CONCEPTUAL MODELS WITH SUPERFLEXPY

1. SuperflexPy

SuperflexPy is an open-source Python framework for constructing conceptual hydrological models for lumped and semi-distributed applications. In these exercises, we will only consider lumped hydrological models.

Information on SuperflexPy can be found in the online documentation https://superflexpy.readthedocs.io/. The following pages are relevant to understand the models used in this exercises session:

- https://superflexpy.readthedocs.io/en/latest/installation.html
- https://superflexpy.readthedocs.io/en/latest/introduction.html (less important)
- https://superflexpy.readthedocs.io/en/latest/components.html (only "elements" and "units")
- https://superflexpy.readthedocs.io/en/latest/numerical_solver.html (less important)
- https://superflexpy.readthedocs.io/en/latest/demo.html (only first three sections)
- https://superflexpy.readthedocs.io/en/latest/popular_models.html
- https://superflexpy.readthedocs.io/en/latest/interfaces.html (less important)
- https://superflexpy.readthedocs.io/en/latest/examples.html

Given that the objective of this session is to understand catchment processes using conceptual models, the models and their calibrated parameters are already provided. Scripts with models and parameters are contained in the folder 'utils' and can be directly imported in Python.

The notebooks (Maimai.ipynb, Huewelerbach.ipynb, Weierbach.ipynb, and Wollefsbach.ipynb) will guide you through the exercises. The remaining of this document illustrates the catchments and the models considered.

2. Description of the catchments and "perceptual" models

The objective of this exercise is to use flexible modelling frameworks to interpret catchment behaviour. We focus on the Maimai catchment in New Zealand and on 3 headwater catchments in Luxembourg on different geologies which behave hydrologically different. All the catchments have been discussed during the lecture on Wednesday.

- The Maimai has an area of 3.8 ha and is underlaid by impermeable bedrock.
- The Huewelerbach catchment has an area of 2.7 km^2 and is located on sandstone underlain by marls.
- The Weierbach catchment has an area of 0.46 km^2 and its geology is dominated by schists.
- The Wollefsbach catchment has an area of 4.5 km^2 and it is located on marls.

Figure 1 illustrates the location of the Luxembourgish catchments and main geological types.

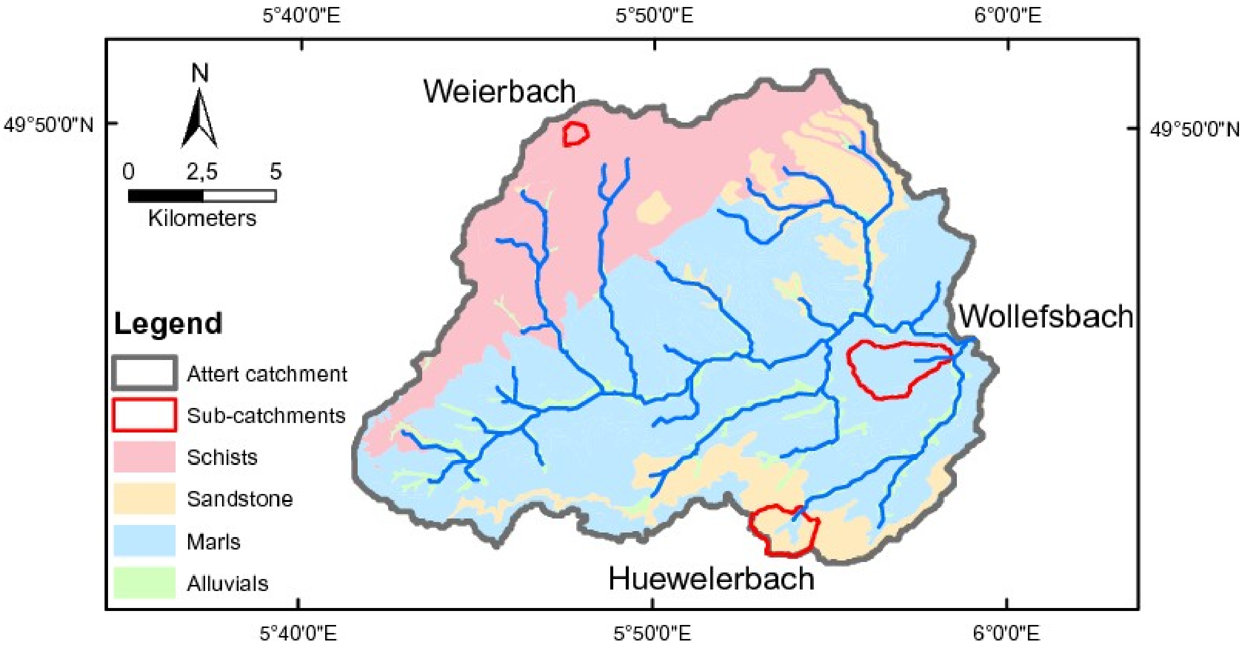

Figure 1: Experimental watersheds on different geological substrata in the Attert catchment in Luxembourg

