

U N I K A S S E L V E R S I T Ä T

Modelling the transfer of pesticide transformation products from agricultural fields to the aquatic environment – *state of knowledge and future challenges*

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- Pesticide transformation products (TPs) are increasingly found in all water bodies such as rivers, lakes, groundwater
- There is a need for modelling tools simulating pesticide and TP concentrations for exposure assessment
- This review analyses...
 - ...currently applied modelling concepts,
 - ...problems occurring during TP model applications...and discusses ways forward for further model development.
- Only models are included with at least one published application in the literature



Leaching models

- | | |
|--------------|-----|
| • GLEAMS | [1] |
| • MACRO | [2] |
| • RZWQM(2) | [3] |
| • PEARL | [4] |
| • PRZM | [5] |
| • Pelmo | [6] |
| • LEACHM | [7] |
| • HYDRUS 1-D | [8] |

Distributed leaching models

- | | |
|------------------|------|
| • GeoPEARL | [9] |
| • LEACHM spatial | [10] |

Catchment models

- | | |
|---------------|------|
| • ZIN-AgriTra | [11] |
| • FRM | [12] |

→ 12 models with 19 published applications for TPs

[x] *References see last slide*

Transformation schemes

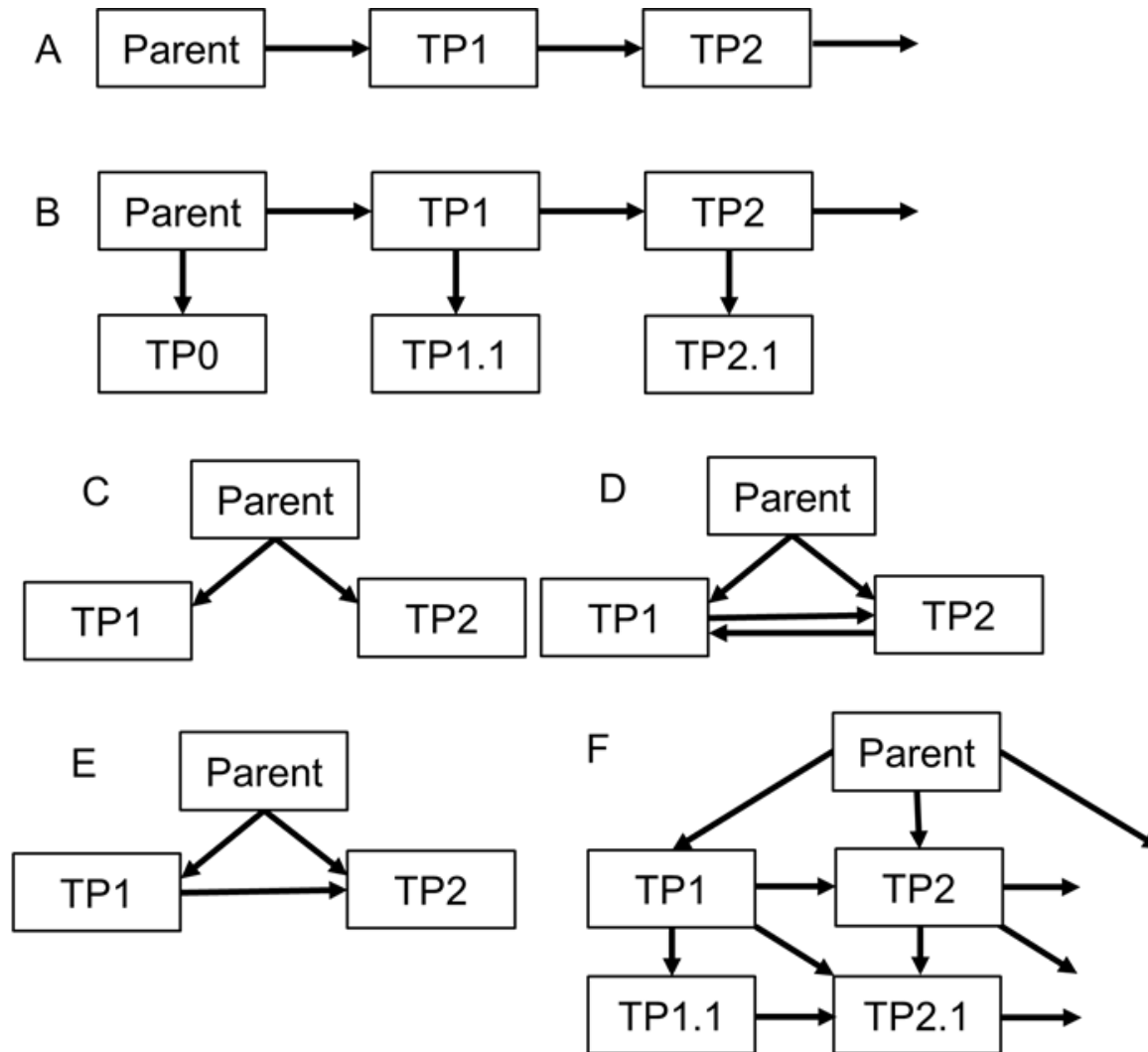


Fig. 1: Different ways models fixed the transformation from parent compounds to TPs. Some models are fully flexible.
→see next slide

