Testing a regional scale pesticide fate model against monitoring data: necessity or endless quest?

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Presentation outline

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- Model purpose.
- MACRO-SE maps and databases.
- MACRO-SE workflow - Example for groundwater
- Simulated scenario (groundwater).
- Results
  - Maps of concentrations.
  - Confusion matrix.
  - Visual examination of the results
- General considerations on the validation of regional models.
- Conclusions.

Model purpose

Providing estimations of the **risks** of **pesticide losses** to **surface- and groundwater**, from **arable-land**, in **Sweden** (21 Swedish counties).

Help **understanding** (*some of*) the **factors affecting pesticide losses** at the regional scale, from **field to catchment**;

for:

1. **Swedish authorities.**
2. Researchers.

Model purpose

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The model MACRO (*in short*)

- MACRO pesticide fate model.
- 1D.
- Water flow micropores (Richards) and macropores (kinematic wave) and convective-dispersive solute transport.
- Percolation (vertical) and losses to the drain (lateral; Houghoudt + seepage potential).
- Freundlich sorption; 1st order degradation.
- Penman-Monteith evapotranspiration.
- No runoff and erosion.
- Long simulation time so no uncertainty assessment (regional).

MACRO-SE maps and databases

(1) **Maps of arable soils.**

(2) **Climate** maps & climate data series.

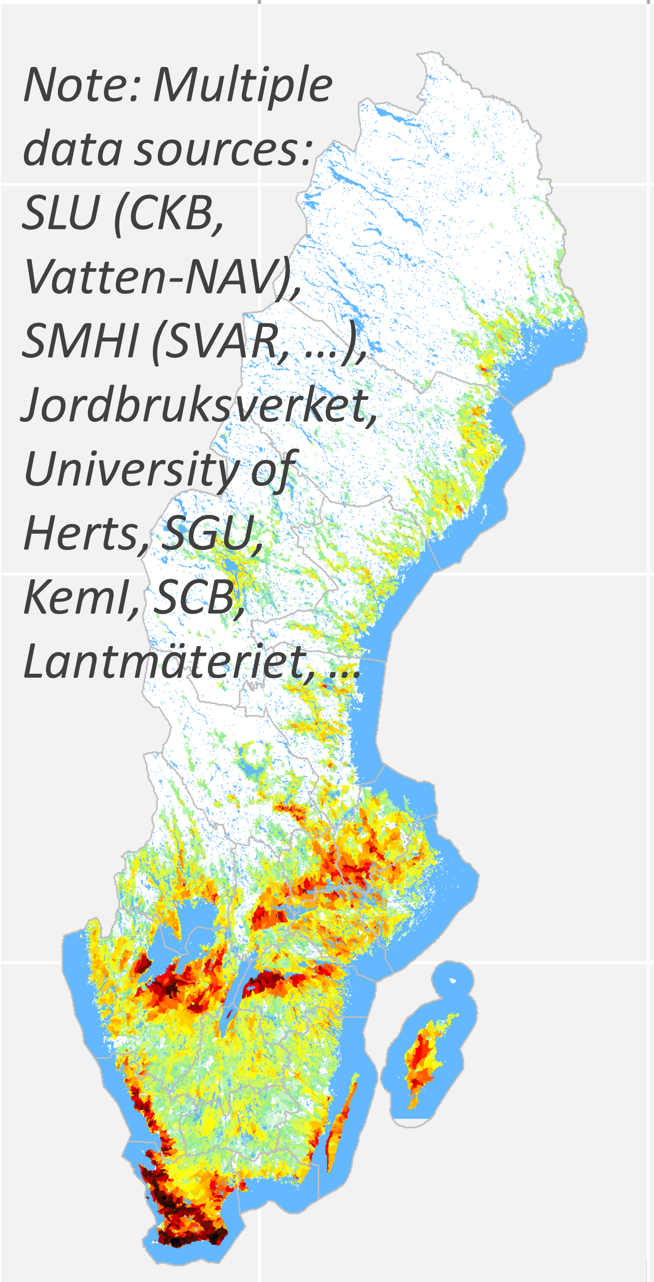
(3) Statistics on **crop area (new)**.

(4) Statistics on **pesticide usage**: What substance? On what crop? What time of the year? What dose? Where?

(5) **Crop physiological stages** (emergence, harvest, …).

(6) Up-to-date **Pesticide Properties Database**.

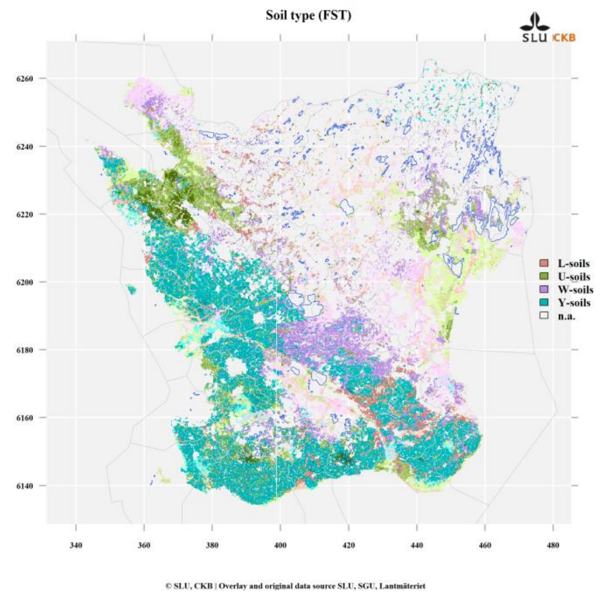
(7) Simulated average water flow in catchment outlet (SMHI S-HYPE)

