

***Interactive comment on “Virtual laboratories: new opportunities for collaborative water science” by S. Ceola et al.***

Response to Hessel Winsemius (Referee)

The authors gratefully acknowledge Hessel Winsemius for his positive and constructive review. In what follows in *italics* are the comments provided by the Referee, and in **bold** fonts the authors response, inclusive of the indication on how the text will be modified within the next days to comply with the Referee’ recommendations and comments.

*In this paper, a much-needed proposition for development of virtual laboratories for collaborative research in hydrology, ensuring reproducibility and repeatability of experiments, is made. The papers focus seems rather trivial, but I agree with the authors that it is not! In fact many hydrological studies to date lack reproducibility due to lack of data sharing, limited metadata, poorly shared and documented experiment protocols and experiment outputs.*

**The authors wish to thank Hessel Winsemius for his recognition of our main goal.**

*I do have a number of comments of which the last one is the most important. I hope the authors find them useful for improving the manuscript. The most important comments are given below. I have also provided an annotated manuscript with some smaller remarks that should be treated.*

**Please see our detailed replies below. The revised manuscript including the suggested changes will be uploaded in the next few days.**

*No reference is made to past or ongoing global model intercomparison studies (some also including social interaction with the natural system) that may also benefit from the methods presented, e.g. ISLSCP, ISIMIP, EU-WATCH. I suggest to add some of these including references. The fact that these studies are global scale rather than local definitely sets this study apart from them as many of the issues raised by the authors (e.g. differences in preprocessing procedures, parameter selection, state handling) are difficult to resolve or less important at global scale, but can be tackled more appropriately at local scales.*

**In response to this comment we have added the following sentence, in which we present and cite the suggested global model intercomparison studies. Thanks for this.**

**“Model inter-comparison studies at a global scale, including social interactions with the natural system, like e.g. ISLSCP ([http://daac.ornl.gov/ISLSCP\\_II/islscp/](http://daac.ornl.gov/ISLSCP_II/islscp/)) EU-WATCH (<http://www.eu-watch.org/>) and ISI-MIP (<https://www.pik-potsdam.de/research/climate-impacts-and-vulnerabilities/research/rd2->**

cross-cutting-activities/isi-mip), but also comparative model inter-comparison experiments in hydrology (i.e. performed by different and independent research groups) such as MOPEX (Duan et al., 2006, Andreassian et al., 2006), DMIP (Reed et al., 2004) or LUCHEM (Breuer et al., 2009), though successful with respect to data sharing, have contributed little to disentangle the causes of performance differences between different models and to increase our understanding of underlying hydrological processes. ”

*The 7 stages mentioned do not seem to be very specific for hydrology (although their implementation in the virtual laboratory of course is hydrology specific) but instead could be applied on any scientific model intercomparison experiment. This raises the question if you are here proposing a general framework for virtual laboratories, showing an application in hydrology, or that you are proposing a hydrology-specific framework. From the remainder of the paper, we can conclude that it is probably the latter. It would be stronger if you can emphasize how these stages are specific to hydrology compared to other scientific fields or change them so that they are hydrology specific.*

**We have now better contextualised the proposed workflow stages as hydrology specific steps. Please refer for instance at STAGE 3: Collect input data, where we included new reference to specific hydrologic data (i.e., precipitation, temperature and river discharge). As kindly suggested by Hessel Winsemius in one of the following comments, we decided to add a new workflow stage as follows. Immediately after the definition of a scientific question/problem (STAGE 1), the involved partners need to clearly outline a protocol (i.e. experiment guideline) in order to ensure experiment reproducibility and therefore reduce and control the degree of freedom of single modellers (STAGE 2: Set up protocols).**

*Stage 3: the reworking of data into model specific inputs. Stage 3 suggests that any modeller can do any preprocessing he/she deems fit. In this transformation process however, much of the intercomparability of the experiments may be polluted by the fact that one modeller does something else with the data than another. I would propose that the degree of freedom is controlled through the proposed protocols and that you clarify this in the description of stage 3.*

**Please refer to our previous reply.**

*An important comment is that the connection between the 7 steps and the description of the collaborative experiment, performed in the SWITCH-ON project is not very clear. Please refer to the steps in the description of the 2 experiments performed so that the reader can make this connection more easily.*

**We acknowledge this lack of information in the original version of**

our manuscript. Accordingly to this useful comment, we have now added some reference to the workflow stages directly in the experiment description.