2.1. Characteristics and responses of the Luxembourgish catchments

Figure 2 shows the soil profiles in the Luxembourgish catchments. Draw the dominant hydrological processes that you expect on these catchments, such as saturation excess overland flow, infiltration excess overland flow, lateral subsurface flow (i.e. roughly parallel to the slope), vertical flow (i.e. deep percolation), groundwater flow.

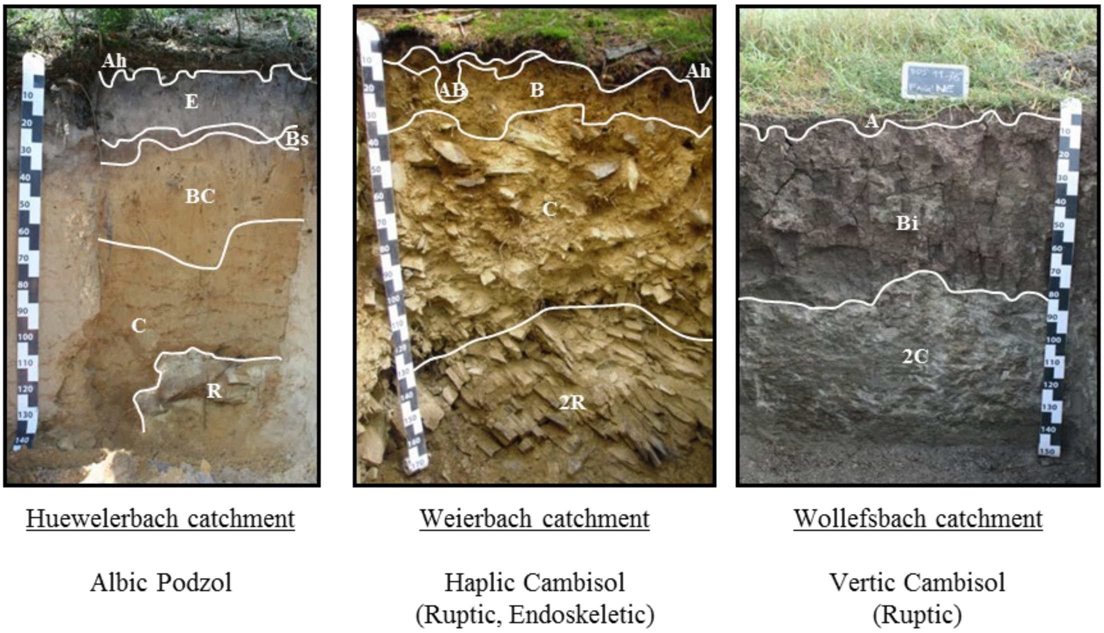

Figure 2: Typical regolith profiles (soil-saprolite-saprock) found in the three catchments including sandstone (left), schist covered by Pleistocene Periglacial Slope Deposits (middle) and marls (right) lithologies. The soils are characterized by a sequence of soil horizons based on pedogenetic processes that occur: the organo-mineral A horizon is impacted by the biological activity of the soil surface (named Ah when it is richer in organic material); the E and B mineral horizons are formed through different pedogenetic processes, these horizons are named according to the loss (E) or gain (B) of material within the soil profile (named Bh for organic enrichment, Bs for metal enrichment and Bv according to vertic properties); the C horizon corresponds to the saprolite (strongly weathered bedrock); the R horizon corresponds to the saprock (slightly weathered bedrock).