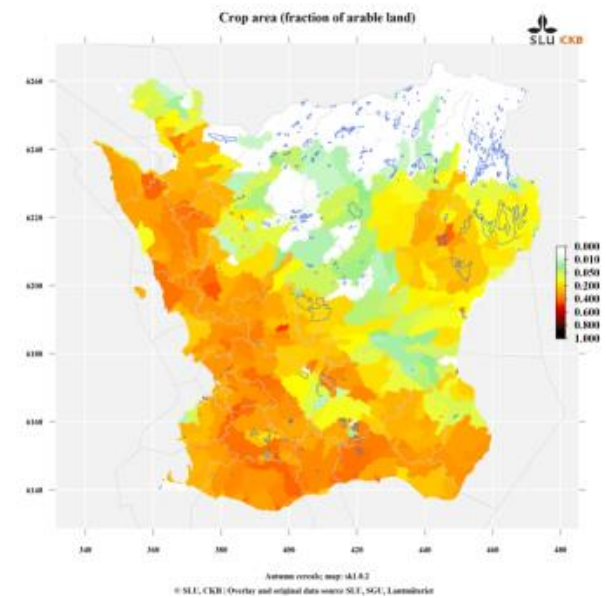


MACRO-SE workflow: example for groundwater

Groundwater risk:

- Scania county.
- Winter cereals.
- Isoproturon.
- ~500 g/ha.
- **Spay: mid-October or mid-April**





MACRO-SE workflow: example for groundwater

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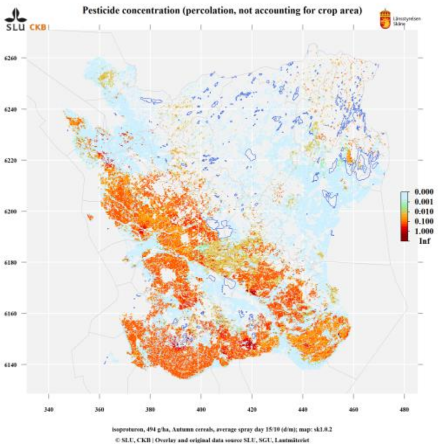
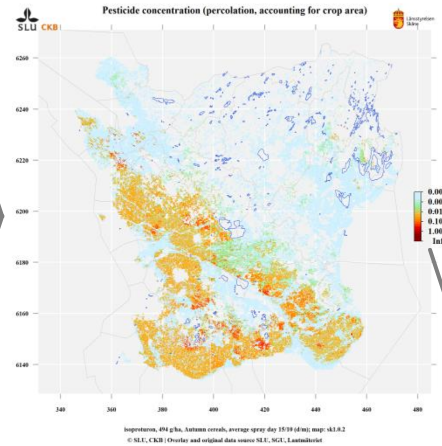
Edge of the field