*Moreover, in the experiment description, a lot of focus is on the protocol design (which I agree is very important) while the protocol design receives very limited attention in the general 7-step description. It is somewhere hidden in step 4. I would emphasize more on the protocol design and describe in the 7-steps more accurately what the protocols should embody. In fact, you could argue that the protocol design should be a concrete separate step. Please consider this option.*

**Thanks for this remarkable advice. Please refer to our previous reply, where we introduce a new workflow step (STAGE 2: Set up protocols).**

*In page 13463, l. 24-25, the authors state that “with different model implementations, the main purpose of the modelling exercise needs to be clearly defined”. Whilst I fully agree with this, strictly speaking, the second experiment design did not adhere fully to this statement. The authors indicate this also in page 13462 l. 17 “we did not specify what model improvement meant a priori”. I can imagine that this observation in fact led to the statement above, however this is not clear from the discussion. Please add a sentence that explains whether the lack of specification of the meaning of model improvement indeed led to the conclusion that the purpose of the experiment needs to be very clearly defined.*

**The original version of our manuscript was not totally clear on this subject. Indeed, the purpose of the second experiment was to profit from researchers personal experience in order to improve model performances. The added value of this second experiment relied on the scientific knowledge of researchers, being capable of exploring alternative modelling options which will be helpful for future hydrological experiments in the VWSL. Therefore, we did not deliberately specify, as in Protocol 1, how to run the experiment. In Protocol 2, researchers could freely choose to improve model performance by either reaching a higher statistical metric, less equifinality among parameters or a more reliable model in terms of realistic internal variables. According to this, in the new version of the manuscript, which will be uploaded soon, we added a couple of sentences providing a thorough explanation.**

*My most important comment: the experiments performed are rather simple (same model structure, same spatial representation, same data, data handling) and perhaps not very representative for the type of collaborative model experiments that the hydrological community would like to perform in the forthcoming decade. Whilst including a more complex experiment is perhaps beyond*

*the scope of this paper, it would make the paper a lot stronger, if the authors can demonstrate that the suggested procedure for protocol establishment indeed applies even when a completely different (more complex) experiment would be performed. For instance, the suggested protocols for the experiments performed amongst the research groups would not yield a satisfactory intercomparability when the science question would be related to differences between model structures, where all groups would use different hydrological models and/or different levels of process or input distribution in their models throughout the 15 catchments, or when e.g. different ways to include man-made interactions in models would be studied. In these examples, models may have very different states and fluxes, and may even have different spatial representations of states and fluxes making their intercomparison a lot more difficult. It would make the framework a lot more convincing if the authors can perform a thought experiment in the discussion that demonstrates the validity of the proposed framework, even in more complex cases that will become important in this decade of Panta Rhei such as mentioned above. I hope these comments prove useful and I am looking very much forward to an improved manuscript.*

**We totally agree with this comment, since this paper presents the results of a relatively simple hydrological exercise run in a collaborative framework. However, the experiments discussed here show that it is important to revisit experiments that are seemingly simpler than existing inter-group model comparisons to understand how small differences affect model performance. What is clear is that it is fundamental to control for different factors that may affect the outcomes of more complex experiments, such as modeller choice and calibration strategy. In more complex situations the virtual experiments could be conducted through comparisons at different levels of detail. For example, if models with different structures were to be compared there will be no one-to-one mapping of the state variables and model parameters and the comparison would applied to a higher level of conceptualizations. There are a number of examples in the literature where comparisons at different levels of conceptualization have been demonstrated to provide useful results. One such example is Chicken Creek model inter comparison (Hollnder et al., 2009, 2014) where the modellers were given an increasing amount of information about the catchment in steps, and in each step the model output in terms of water fluxes were compared. The Chicken Creek inter comparison involved models of vastly different complexities, yet provided interesting insights in the way models made assumptions about the hydrological processes in the catchment and the associated model parameters. Another example is the Predictions in Ungauged Basins (PUB) comparative assessment (Blöschl et al., 2013) where a two step process was adopted. In a first step (Level 1 assessment), a literature survey was performed and publications in the international refereed literature were scrutinised for results of the predictive per-**



