

Use of Free Open Source Spatial Analysis tools II: Pesticide modelling

Mira Kattwinkel, Andreas Scharmüller, Jörg Rapp

RALF B. SCHÄFER
SUMMER ACADEMY SPATIAL ECOTOXICOLOGY 2017

Short introduction (Ralf Schäfer)

- Professor for Quantitative Landscape Ecology
- Current teaching: Statistics (M.Sc.); GIS (B.Sc./M.Sc.);
 Environmental Modelling (B.Sc./M.Sc.); Aquatic
 Ecotoxicology (M.Sc.); Environmental Philosophy (B.Sc.)
- Current research projects:
 - Effects of toxicants in freshwater ecosystems
 - Trait-based aquatic ecology (focused on anthropogenic stressors and climate change)
 - Trophic linkages between aquatic & terrestrial systems
- Primarily field studies/experiments and data analyses/ modelling

Short introduction Mira Kattwinkel

- Scientist in Quantitative Landscape Ecology group
- Current teaching: Environmental Modelling (B.Sc./M.Sc.);
 Human-Environment Interactions (M.Sc.), Introduction to R (PhD students)
- Current research projects and methods:
 - Effects of toxicants and other anthropogenic stressors on freshwater ecosystems
 - Population modelling and Bayesian parameter inference
 - Spatial statistics on river networks, GIS
- Primarily data analyses / modelling

Short introduction Andreas Scharmüller

- PhD student in Quantitative Landscape Ecology group
- Current teaching: tutor statistic courses
- Current research projects and methods:
 - Effects of pesticides on freshwater ecosystems
 - Spatial statistics on river networks, GIS
- Primarily data analyses / modelling

Course organisation

- Course material under https://github.com/andreasLD/Sum_acad_spatmod/tree/changes_andreas
- Password for literature: "landau"
- Simplified runoff modelling (in R)

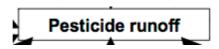
Learning targets

- Understand the basics of pesticide modelling
- How to model chemical exposure under data scarcity (Theory and Practice)
- Overview on global GIS data
- Practical training in GIS functions in R

Pesticide surface runoff modelling: Relevant processes

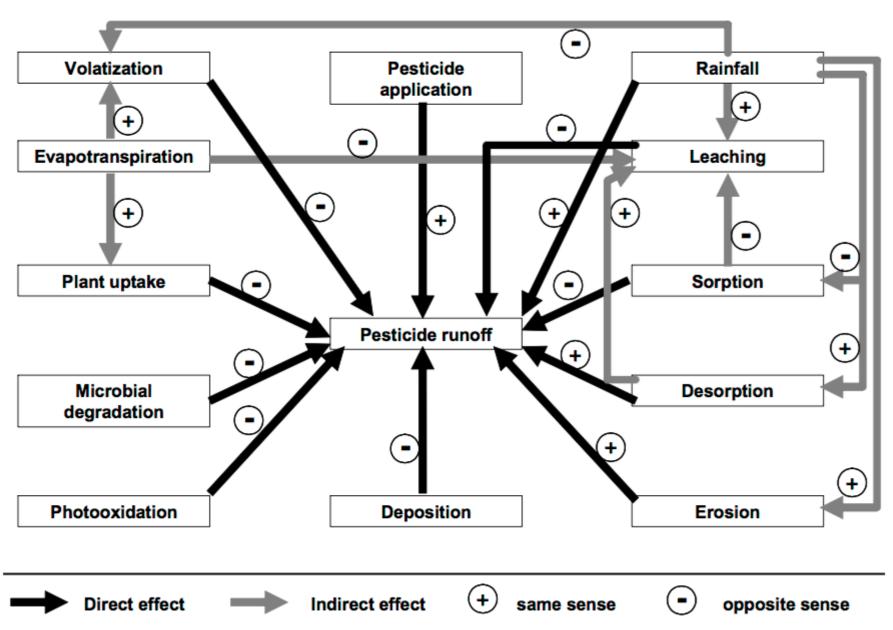
Plot and reach scale





Pesticide surface runoff modelling: Relevant processes

Plot and reach scale



Pesticide modelling: Relevant processes

Plot, reach and (sub)catchment scale

Processes	MIKE SHE ADM	LEACHM- runoff	GR5- pesticides	SACADEAU	SWAT	STREAM- pesticide	FLOWT	VESPP	I-Phy- BVci	PHYLOU
Air										
Drift	_	_	_	_	_	_	_	_	x	_
Deposition	_	_	_	_	_	_	_	_	X	_
Plant										
Plant growth	X	X	_	X	X	X	X	_	X	_
Water cycle										
Interception	X	_	_	_	X	_	X	x	_	_
Foliar evaporation	X	X	_	_	X	_	_	_	_	_
Roots uptakes	X	X	_	_	X	_	_	_	_	_
Pesticide fate										
Volatilisation	_	_	_	_	x	x	_	_	_	_
Washoff	_	_	_	_	x	_	_	_	_	_
Degradation	_	_	_	_	x	x	_	_	X	X
Soil (unsaturated zone)										
Water cycle										
Horton runoff	X	X	x	x	x	x	x	x	X	X
Saturation excess runoff	X	_	_	x	_	_	_	_	_	_
Infiltration	X	X	X	X	X	X	x	_	X	X
Evaporation	X	X	X	X	X	_	X	_	_	_
Percolation	X	X	X	X	X	_	X	_	_	_
Lateral sub-surface flow	_	_	_	X	X	_	X	_	_	_
Capillary fringe	X	_	_	_	X	_	_	_	_	_
Fate of dissolved pesticides										
Soil/water exchanges	x	x	x	x	x		x	х		x
Advection/dispersion	X	X	X	_	_	_	_	_	_	_
Degradation	X	X	_	x	x	_	_	X	_	X
Volatilisation	_	_	_	_	X	_	_	_	x	_
Fate of particular pesticides	_	_	_	_	Α.	_	_	_	Λ.	_
Erosion					x	x				
	_	_	_	_	X	X	_	_	_	_
Deposition on vegetated strips	-	_	_	_	Λ.	Λ.	_	_	_	-
Aquifer										
Water cycle	v	v	v	v					v	
Flows	X X	X	X X	X X	X	_	_	-	X	-
River/aquifer exchanges	Х	-	Х	х	X	-	_	_	_	-
Pesticide fate										
Volatilisation	-	-	-	_	_	-	-	-	_	-
Advection/dispersion	X	-	-	_	_	-	-	-	_	-
Adsorption	X	-	-		-	-	-	-	_	-
Degradation	X	-	-	X	_	-	-	-	-	-
River										
Water cycle										
Flows	X	-	X	-	X	-	-	-	-	X
Pesticide fate										
Deposition	-	-	-	-	X	-	-	-	-	-
Resuspension	-	-	-	-	X	-	-	-	-	-
Volatilisation	-	-	-	-	X	-	-	-	-	-
Advection/dispersion	X	-	-	-	X	-	-	-	-	-
Degradation	X	-	-	-	X	-	-	-	X	X
Landscape mitigation objects										

