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► To cite this version:

Guillaume Metayer, Jean-Stéphane Bailly, Marc Voltz, Cécile Dagès. A mechanistic-AI hybrid approach to meta-model pesticide transport in landscapes. 18. Symposium in Pesticide Chemistry, Sep 2026, Cremona, Italy. <hal-05738649>

HAL Id: hal-05738649

<https://hal.inrae.fr/hal-05738649v1>

Submitted on 4 Sep 2026

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A mechanistic-AI hybrid approach to meta-model pesticide transport in landscapes

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INTRODUCTION

Predicting water flows and contaminant transport in a catchment is crucial for designing sustainable land-use strategies. We need spatially explicit models that show how local farming practices influence both immediate and delayed outcomes—whether at the treated field or at a distance.

These approaches can be hard to implement. Numerical instability, parameterisation problems, and long run times are common issues. As a result, it becomes difficult to explore many scenarios, especially over wide areas or long time periods.

Metamodeling can reduce the computation time of complex model while preserving its predictive skill. Many techniques exist. Recent studies¹⁻⁵ demonstrated the

effectiveness of Long Short-Term Memory (LSTM) neural network for simulating streamflow at the catchment scale.

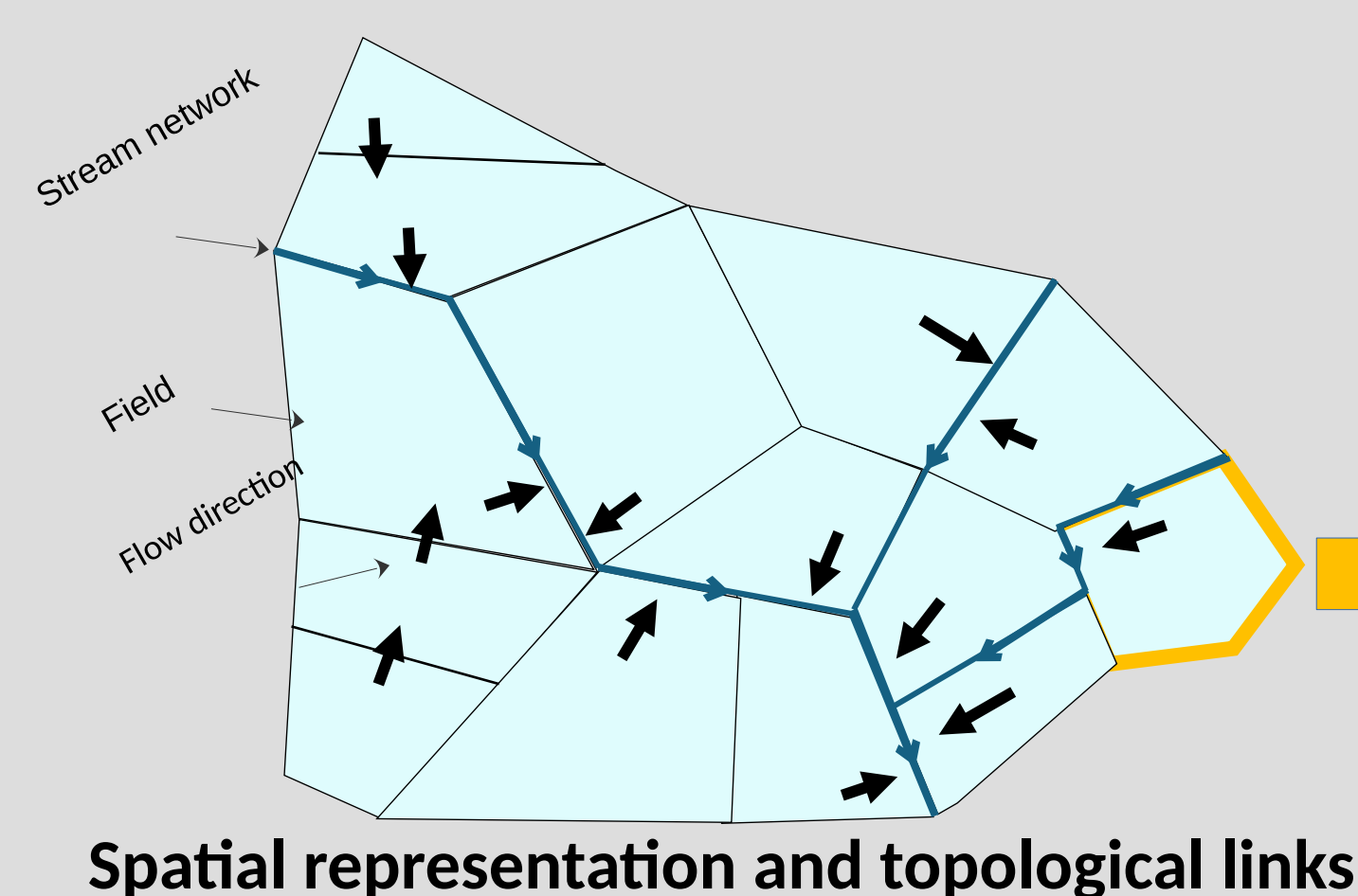
However, these metamodels were site-specific. Their training uses data from a single catchment. Creating a generic catchment-scale metamodel would mean training on many catchments with very different flow structures. Such a training would be prohibitive in terms of both computing time and data volume storage needs.