formance of runoff, i.e. a meta-analysis of prior studies performed by the hydrological community. In a second step (Level 2 assessment) some of the authors of the publications from Level 1 were approached with a request to provide data on their runoff predictions for individual ungauged basins. At Level 2 the overall number of catchments involved was smaller than in the Level 1 assessment but much more detailed information on individual catchments was available. Level 1 and Level 2 were therefore complementary steps. In a similar fashion, virtual experiments could be conducted using the protocol proposed in this paper at different, complementary levels of complexity. The procedure for protocol development (Figure 5), which notably checks on independent model choices between partners and feedbacks to earlier stages in protocol development, will help in developing protocols for more complex collaborative experiments, addressing real science questions on floods, droughts, water quality and changing environments. As such more elaborated experiments are part of ongoing collaborative work, we are not able to present their outcomes in the manuscript, but we will certainly upload their description in the Virtual Water-Science Lab space of the SWITCH-ON website (<http://www.water-switch-on.eu/lab.html>), accessible to all HESS Readers, in the next months, as soon as they are completed. As this is a learning process, the adequacy of the protocol development procedure itself will be evaluated during these experiments. The modelling study presented in this paper therefore represents a relatively simple, yet no less important first step towards collaborative research in the Virtual Water-Science Laboratory. Finally, we thank Hessel Winsemius for his detailed and helpful review.

*Please also note the supplement to this comment: <http://www.hydrol-earth-syst-sci-discuss.net/11/C6069/2015/hessd-11-C6069-2015-supplement.pdf>*

We modified the manuscript according to the proposed suggestions. Thank you. Please also see below our reply to one of Hessel Winsemius's comments.

Hessel Winsemius's comment at page 13454: *This would in terms of calibration/validation yield the same as NSE, why did you use both?*

The metrics we selected to measure the goodness-of-fit of the TUWmodel are widely employed indicators that separately focus on high, low and ordinary flows. Even though we are well aware that NSE and RMSE provide comparable information on model performance, we deemed important to compute both.

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***Interactive comment on “Virtual laboratories: new opportunities for collaborative water science” by S. Ceola et al.***

Response to Anonymous Referee #2

The authors gratefully acknowledge the Referee for his/her fully supportive review. In what follows in *italics* are the comments provided by the Referee, and in **bold** fonts the authors response, inclusive of the indication on how the text will be modified within the next days to comply with the Referee’ recommendations and comments.

*The paper presents the main results of an innovative collaborative work on virtual laboratories for hydrological science within the framework of the EU funded project SWITCH-ON. The topic is of interest for HESS readers and the paper is very well written, presented and structured. After reviewing the paper, I strongly support its final publication in HESS.*

**We wish to thank the Referee for his/her important appreciation.**

*I only would like to suggest two ideas which in my opinion could improve the paper. 1. The title of the paper states “new opportunities for collaborative water science”. Nevertheless, the focus of the paper (or at least, the case study presented) is on hydrology as the two main questions to be addressed (page 13448 lines 21-23) point out. Have the authors considered a more concise title, writing hydrological science instead of “water science”? In my opinion, even if the general framework could be useful for other water science experiments, the focus of the paper is on hydrology.*

**As the Referee properly noticed, the experiment we present in this paper is exclusively focused on hydrology. However, we believe to keep the title in its original form since our aim was to present a first example of comparative research in the water science context. Further experiments, some of them already started, are planned to include ecohydrological and social features not originally embedded in a hydrological context. In addition, we prefer not to change the title length, since we found it as the most synthetic version.**

