33	0.02872	5869	0.8525566
75	0.03205	5871	0.8528472
35	0.03232	5910	0.8585125
36	0.03732	5944	0.8634515

Output

80th temporal percentile PECgw at bottom of profile (Scenario: AU x Soil(Crop), FOCUS Pearl 3.3.3)

- **PECgw = $\Sigma^{\text{over rotation}}$ mass leached / $\Sigma^{\text{over rotation}}$ water percolation**

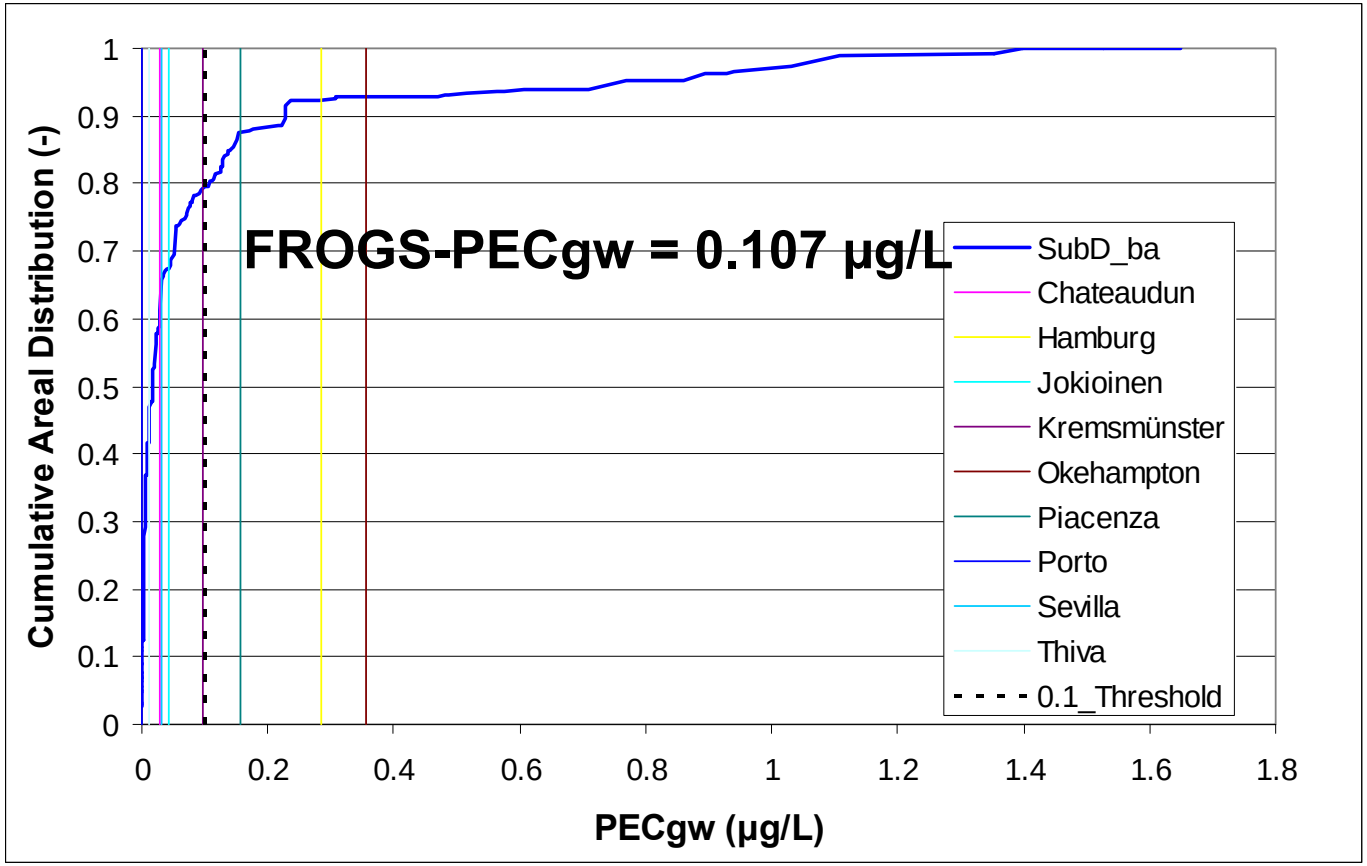
Order scenarios by PECgw (ascending)
Calculate areal probabilty (cumulative area / total area)
Select 80th areal percentile PECgw