To ensure more genericity, we developed a hybrid solution to model pesticide transport in landscapes that combines an AI meta-model with a mechanistic model to simulate pesticide concentrations in runoff water at the catchment scale

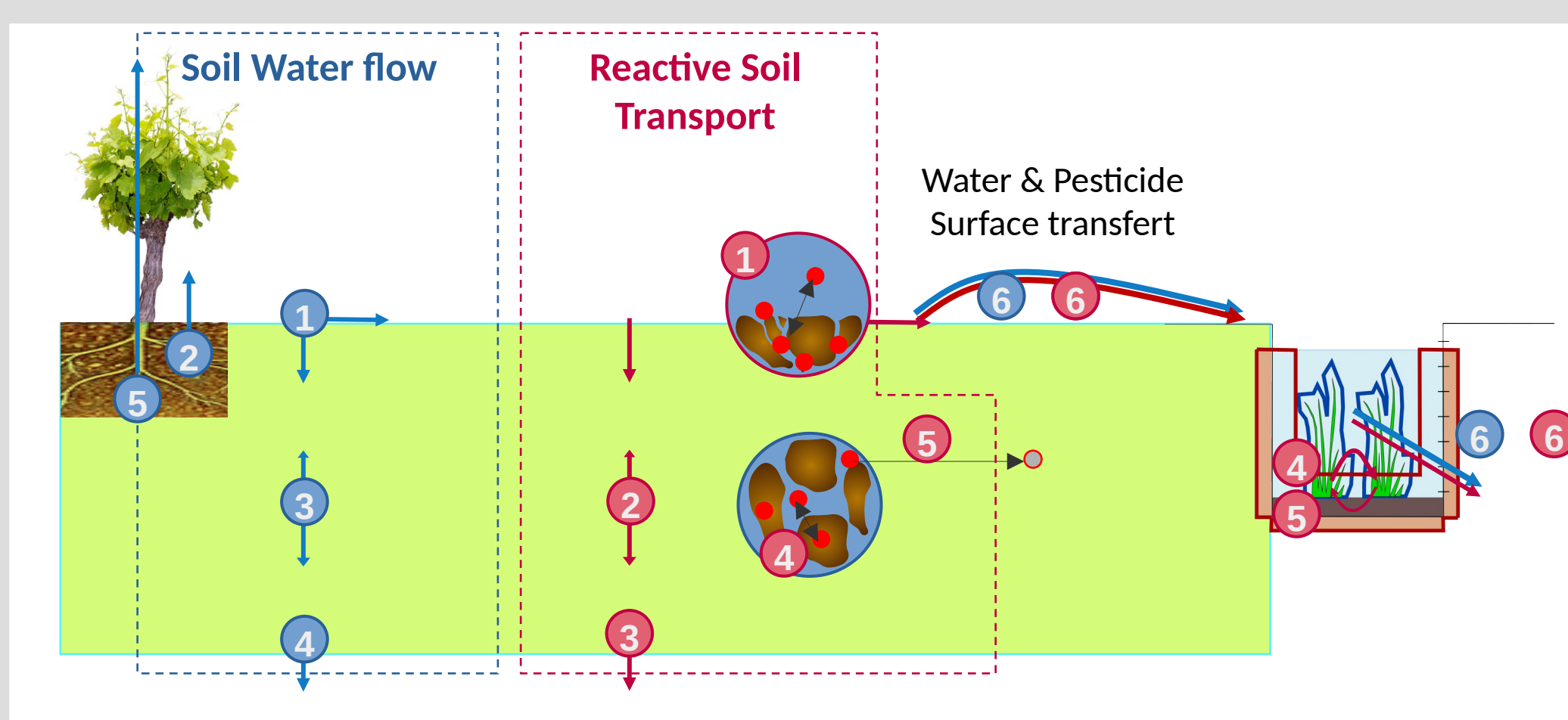
MODEL DEVELOPMENT

1- Original mechanistic MHYDAS-Pesticide model⁶

MHYDAS Pesticide 1.0 is a hydrological model that simulates the behaviour of pesticides in soil and water. Its accuracy in simulating the temporal variability of pesticide concentrations in runoff was assessed over a 20-year period for two compounds: diuron and glyphosate⁷.