*2. 15 catchments have been considered to develop the experiment. According to data provided in Table 1, mean catchment annual rainfall correspond to wet or very wet conditions and mean catchment temperatures to cold or very cold climates. Do the authors think that this homogeneity could influence the results? Would a much varied range of catchment conditions imply a lower reproducibility?*

**Thank you for this comment, which allows us to better explain our choice. The main goal of our experiment was to verify experiment**

reproducibility, as outlined in the Introduction. Indeed, “The paper aims to address the following questions: 1. What factors control reproducibility in computational scientific experiments in hydrology? 2. What is the way forward to ensure reproducibility in hydrology?”. Therefore, in order to limit the degrees of freedom of our analysis, we decided to select catchments having comparable hydro-climatic features, similar drainage areas and a minimum of 10 years as observation period.

*Typographic errors*

*1. Page 13454, line 7. Is superscript “-1” correct after “years”? 2. Page 13454, line 26. Is superscript “-1” correct after “years”?*

**No, the superscript “-1” should be removed from text. Thanks!**

# Virtual laboratories: New opportunities for collaborative water science

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**Abstract.** Reproducibility and repeatability of experiments are the fundamental prerequisites that allow researchers to validate results and share hydrological knowledge, experience and expertise in the light of global water management problems. Virtual laboratories offer new opportunities to enable these prerequisites since they allow experimenters to share data, tools and pre-defined experimental procedures (i.e., protocols). Here we present the outcomes of a first collaborative numerical experiment undertaken by five different international research groups in a virtual laboratory to address the key issues of reproducibility and repeatability. Moving from the definition of accurate and detailed experimental protocols, a rainfall-runoff model was independently applied to 15 European catchments by the research groups and model results were collectively examined through a web-based discussion. We found that a detailed modelling protocol was crucial to ensure the comparability and reproducibility of the proposed experiment across groups. Our results suggest that sharing comprehensive and precise protocols and running the experiments within a controlled environment (e.g., virtual laboratory) is as fundamental as sharing data and tools for ensuring experiment repeatability and reproducibility across the broad scientific community and thus advancing hydrology in a more coherent way.

## 1 Introduction

Global water resources are increasingly recognised to be a major concern for a sustainable development of the society (e.g., Haddeland et al., 2014; Schewe et al., 2014; Berghuijs et al., 2014).

Ongoing changes in demography, ~~land-use~~ land use and climate will likely exacerbate the current  
20 circumstances (Montanari et al., 2013). Water availability and distribution support both ecosystem  
(Ceola et al., 2013, 2014a) and human demand for drinking water, food, sanitation, energy, industrial  
production, transport and recreation. Water is also recognised as the most important environmental  
hazard: floods (Ceola et al., 2014), droughts and water-borne diseases (Rinaldo et al., 2012) cause  
thousands of casualties, famine, significant disruption and damage worth billions every year (e.g.,  
25 Jongman et al., 2012; UNISDR, 2013; Ward et al., 2013). Efficient water management is thus cru-  
cial for sustainable development of human society. As a consequence, a sound coherent science  
underpinning decision making is urgently needed. Many studies have already acknowledged the  
needs for a scientific advancement in water resources management and improved computational  
models for decision support, which should be capable of predicting the implications of a chang-  
30 ing world (Milly et al., 2008; Montanari and Koutsoyiannis, 2012, 2014a, b; Montanari et al., 2013;  
Koutsoyiannis and Montanari, 2014; Wagener et al., 2010; Gao et al., 2014; Ceola et al., 2014b).  
Unfortunately, the large diversity of hydrological systems (i.e., catchments) makes it very diffi-  
cult to identify overarching, scale independent organizing principles of hydrological functions that  
are required for sustainable and systematic global water management (Beven, 2000; Wagener et al.,  
35 2007; Hrachowitz et al., 2013). Blöschl et al. (2013, p. 4) noted that, as hydrologists, we do not  
have a single object of study. Many hydrological research groups around the world are studying  
different objects, i.e., different catchments with different response characteristics, thus contribut-  
ing to the fragmentation of hydrology at various levels. In addition, environmental data are of-  
ten not easily accessible for hydrological comparisons to enable universal principles to be iden-  
40 tified (Viglione et al., 2010). Data are often not provided in appropriate formats, quality checked  
and/or adequately documented. The hydrological community has therefore recently started to urge  
for more collaboration between different research groups, to establish large data samples, improve  
interoperability and comparative hydrology (Duan et al., 2006; Arheimer et al., 2011; Blöschl et al.,  
2013; Gupta et al., 2014). Sharing data and tools, embedded within virtual observatories, may be a  
45 way forward to advance hydrological sciences in a coherent way. In Europe, a major recent de-  
velopment has been the implementation of the INSPIRE Directive (2007/2/EC) in 2007, which  
provides a general framework for Spatial Data Infrastructure (SDI) in Europe. This directive re-  
quires that common implementing rules are adopted in all member states for a number of specific  
areas (e.g., metadata, data specifications, network services, data and service sharing, monitoring and  
50 reporting) by 2020. Worldwide, similar initiatives can be found by the World Meteorological Or-  
ganisation, WMO (<http://www.whycos.org/whycos/>), the Earth Observation Communities, GEOSS  
(<http://www.earthobservations.org/geoss.php>), and the World Water Assessment Programme by UN-  
ESCO (2012). However, sharing of open data and source codes does not automatically lead to good  
research and scientific advancement.