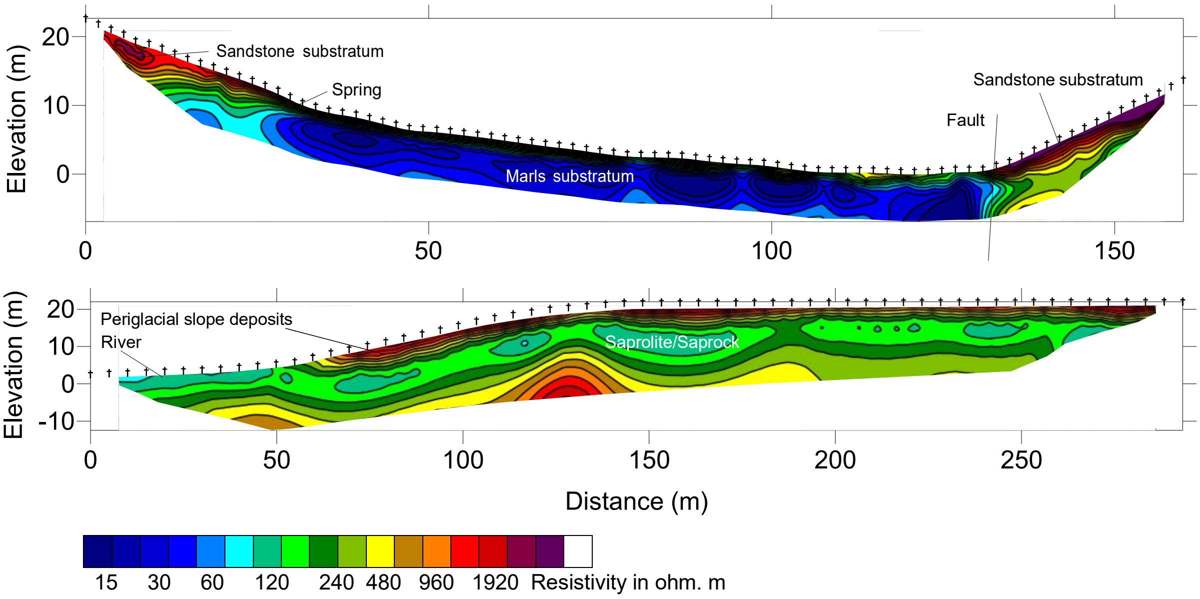

Figure 3: Typical resistivity transects of the Huewelerbach (top) and Weierbach (bottom) catchment. Features are outlined.

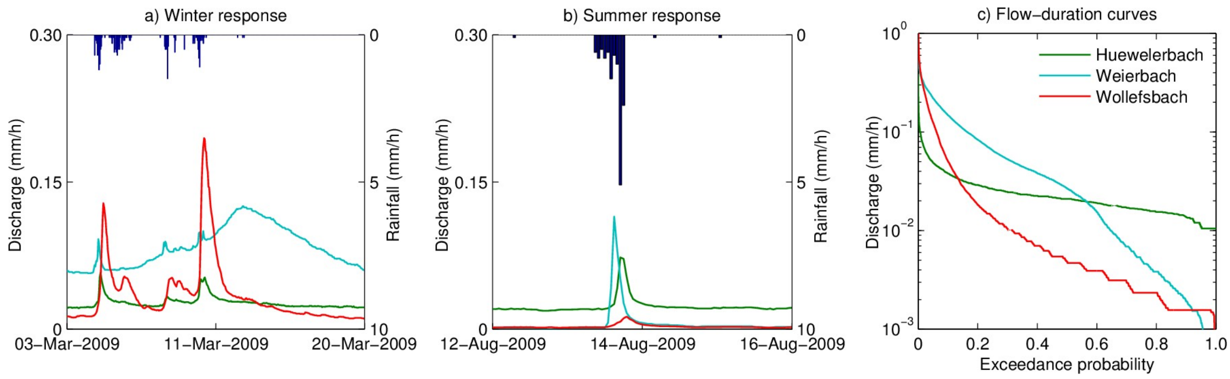

Figure 4: Typical hydrological responses of the three catchments in winter (wet) and summer (dry) conditions, and flow duration curves based on five years of discharge data (2005-2009).