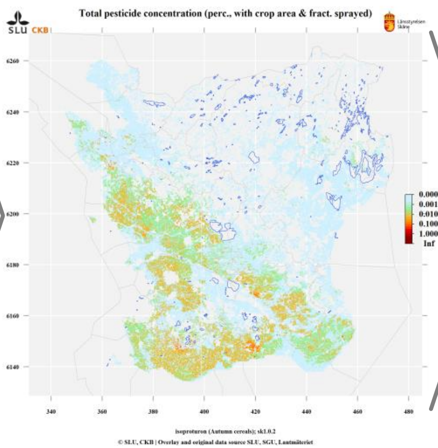
+ crop area

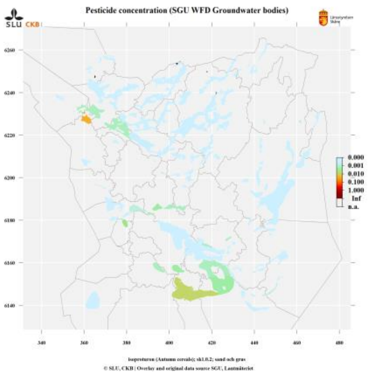
sum + fraction sprayed

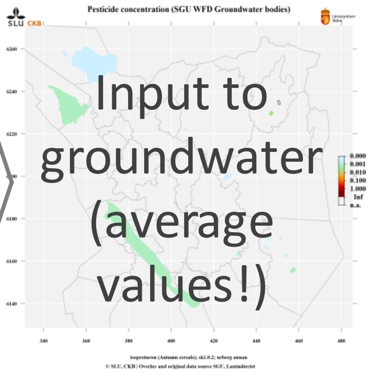
Autumn



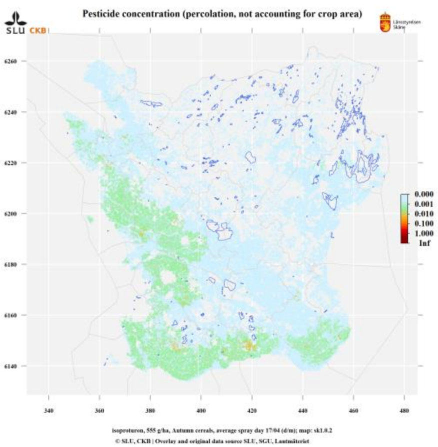


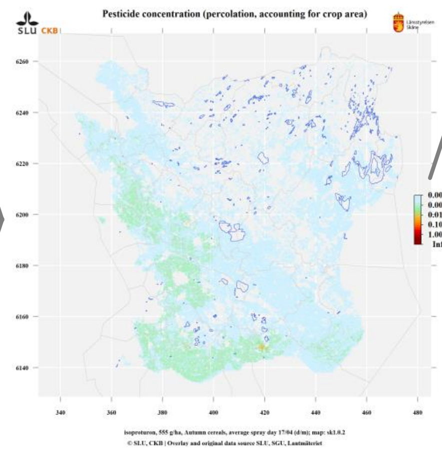






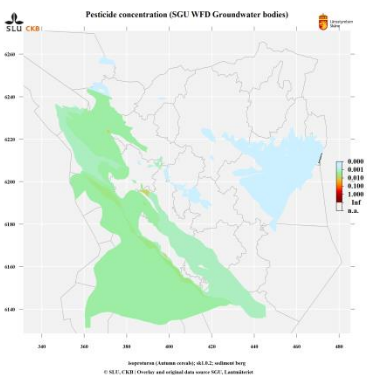
Input to groundwater (average values!)





Spring

Note: 2 meters depth!



Simulated scenario (groundwater)

Monitoring: 128 water wells (georeferenced), in Scania, with one or several measurement, for one or several pesticides. Long term.

Substance	Type	Crop	Spray-season	Dose g/ha	% sprayed
bentazone	H	Peas and beans	Spr: 7 – 21 jun	435	95
Isoproturon	H	Win. cereals	Spr: 14 – 28 apr	555	4
Isoproturon	H	Win. cereals	Aut: 9 – 23 oct	494	23
MCPA	H	Spr. cereals	Spr: 19 may – 02 jun	500	63
MCPA	H	Win. cereals	Spr: 6 – 20 may	850	9
metazachlor	H	Spr. rapes	Spr: 15 – 29 may	950	20
metazachlor	H	Win. Rapes	Aut: 2 – 16 sep	888	62
quinmerac	H	Sugar beets	Spr: 11 – 25 may	150	1
quinmerac	H	Win. Rapes	Spr: 26 aug – 9 sep	250	56
metribuzin	H	Potatoes	Spr: 24 may - 7 jun	245	91

Statistics from 2 CKB monitoring catchments

Note: isoproturon & metazachlor: not re-registered (in *2014 and 2015, resp.*)

Results: maps of concentrations (*2 m depth*)

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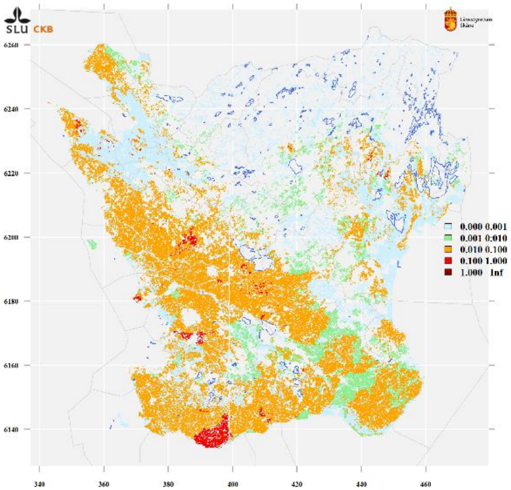
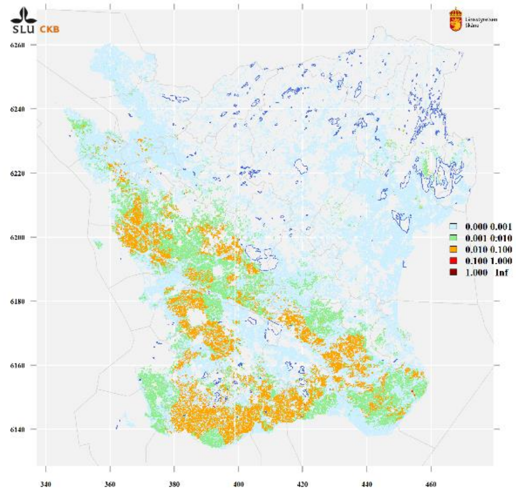
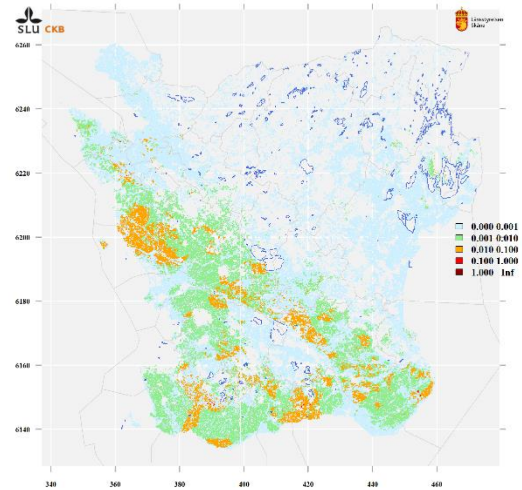
bentazone