Payraudeau & Gregoire 2012 Agron. Sustain. Dev. 32: 479–500

Pesticide modelling: Relevant processes

Plot, reach and (sub)catchment scale

iot, reach a	and (3	abju	aton	IIICIII	Proc	esses	MIKE ADM	SHE LEACH runoff	IM- GR5- pesticio	SACADEAU	SWAT	STREAM- pesticide	FLOWT	VESPP	I-Phy- BVci	PHYLO
					Air	2 :0									1/	
						Orift Deposition	_	_	_	_	_	_	_	_	X X	_
					Plant											
						Plant growth ter cycle	х	х	-	Х	Х	Х	Х	-	Х	-
						interception	x	-	-	-	X	-	X	X	-	-
					I	Foliar evaporation	X X	X X		_	X	-	_	_	_	-
Processes	MIKE SHE	LEACHM-	GR5-	SACADEAU	SWAT	STREAM-	FLOWT	VESPP	I-Phy-	PHYLOU		x	_	_	_	-
	ADM	runoff	pesticides			pesticide			BVci			x	_	_	x	x
vegetated diten											4					
Degradation	_	_	_	_	_	_	_	X	_	_		X -	X -	X -	X -	X -
Grass strips												X	X	-	X	X
Infiltration	_	_	_	X	_	X	X	X				_	X X	_	_	_
Degradation	_	_	_	_	X	_	_	X	X	X		-	X	-	-	-
Wetlands												-	-	-	-	_
Degradation	_	_	_	_	_	_	_	_	X	_		-	X	X	-	X
Ponds, lakes	_	_	_	_								_	_	X	_	X
Deposition	_	_	_	_	X	_	_	_	_	_		-	-	-	Х	-
Resuspension	_	_	_	_	X	_	_	_	_	_		x	-	_	-	_
Volatilisation	_	_	_	_	X	_	_	_	_	_		X	-	-	-	-
Advection/dispersion	_	_	_	_	X	_	_	_	_	_						
Degradation	_	_	_	_	X	_	_	_	_	_		_	_	_	X	_
Number of processes	21	11	9	13	32	8	8	7	12	8	1	_	_	_	_	_
												-	-	-	-	-
						Degradation	x	_	_	x	_	_	_	_	_	_
\\/ida	Voriot	v of r		rad	Rive											
vvide	variety	y Oi f	equi	rea		ter cycle Flows	x	_	x	_	x	-	-	-	_	X
input parameters						sticide fate										
						Deposition Resuspension	_	_	_	_	X	_	_	_	_	_
						Volatilisation	_	-	_	-	X	_	-	-	_	-
					A	Advection/dispersion	X	_	_	_	X	_	_	_	_	_

Payraudeau & Gregoire 2012 Agron. Sustain. Dev. 32: 479–500

Classification: Pesticide model type

Model type	Model name	Case studies references	Objectives and scope
Type 1: physically based model	MIKE SHE ADM	De Bruyn 2004; De Bruyn et al. 2006	Hydrological modelling in order to mechanistically represent the karstic aquifers and the fate of point and non-point source pollution
	LEACHM-runoff	Maison 2000	Hydrological modelling in order to mechanistically represent the quantitative and qualitative regime of the catchment
	GR5-pesticides	Madier 2007	Using a pesticide fate model to define robust sampling strategies with reduced cost, i.e. with a minimum of analyses
	SACADEAU	Tortrat 2005; Gascuel- Odoux et al. 2009	Building a decision-aid tool to help specialists in charge of the catchment's management to preserve the stream water quality
Type 2: conceptual model	SWAT	Holvoet et al. 2005; 2008	Modelling the impact of land management practices on water and pesticide loads in large catchments with varying soils, land uses and management conditions over long time periods
	STREAM- pesticides	Lecomte 1999	Modelling the behaviour of pesticides driven by runoff and erosion from the cultivated plots to the catchment area
	FLOWT	Gregoire 2006; Madier 2007	Modelling the impact of land management practices on water and pesticide loads in small catchments with varying soils, land uses and management conditions over long time periods
Type 3: environmental indicator	VESPP	De Bruyn 2004; 2006	Evaluating the vulnerability of surface water to pesticides
	I-Phy-BVci	Thiollet-Scholtus 2004	Evaluating the vulnerability of surface water to pesticides
Type 4: multi-agent system	PHYLOU	Barreteau and Cernesson 2003	Facilitate communication between stakeholders by using an agent-based model of pesticide transfer in order to preserve the stream water quality

Classification: Scales

Catchment models	Field-scale pesticide models	Field-scale crop models			
annAGNPS	CREAMS	EPIC			
geoPEARL	PEARL	WOFOST			
HSPF	Included/PRZM	Generic			
I-phyBV	I-pest	None			
MHYDAS	Included	None			
MIKE SHE	MIKE SHE AD/ MACRO/DAISY	Included/MACRO/ DAISY			
SoilFug	Included	Simple			
SWAT	GLEAMS	EPIC			

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Choose model depending on

- question to be answered / problem to be solved!
- resources

Example model in this course: Runoff potential

- Field-scale pesticide model
- Indicator



Available online at www.sciencedirect.com



CHEMOSPHERE

Chemosphere 68 (2007) 2161-2171

www.elsevier.com/locate/chemosphere

Estimating pesticide runoff in small streams

Carola A. Schriever a,*, Peter C. von der Ohe b, Matthias Liess a

^a Department of System Ecotoxicology, UFZ – Helmholtz Centre for Environmental Research, Permoserstrasse 15, 04318 Leipzig, Germany ^b Department of Effect Directed Analysis, UFZ – Helmholtz Centre for Environmental Research, Permoserstrasse 15, 04318 Leipzig, Germany

Example model in this course: Runoff potential

- Field-scale pesticide model
- Indicator



- Runoff potential (RP)
- Generic organic substance
- Considers rainfall pattern instead of single event
- Basic formula:

$$RP = \log_{10} \left(\max_{h} \left(\sum_{i} \sum_{j} A_{i,j} D_{j} \left(1 - \frac{I_{j,h}}{100} \right) \frac{1}{1 + \frac{K_{OC} OC_{i}}{100}} f(s_{i}) \frac{f(P_{h}, T_{i})}{P_{h}} \right) \right)$$