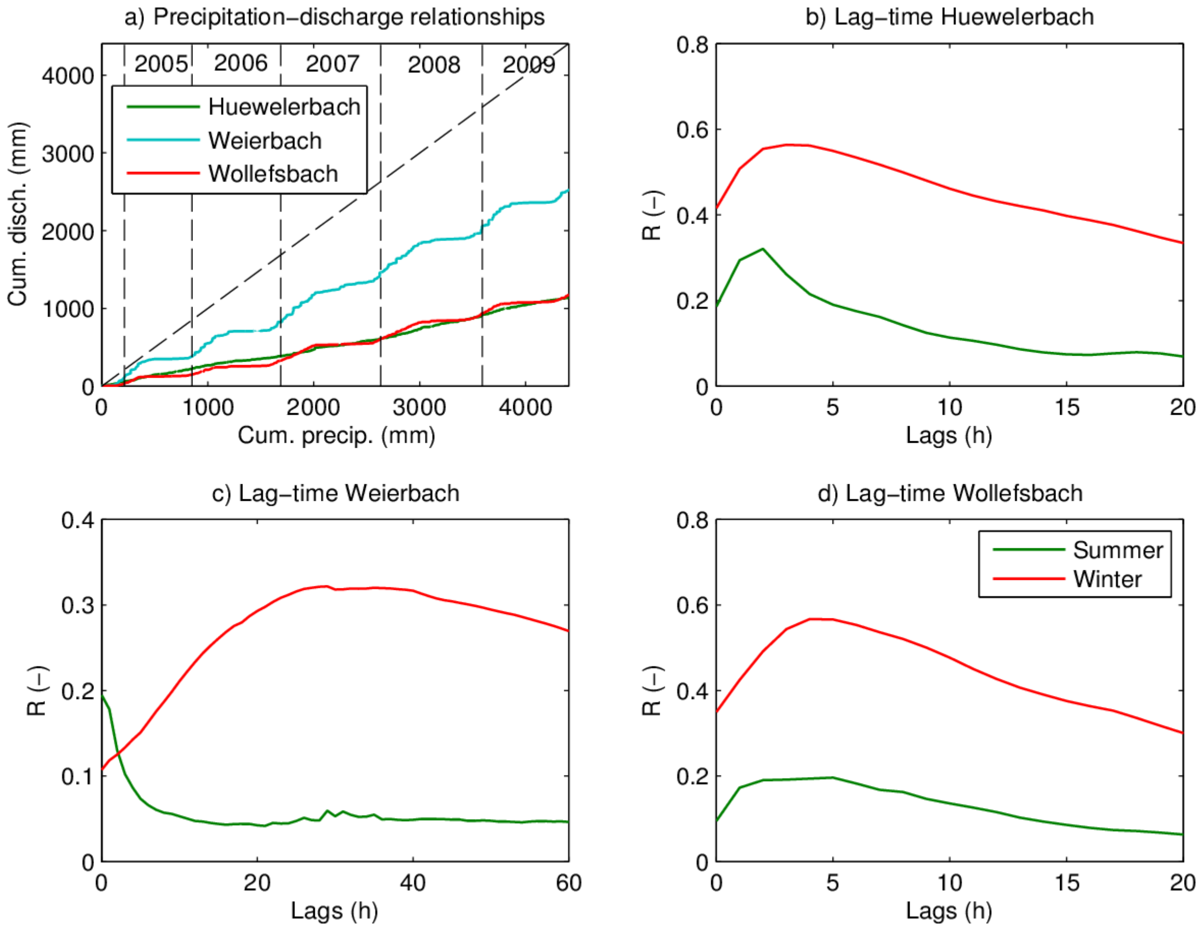

Figure 5: Double mass curves of cumulated discharge and precipitation for the period 2005-2009 (a). Panels (b) through (d) display lag times for the three catchments under summer and winter conditions, derived from stepwise cross correlation of the precipitation and discharge time series.

2.2. *Perceptual models of the Luxembourgish catchments*

Figure 6 illustrates the perceptual models of the 3 catchments. You can observe the different structures of the catchments based on the different geologies, and the perceived dominant processes.