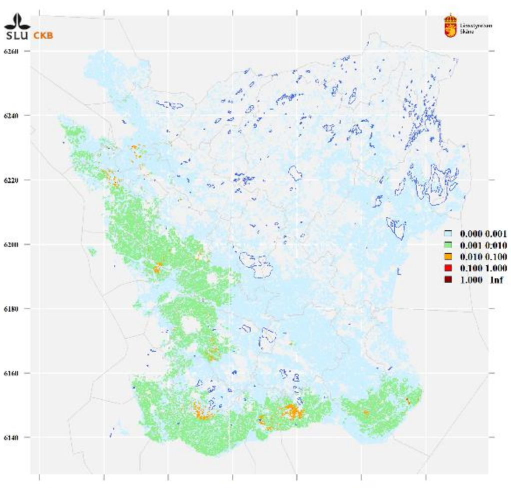
isoproturon (2)



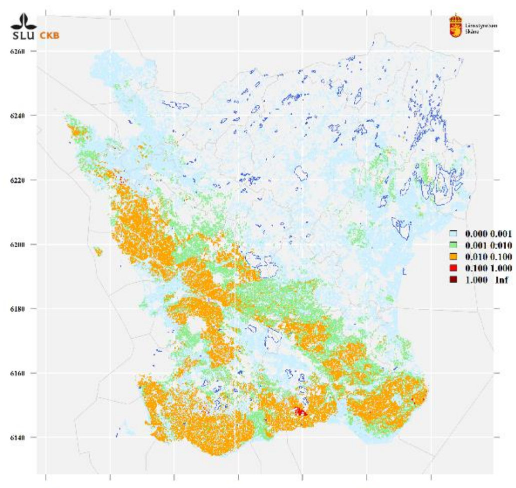
quinmerac (2)



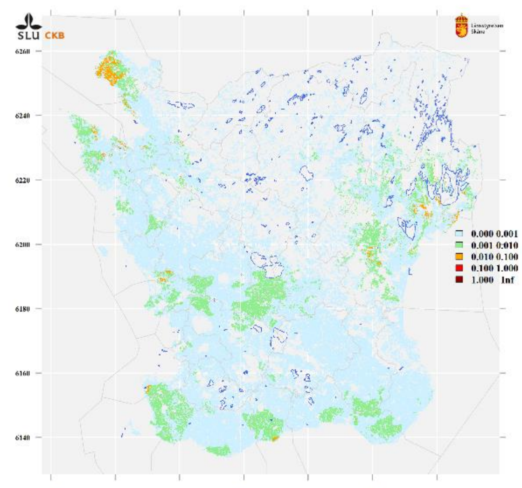
MCPA (2)



metazachlor (2)



metribuzin



Results: confusion matrix (correct / incorrect classif.)

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	Measured value	Simulated value		%tage correct clas.
		Detected	N. detected	
bentazon	Detected	6 (5%)	10 (8%)	
	N. detected	31 (24%)	81 (63%)	68%
isoproturon	Detected	0 (0%)	4 (3%)	
	N. detected	6 (5%)	118 (92%)	92%
kvinmerak	Detected	1 (1%)	1 (1%)	
	N. detected	4 (3%)	122 (95%)	96%
MCPA	Detected	0 (0%)	3 (3%)	
	N. detected	0 (0%)	95 (97%)	97%
metazaklor	Detected	0 (0%)	2 (2%)	
	N. detected	14 (11%)	112 (88%)	88%
metribuzin	Detected	0 (0%)	2 (2%)	
	N. detected	2 (2%)	93 (96%)	96%

Green: correct classification; Red: incorrect classification.

→ High percentage of correct classification (also) because **low detection frequency** in observations: only 29/128 detections!