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precipitation

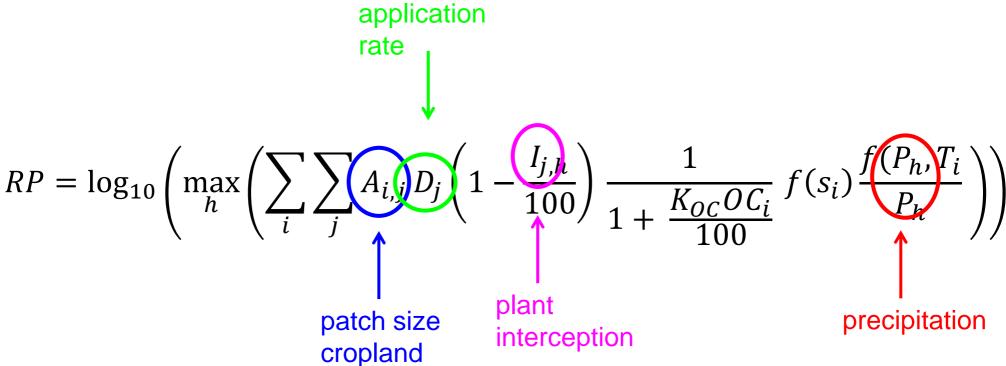
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patch size
cropland

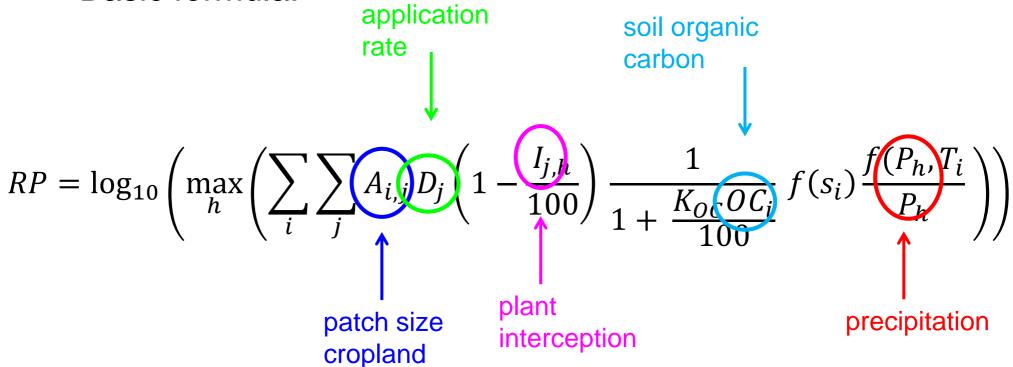
- Runoff potential (RP)
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- Considers rainfall pattern instead of single event
- Basic formula:

application rate
$$RP = \log_{10} \left(\max_{h} \left(\sum_{i} \sum_{j} A_{i,j} D_{j} \left(1 - \frac{I_{j,h}}{100} \right) \frac{1}{1 + \frac{K_{OC}OC_{i}}{100}} f(s_{i}) \frac{f(P_{h}, T_{i})}{P_{h}} \right) \right)$$
patch size cropland

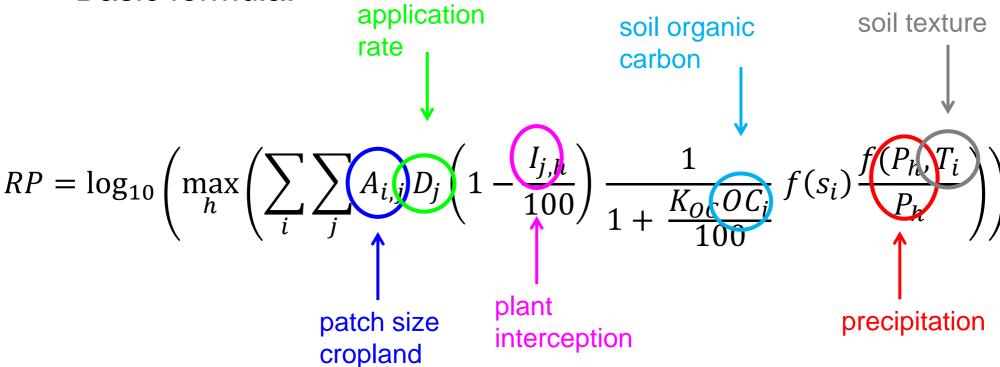
- Runoff potential (RP)
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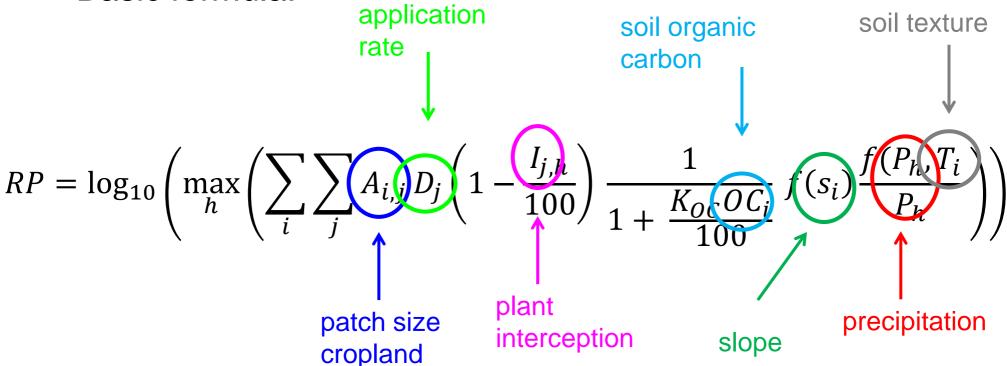
- Runoff potential (RP)
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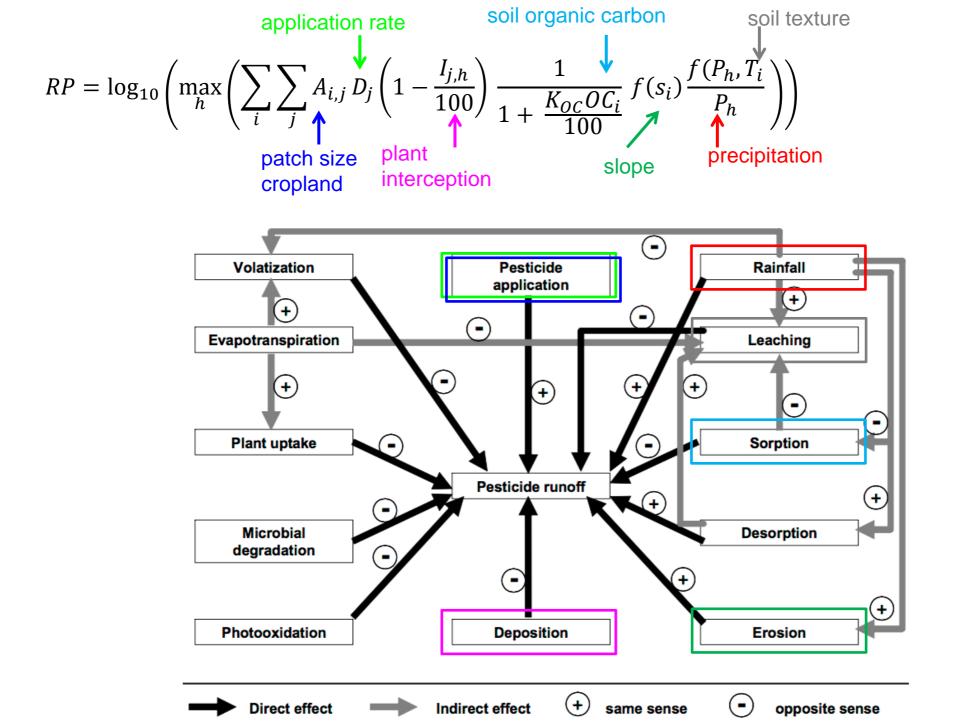