Transformation concepts



Model	Transformation scheme	Influences on transformation						Formation in solute and solid domain	Different TPs in compartments	No. transformation processes
		Soil moisture	Soil temperature	Soil depth	pH	Organic carbon	Clay content			
GLEAMS	B	X	X							1
MACRO	A	X	X	X				X		1
RZWQM	A, C	X	X	X					X	5
PEARL	flex	X	X	X						1
PRZM	E		X					X	X	1
Pelmo	F	X	X	X				X	X	2
LEACHM	A	X	X	X				X		1
HYDRUS 1D	B	X	X					X		1
GeoPEARL	flex	X	X	X	X	X	X			1
ZIN-AgriTra	D	X	X	X				X		1
FRM	E									1

Tab. 1: Overview of transformation concepts in considered models.

flex – fully flexible transformation scheme

Process details of the models

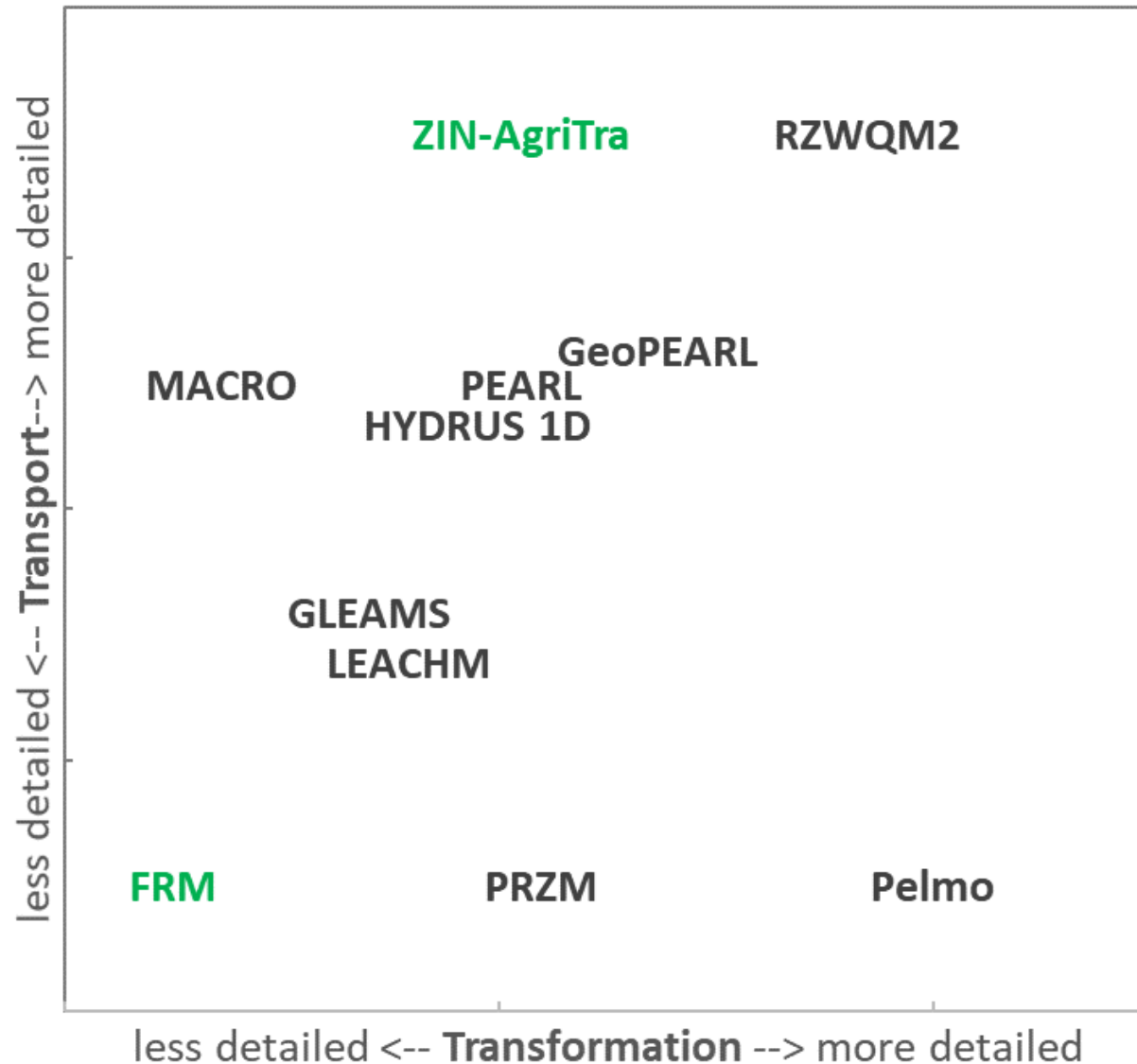


Fig. 2: Results of a numerical rating scheme considering the complexity/process detail of transformation equations and hydrological equations of each model.