55     Reproducibility and repeatability of experiments are the core of scientific theory for ensuring  
scientific progress. Reproducibility is the ability to perform and reproduce results from an experi-  
ment conducted under near identical conditions by different observers in order to independently test  
60     findings. Repeatability refers to the degree of agreement of tests or measurements on replicate spec-  
imens by the same observer under the same control conditions. Thus, only providing data through  
open online platforms (or any other way) is not enough to ensure that reproducibility objectives can  
be met. In fact, the inference previously drawn may be ambiguous to different observers if insuffi-  
cient knowledge of the experimental design is available. Holländer et al. (2009, 2014) highlighted  
the impact of modellers' decisions on hydrological predictions. Hydrology is therefore likely to  
be similar to other sciences that have not yet converged to a common approach to modelling their  
65     entities of study. In such cases, meaningful interpretations of comparisons are problematic, as illus-  
trated by many catchment – or model – inter-comparison studies in the past. Comparative Model  
inter-comparison studies at a global scale, including social interactions with the natural system, like  
e.g. ISLSCP (<http://daac.ornl.gov/ISLSCP>  
[SUBSCRIPTNBII/islscpii.shtml](http://www.eu-watch.org/)), EU-WATCH (<http://www.eu-watch.org/>) and ISI-MIP (<https://www.pik-potsdam.de/research/climat>  
70     but also comparative model inter-comparison experiments in hydrology (i.e. ~~r~~performed by different  
and independent research groups) such as MOPEX (Duan et al., 2006; Andreassian et al., 2006), ~~but~~  
~~also in~~-DMIP (Reed et al., 2004) or LUCHEM (Breuer et al., 2009), though successful with respect  
to data sharing, have contributed little to disentangle the causes of performance differences between  
different models and to increase our understanding of underlying hydrological processes. This was  
75     ultimately often rooted in the problems that (see e.g., Clark et al., 2011; Gudmundsson et al., 2012):  
(i) there are considerable differences in model structures which hinder the identification of particular  
features that make it perform better or worse; (ii) different research groups make various different  
decisions for pre-processing data and calibrating models (although often thought to be negligible,  
this may, cumulatively, prevent a valid comparison of differences in the results); and (iii) compar-  
80     ing model outputs without analysis of model states and internal fluxes provides limited insight into  
the workings of a model. Hence, greater acknowledgement is required of the dependency of sci-  
entific experiments on the applied procedure and choices made in observation and modelling to  
identify causal relationships (e.g., setting up of boundary conditions, forcing conditions, narrowing  
of degrees of freedom), both in empirical field work (Parsons et al., 1994) and modelling studies  
85     (Duan et al., 2006; Gudmundsson et al., 2012). This would ensure more transparency in the data and  
methods used in experiments. In particular, hydrology suffers from the perceived difficulty of report-  
ing detailed experiment protocols in the research literature, largely under-exploiting the convenient  
option to provide supplementary information in scientific journals. Thus, in the presence of open  
data platforms, setting up strategies to guarantee experiment reproducibility and thereby a means for  
90     meaningful inter-experiment comparison is a challenging target. It requires a concerted and interdis-  
ciplinary effort, involving information technology, environmental sciences and dissemination policy

in developing and communicating strict, detailed, coherent and generally unambiguous experiment protocols.

