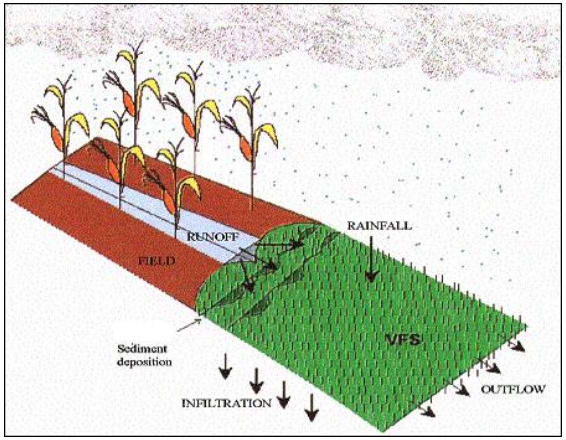
Evaluation of a new VFSMOD version with upgraded pesticide trapping equations against field data

Stefan Reichenberger, Robin Sur, Carolin Kley, Sebastian Multsch, Stephan Sittig



9th European Modelling Workshop, 9-11 Oct 2018, Copenhagen

Introduction

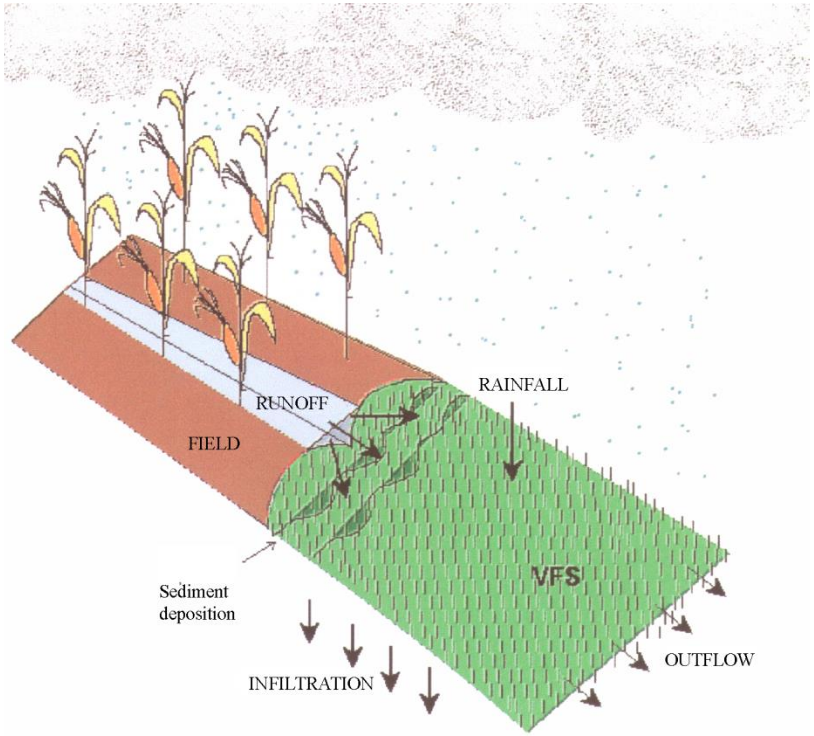
- Surface runoff from agricultural fields is a major input pathway of pesticides into surface waters (e.g. Wauchope, 1996).
- The most widely implemented mitigation measure to reduce transfer of pesticides and other pollutants to sw via surface runoff are vegetative filter strips (VFS).
- These are densely vegetated areas designed to intercept surface runoff, often located at the downslope field border.
- The effectiveness of VFS in reducing surface runoff volumes and associated eroded sediment and pesticide loads has been demonstrated in general, but also found very variable.
- Experimental VFS studies (e.g. Poletika et al., 2009) have shown that the most important factor influencing VFS efficiency for a given runoff event is the hydraulic load (incoming water volume per VFS area).
  → Fixed reduction fractions (e.g. such as proposed by FOCUS L&M) will under-estimate VFS efficiency for small runoff events and overestimate it for large ones.
  → To model the reduction of surface runoff, eroded sediment and pesticide inputs into surface water by VFS in a risk assessment context, an event-based, dynamic model is needed.

The model VFSMOD

- The most widely used dynamic, event-based model to simulate the reduction of surface runoff volumes, eroded sediment and pesticide loads by VFS is VFSMOD (Muñoz-Carpena and Parsons, 2014).

- While VFSMOD simulates infiltration and sedimentation mechanistically, the reduction of pesticide load by the VFS (ΔP) has – until recently – been calculated exclusively with the empirical multiple regression equation of Sabbagh et al. (2009).

- The Sabbagh equation (in its original formulation) has not been widely accepted by regulatory authorities, because its reliability had not been sufficiently demonstrated.
  - Major drawback: small number of calibration data points (n = 47).



Muñoz-Carpena and Parsons (2014)

Previous work: study of Reichenberger et al. (2019)

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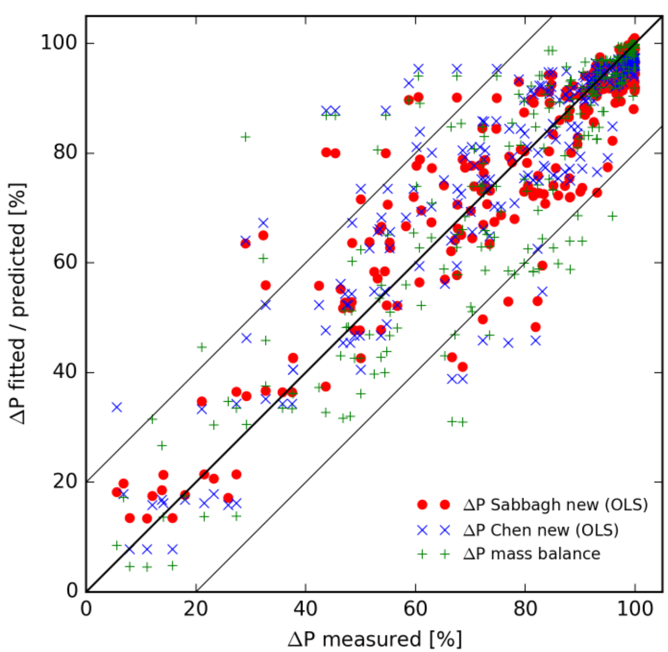
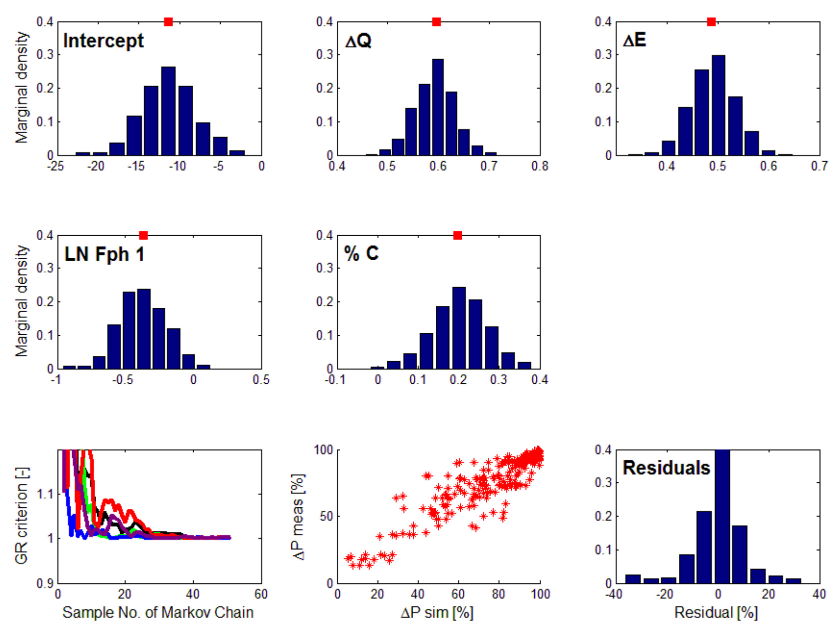
- To corroborate and improve the predictive capability of the Sabbagh equation, additional experimental VFS data were compiled from the available literature.
- The enlarged dataset (n = 244) was used to recalibrate the Sabbagh equation and the equation of Chen et al. (2016) and to test an alternative, regression-free mass balance approach (Reichenberger et al., 2017)
- A k-fold cross validation analysis with 2100 individual tests was performed to assess the predictive capability of the Sabbagh and Chen equations.
- A maximum-likelihood-based calibration and uncertainty analysis were performed for the Sabbagh equation using the DREAM_ZS algorithm (Vrugt, 2016)





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Recalibration and cross-validation of pesticide trapping equations for vegetative filter strips (VFS) using additional experimental data

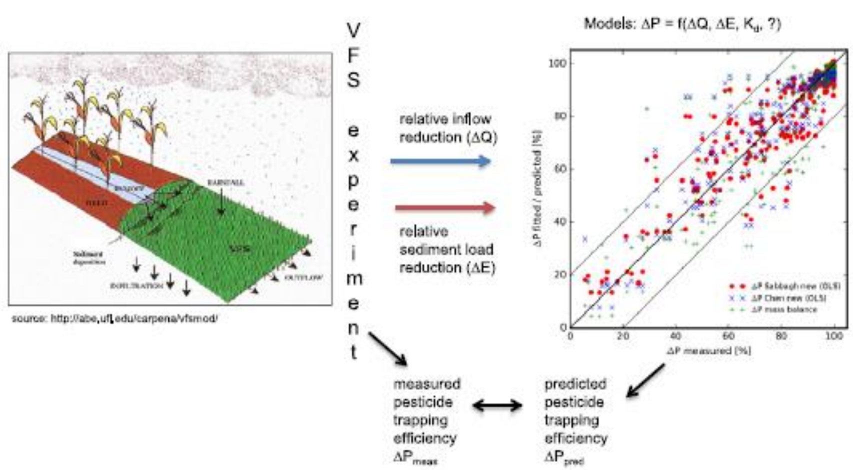
Stefan Reichenberger [a,*], Robin Sur [b], Carolin Kley [b], Stephan Sittig [a], Sebastian Multsch [a]

[a] *knoell Germany GmbH, Konrad-Zuse-Ring 25, 68163 Mannheim, Germany*
[b] *Bayer AG, 40789 Monheim, Germany*

HIGHLIGHTS

- Lack of parsimonious mechanistic approaches for modelling pesticide trapping in filter strips
- Sabbagh regression equation needed broader data basis and rigorous evaluation
- Experimental data basis has been considerably widened
- Suitability of Sabbagh equation for modelling pesticide trapping in vegetative filter strips has been confirmed
- Regression-free mass balance approach is viable alternative

GRAPHICAL ABSTRACT



Previous work (2)

Conclusions of Reichenberger et al. (2019):

- The study confirmed the suitability of the Sabbagh equation for modelling pesticide trapping in VFS.
- The new parameter set obtained with OLS regression has been corroborated by both the cross-validation analysis and the DREAM_ZS simulations.
  - It can be recommended for use in regulatory modelling with VFSMOD.
  - It constitutes a major improvement in terms of predictive capability and statistical justification compared with the original coefficients of Sabbagh et al. (2009)
- Because of being mechanistic and its overall good predictive performance, the mass balance approach can be recommended as a viable alternative to the Sabbagh eq.