- Runoff potential (RP)
- Generic organic substance
- Considers rainfall pattern instead of single event
- Basic formula:



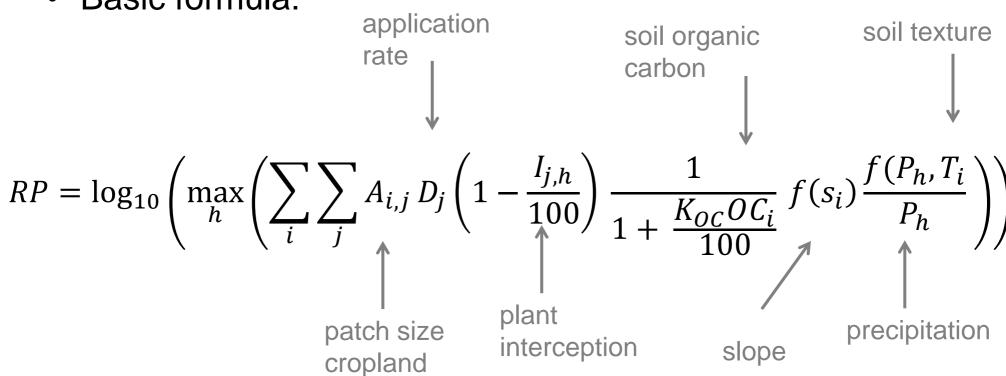
- Runoff potential (RP)
- Generic organic substance
- Considers rainfall pattern instead of single event
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Schulz & Matthies 2007 Living Reviews in Landscape Research 1

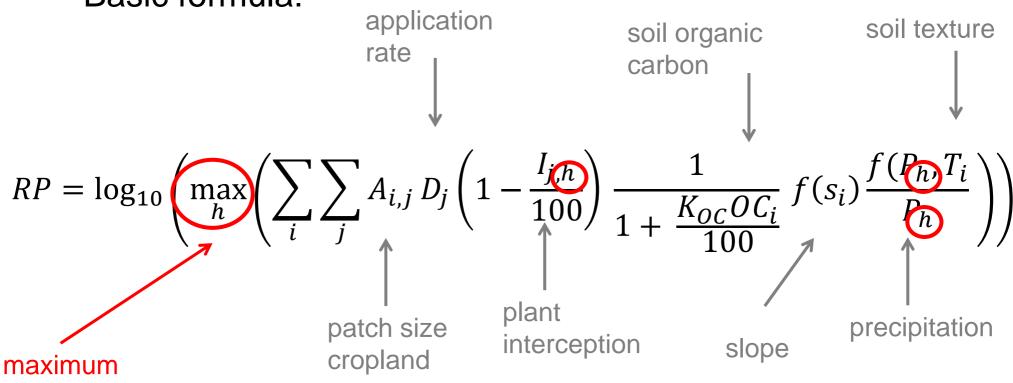
- Runoff potential (RP)
- Generic organic substance
- Considers rainfall pattern instead of single event
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- Runoff potential (RP)
- Generic organic substance
- Considers rainfall pattern instead of single event
- Basic formula:

precipitation

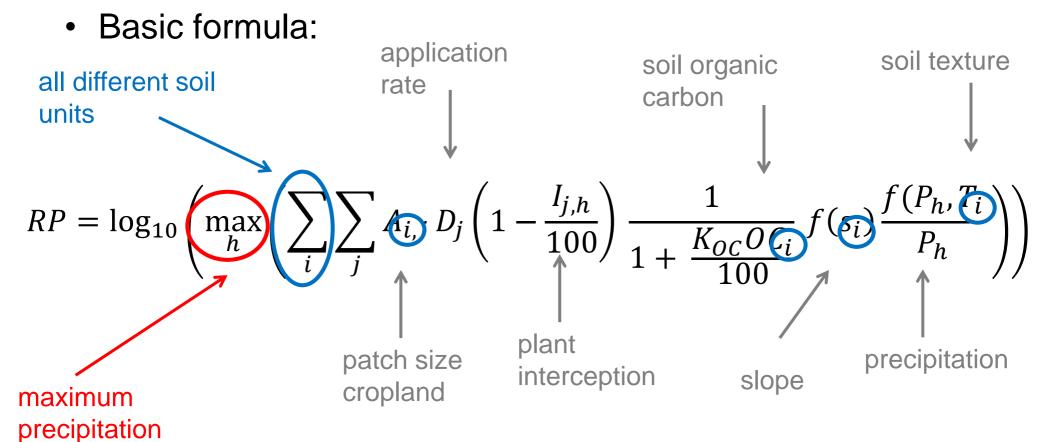
event



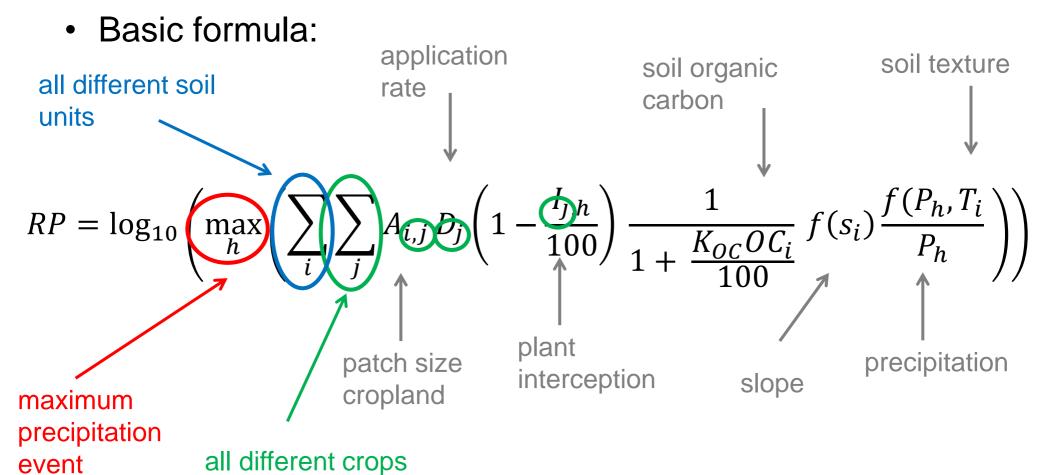
Runoff potential (RP)

event

- Generic organic substance
- Considers rainfall pattern instead of single event



- Runoff potential (RP)
- Generic organic substance
- Considers rainfall pattern instead of single event