In this paper we explore the potential of a virtual water-science laboratory to overcome the aforementioned problems. A virtual laboratory provides a platform to share data, tools and experimental protocols (Ramasundaram et al., 2005). In particular, experimental protocols constitute an essential part of a scientific experiment, as they guarantee quality assurance and good practice (e.g., Refsgaard et al., 2005; Jakeman et al., 2006) and, we argue, are at the core of repeatability and reproducibility of the scientific experiments. More specifically, a protocol is a detailed plan of a scientific experiment that describes its design and implementation. Protocols usually include detailed procedures and lists of required equipment and instruments, information on data, experimenting methods and standards for reporting the results through post-processing of model outputs. By including a collection of research facilities, such as e-infrastructure and protocols, virtual laboratories have the potential to stimulate entirely new forms of scientific research through improved collaboration. Pilot studies, such as the Environmental Virtual Observatory (~~EVO~~p-EVO - <http://www.evo-uk.org>), have already explored a number of these issues and, additionally, the legal and security challenges to overcome. Other example projects related to hydrology ~~that~~, which are exploring community data sharing and interoperability, include DRIHM (<http://www.drihm.eu>), NEON in the USA (<http://www.neoninc.org>), and the Organic Data Science Framework (<http://www.organicdatascience.org/>).

To sum up, virtual laboratories aim at (i) facilitating repetition of numerical experiments undertaken by other researchers for quality assurance, and (ii) contributing to collaborative research. Virtual laboratories therefore provide an opportunity to make hydrology a more rigorous science. However, virtual laboratories are relatively novel in environmental research and their essential requirements to ensure the repeatability and reproducibility of experiments are still unclear. Therefore, we have undertaken a collaborative experiment, among five universities and research institutes, to explore the possible critical issues that may arise in the development of virtual laboratories. This paper presents a collaborative simulation experiment on reproducibility in hydrology, using the Virtual Water-Science Laboratory, established within the context of the EU funded research project "Sharing Water-related Information to Tackle Changes in the Hydrosphere – for Operational Needs (SWITCH-ON)", (<http://www.water-switch-on.eu/>), which is currently under development. The paper aims to address the following questions:

1. What factors control reproducibility in computational scientific experiments in hydrology?
2. What is the way forward to ensure reproducibility in hydrology?

After presenting the structure of the Virtual Water-Science Laboratory (VWSL), we describe in detail the collaborative experiment, carried out by the research groups in the VWSL. We deliberately decided to design the experiment as a relatively traditional exercise in hydrology in order to better identify critical issues that may arise in virtual laboratories development and dissemination and that



are not associated with the complexity of the considered experiment. This experiment therefore supports subsequent research within the VWSL, and provides an initial guidance to design protocols and share evaluation within virtual laboratories by the broad scientific community.

## 2 The SWITCH-ON Virtual Water-Science Laboratory

The purpose of the SWITCH-ON VWSL is to provide a common workspace for collaborative and meaningful comparative hydrology. The laboratory aims to facilitate the, through the development of detailed protocols, the sharing of data tools, models and any other relevant supporting information, thus allowing experiments on a common basis of open data and well defined ~~protocols~~ procedures. This will not only enhance the general comparability of different experiments on specific topics carried out by different research groups, but the available data and tools will also facilitate researchers to more easily exploit the advantages of comparative hydrology and collaboration, which is widely regarded as a prerequisite for scientific advance in the discipline (Falkenmark and Chapman, 1989; Duan et al., 2006; Wagener et al., 2007; Arheimer et al., 2011; Blöschl et al., 2013; Gupta et al., 2014). In addition, the VWSL aims to foster cooperative work by actively supporting discussions and collaborative work. Although the VWSL is currently used only by researchers who are part of the EU FP7-project SWITCH-ON, it is also open to external research groups to obtain feedback and to establish a sustainable infrastructure that will remain after the end of the project. Any experiment formulated within the VWSL needs to comply with specific stages, shown as ~~a 7-point~~ an 8-point workflow described in detail below, which outline the scientific process and the structure for using the facilitating tools in the VWSL.