The latest version of VFSMOD (v.4.4.0; 08/2018) includes 4 pesticide trapping options:

- original Sabbagh eq. (original coefficients)
- Sabbagh eq. with user-defined coefficients
- mass balance approach
- Chen eq. (original coefficients)

The new options have not been included in SWAN yet.

Overview of Sabbagh eq. and mass balance approach

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- Sabbagh:
  - old: $\Delta P = 24.79 + 0.54 * \Delta Q + 0.52 * \Delta E - 2.42 * \ln(Fph+1) - 0.89 * \%C$
  - new: $\Delta P = -11.514 + 0.595\ \Delta Q + 0.489\ \Delta E - 0.375\ \ln(Fph+1) + 0.204\ \%C$

where ΔP = relative reduction (%) of total pesticide load, ΔQ = relative reduction (%) of total inflow, ΔE = relative reduction (%) of incoming sediment load, F_{ph} = phase distribution coefficient (ratio of dissolved and particle-bound pesticide mass in inflow), and %C = clay content (%) of field topsoil (as a proxy for the clay content of the eroded sediment). The phase distribution coefficient is given as:

$$F_{ph} = \frac{Q_i}{K_d E_i}$$

where Q_i = total water inflow into the VFS (run-on + rainfall + snowmelt (L)), E_i = incoming sediment load (kg), K_d = linear sorption coefficient (L kg^{-1}).

- Mass balance approach:

$$\frac{\Delta P}{100\%} = \frac{\min[(V_i+K_d E_i);\left(\frac{\Delta Q}{100\%}V_i+\frac{\Delta E}{100\%}K_d E_i\right)]}{(V_i+K_d E_i)}$$

with Vi = incoming run-on volume (L)

Follow-up study

- Idea: Simulate real runoff events with the full VFSMOD model

- Objectives
  - ➢ compare the performance of the different trapping equations
    - original Sabbagh
    - Sabbagh with new coefficients from Reichenberger et al. (2019)
    - mass balance approach
  - ➢ assess the relative importance of the choice of the trapping equation compared with other factors, notably
    - input hydrographs (rainfall; run-on)
    - initial and boundary conditions
    - hydraulic parameters

Materials and Methods

Preliminary considerations

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- Since ca. 2011 VFSMOD is able to simulate shallow water tables (e.g. Muñoz-Carpena et al., 2011 and 2018).
- This feature is especially relevant for VFS adjacent to surface water bodies or for soils with poorly permeable or impermeable horizons.

- Global Sensitivity Analyses for VFSMOD are available (e.g. Lauvernet and Muñoz-Carpena, 2018)
  → Sensitivity of model parameters well known for situations with and without shallow water table (WT)

- For real VFS experiments, VFS dimensions are fixed → most important parameters will be
  - vertical saturated conductivity VKS (no WT and WT)
  - water table depth (WT only)

Study / event selection

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- 4 studies with 16 hydrological events were selected from the data compiled by Reichenberger et al. (2019)
- 1 hydrological event = unique combination of site, treatment and date
- 31 combinations of hydrological event and compound
- different levels of data availability and uncertainty in experimental data
- no information on presence/depth of a shallow water table available

Study	country	site	event dates	surface runoff generation	nb hydrol. events	compounds	availability of hydrographs
Arora et al. (1996)	USA	Ames, Iowa [1)]	06/1993	natural rainfall	2	atrazine, cyanazine, metolachlor	run-on; outflow (partly)
Boyd et al. (2003)	USA	Ames, Iowa [1)]	06/1999	natural rainfall	2	acetochlor, atrazine, chlorpyrifos	rainfall duration; run-on; outflow
Réal (1997)	FR	Bignan, Bretagne [2)]	12/1994 – 02/1995	natural rainfall	7	diflufenican, isoproturon	none
White et al. (2016)	USA	St. Paul, Minnesota	06/2015-07/2015	Simulated run-on + simulated rainfall on VFS	5	tebuconazole, trichlorfon eq.	rainfall, run-on, outflow

[1)] same site, same experimental device

[2)] run-on, sediment and pesticide inputs into VFS estimated as outflow from control plots

Preparation of model input

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- Parameterisation largely according to SWAN scenario report (Brown et al., 2012)
  - HYPRES pedotransfer functions for water retention (Van Genuchten) and saturated hydraulic conductivity VKS
  - if unknown, estimate bulk density according to Rawls (1983)
  - initial soil water content (relevant for no WT only) estimated using ThetaFAO tool and available weather time series
  - SWAN-VFSMOD default values for overland flow (RNA) and sediment filtration parameters (COARSE, DP; SS, VN, H, VN2); exception: filter media height (H) was given in White et al. (2016)

- Rainfall hydrograph (hyetograph):
  - if no real hydrograph available, use generic rectangular one
  - if both duration and intensity are unknown, estimate one of them

- Run-on hydrograph:
  - if no real hydrograph available, use generic triangular one
  - estimate onset of run-on if unknown

Simulation setup, running and postprocessing

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- Variation:
  - ➢ multiply estimated VKS with constant factor: 1, 5, 10, 20, 50, 100
  - ➢ different levels of water table depth: none, 0.5 m, 1.0 m, 1.5 m
  - ➢ test effect of ICO switch (= feedback of sedimentation on infiltration or not): 0 or 1
- Final number of simulations:

  31 combinations of hydrological event and chemical *

  2 (ICO switch on/off) *

  4 WTD values (none, 0.5 m, 1.0 m, 1.5 m) *

  6 VKS factors (1, 5, 10, 20, 50, 100)

  → 1488 VFSMOD simulations
- target output variables for comparison with measured values:
  - ➢ relative reduction of total water inflow (rainfall + run-on) (ΔQ)
  - ➢ relative reduction of incoming sediment load (ΔE)
  - ➢ relative reduction of total pesticide load (ΔP)
  - ➢ (relative reduction of surface runoff volume (ΔR))
- VFSMOD running and postprocessing were performed with a tool programmed by S. Multsch in Python

Results and Discussion

Hydrology and sediment trapping: Overall performance

variable	Mean difference predicted - measured ΔQ and ΔE (%)			
	over all 16 * 48 hydrologically unique simulations	over the „default" simulations (VKSfac = 1, no WT)	over the best hydrological simulations for each event	over the best hydrological simulations for each event with ΔQ pred < 100 %
	(n = 768)	(n = 16)	(n = 16)	(n = 10)
	%	%	%	%
ΔQ	-19.03	-24.15	**-1.66**	-4.93
ΔE	18.52	18.45	18.51	26.04

Summary for hydrology and sediment trapping

- Sensitivity of ICO switch was found very low (for both ΔQ and ΔE)
- On average, the „default" parameterisation (VKS according to HYPRES; no WT) did not yield good ΔQ estimates.
- Effect of varied factors on ΔE was very small

- Best hydrological simulations
  - determined by
    - simulated vs. measured ΔQ
    - visual fit of outflow hydrograph (if measured hydrograph available)
  - ΔQ well predicted
    - best parameterisations (VKS / WTD) relatively consistent between events of the same study
    - however, very different best parameterisation between the 2 studies from the same site
  - ΔE generally overestimated
    - especially for the two hydrologic events of Arora et al. (1996)
    - however: „blind" simulation with only default values for overland flow and sediment filtration → results could surely be improved with more site-specific parameter values

Observed vs. predicted ΔQ and ΔE for best hydrological simulations

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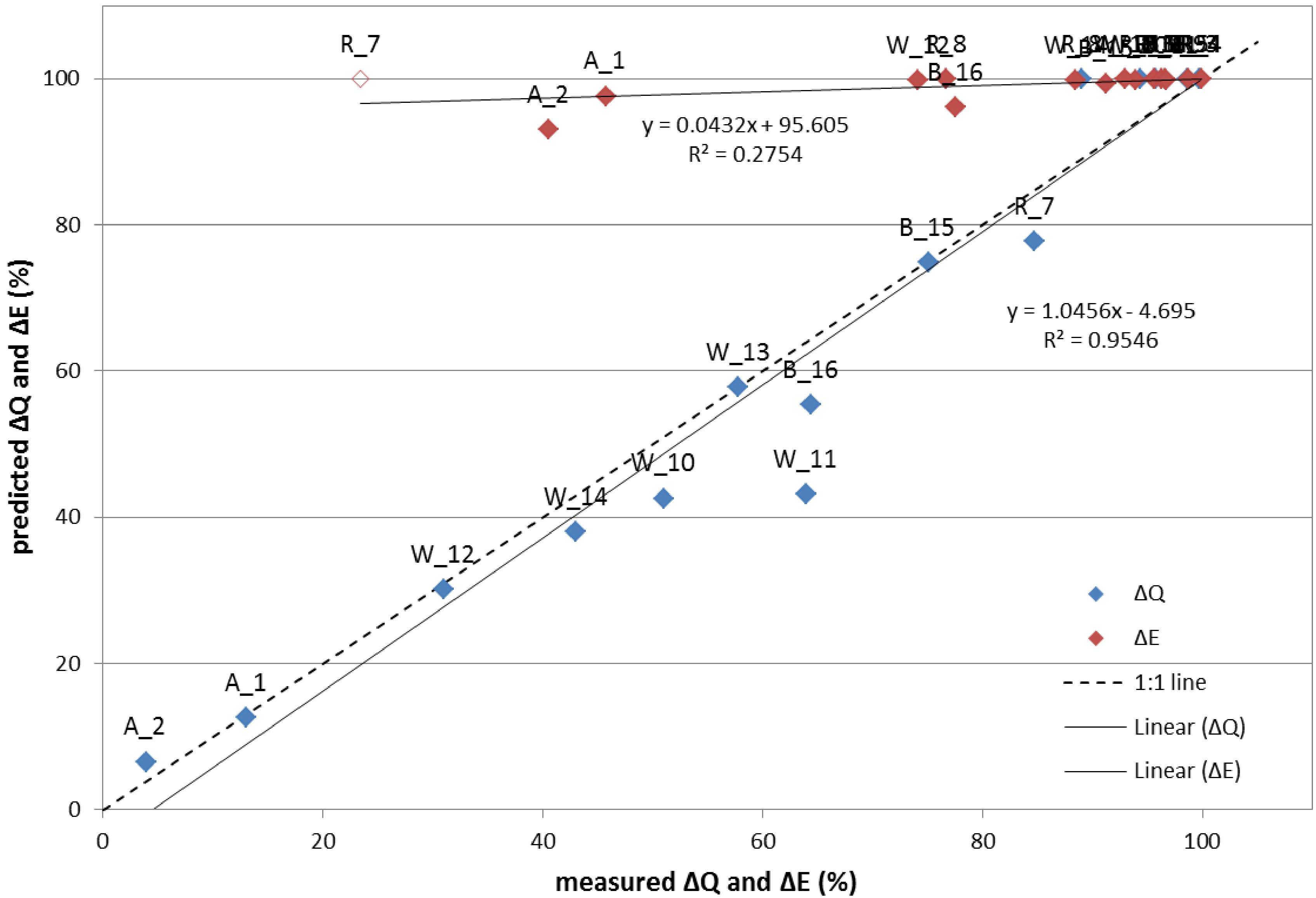