- We need spatially resolved:
 - Precipitation data
 - Crop production area
 - Pesticide application rate (and K_{oc})
 - Plant interception
 - Soil Organic Carbon content
 - Soil Texture
 - Slope
 - Hydrological network

application rate soil organic carbon soil texture
$$RP = \log_{10} \left(\max_{h} \left(\sum_{i} \sum_{j} A_{i,j} D_{j} \left(1 - \frac{I_{j,h}}{100} \right) \frac{1}{1 + \frac{K_{OC} OC_{i}}{100}} f(s_{i}) \frac{f(P_{h}, T_{i})}{P_{h}} \right) \right)$$
patch size plant interception slope

Where do we get all these data from?

→ Case study Malawi



- We need spatially resolved:
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Precipitation data

ftp://ftp.cpc.ncep.noaa.gov/fews/fewsdata/africa/arc2

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JOURNAL OF APPLIED METEOROLOGY AND CLIMATOLOGY

VOLUME 52

African Rainfall Climatology Version 2 for Famine Early Warning Systems

NICHOLAS S. NOVELLA

NOAA/National Centers for Environmental Prediction/Climate Prediction Center, Camp Springs, Maryland, and Wyle Information Systems, McLean, Virginia

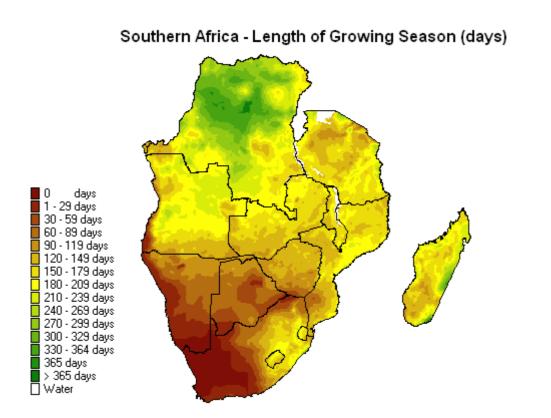
WASSILA M. THIAW

NOAA/National Centers for Environmental Prediction/Climate Prediction Center, Camp Springs, Maryland

(Manuscript received 22 November 2011, in final form 8 August 2012)

Precipitation data

- Download data for pesticide application period.
- → How to determine the latter:
 - Review country information and/or contact authorities
 - Information on length of growing season in Africa http://www.fao.org/nr/climpag/cropfor/lgp_en.asp

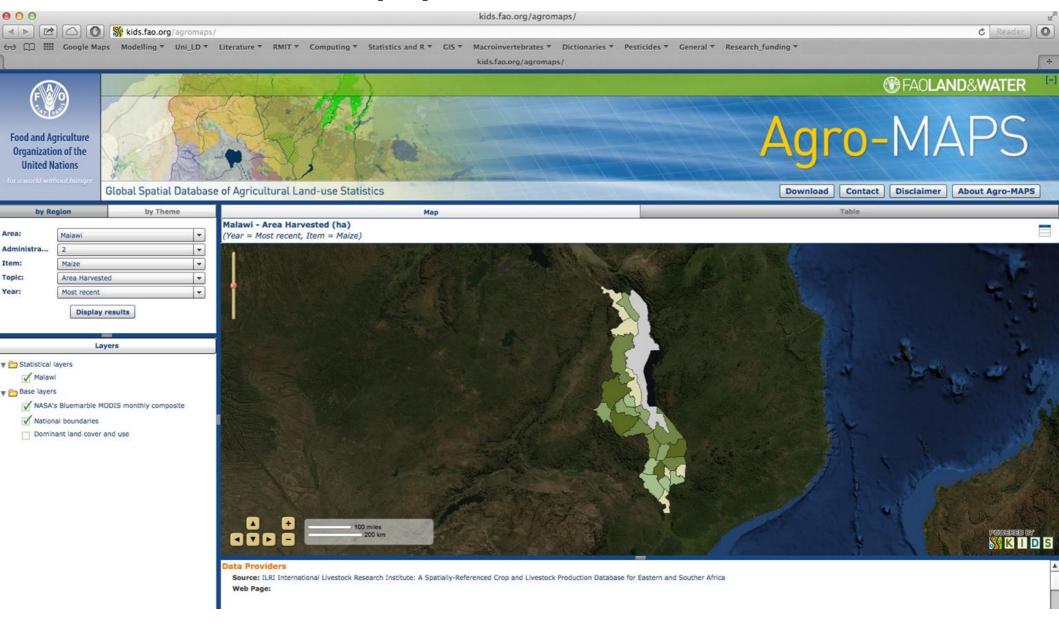


Precipitation data

- Download data
 - → provided with course materials
- 2. Processing in R
 - → load rasters, clip, identify maximum

- We need spatially resolved:
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Crop production area



Could be used for detailed crop information

Crop production area

- For sake of simplicity, we consider only the aggregated crop production area
- Land cover data for many countries provided by: FAO GeoNetwork