Results: visual examination of the results

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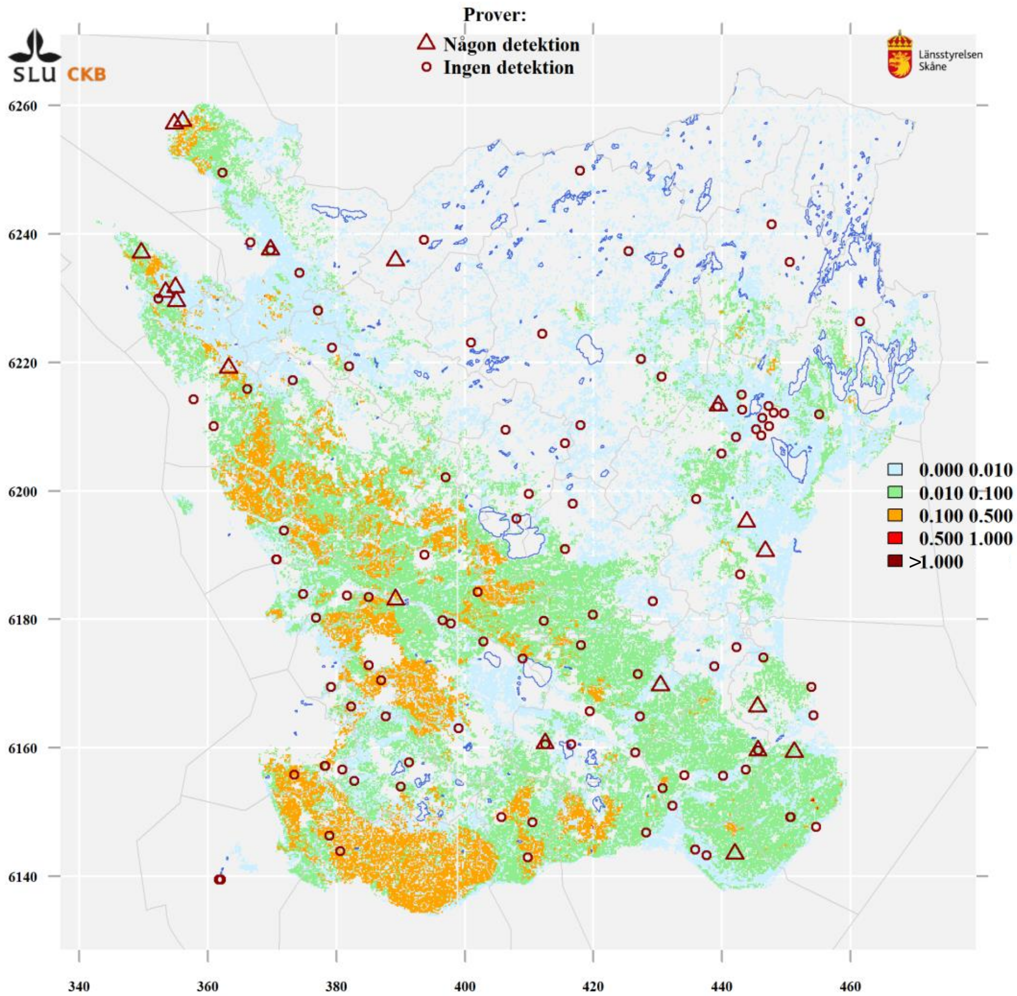

Cumulated concentration [µg/L] of all simulated herbicides at 2 m depth.

Red circles indicate wells where no pesticide was detected, triangles indicate wells with at least one detection.

Results: visual examination of the results

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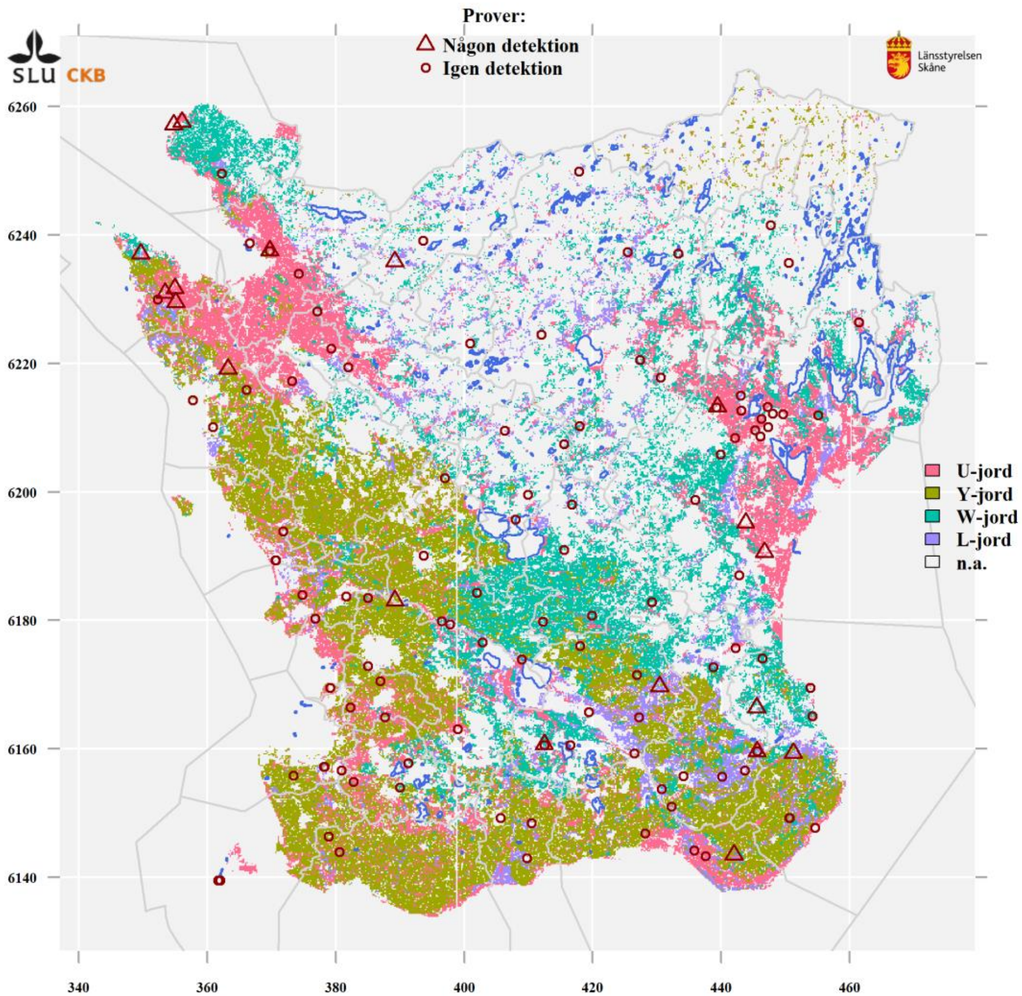

Map of hydrological classes for arable soils. “U” (pinkish) indicates soils with losses to drainage only. “L” (purple) indicates losses to groundwater only. “Y” and “W” (yellowish; blue-green) indicate losses to both.