Best simulation h_event 1, Arora et al. (1996)

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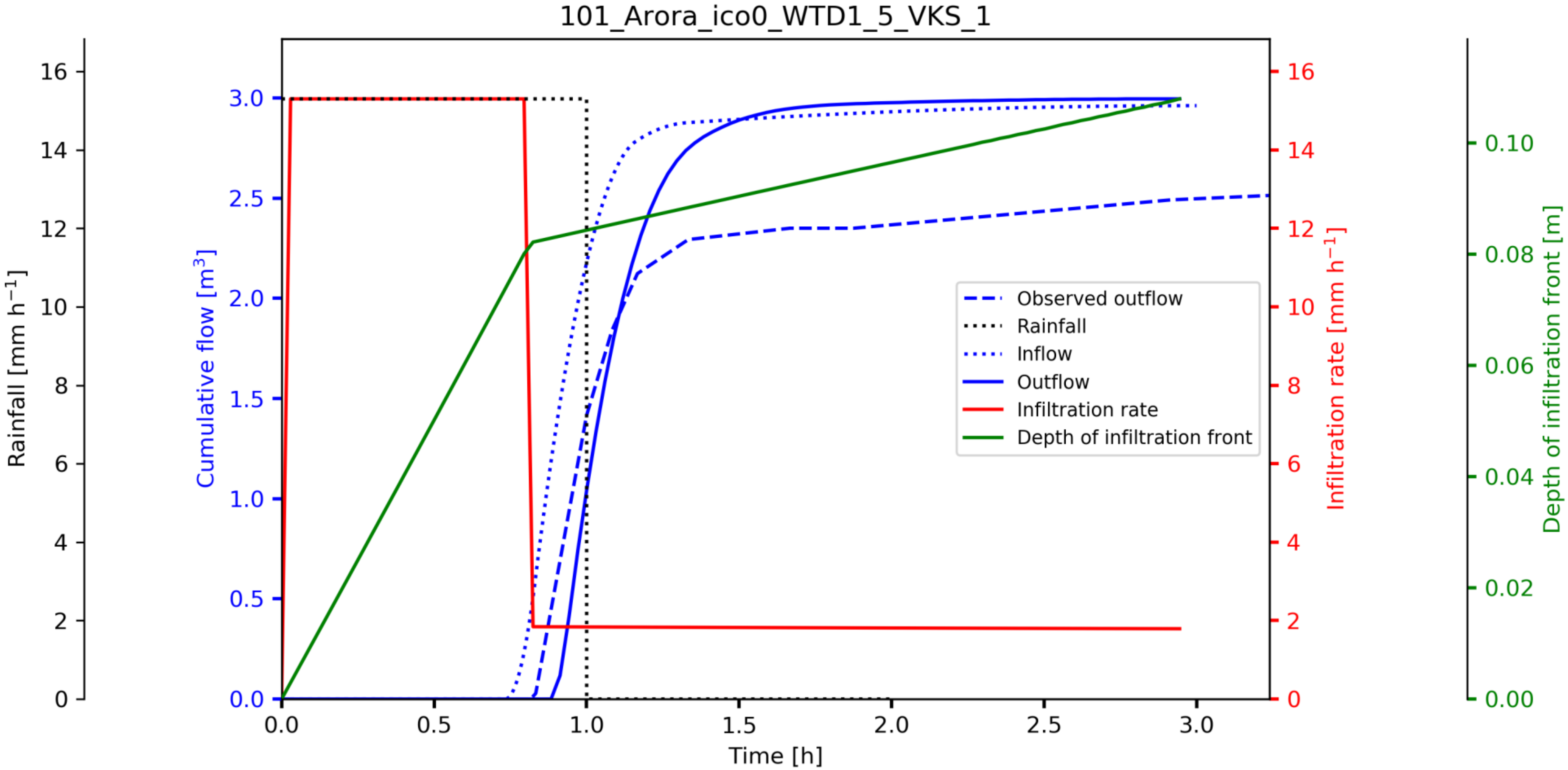
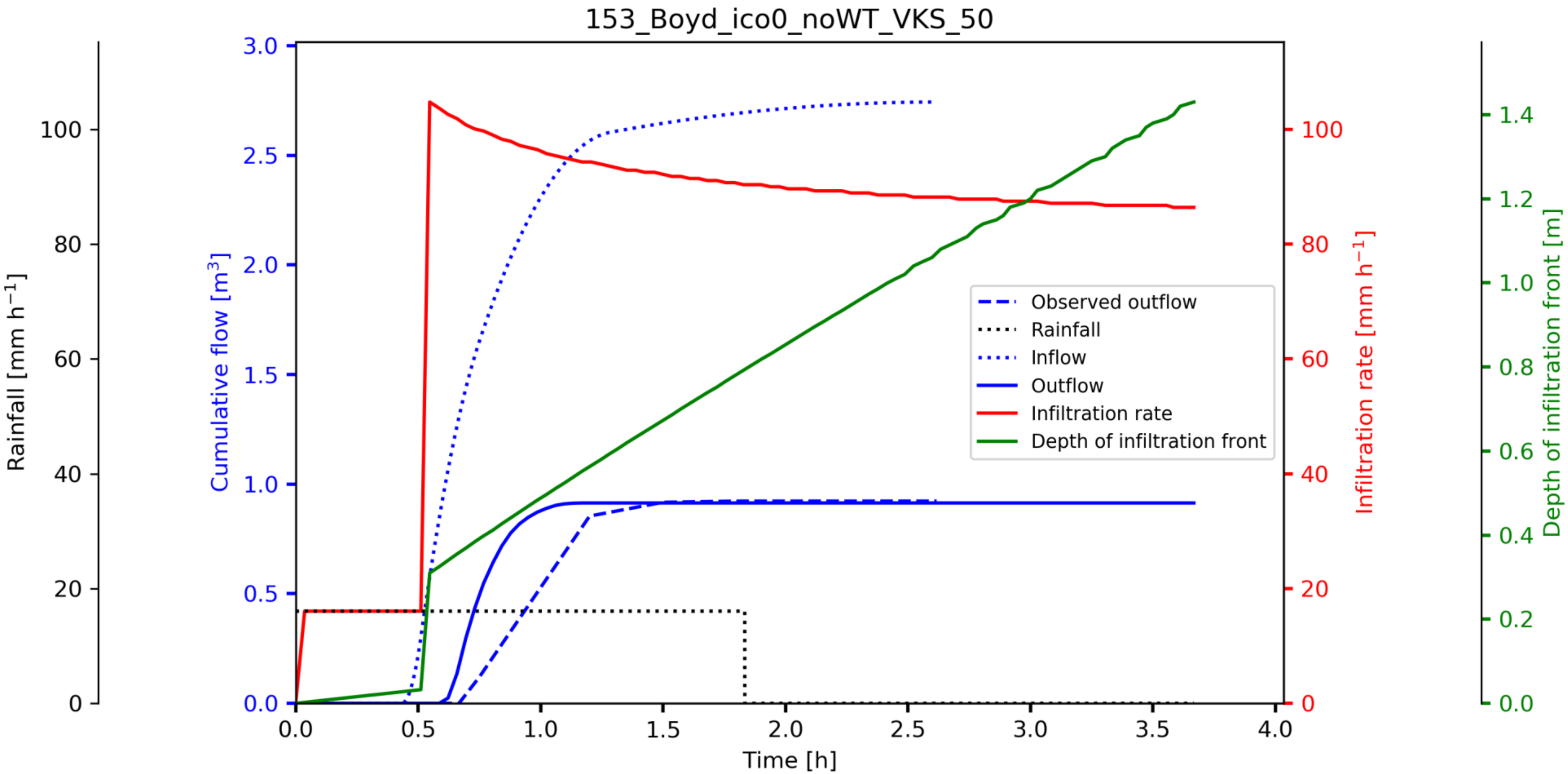


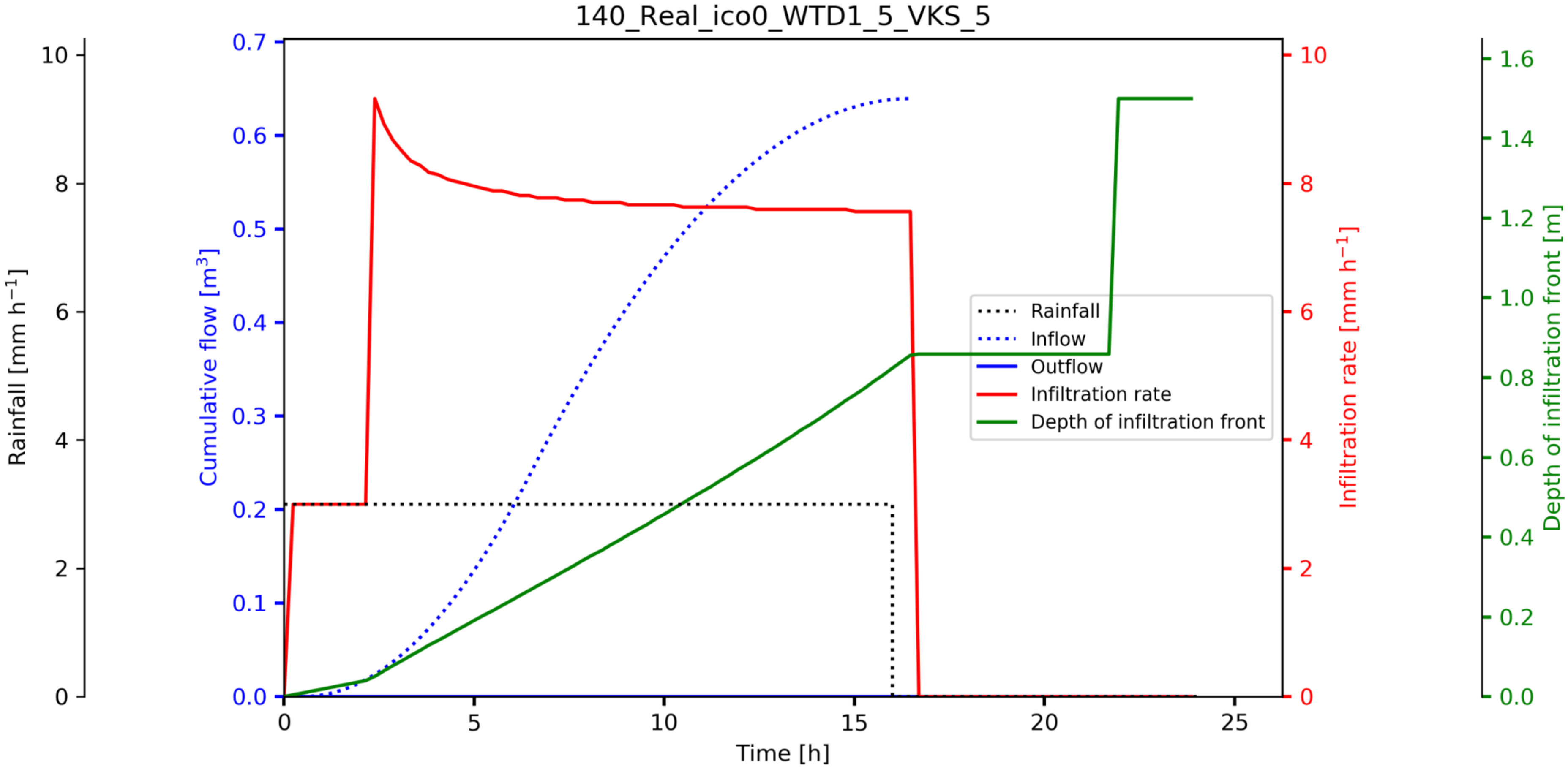
- VL = 20.12 m; FWIDTH = 1.52 m
- run-on dominated event: V_i/Q_i = 86.35 %
- outflow hydrograph reported only for one replicate: actual mean Q_o meas = 2.982 m^3
- ΔQ meas = 13.05 %; ΔQ pred = 12.57 %; ΔE meas = 45.76 %; ΔE pred = 97.62 %
- similar results for different water table depths → infiltration front does not reach water table → infiltration limited by VKS (1.627 mm/h) and initial soil water content