Black: leaching models
Green: catchment models

Spatio-temporal resolution

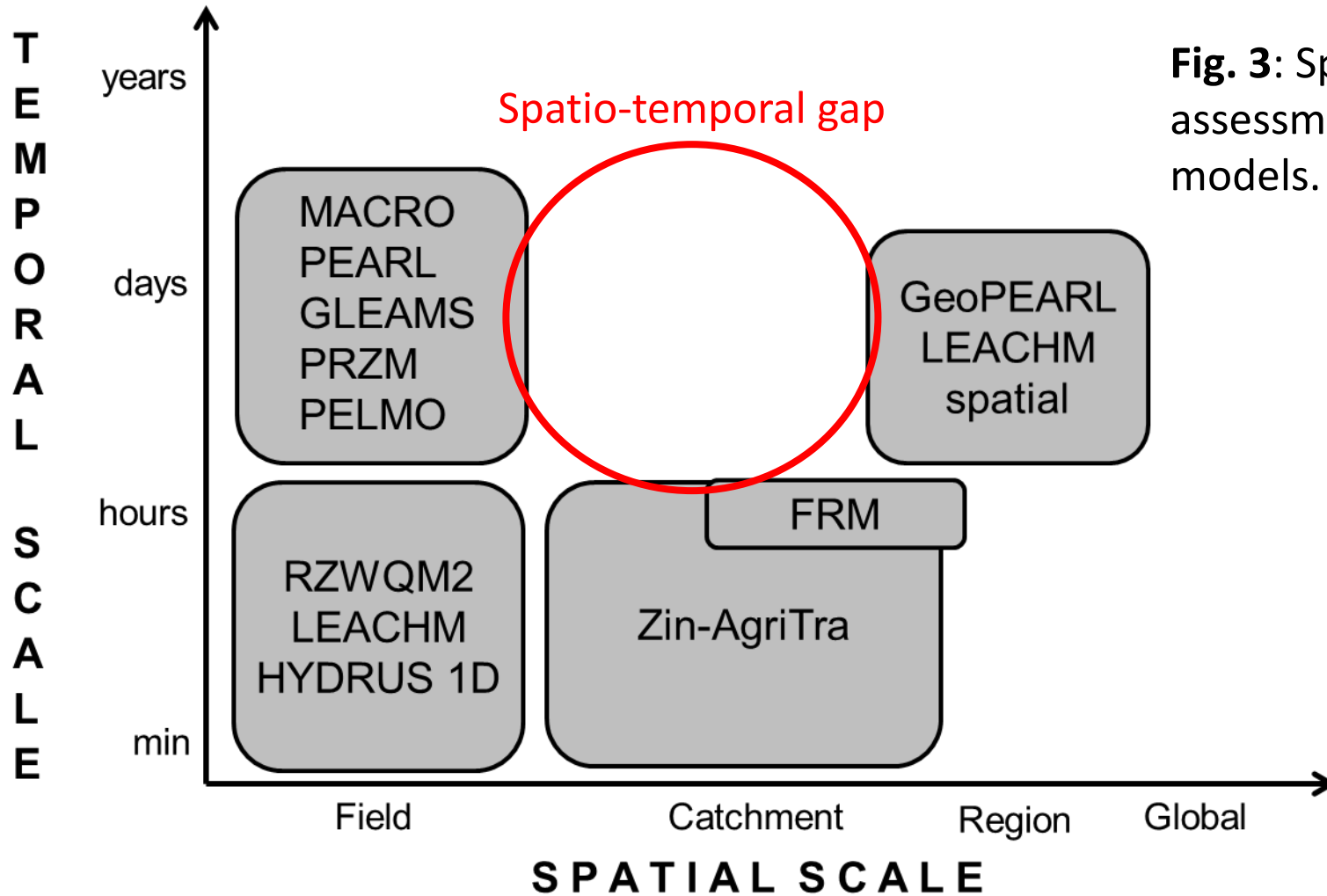


Fig. 3: Spatio-temporal assessment of analysed models.