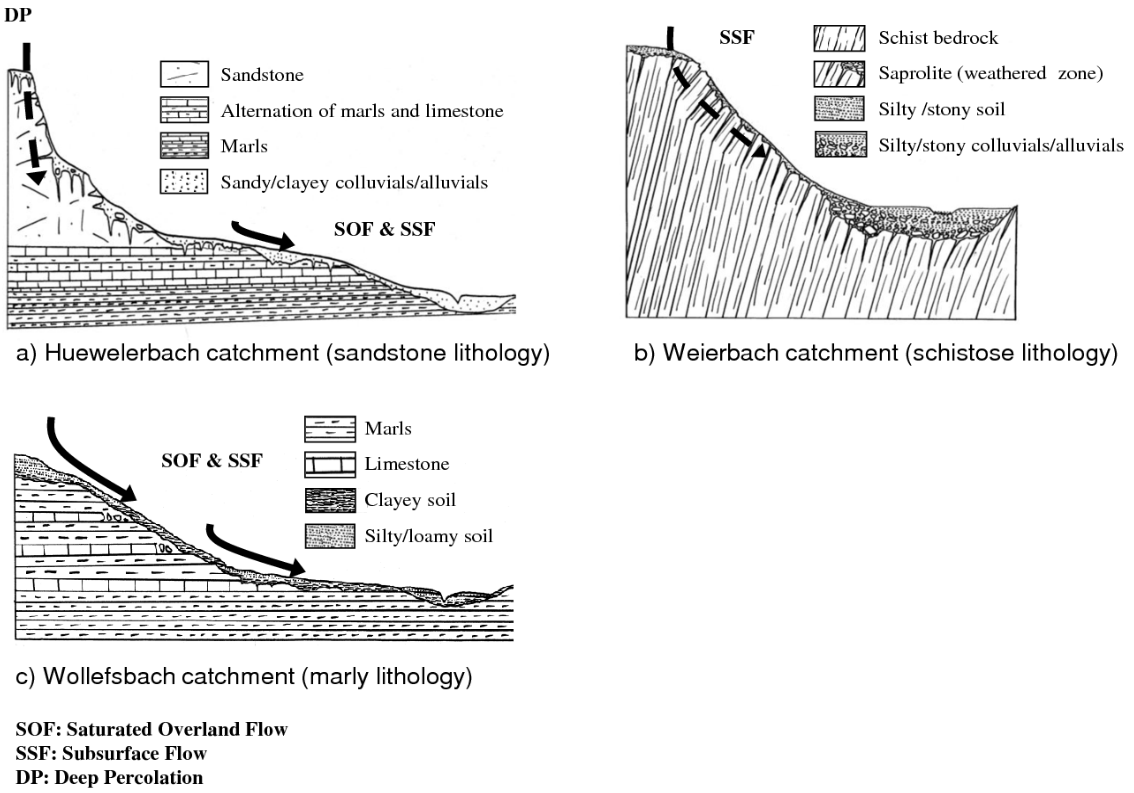

Figure 6: Schematics of the perceptual model of runoff generation processes in the three headwater catchments, presented as geological cross-section with arrows indicating the main flow pathways in the catchments.

3. Summary of hydrological case studies

In previous research, the SUPERFLEX model has been applied in several case studies based on Luxembourgish and New Zealand catchments. We will use daily data for computational speed.

The exercise consists of applying 4 models to 3 catchments. By examining the difference in performance between different model structures, we try to gain insights on catchment behaviour.

The models differ in a “controlled” way, so that we can easily associate the difference in performance to the presence or absence of some model components. This is one of the advantages of performing model comparison in a multi-hypothesis framework, with respect to comparing models that differ in several respects. In the latter case, it is more difficult to understand why models perform differently.

While trying different model structures, you may ask yourself different questions, which can help you understand what models do, how different structures behave, and how different catchments respond. First of all, while applying the structures, try to understand the effect of different components and parameters on the hydrograph, by changing the parameter vales using the ‘set_parameters’ method.

1. What is the effect of different parameters on the hydrograph?
2. Could these effects be anticipated?
3. Is the model parameter or model component doing what it is supposed to do?
4. Are parameters sensitive or not?

Then, while comparing the performance of different models on the same catchment, you may ask yourself the following questions:

1. Why do different models perform differently?
2. Which model components are responsible?
3. Can the effect of these model components be justified in terms of process understanding?
4. Does it make sense to use a more complex model instead of a simpler one? Why?

Similarly, we should be prepared to think about why certain model modifications do not give any improvement.

1. Why do different models perform similarly?
2. Why the addition of certain model components does not improve results?
3. Does this make sense experimentally?
4. Can the objective function / error model be responsible for this?

We should also take advantage of the fact that we are comparing different models on different catchments. As the Luxembourgish catchments are closely spaced, they share similar climatology.

1. Are different structures best suited for different catchments? Why?
2. Why a structure that behaves poorly on a certain catchment does well in another?

And finally, always try to relate model results to process understanding. This way, you can use modelling as a learning tool.