Best simulation h_event 15, Boyd et al. (2003)



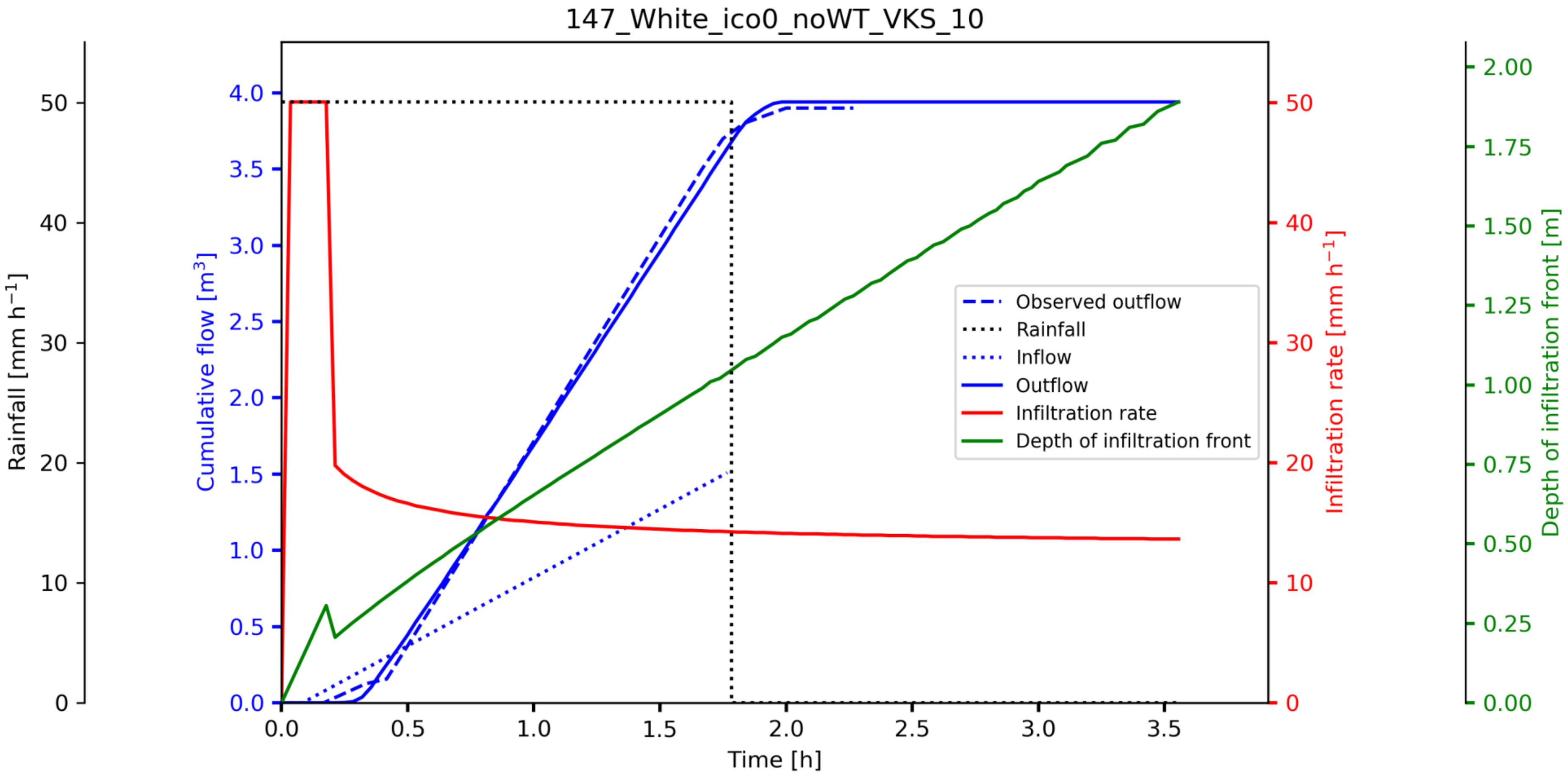
- VL = 20.12 m; FWIDTH = 1.52 m
- event somewhat less dominated by run-on: V_i/Q_i = 74.16 %
- ΔQ meas = 75.06 %; ΔQ pred = 74.88 %
- ΔE meas = 91.27%; ΔE pred = 99.33 %
- 50-fold higher saturated hydraulic conductivity (VKS = 81.36 mm/h) and no WT needed to match ΔQ → VFS system must have changed in six years (biopores?)

Best simulation h_event 5, Réal (1997)



- VL = 12 m; FWIDTH = 5 m
- event dominated by rainfall (48 mm): V_i/Q_i = 18.18 %
- ΔQ meas = 94.31 % (slightly underestimated due to tank overflow for control plot); ΔQ pred = 100 %
- ΔE meas = 98.80 %; ΔE pred = 100 %
- 6 simulations yielded ΔQ = 100 %: no WT / VKSfac ≥ 5; WTD = 1.5 / VKSfac = 5 → nonuniqueness

Best simulation h_event 12, White et al. (2016)



- VL = 15.24 m; FWIDTH = 3.05 m
- event dominated by rainfall (89 mm): V_i/Q_i = 26.71 %
- ΔQ meas = 30.98 %; ΔQ pred = 30.11 %
- ΔE meas = 74.16 %; ΔE pred = 99.82 %
- 10-fold higher saturated hydraulic conductivity (VKS = 12.89 mm/h) and no WT needed to match ΔQ

Pesticide trapping efficiency (ΔP): Comparison of overall performance

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Trapping equation	Mean difference predicted - measured ΔP (%)			
	over all 31 * 48 simulations	over the „default“ simulations	over the simulations with best ΔP for each event	over the best hydrological simulations for each event with ΔQ pred < 100 %
	(n = 1488)	(n = 31)	(n = 31)	(n = 24)
Sabbagh_old	**-4.64**	**-9.54**	3.34	7.38
Sabbagh_new	-6.10	-11.99	5.45	**3.10**
mass balance	-25.10	-33.60	**-1.76**	-15.4

Note: For Boyd et al. (2003) and Réal (1997) there are uncertainties in the measured ΔP because of unknown residues in the VFS topsoil from previous events; for Réal (1997) an approximate residue estimation could be made

Observed vs. predicted ΔP for the best hydrologic simulations for each event with predicted ΔQ < 100 %

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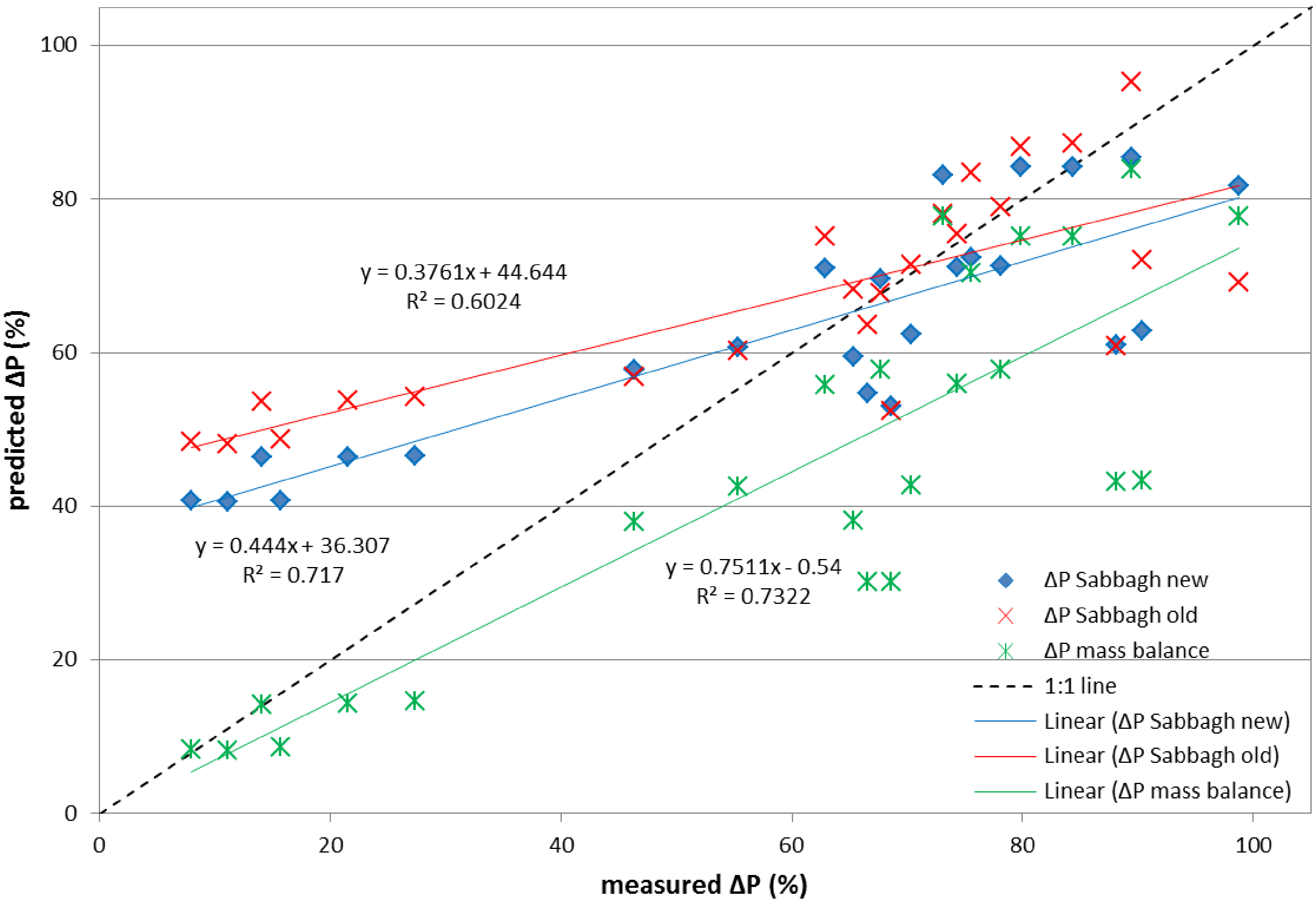