Red circles indicate wells where no pesticide was detected, triangles indicate wells with at least one detection.

→ Several detections in area where we don’t predict flow to groundwater. Map error or **lateral flow towards the groundwater**?

Results: visual examination of the results

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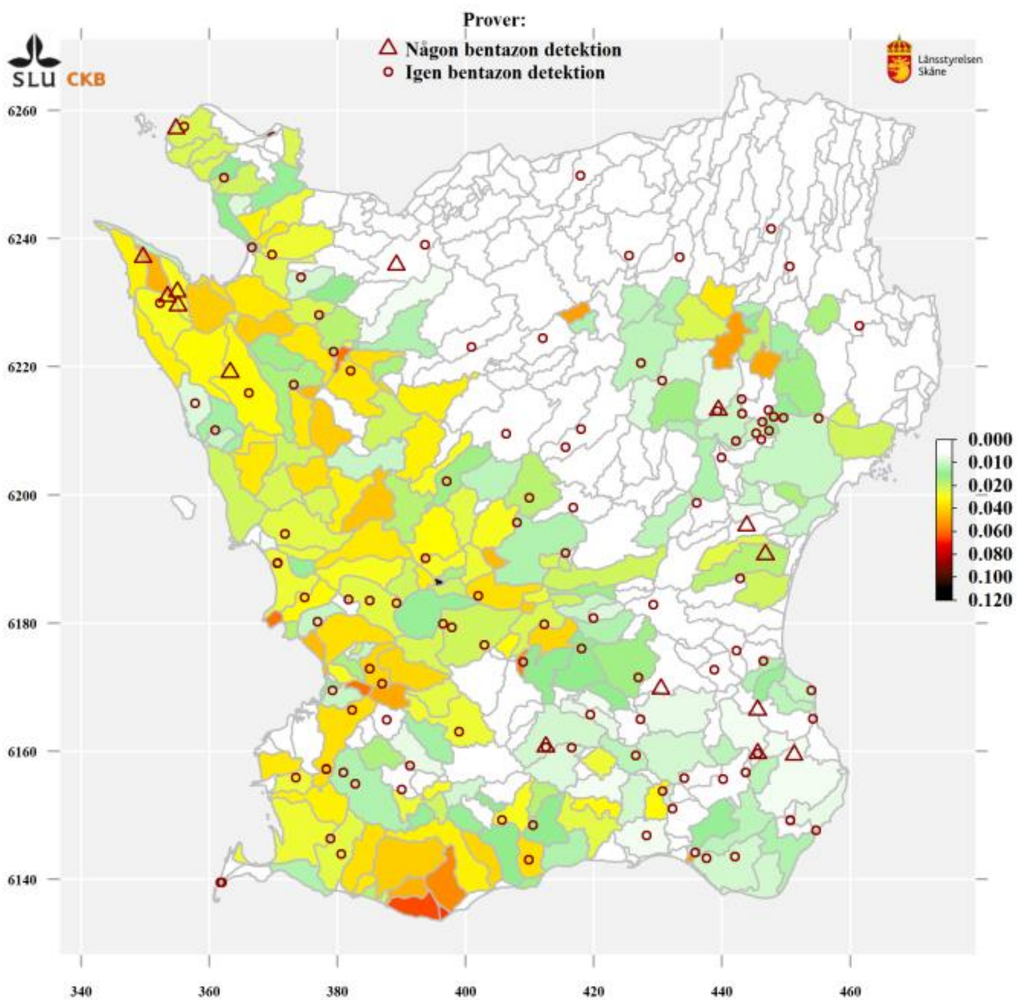

Map of peas and beans area, as a fraction of the arable area in the catchment (average-statistics over 9 years).

Red circles indicate wells where no bentazone was detected, triangles indicate wells with at least one detection.

→ Several detections in area where we don’t observe a high fraction of peas or beans in the arable area. **Historical** or other usage?