3.1. *Specific SuperflexPy configurations*

3.1.1. General description

It does not take long to ascertain that attempting to infer the parameters of very complex model structures is a hopelessly non-identifiable problem [e.g., see the classic work of Jakeman and Hornberger, WRR1990]. Instead, SuperflexPy is intended to be used to hypothesize, build and test much more parsimonious configurations. In some cases, independent insights into the catchment dynamics can guide the selection of the model structure, whereas in other cases empirical trial-and-error approaches may be necessary. The best ways to accomplish this are the subject of ongoing research.

For the purposes of this tutorial, we created 4 distinct model configurations M01, M02 and M03 and M04, that can be directly imported (refer to the notebooks). Schematic representations of these models are shown in Figure 7.

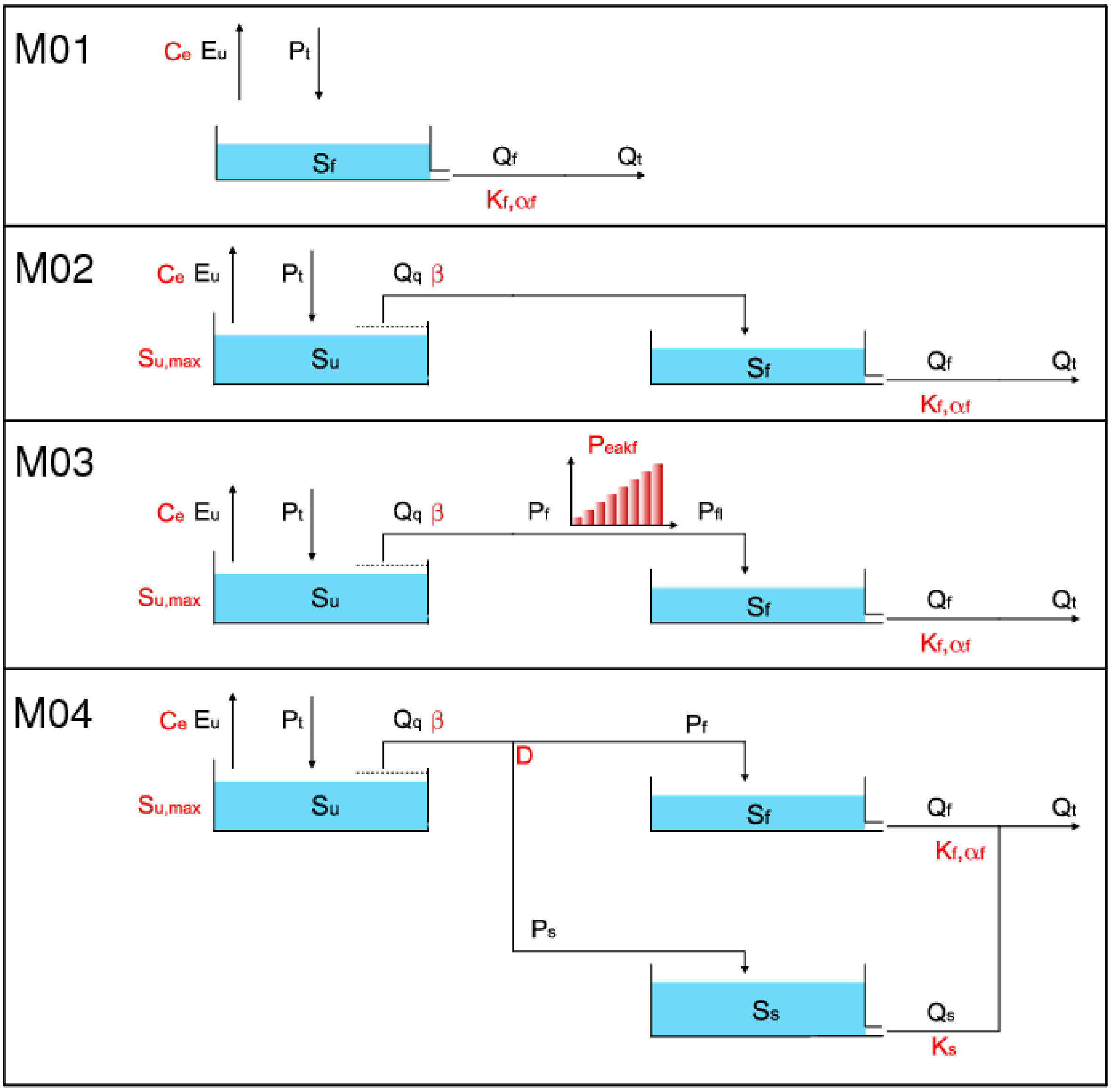

Figure 7. Schematic of model structures. M01: 1-bucket model (non-linear reservoir). M0: 2-bucket model without a lag function. M03: 2-bucket model with a lag function. M04: 3-bucket model.