Observed vs. predicted ΔP for the best hydrologic simulations for each event with predicted ΔQ < 100 %; label: study + hydrol_event

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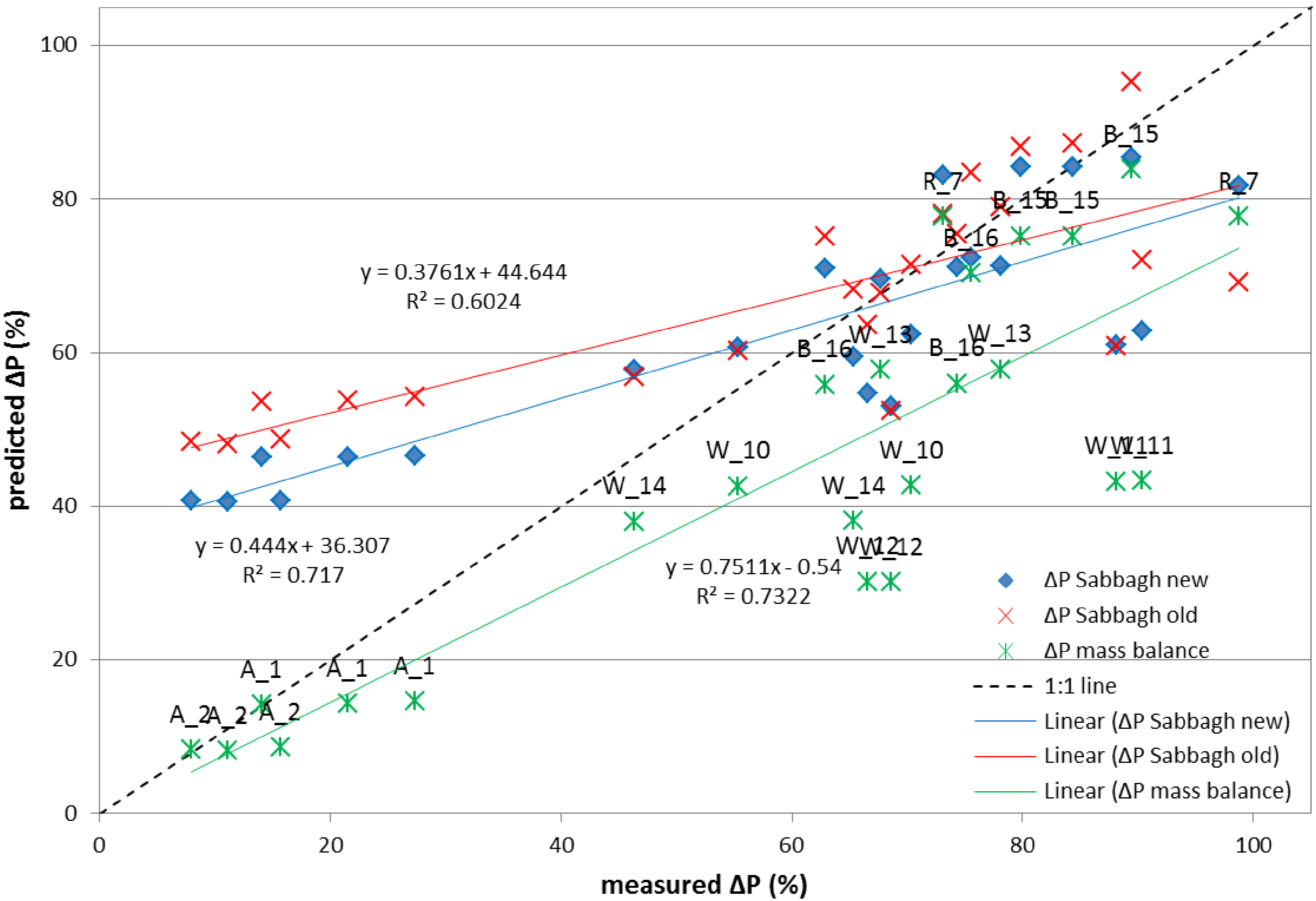

Observed vs. predicted ΔP for the best hydrologic simulations for each event with predicted ΔQ < 100 %; label: K_{OC} (L/kg)

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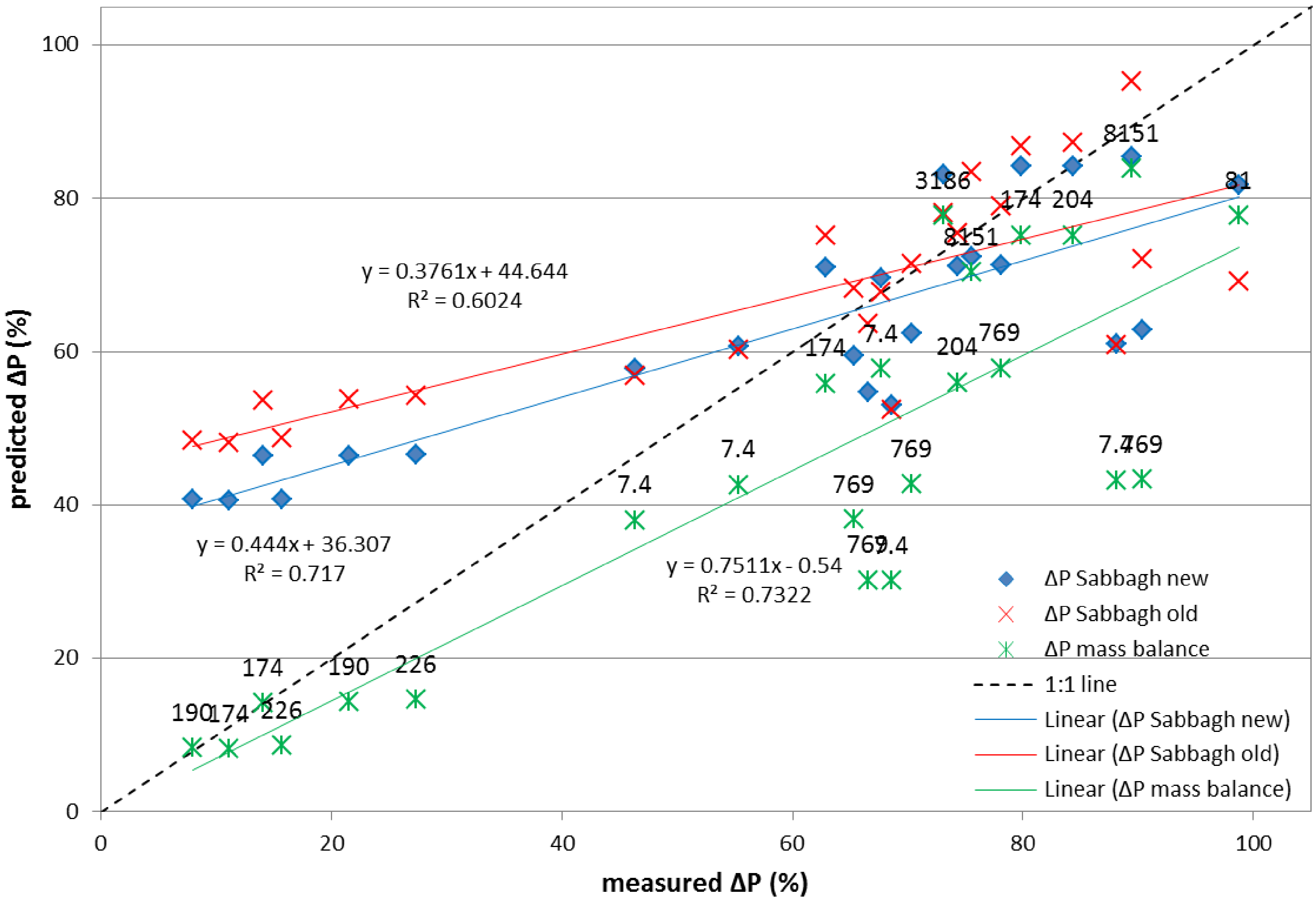

Observed vs. predicted ΔP for the best hydrologic simulations for each event with predicted ΔQ < 100 %; label: K_{OC}; add ΔQ pred