**STAGE 1: Define science questions.** This stage allows researchers to discuss through a dedicated on-line forum (available at <https://groups.google.com/forum/#!forum/virtual-water-science-laboratory-forum>) specific ~~scientific~~ hydrological topics to be elaborated upon by different research groups in a collaborative context. Templates are available to formulate new experiments.

**STAGE 2: Set up experiment protocols.** In this step a recommended protocol for collaborative experiments needs to be developed. This protocol formalises the main interactions between project partners and acts as a guideline for the experiment outline in order to ensure experiment reproducibility and thus controlling the degree of freedom of single modellers.

**STAGE 3: Collect input data.** The VWSL contains a catalogue of relevant external data available as open data from any source on the Internet in a format that can be directly used in experiments. Stored data are organised in Level A (pan-European scale covering the whole of Europe) and Level B (local data covering limited or regional domains). Currently Level A includes input data to the E-HYPE model (Donnelly et al., 2014) with some 35,000 sub-basins

covering Europe ~~;~~ such as precipitation, evaporation, soil and land use, river discharge and nutrients data, while Level B includes hydrological data (i.e. precipitation, temperature and river discharge) for 15-20 selected catchments across Europe. In addition, a Spatial Information Platform (SIP) has been created. This platform includes a catalogue with a user interface for browsing among metadata from many data providers. So far, the data catalogue has been filled with 6990 items of files for download, data viewers and web pages. The SIP also includes functionalities for linking more metadata, and visualisation of datasets. Therefore, through stored data and the SIP, researchers can easily find and explore data deemed to be relevant for ~~an experiment.~~ a hydrological experiment.

**STAGE 4: Repurpose data to input files.** In this step, raw original data from STAGE 2 can be processed (i.e., transformed, merged, etc.) to create suitable input files for hydrological experiments or models. For example, the World Hydrological Input Set-up Tool (WHIST) can tailor data to specific models or resolutions. An alternative example, planned to be used for future activities in the VWSL, is provided by land use data, which can be aggregated to relevant classes and adjusted to specific spatial discretisations (e.g., model grid or sub-basin areas across Europe). Both raw original and repurposed data (STAGES 2 and 3) should be accompanied by detailed metadata (i.e., a protocol), which specify e.g., data origin, spatial and temporal resolution, observation period, description of the observing instrument, information on data collection, measures of data quality, coherency of the measured method and instrument, and any other relevant information. Data should be provided to international open source data standards (i.e., <http://www.opengeospatial.org>) and, for water related research in particular, it should be compliant with the WaterML2 international initiatives (see above site for more information).

**STAGE 5: Compute model outputs.** By employing open source model codes, freely available via the VWSL, or through links to model providers, researchers can perform hydrological model calculations using the same tools. Results can then be compared, evaluated, reused and/or repurposed for new experiments. In addition, templates for protocols are available to ensure the reproducibility and repeatability of model analysis and results. The protocol may include, for instance, a description of the hydrological experiment, and information on the model, input data and metadata, employed algorithms and temporal scales. Protocols for model experiments will thus create a framework for a generally accepted, scientifically valid and identical environment for specific types of numerical experiments within the VWSL, and will promote transparency and data sharing, therefore allowing other researchers to download and reproduce the experiment on their own computer.

**STAGE 6: Share results.** Links to model results are uploaded to the VWSL in order to ensure the post audit analyses and transparency of the performed experiments, which can be reproduced by other research groups.