3.1.2. Water balance equations and constitutive functions

The water balance equations and constitutive functions are described in Tables 1 and 2 below.

Table 1. Properties of model structures M1-M4. N_θ is the number of parameters and N_s is the number of states. UR, FR, and SR denote the unsaturated, fast, slow reservoirs. LF is the lag function.

Model			Components				Parameters							
	N_θ	N_s	UR	FR	SR	LF	C_e (-)	$S_{u,max}$ (mm)	β (-)	T_f (h)	K_f ($mm^{1-\alpha}/h$)	α (-)	D (-)	K_s (1/h)
M01	3	1	-	✓	-	-	✓	-	-	-	✓	✓	-	-
M02	5	2	✓	✓	-	-	✓	✓	✓	-	✓	✓	-	-
M03	6	3	✓	✓	-	✓	✓	✓	✓	✓	✓	✓	-	-
M04	7	3	✓	✓	✓	-	✓	✓	✓	-	✓	✓	✓	✓

Table 2. Water balance equations and constitutive functions of model structures M01-M04 (✓ and "-" indicate presence or absence respectively). The operator * denotes the convolution.

Water balance equations:	M 01	M 02	M 03	M 04	Constitutive relationships	M 01	M 02	M 03	M 04
$dS_u/dt = P_t - Q_q - E_u$	-	✓	✓	✓	$Q_q = P_t f_p(\bar{S}_u \| \beta)$	-	✓	✓	✓
$dS_f/dt = P_t - Q_f - E_f$	✓	-	-	-	$E_u = C_e E_p f_e(S_f \| m_1)$	✓	-	-	-
$dS_f/dt = P_f - Q_f$	-	✓	-	✓	$E_u = C_e E_p f_m(\bar{S}_u \| m_2)$	-	✓	✓	✓
$dS_f/dt = P_{fl} - Q_f$	-	-	✓	-	$P_{fl} = (P_f * h_f)(t)$	-	-	✓	-
$dS_s/dt = P_s - Q_s$	-	-	-	✓	$h_f = \begin{cases} 2t/T_f^2, & t < T_f \\ 0, & t > T_f \end{cases}$	-	-	✓	-
$Q_q = P_f + P_s$	-	-	-	✓	$P_s = DQ_q$	-	-	-	✓
$Q_t = Q_f$	✓	✓	✓	-	$Q_f = k_f S_f^\alpha$	✓	✓	✓	✓
$Q_t = Q_f + Q_s$	-	-	-	✓	$Q_s = k_s S_s$	-	-	-	✓

Table 3. Details of functions referred to in Table 2.

Function	Name
$\bar{S}_u = S_u / S_{u,max}$	Scaled storage (relative to a maximum capacity)
$f_p(x \| m) = x_m$	Power function
$f_e(x \| m) = 1 - e^{-x/m}$	Tessier function (note that fe(x|m) → 1 as x → ∞)
$f_m(x \| m) = (1+m)\frac{x}{x+m}$	Monod-type kinetics, adjusted so that $f_m(1 \| m)=1$

4. Case studies

After a first group discussion of the performance of the models on the Maimai catchment, you will be working on the three Luxemburgish catchments. While doing that, try to address the following questions.

BEFORE RUNNING THE MODELS

1. Based on the information contained in this document and on what discussed on Wednesday, how do you expect the response of the catchments to be?
2. Which models should perform better in the catchments? Why?

WHILE RUNNING THE MODELS

1. Is the result coherent with your expectations?
2. Is seasonality captured by the models?
3. What about the representation of high and low flows?
4. Is the timing of the peaks right?
5. Can you motivate the deficiencies that you find? (e.g. model X cannot represent low flows because it does not have an element to simulate groundwater)
6. What are the improvements that more complex model structures bring?
   a. Is adding the representation of soil processes useful? (compare M01 to M02)
   b. Is adding a lag useful? (compare M03 to M02)
   c. Is adding the representation of groundwater useful? (compare M04 to M02)
7. Look at the internal states of the reservoirs and at the internal fluxes: do they behave correctly?