Spatial representation and topological links

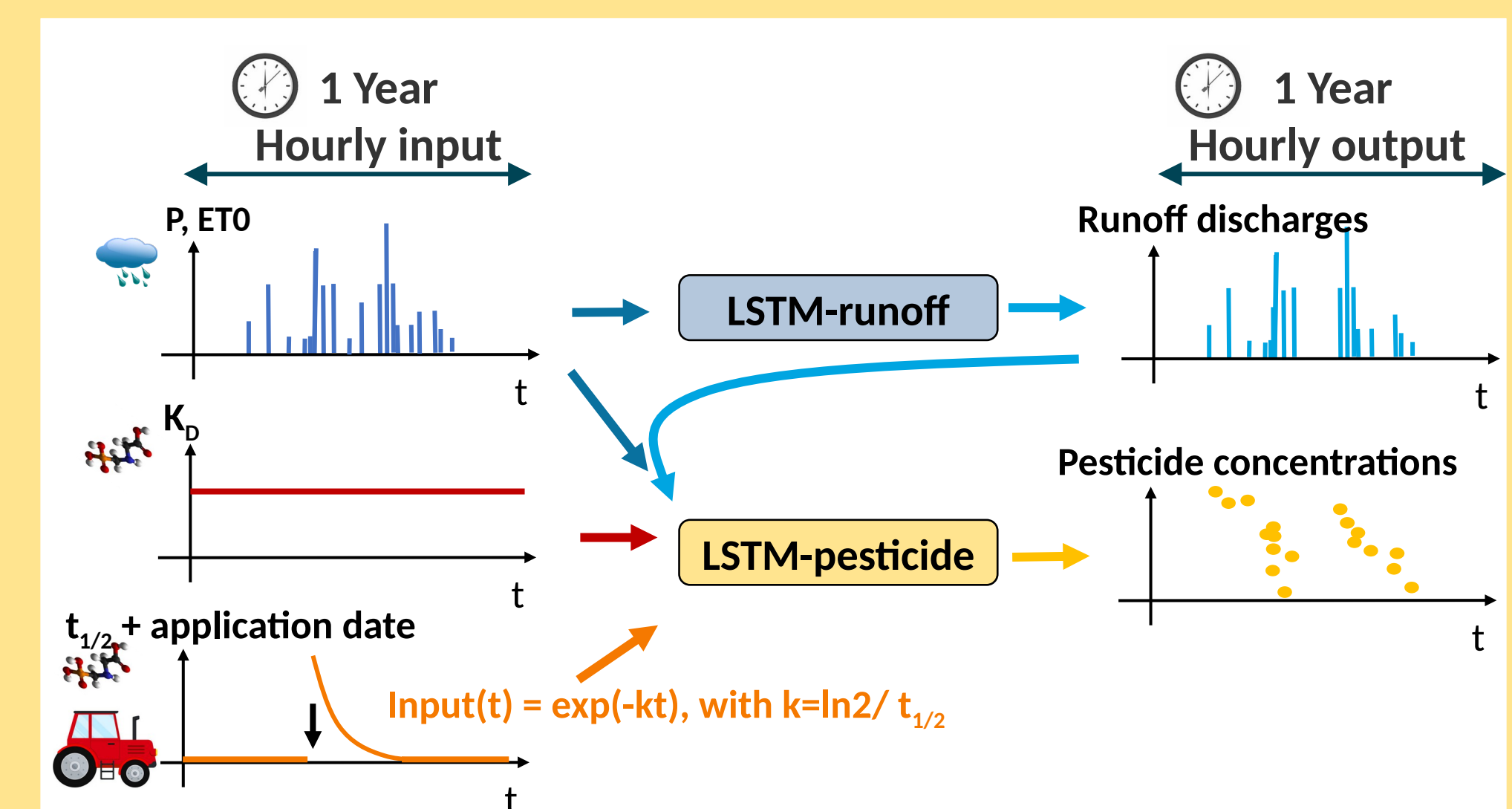


Main processes of MHYDAS-Pesticide model⁶ and their formalism^{8,9}

Simulated processes	Formalism
1 Runoff/infiltration partition	Richards' equation (Ross solution)
2 Soil evaporation	Feddes eq. Diffusive wave (Hayami solution)
3 Within soil water fluxes	uniform mixing
4 Deep percolation	CDE