Exercise

 Search and download the global land cover (Globcover regional) data for Malawi

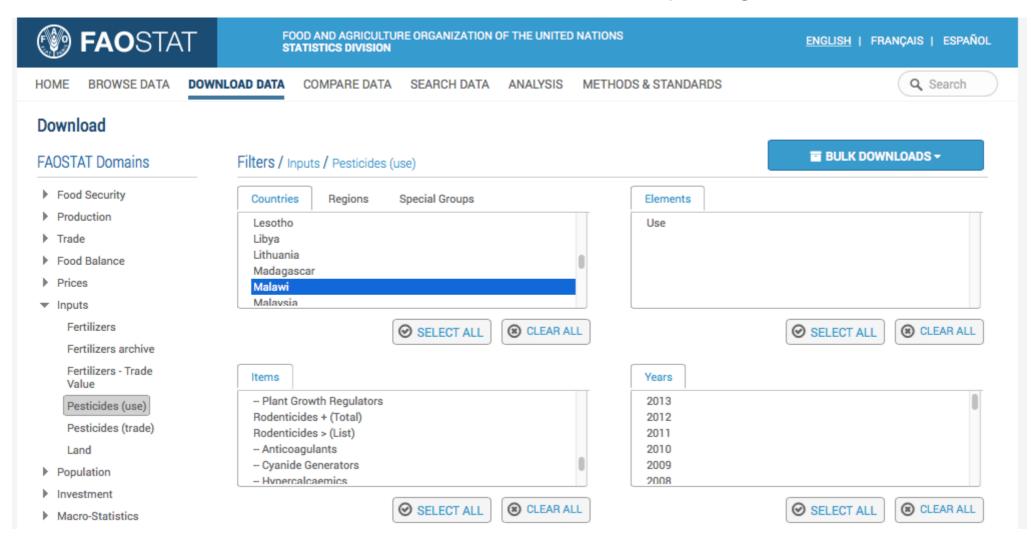
Demonstration in R

- Aggregation of all crop land into one land cover class and dissolving polygon boundaries
- Projection into an appropriate UTM and saving file

- We need spatially resolved:
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Pesticide application rate: Insecticides

- FAO provides pesticide use information http://www.fao.org/faostat/en/#data/RP
- More sophisticated method presented by Jörg Rapp



Pesticide application rate: Insecticides

Result

Domain	Country	Element	Item	Year	Unit	Value	Flag	Flag Description
Pesticides (use)	Malawi	Use	Insecticides	1997	tonnes of active ingredients	263.00	Q	Official data reported on FAO Questionnaires from countries
Pesticides (use)	Malawi	Use	Insecticides	1998	tonnes of active ingredients	221.00	Q	Official data reported on FAO Questionnaires from countries
Pesticides (use)	Malawi	Use	Insecticides	1999	tonnes of active ingredients	202.00	Q	Official data reported on FAO Questionnaires from countries
Pesticides (use)	Malawi	Use	Insecticides	2000	tonnes of active ingredients	257.00	Q	Official data reported on FAO Questionnaires from countries
Pesticides (use)	Malawi	Use	Insecticides	2004	tonnes of active ingredients	7.00	Q	Official data reported on FAO Questionnaires from countries
Pesticides	Malawi	Hee	Insecticides	2005	tonnes of active	177 49	0	Official data reported on FAO

- Download the data
- Compute the average application rate since 2007
- Calculate the rate per hectar using the crop area

$K_{\rm oc}$

- Depends on compound
- Review country information on imported and/or used compounds and contact authorities

Example: Kidd et al. 1999 refer to import survey of Ministry for Agriculture and Livestock Development

- Simple approach:
 - Set to use-weighted average K_{oc}
- Retrieve K_{oc} from <u>Pesticide Properties Database</u>
- We set K_{oc} to 1000 (mixture of carbamate and OPs)

Kidd et al. 1999 in Bootsma & Hecky: Water Quality Report. Lake Malawi/NYASA biodiversity conservation project. 243-282

University of Hertfordshire 2017. Pesticide Properties DataBase (PPDB)

- We need spatially resolved:
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Plant interception

- Depends strongly on crop type and growth phase
- Review country information (e.g. <u>FAO AgroMaps</u>) and/or contact authorities
- Use spatially resolved crop harvest area and derive average plant interception per administrative level
- Consider growth phases (time-dependent plant interception)
- Simple approach:
 - Set to average of growth phases and crop type weighted by harvested area

Plant interception

Pure Appl. Chem., Vol. 72, No. 11, pp. 2199–2218, 2000. © 2000 IUPAC

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

DIVISION OF CHEMISTRY AND THE ENVIRONMENT COMMISSION ON AGROCHEMICALS AND THE ENVIRONMENT*

FOLIAR INTERCEPTION AND RETENTION VALUES AFTER PESTICIDE APPLICATION. A PROPOSAL FOR STANDARDIZED VALUES FOR ENVIRONMENTAL RISK ASSESSMENT

(Technical Report)

Prepared for publication by
J. LINDERS¹, H. MENSINK¹, G. STEPHENSON², D. WAUCHOPE³, AND K. RACKE⁴

Plant interception

Exercise

 Search and download the area harvested per crop for Malawi

Trick: Download all data

- 2. Identify the dominant crop in 2006 (latest year of reporting) → even more simplification
- 3. Retrieve plant interception (harmonised values) from Linders et al. (2000) for first growth phase.

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Lecture of Avit Bhowmik

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Soil texture

- Influences runoff (e.g. less runoff from sandy soils)
- Review global data from <u>ISRIC</u> World Soil Information, country information and/or contact authorities
- Simple runoff models only discriminate between sandy and loamy soils
 - → base classification on infiltration capacity

- Case study Malawi: Check %sand content
- R script is provided

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Slope

- Runoff increases with slope
- Derived from Digital Elevation Models (DEM)
- ASTER Global DEM 2 available (30 m resolution)
- Review country information for better resolution



Slope

- For case study lower resolution sufficient:
 - → SRTM 90m data (available within R)



Data

Portfolio

Meetings

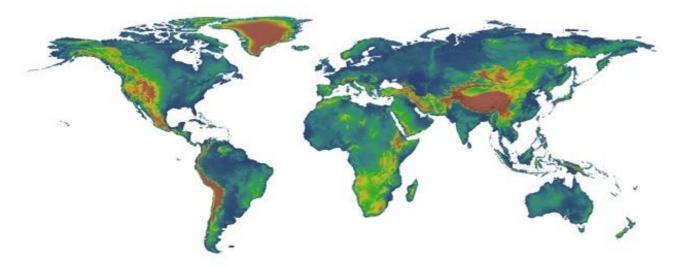
Blog

Publications

Forum



SRTM 90m Digital Elevation Database v4.1



The SRTM digital elevation data, produced by NASA originally, is a major breakthrough in digital mapping of the



Q



- Introduction
- Methodology
- Download
- Acknowledgements
- Citation
- Version History

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Hydrological network

- Buffered stream network to identify raster cells for runoff calculation
- Hydrological network available from:
 - Global network (e.g. HydroSHEDS, see next slide)
 - National or regional networks (e.g. from authorities)
 - DEM through flow accumulation algorithm (see example in course script)
- Buffer could be adjusted to stream size
- Derivation of network from DEM more efficient in GRASS GIS than R