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Some consideration regarding the evaluation of regional models:

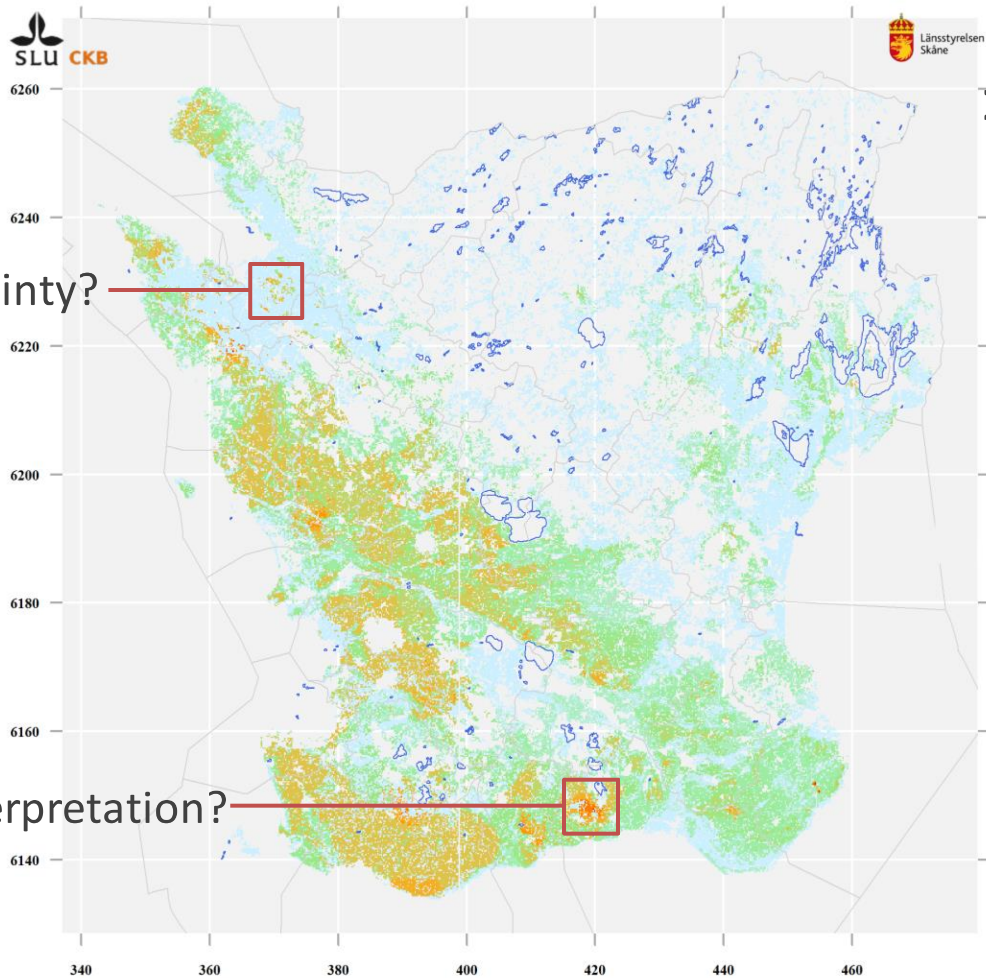
- Risk assessment models are **validated for a certain purpose**.
- Regional scale models are **not just numerical models**.
  1. Numerical model: collection of solutions.
  2. Model of the environment: collection of maps and databases.
  3. Parameter estimation routines.
- **Observations**, “ground-truth”, are **scarce and heterogeneous** (normalisation and aggregation needed?).
- Methodology for **matching simulation results and observations**:
  1. Aggregating and censoring simulated values.
  2. Evaluating (*or not*) ‘influence area’ around groundwater wells.
- Forecast vs history matching (historical maps & stats needed too).
- The regulatory framework, and practices, have changed.

Conclusions

→ **It's complicated!** We can discriminate leachable from non-leachable compounds (*Steffens et al. 2015*). But how accurate the results are is difficult to say (*blame the models, historical issues, …?*)

Uncertainty?

Interpretation?



>> Need to **define acceptable model usage.**

>> Model as a complex indicator?

>> Combine with other sources of information?

Thank you for you attention!

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Länsstyrelsen Skåne

Further references

Gustaf Boström, Julien Moeys, Nicholas Jarvis, Mikaela Gönczi och Jenny Kreuger, 2015. Riskkartering av bekämpningsmedel i Skånes Grundvatten - Simuleringar med MACRO-SE. CKB rapport 2015:1. (*in Swedish*).
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Supplementary materials