5 Root water uptake	linear, instantaneous
6 Water surface transfer ²	first order rate
	Diffusive wave (Hayami solution)

2- Metamodeling Field Runoff Flow & Concentrations¹⁰

APPROACH : TWO LSTM NEURAL NETWORKS CONNECTED IN SERIES



TRAINING DATABASE = MHYDAS PESTICIDE SIMULATION DATASETS

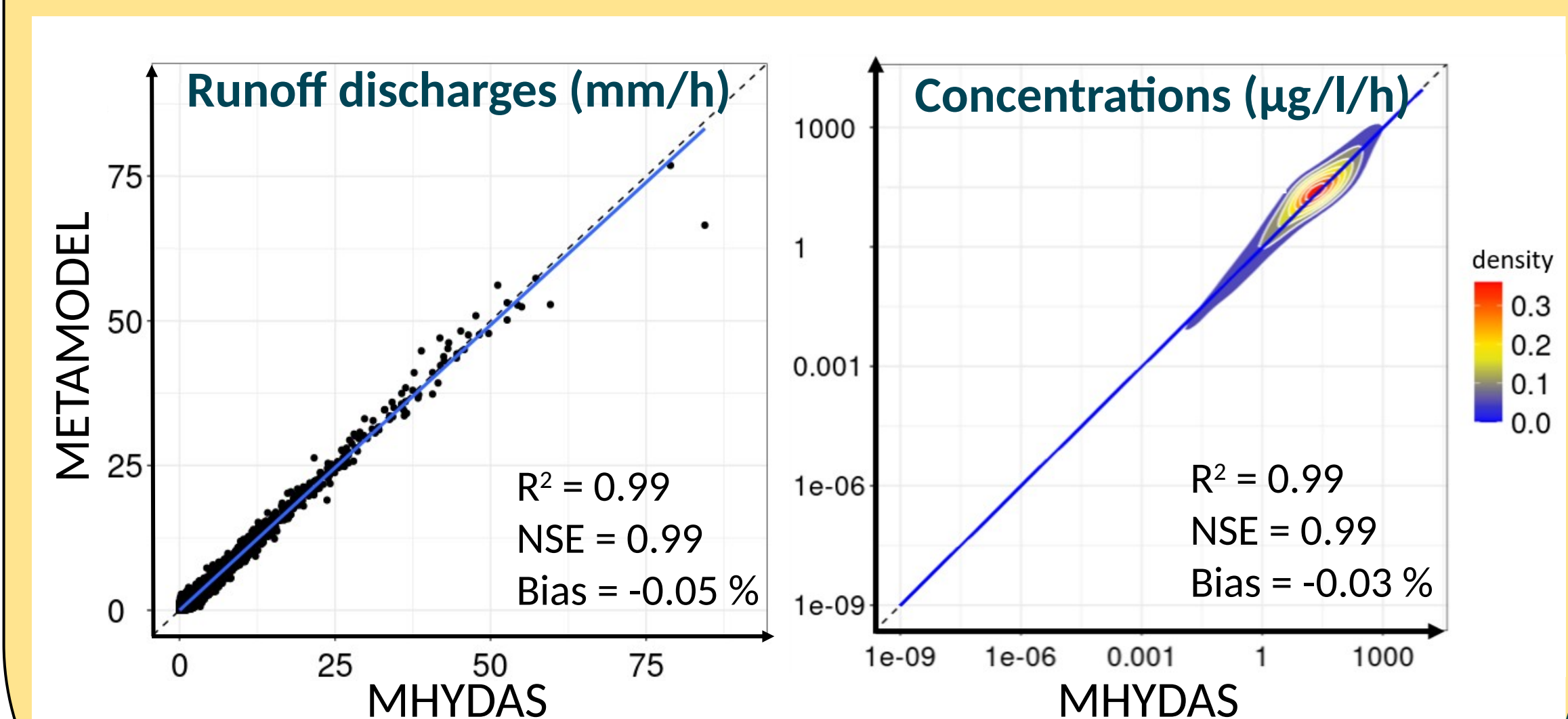
~ 550 000 simulations, resulting from the combination of :