Hydrological network

 HydroSHEDS used in case study, data is provided because registration required



Register Sign In Contact Us

Overview Development Availability Links FAQs License Download

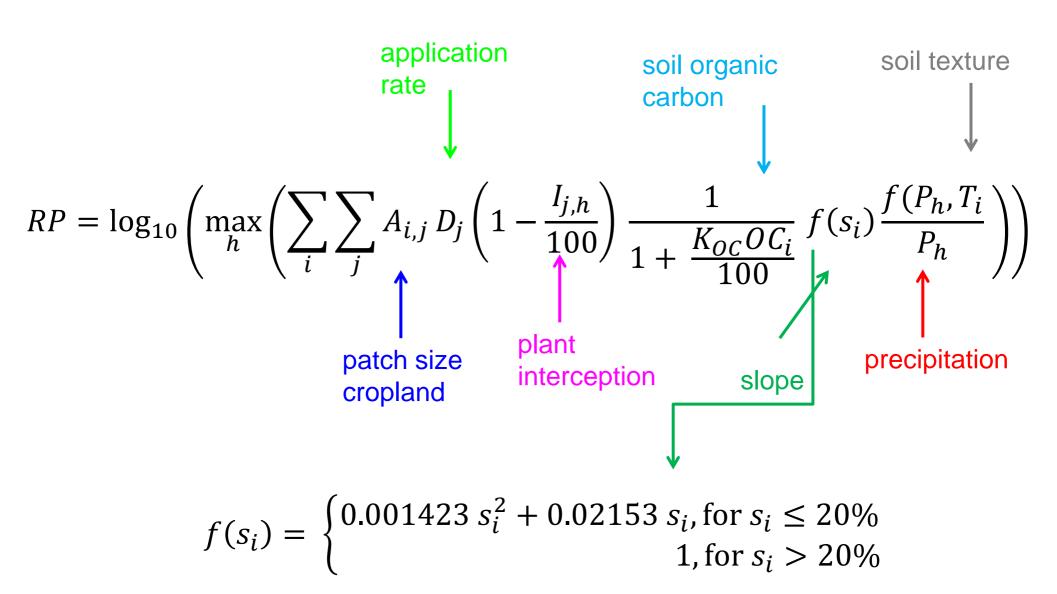
Overview / Acknowledgement / Citation

Overview

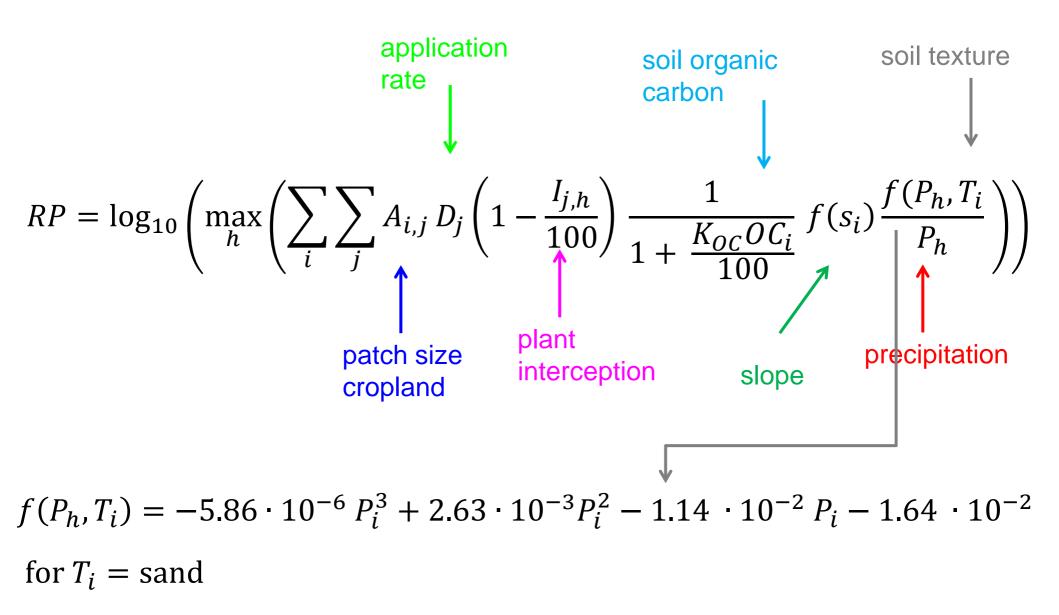
HydroSHEDS (**Hydro**logical data and maps based on **SH**uttle Elevation **D**erivatives at multiple **S**cales) provides hydrographic information in a consistent and comprehensive format for regional and global-scale applications. HydroSHEDS offers a suite of geo-referenced data sets in raster and vector format, including stream networks, watershed boundaries, drainage directions, and ancillary data layers such as flow accumulations, distances, and river topology information.



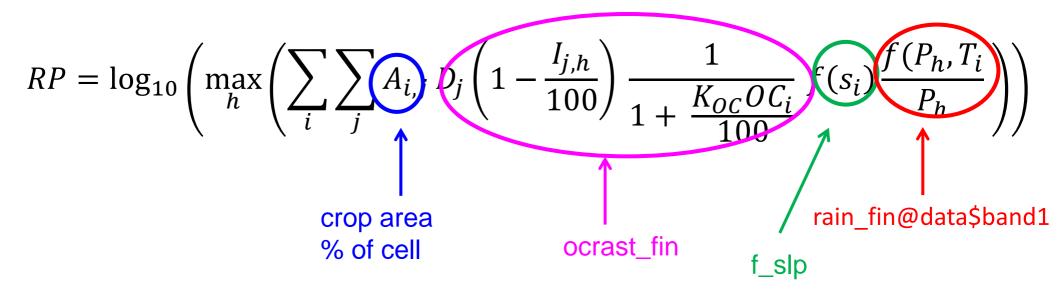
Fill in our first results and check units