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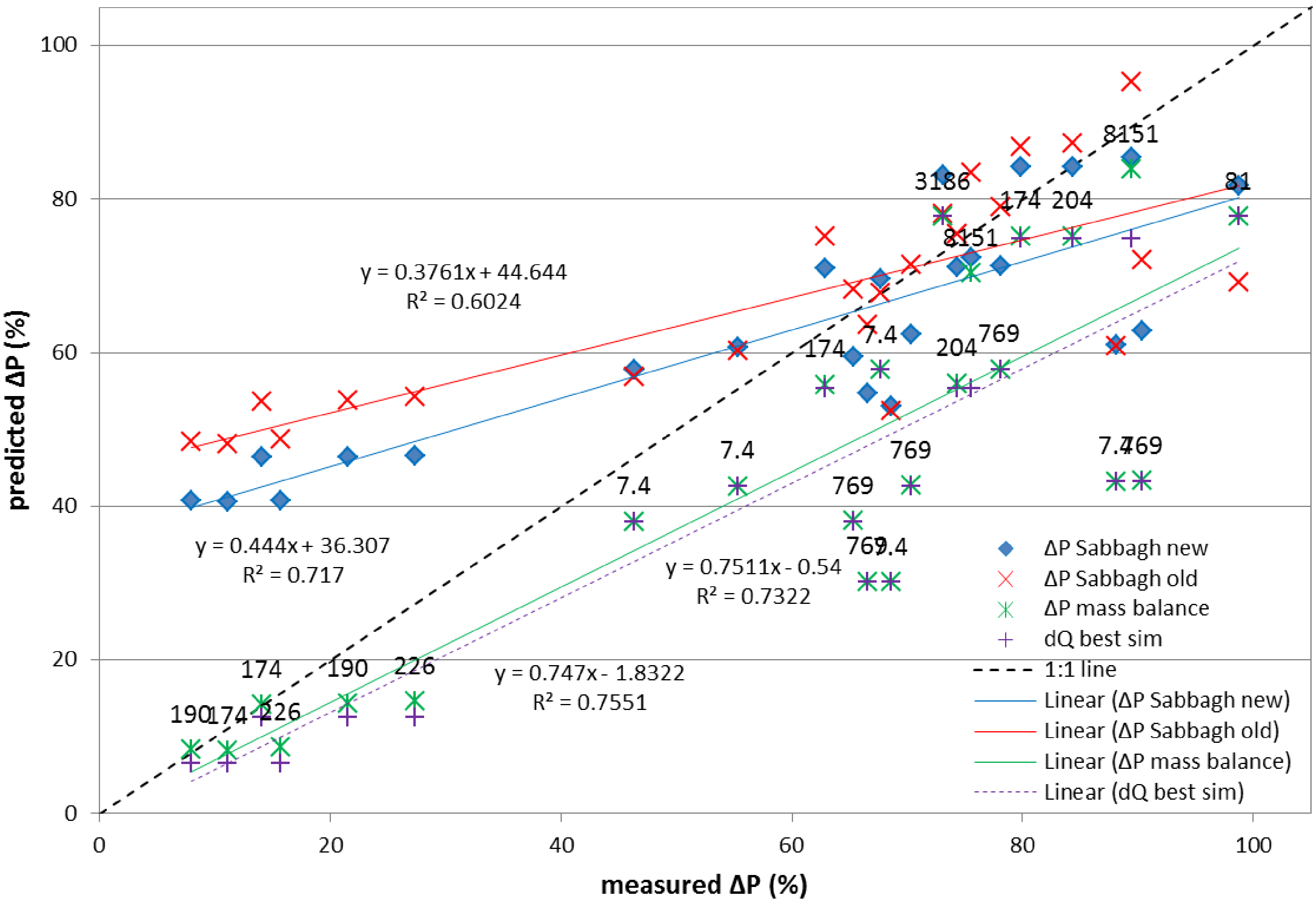

Conclusions and Outlook

Conclusions: Hydrology and sediment trapping

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- ΔQ could be well matched after adjusting vertical hydraulic conductivity (VKS) and water table depth (WTD).
- VKS estimated with HYPRES too low in many cases (ptf does not account for preferential flow)
- ΔE was generally overestimated (but then only default values for overland flow and sediment filtration were used)
- Rainfall and run-on hydrographs (notably duration and intensity) do affect the predicted ΔQ → hydrographs should be carefully established

Implications for SWAN-VFSMOD:

- parameterisation of VKS seems to be too conservative
- parameterisation of sediment filtration seems to be too optimistic (need to look into that)
- rainfall and run-on hydrographs should be made more realistic (intensity, duration, time lag)
- Under the current SWAN scenario assumptions, the mathematical effect of ΔR on PECsw is small, and ΔPECsw ≈ ΔP. However, I personally think that it would not be sufficient to get only ΔP right while the hydrology is wrong.

Conclusions: Pesticide trapping efficiency (ΔP)

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- Sabbagh equation:
  - The new Sabbagh equation performed best of the three approaches
  - However, old and new Sabbagh equations rely on well predicted ΔQ and ΔE

- Mass balance approach:
  - was the most conservative of the three (however, this cannot be generalised; cf. Reichenberger et al. (2019))
  - generally underestimated ΔP
  - but turned out less sensitive to errors in ΔE than Sabbagh (however, this is because there were only substances with Koc $\leq 10^4$ L/kg simulated)
  - → seems safe option for situations where most of the pesticide mass in the run-on is in the dissolved phase

- Outlook: Upgrade of the mass balance approach under discussion

Many thanks for your attention!

Supplementary slides

Outlook – Potential upgrades of mass balance approach

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- The mass balance approach is mechanistic, but
  - it only considers mixing, infiltration and sedimentation
  - it does not consider processes such as sorption of dissolved pesticide to soil or plant material in the VFS

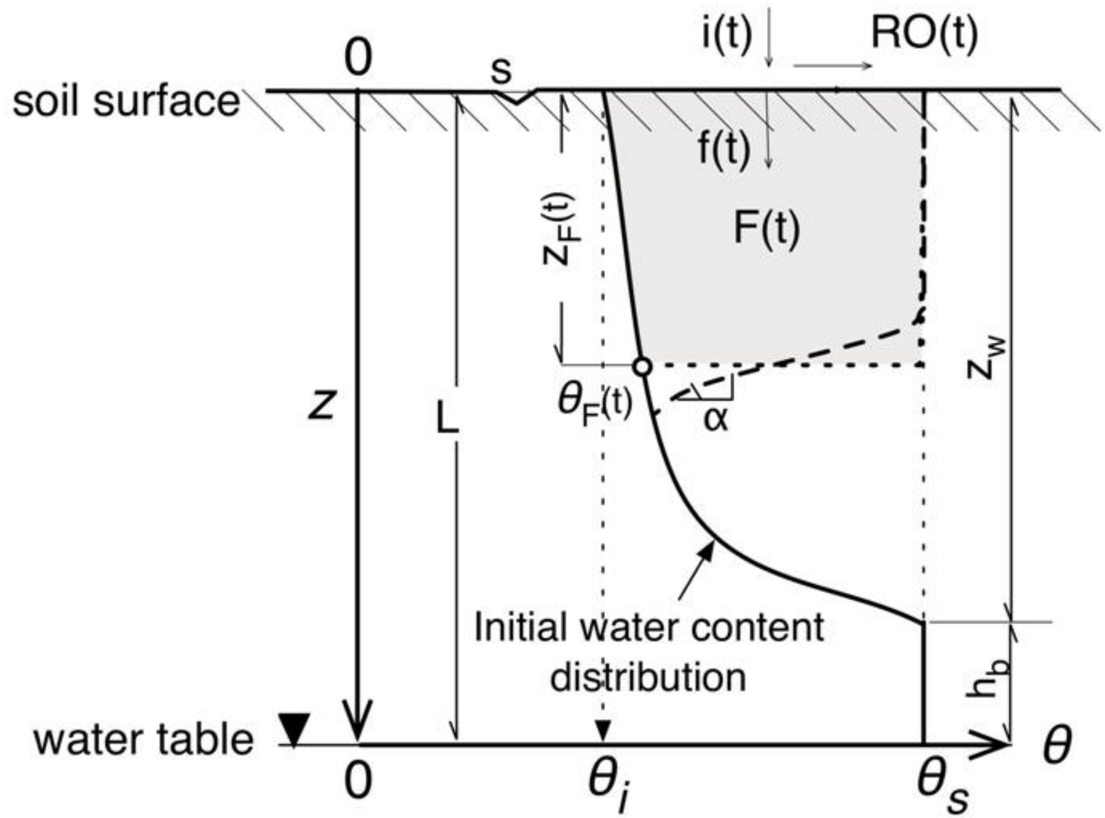
- Moreover, the lumped mixing assumption ($C' = Ci * V_i/Q_i$) is probably too coarse.
  - spatial and temporal discretisation of C‘ may help
  - The approach could be upgraded in a relatively straightforward manner to a simple dynamic and spatially explicit convective model which uses only existing VFSMOD output files (under discussion with VFSMOD developer).

Infiltration and redistribution in VFSMOD before water table is reached

- At the beginning of the event, the soil above the shallow water table is in hydrostatic equilibrium with the shallow water table.

- The wetting front proceeds from the surface (according to Green-Ampt) and fills up the profile from the top.

- Once the wetting front reaches the upper boundary of the capillary fringe (t = tw), the profile is completely saturated and the boundary condition changes.



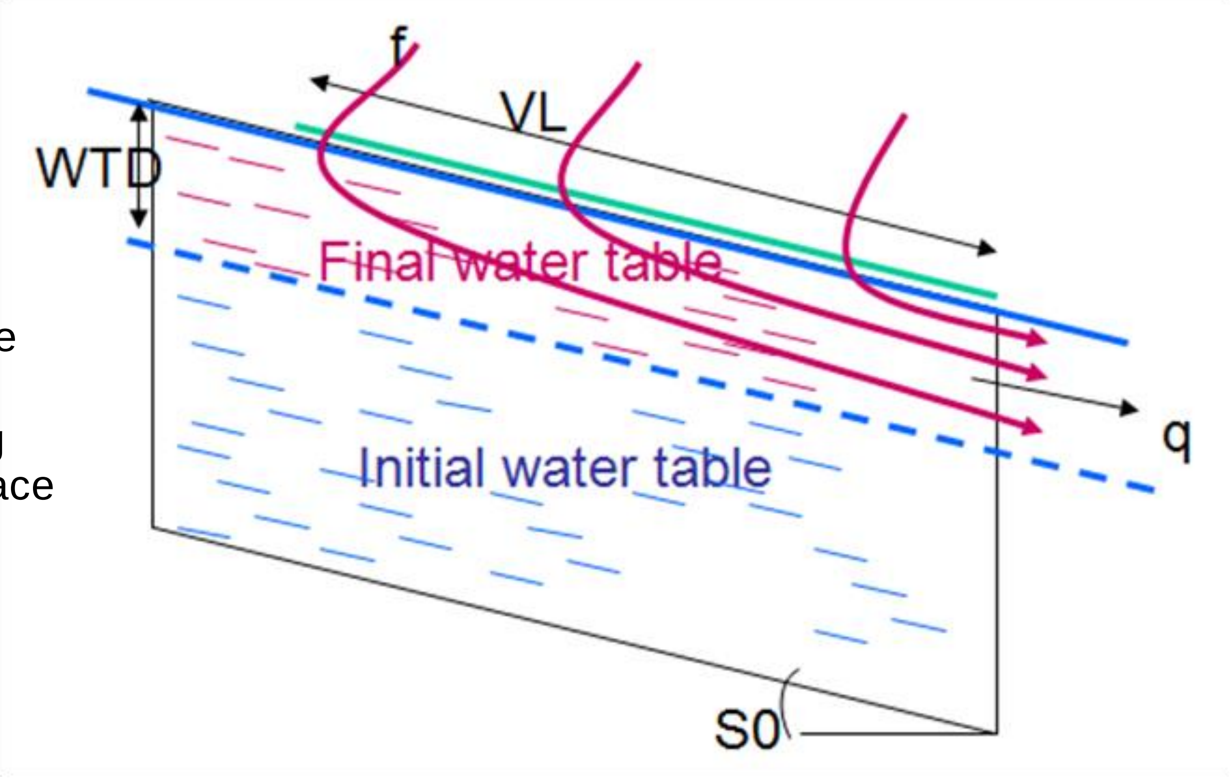
Source: Rafael Muñoz-Carpena

Water flow in VFSMOD for BC1 once soil profile is saturated

- For t ≥ tw the initial water table is a no-flux boundary condition (due to a zero hydraulic gradient).
- Infiltration flow at the surface (Q_f) is only allowed by lateral flow (Q_L) at the downslope boundary of the simulated soil elementary volume.
- The infiltration rate is then given as f = VKS/RVH * WTD/VL * S_0.