- 286 climate time series
- 40 application dates per climate time series
- 7 levels of K_D values $\in [0.05 ; 500 \text{ l/kg}]$
- 7 levels of $t_{1/2}$ values $\in [0.1 ; 400 \text{ days}]$

Dataset : 70 % for training 70 % ; 30% for validation.

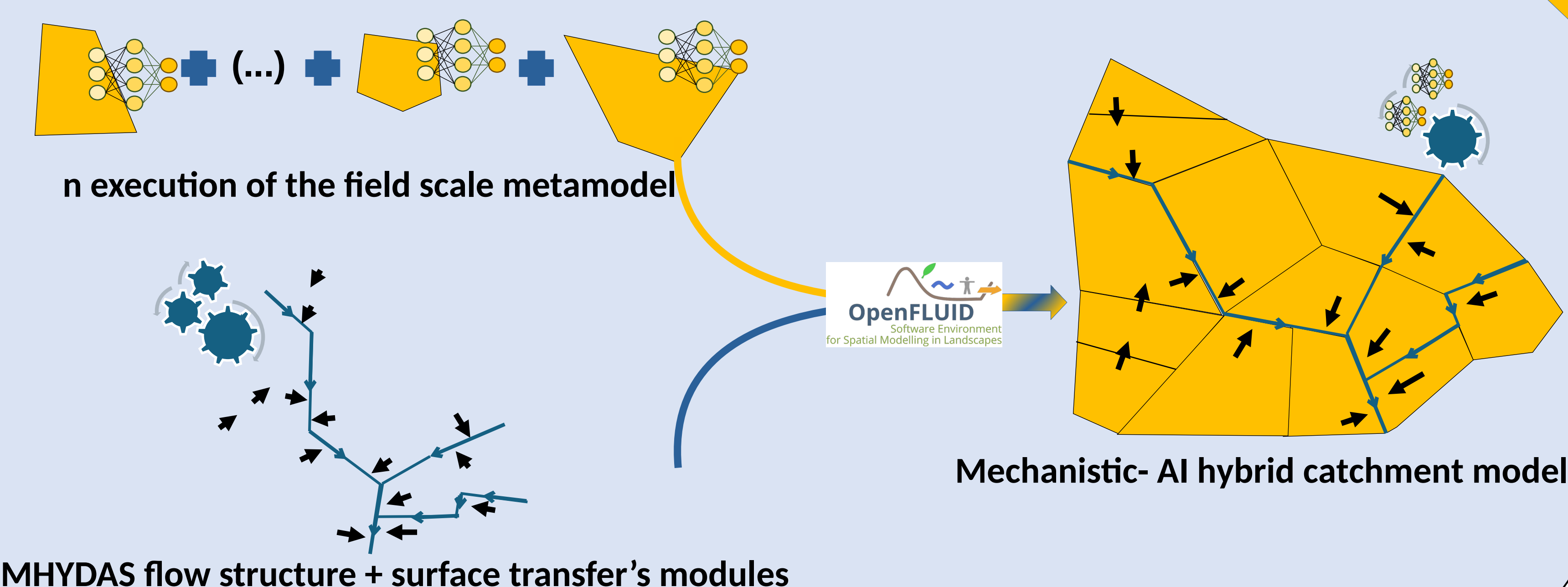
PERFORMANCE

- Very good overall performance of the field scale metamodel, but difficulties in simulating non-runoff hourly events
- Significant reduction in computation time (~90%)



Comparison of simulated runoff discharges and concentration with MHYDAS and its metamodel, for the validation data set.