Fill in our first results and check units



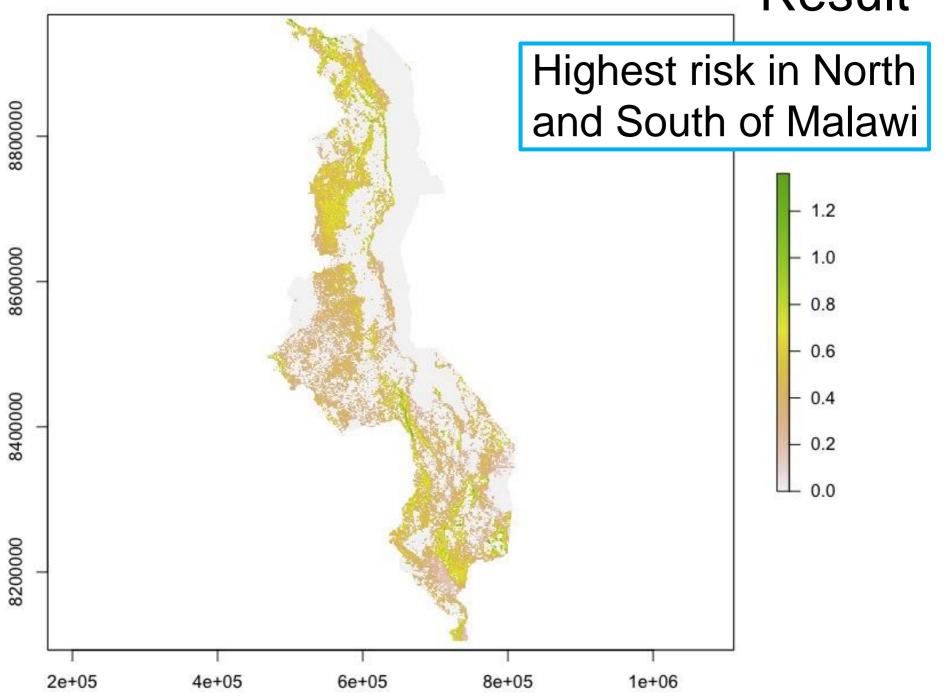
R object from calculations:



Next steps:

- Calculate proportion of crop area
- Convert all data to raster with same projection, extent and resolution

Result



How good is the model?

- A model cannot be better than its input data:
 - → Critical assessment required
 - "Garbage in Garbage out!" (GIGA)

Example:

- Suitability of land use data? (from 2005, 300 m resolution)
- Equal application rate across crops?
- Model parts calibrated for German/European conditions (e.g. runoff from precipitation)
- Model not validated for global use
- More sophisticated models available, which require more input data

Nevertheless!

- Parameterisation difficult for sophisticated models
- Good match with pesticide-related biotic metrics in previous studies (sample sizes > 100)
- Regional application of RP in:
 - Germany
 - Sweden
 - South-East Australia
 - Denmark
- Large-scale application of RP for Europe and World
- See literature for respective papers

Example: change of RP under climate change

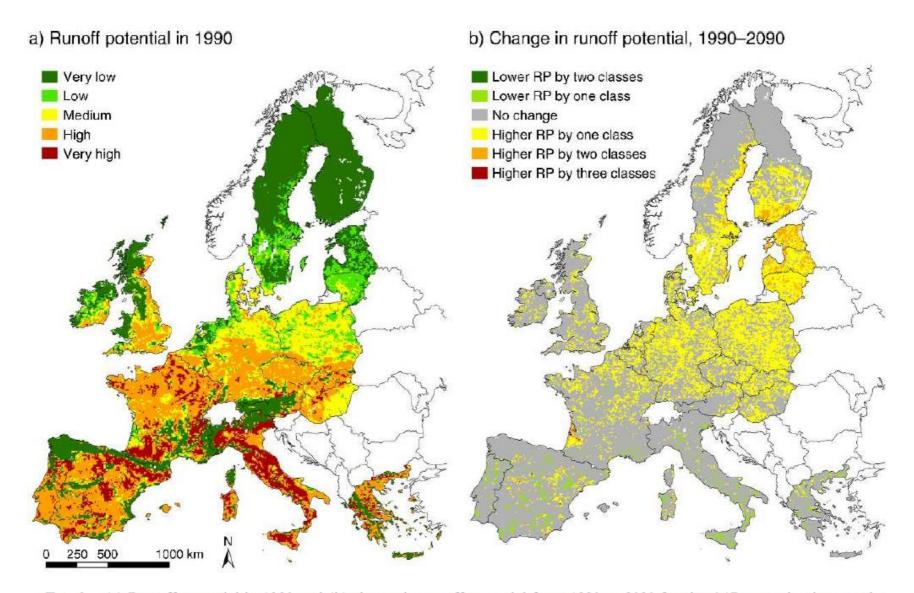


Fig. 3. (a) Runoff potential in 1990 and (b) change in runoff potential from 1990 to 2090 for the A1B scenario given as the change in RP class. RP indicates a logarithmic decrease from class to class in the amount of insecticide runoff. The change in RP is given as the difference between the classes in 2090 and 1990. Hence, an increase in the RP by two classes could represent an increase from low to high (see *Material and methods: GIS modeling*).

Example: Global RP calculation

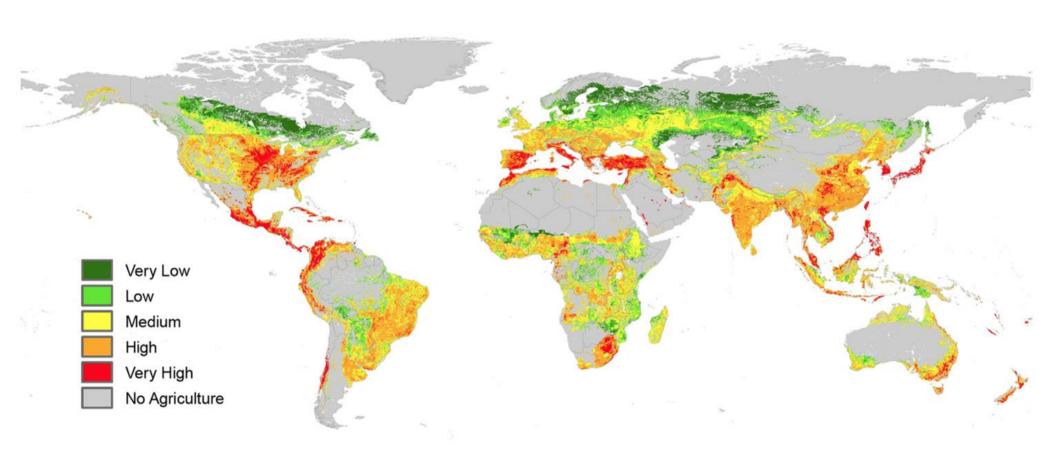


Fig. 3. Global insecticide RP map. The map shows the spatial distribution of potential insecticide runoff to stream ecosystems. According to this estimation, the surface waters in 43% of the total global land area are potentially subject to insecticide load as a consequence of current agricultural practices. The class boundaries (-3;-2;-1;0) are the same as those used in previous studies (Kattwinkel et al., 2011). Gray areas indicate the absence of any relevant agricultural activity.

Ippolito et al. 2015 Environmental Pollution 198: 54-60

Essentially, all models are wrong, but some are useful!

George E.P. Box

What is a model?

- A model is a purposeful representation of a system.

 Starfield et al. 1990
 - → Model choice / construction depends on question to be answered
- A model is an abstraction of reality. This abstraction represents a complex reality in the simplest way that is adequate for the purpose of the modelling.
 Wainwrigt & Mulligan 2004
 - → Not the more complex the better, but as simple as possible (but no simpler)

Questions?

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