Dupuit-Forchheimer assumptions:

- The flow is horizontal at any vertical cross-section.
- The velocity is constant over the depth.
- The velocity is calculated using the slope of the free water surface as the hydraulic gradient.
- The slope of the water table is relatively small.



Source: N. Carluer, provided by Rafael Muñoz-Carpena

Soil properties of the three VFS sites

Study	site	soil description	USDA texture class	clay	silt	sand	OM	BD
				%	%	%	%	kg/dm^3
Arora et al. (1996); Boyd et al. (2003)	Ames, Iowa	Clarion loam	loam	21.0	34.0	45.0	5.17	1.16 [1)]
Réal (1997)	Bignan, Bretagne	silt loam	loam	17.2	46.2	36.6	7.0	1.02 [1)]
White et al. (2016)	St. Paul, Minn.	Mollic Hapludalf	sandy loam	12.0 [2)]	33.0 [2)]	55.0 [2)]	3.25 [2)]	1.54 [3)]

[1)] estimated according to Rawls (1983)

[2)] properties averaged over the top two layers (0-3‘‘ and 3-6‘‘); these two layers were also used for the run-on matrix

[3)] undisturbed soil cores

Sabbagh equation

The Sabbagh equation with the original coefficients by Sabbagh et al. (2009) is given as:

$$\Delta P = 24.79 + 0.54\ \Delta\mathrm{Q} + 0.52\ \Delta\mathrm{E} - 2.42\ \ln\left(F_{ph} + 1\right) - 0.89\ \%\mathrm{C}$$

where ΔP = relative reduction (%) of total pesticide load, ΔQ = relative reduction (%) of total inflow, ΔE = relative reduction (%) of incoming sediment load, F_{ph} = phase distribution coefficient (ratio of dissolved and particle-bound pesticide mass in inflow), and %C = clay content (%) of field topsoil (as a proxy for the clay content of the eroded sediment). The phase distribution coefficient is given as:

$$F_{ph} = \frac{Q_i}{K_d E_i}$$

where Q_i = total water inflow into the VFS (run-on + rainfall + snowmelt (L)), E_i = incoming sediment load (kg), K_d = linear sorption coefficient (L kg^{-1}).

→ 5 regression parameters and 6 independent variables: ΔQ, ΔE, Q_i, E_i, K_d and %C

Chen equation

The Chen equation with the original coefficients by Chen et al. (2016) is given as:

$$\Delta P = 101 - (8.06 - 0.07\,\Delta Q + 0.02\,\Delta E + 0.05\,\%C - 2.17\,Cat + 0.02\,\Delta Q\,Cat - 0.0003\,\Delta Q\,\Delta E)^2$$

where Cat is a categorical variable with Cat = 1 for Koc > 9000 L kg^{-1} and Cat = 0 for Koc ≤ 9000 L kg^{-1}.

- For the Chen equation the fit is not performed against ΔP directly, but against the transformed variable $(101 - \Delta P)^{0.5}$.
- The Chen equation has 7 regression parameters, but only 4 independent variables: ΔQ, ΔE, %C and K_{oc}.
- The actual mass distribution between the liquid and the solid phase of the surface runoff is not taken into account.

Mass balance approach (Reichenberger et al., 2017)

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Three key assumptions:

1) instantaneous and complete mixing of incoming run-on and incoming rainfall on the VFS (prerequisite: time lag between rainfall and run-on is short)
2) constant particle-bound pesticide concentration in surface runoff during the event
3) infiltration and sedimentation are the only relevant pesticide trapping mechanisms in the VFS, i.e. sorption of dissolved pesticide to soil or plant material in the VFS is negligible.

The approach can be written as a single equation

$$\frac{\Delta \mathrm{P}}{100\%} = \frac{\min[(V_i + K_d E_i);\left(\frac{\Delta Q}{100\%}V_i + \frac{\Delta E}{100\%}K_d E_i\right)]}{(V_i + K_d E_i)}$$

with Vi = incoming run-on volume (L)

- ΔP is expressed as a function of V_i, K_d, E_i, ΔE and ΔQ. → 5 independent variables
- In contrast to the Sabbagh and Chen equations, there is no dependence on clay content.

Old vs. new regression coefficients

- Sabbagh:
  - old: $\Delta P = 24.79 + 0.54 * \Delta Q + 0.52 * \Delta E - 2.42 * \ln(Fph+1) - 0.89 * \%C$
  - new: $\Delta P = -11.514 + 0.595\ \Delta Q + 0.489\ \Delta E - 0.375 \ln(Fph+1) + 0.204\ \%C$

→ decreased intercept

→ much smaller effect of phase distribution coefficient Fph

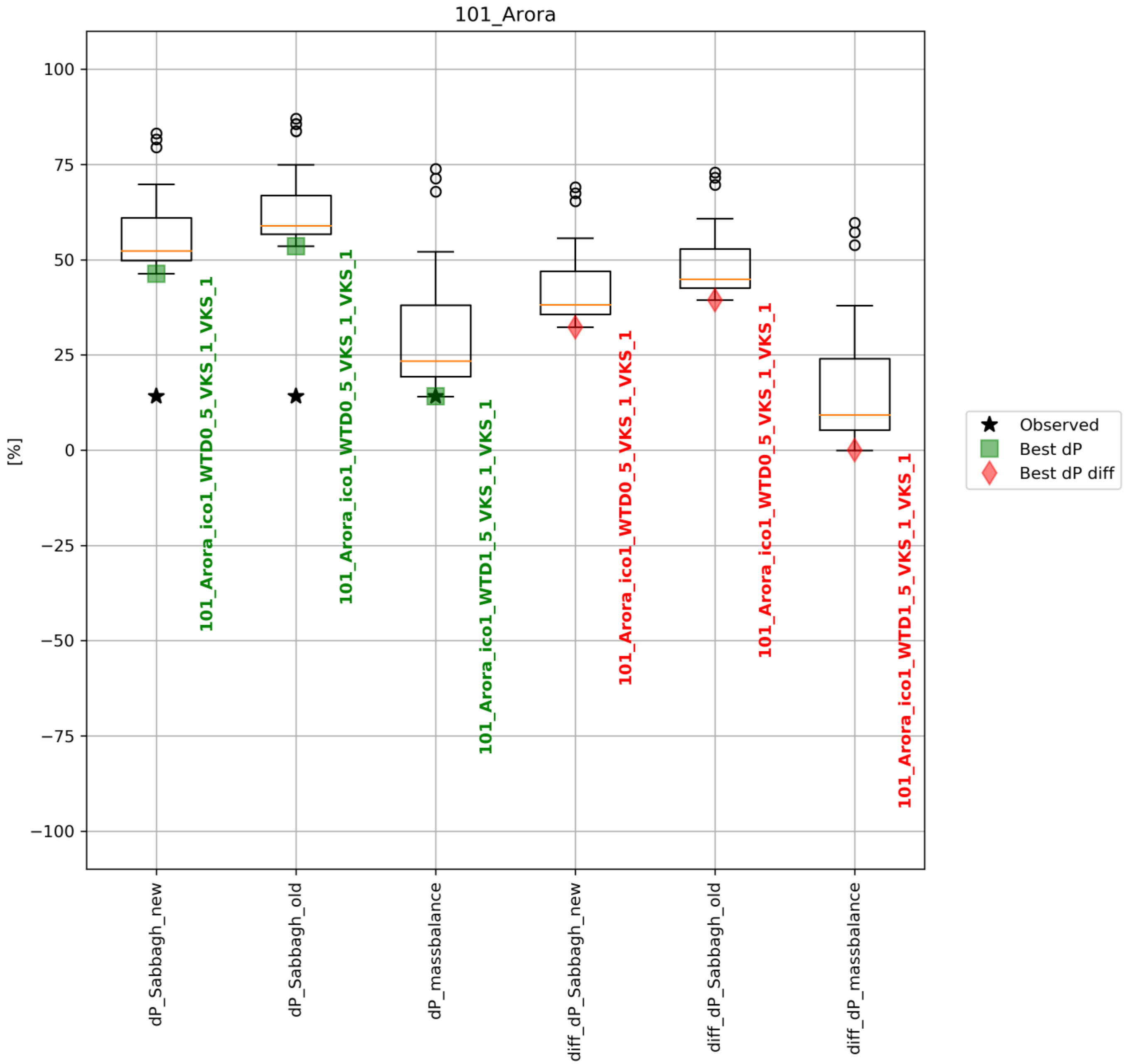
→ effect of clay now much smaller and positive (no explanation yet)

- Chen:
  - old: $\Delta P = 101 - (8.06 - 0.07\ \Delta Q + 0.02\ \Delta E + 0.05\ \%C - 2.17\ Cat + 0.02\ \Delta Q{*}Cat - 0.0003\ \Delta Q{*}\Delta E)^2$
  - new: $\Delta P = 101 - (10.441 - 0.0165\ \Delta Q - 0.00620\ \Delta E - 0.0179\ \%C - 1.704\ Cat + 0.0184\ \Delta Q{*}Cat - 0.000596\ \Delta Q{*}\Delta E)^2$