3-Assembling the mechanistic- AI hybrid catchment model within OpenFLUID framework¹¹



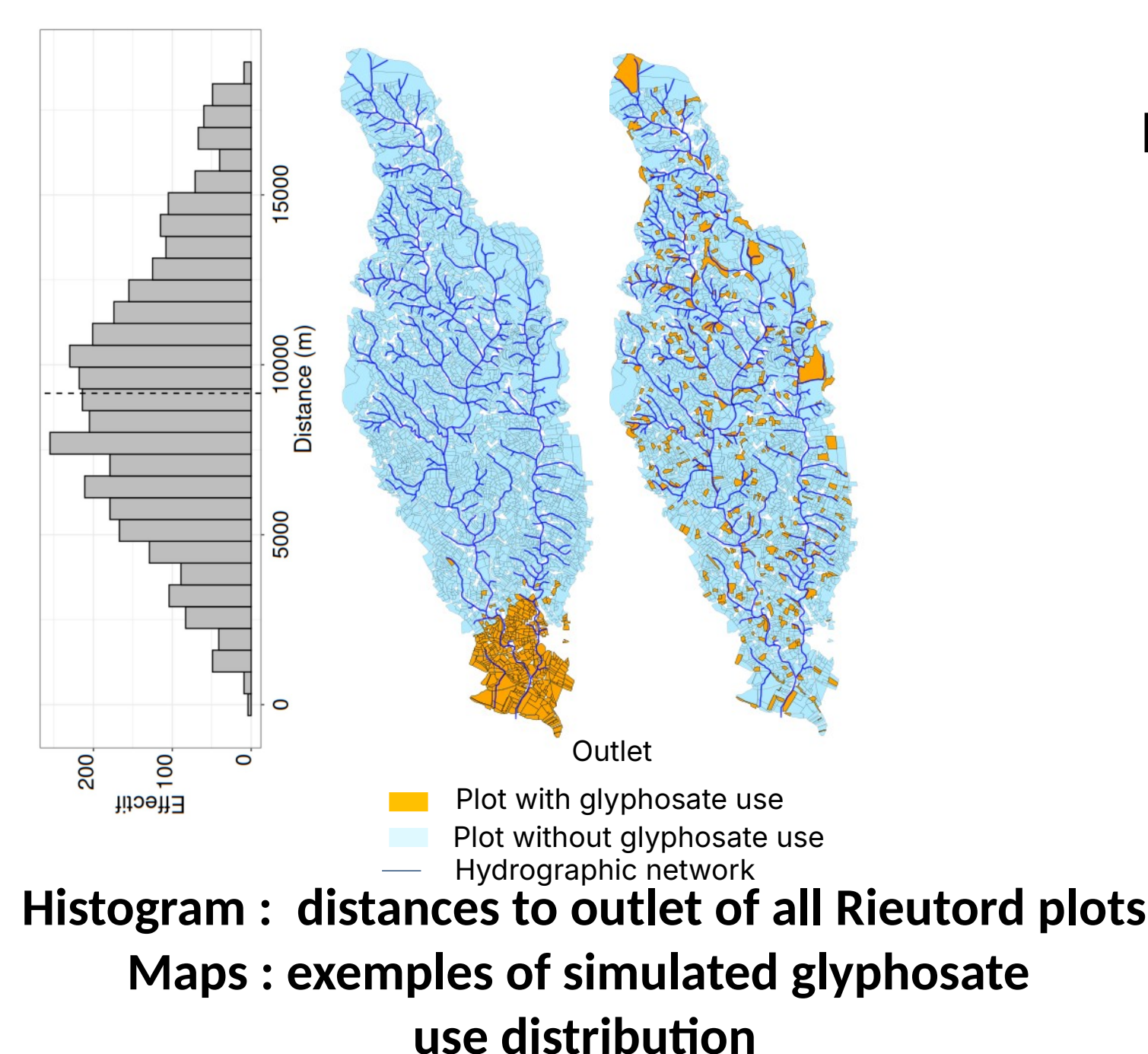
Mechanistic- AI hybrid catchment model

MHYDAS flow structure + surface transfer's modules

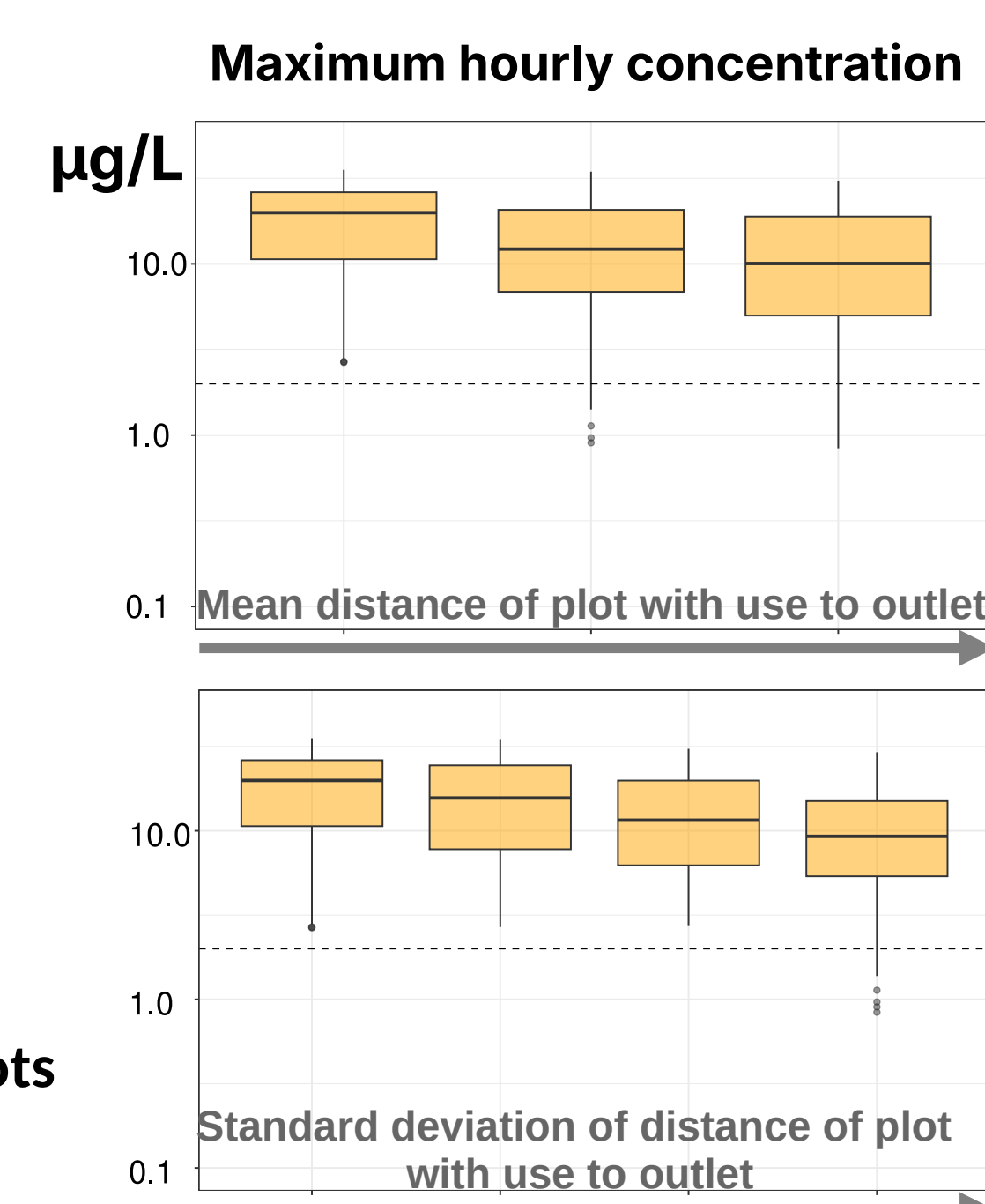
APPLICATION : SIMULATING GLYPHOSATE TRANSPORT IN A VINE-GROWING CATCHMENT¹²

NUMERICAL DESIGN :

- Site support : Rieutord catchment, South France
 - 45 km² and 3645 plots
 - Simplification of soil map (1 soil type)
- Evaluation of glyphosate concentration variation with spatial pattern of use : 1800 simulations
 - 30 spatial distributions of glyphosate use
 - upstream/downstream ; aggregated/scattered
 - Applied dose of glyphosate : 1kg/ha
 - percentage of the catchment treated : [20;80]
 - 20 meteorological datasets
 - Simulated period : 6 month (warm-up) + 12 months



Histogram : distances to outlet of all Rieutord plots
Maps : examples of simulated glyphosate use distribution



RESULTS :

- Reduction in computation time (~70%) enables intensive simulations
- First results show a significant effect of spatial distribution on contamination with a decrease in glyphosate concentration with :
 - Scattered use
 - Distance of use to outlet
- This can be explained by
 - Timing of arrival to the hydrographic network
 - Duration of retention processes

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ACKNOWLEDGEMENTS

This work was carried out as part of the PhD thesis of Guillaume Métayer, funded by the AgroEcoSystem Department of INRAE and the Occitanie Region.