MACRO-SE workflow

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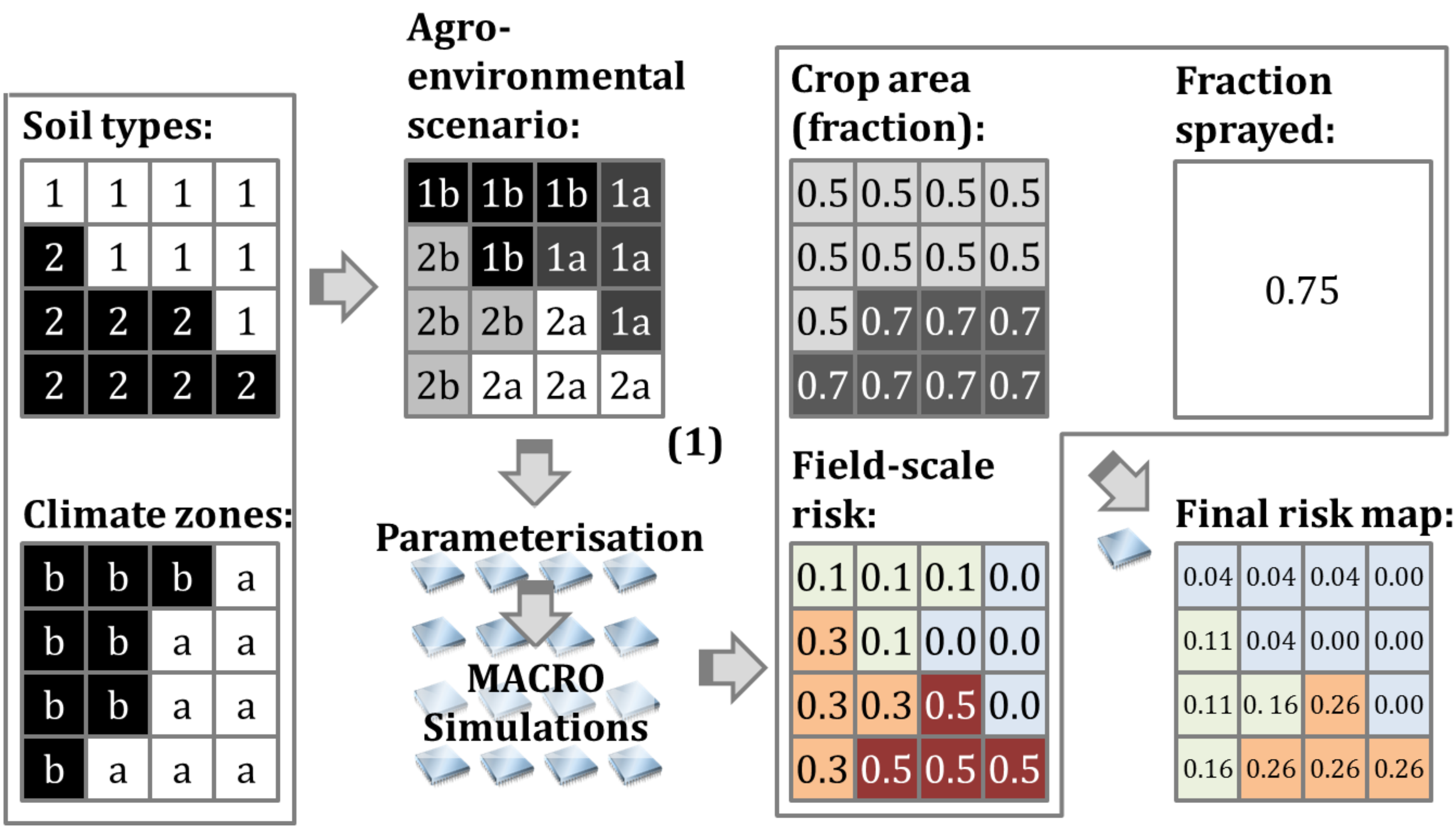

+ additional aggregation
& post-processing

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Components of a regional scale pesticide fate model:

- **Numerical model of pesticide fate** (here MACRO, 1D).
  - Different processes → different sub-models.
  - More or less mechanistic or empirical.
  - More or less dynamic.
- **Model of the environment** (maps and databases).
  - Several variables (soil, climate, crop, pesticide).
  - **Discretised** time and space. Various resolutions, scales and levels of **aggregation**.
  - Note: Too few studies on its impact on model 'validity'.
- **Parameter estimation routines**.
  - Continuous vs class-based?
  - Fitted statistics vs expert judgment?
  - Sensitive parameter?

→ Testing regional models = testing a local model-setup.

Testing models: observations

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Observations ("ground truth") against which models are tested are **also heterogeneous:**

- Sampling design & frequency? Purpose?
- Different operators, laboratories, authorities.
- Observation replica: how to aggregate? min, max, average?
- Different detection limits (variable in time?). How to normalise?
- Different types of aquifer, different streams.
- Different depth (for groundwater).
- Poorly known historical pesticide usage crop area & groundwater 'age' (simplest: time stationarity is assumed)

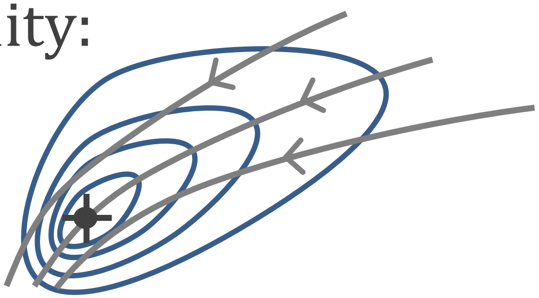
Testing models: matching with observations

Processing observations and simulated concentrations to make them comparable:

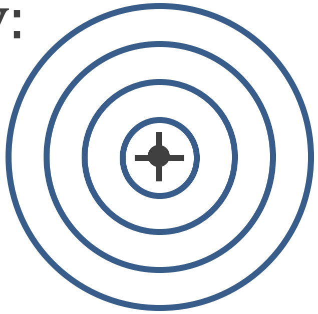
- Selecting a common detection limit (global, well-specific? …).
- Censoring simulations (under detection → non-detect).
- Re-censoring observations (if necessary).

Problem of the (unknown) groundwater influence area:

Reality:



Study:



Surface water: catchment outlet (estimation) vs observation point in the catchment; Only one sampling season.

The MACRO models