Reasons for model failure



- 13 out of 20 studies discussed reasons for model failure

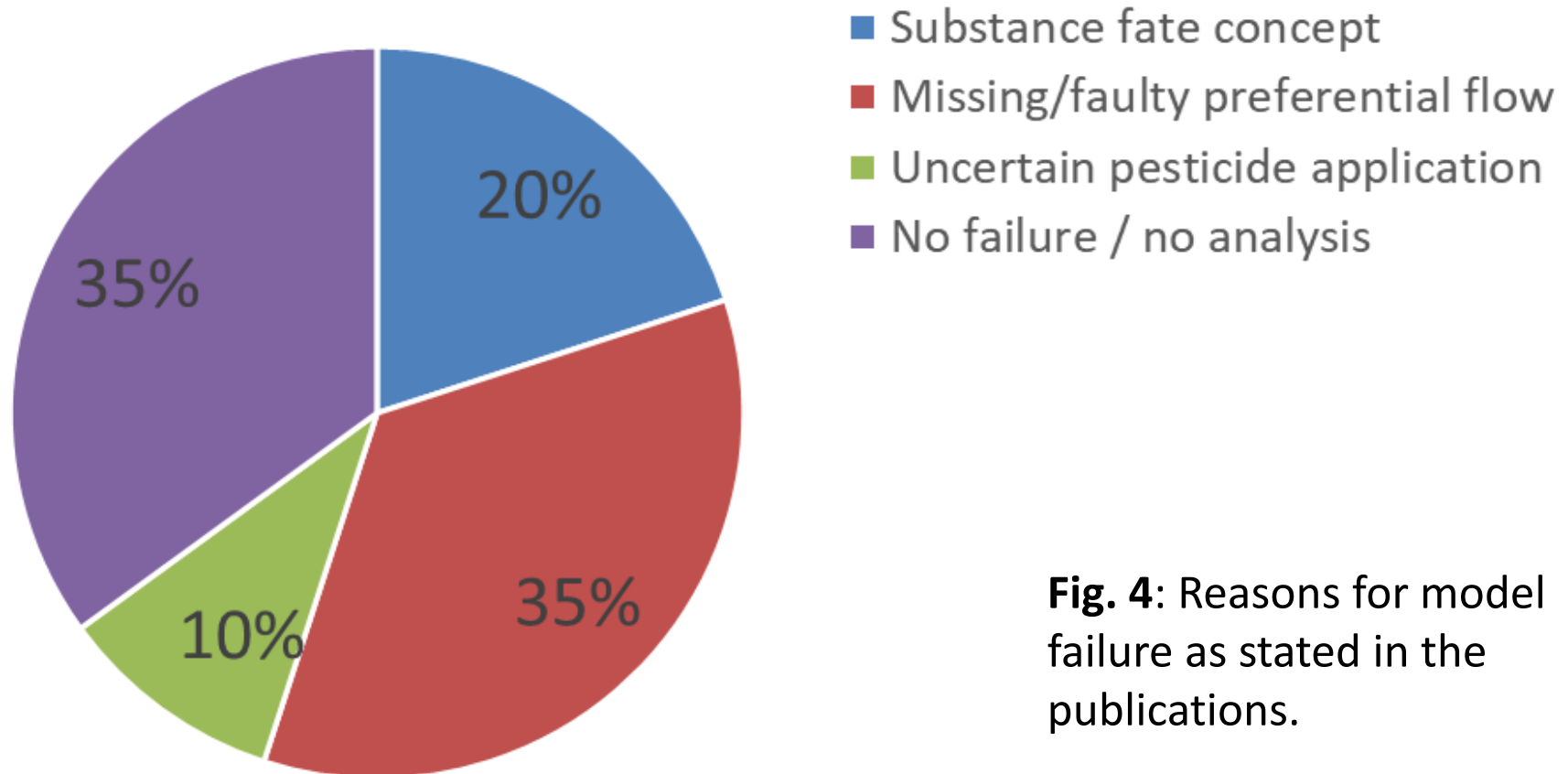


Fig. 4: Reasons for model failure as stated in the publications.



Model structure

- Most models are not able to build different TPs by different transformation processes (e.g. microbial vs. photolysis)
- Most models have fixed transformation schemes
- Spatio-temporal gap at one-day at catchment scale

Model applications

- Model failure was rarely blamed to environmental fate concepts – but the concepts were mostly not even discussed.
- Preferential flow is still an issue in leaching models



- Adequate number of leaching models (8) but low number of catchment models (2)
- Large variety in transformation process detail between models
- Recommendations for model development
 - Existing catchment models at one day resolution should be updated for TPs
 - More flexible transformation schemes
 - Build-up of TPs in different domains (plant, soil)
 - Critical assessment of implemented transformation schemes required
- Outlook
 - An integration with a pathway prediction model could add to a more comprehensive exposure assessment

The end?



Please contact me if I included any wrong assumptions about the model concepts – it was not always easy to find information about the implemented equations.

Please contact me also for any further questions.

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