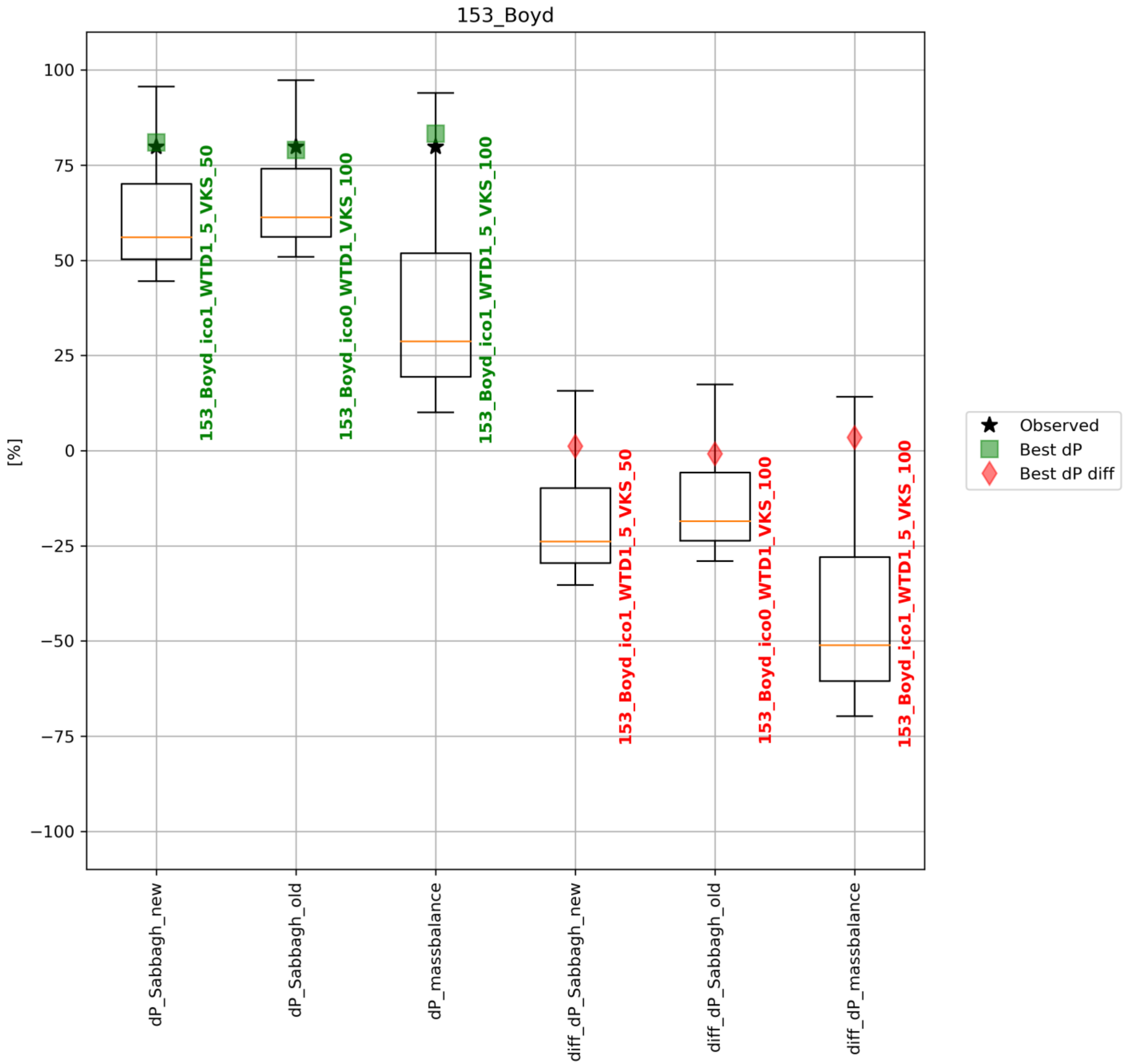
→ p-values for ΔQ, ΔE and $\Delta Q{*}Cat$ are now > 0.05 → overparameterisation → limitation of predictive capability

Box plots of ΔP per event

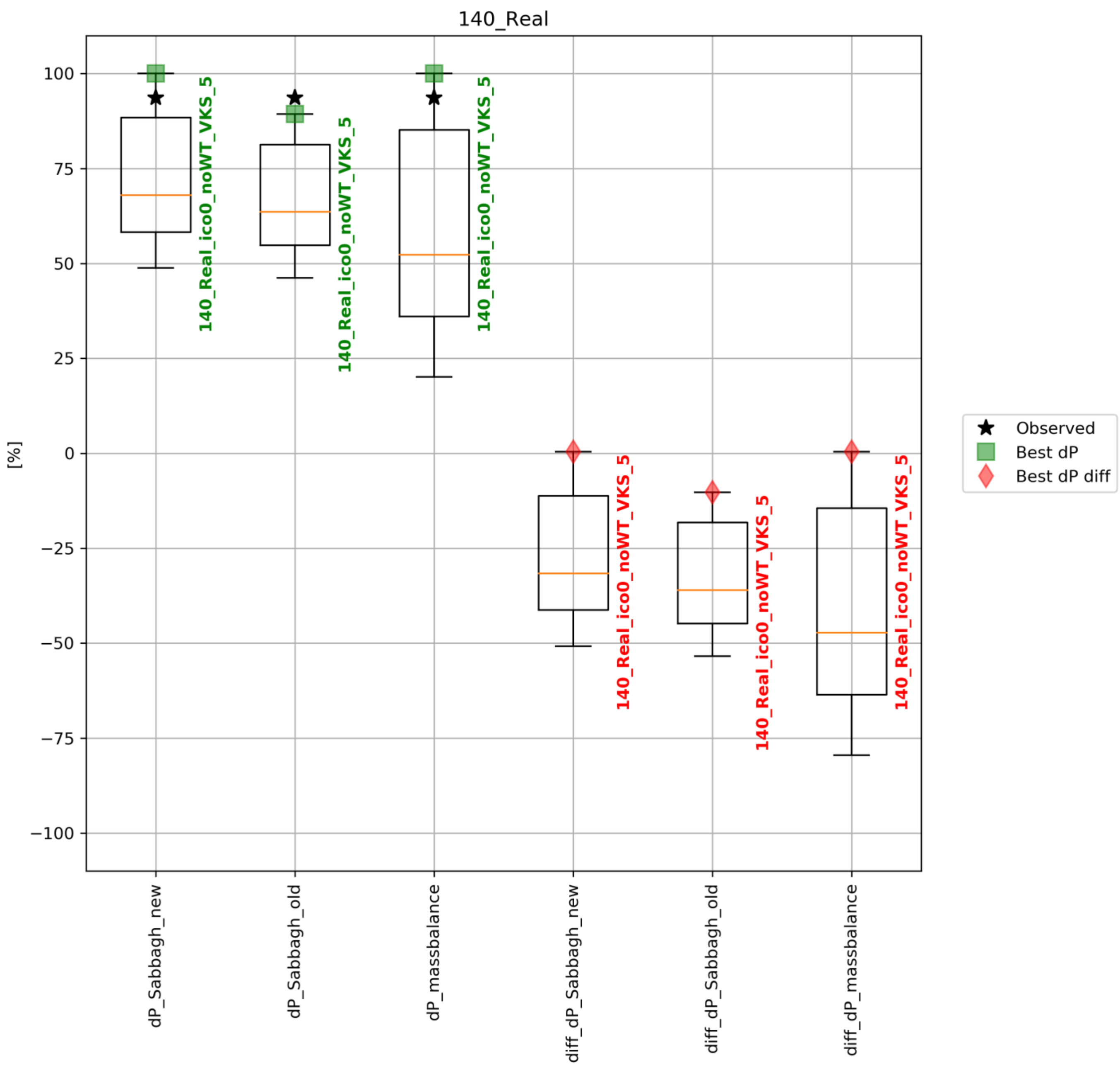
Boxplot ΔP predicted and difference ΔP pred - ΔP meas; n =48



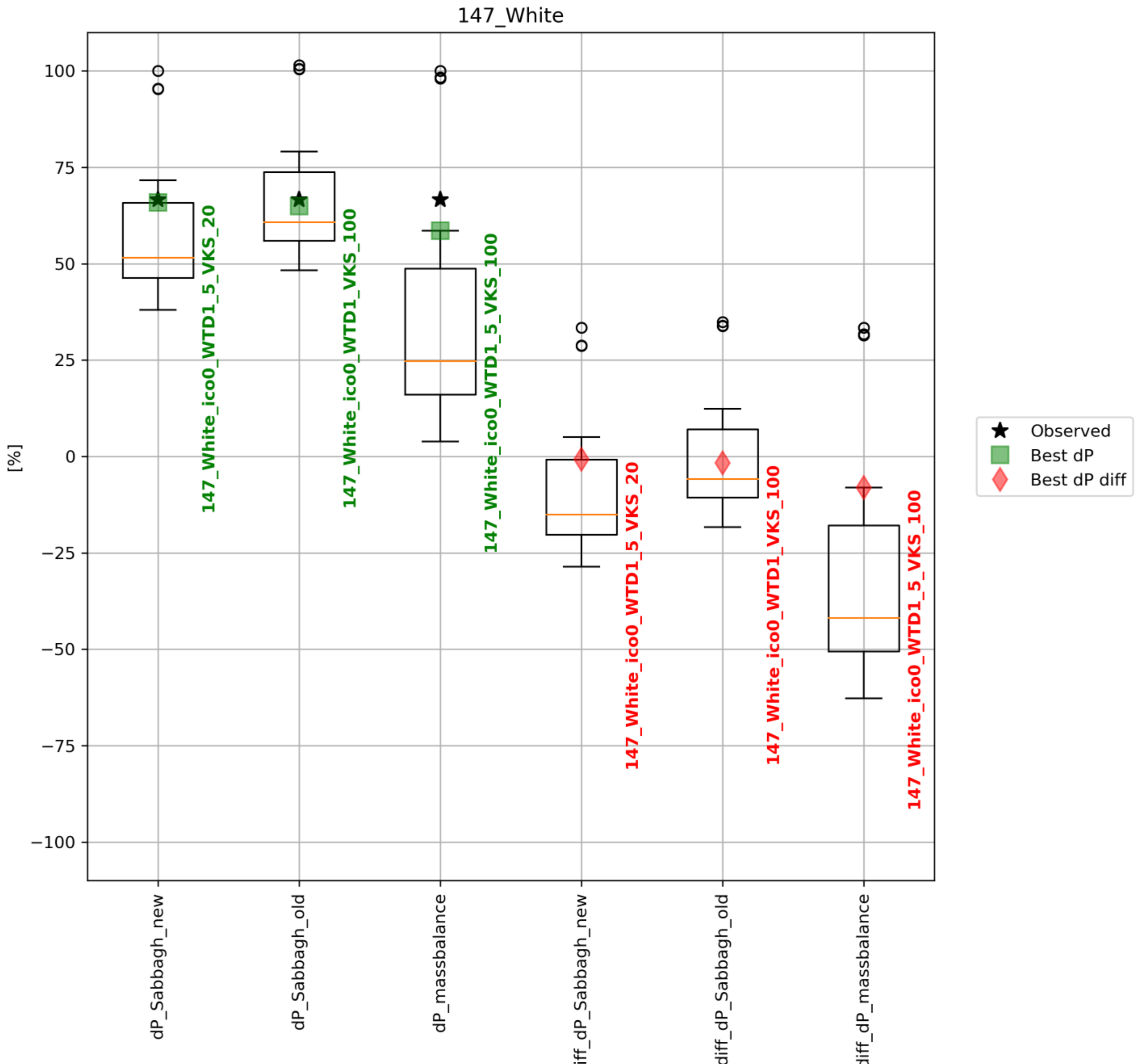
Boxplot ΔP predicted and difference ΔP pred - ΔP meas; n =48



Boxplot ∆P predicted and difference ∆P pred - ∆P meas; n =48



Boxplot ∆P predicted and difference ∆P pred - ∆P meas; n =48



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