Represents overall 90th percentile PECgw
In analogy to FOCUS GW

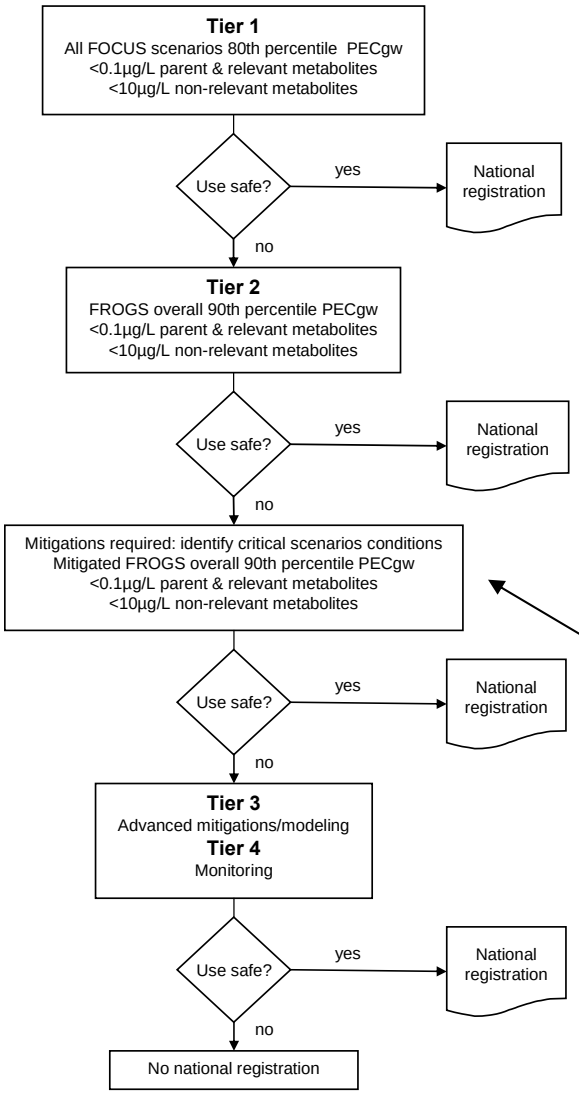
Area (Scenario)

Exemplary Results - FOCUS Dummy D in Barley

Cumulative aerial distribution of FROGS-PECgw for Substance D following application to winter cereals (barley and wheat)



French Refinement Of Groundwater Scenarios
Groundwater Assessment Scheme



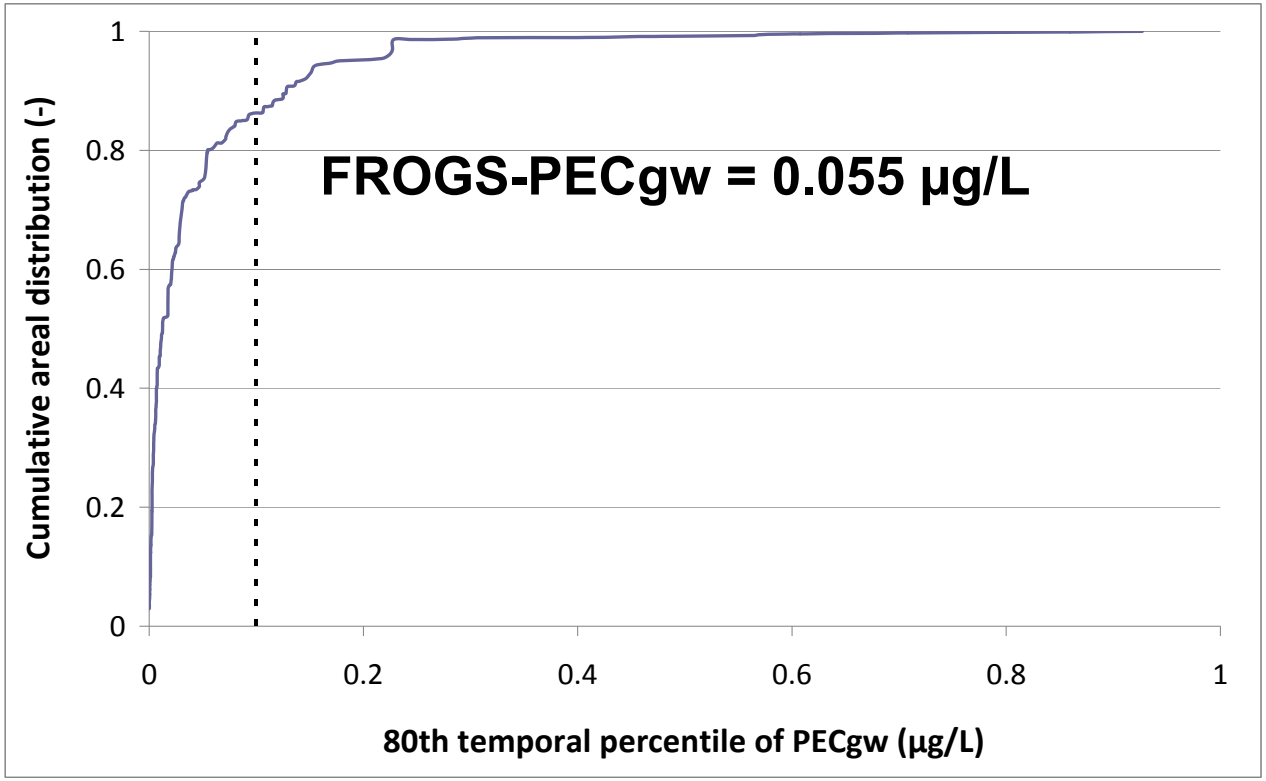
FROGS allows analysis of PECgw exceedances (Weather, soil, ...)

Mitigation options

Exemplary Results - Mitigation

Cumulative aerial distribution of FROGS-PECgw for Substance D following application to winter cereals (barley and wheat) with mitigation: AWC (available water capacity) < 100 mm

→ eliminates sandy/shallow profiles)



Conclusions

Realistic environmental conditions in terms of climate, soils and management derived from readily available data

Compliant with FOCUS principles (FOCUS-Pearl, 90th percentile threshold)

Straightforward and easy-to-use program shell

Flexible (scenarios can be added if needed) and transparent (all input parameters can be accessed via database)

Causal analysis of PECgw exceedances enables implementation of mitigation options

Main limitations are due to limited availability of environmental data at sufficient spatial resolution. Most severe is high aggregation of soil data.

Thank you very much for your kind attention.