200 **STAGE 7: Explore the findings.** Here, researchers can extract, evaluate and visualise experiment results gathered at STAGE 5. A separate space for discussion and comparisons of results, through the on-line forum, additionally facilitates direct and open knowledge exchange between researchers and research teams.

205 **STAGE 8: Publish and access papers.** Links to scientific papers and technical reports on comparative research resulting from collaboration and experiments based on data in the VWSL will be found in the VWSL.

### 3 The first collaborative experiment in the SWITCH-ON Virtual Water-Science Laboratory

#### 3.1 Description and purpose of the experiment

The first pilot experiment of the SWITCH-ON VWSL aims to assess the reproducibility of the calibration and validation of a lumped rainfall-runoff model over 15 European catchments (Fig. 1) by different research groups using open software and open data ([STAGE 1](#)). Calibration and validation of rainfall-runoff models is a fundamental step for many hydrological analyses (Blöschl et al., 2013), including drought and flood frequency estimation (see, for instance, Moretti and Montanari, 2008). The rainfall-runoff model adopted in the experiment is a HBV-like model (Bergström, 1976) called TUVmodel (Parajka et al., 2007; Parajka and Viglione, 2012), which is designed to estimate daily streamflow time series from daily rainfall, air temperature and potential evaporation data ([STAGE 5](#)). ~~The TUVmodel code~~ (see Supplementary Material for further information). ~~The TUVmodel code~~, written as a script in the R programming environment (R Core Team, 2014), is run for each of the selected catchments by five research groups, based at the Swedish Meteorological and Hydrological Institute (SMHI), University of Bologna (UNIBO), Technical University Wien (TUW), 220 Technical University Delft (TUD), and University of Bristol (BRISTOL). The R script is run by the five research groups using different operating systems (i.e., Linux by UNIBO, TUW and TUD; Windows 7 by SMHI and BRISTOL). The groups a priori agreed on a rigorous protocol for the experiment ([STAGE 2](#)), which is described in detail below, conducted the experiment ([STAGES 3, 4, 5](#)), and subsequently engaged in a collective discussion of the results ([STAGES 6, 7](#)). Despite 225 the relatively simple hydrologic exercise, this experiment is expected to benefit from a comparison of model outcomes, an exchange of views and modelling strategies among the research partners in order to identify and assess potential sources of violations of the condition of reproducibility. Indeed the experiment has the purpose of bringing scientists to work together collaboratively in a well-

defined and controlled hydrological study for result comparison. By exploring reproducibility, this  
230 experiment places itself as a base-line for comparative hydrology.

### 3.2 Study catchment and hydrological data

European catchments characterised by a drainage area larger than 100 km<sup>2</sup> with at least 10 years  
of daily hydro-meteorological data, as lumped information on rainfall, air temperature, potential  
evaporation and runoff are considered ([STAGE 3](#)). The selected 15 catchments are located in Swe-  
235 den, Germany, Austria, Switzerland and Italy (Fig. 1). Daily time series of rainfall, temperature and  
streamflow, gathered from national environmental agencies and public authorities (see Acknowl-  
edgements for more details), are pre-processed by the partner who contributed the data set to the  
experiment (e.g., to homogenise units of measurement) to be employed in the TUWmodel ([STAGE](#)  
[4](#)). Potential evaporation data are derived, as repurposed data ([STAGE 4](#)), from hourly temperature  
240 and daily potential sunshine duration by a modified Blaney-Criddle equation (for further details, see  
Parajka et al., 2003). Table 1 reports the foremost features of the 15 study catchments investigated.

### 3.3 Experiment protocols

As detailed above, the objective of this experiment is to test the reproducibility of the TUWmodel  
results on the 15 study catchments when implemented and run independently by different research  
245 groups. Consequently, the experiment provides an indication of the experimental implementation  
uncertainty (see e.g., Montanari et al., 2009) due to combined effects of insufficiently developed  
protocols, human error or computational architecture. To this aim, identical implementations (the  
R code) of the TUWmodel are distributed to the research groups, and two different protocols (i.e.,  
Protocol 1 and Protocol 2) establishing how to perform the experiment are defined ([STAGES 2, 5](#)).  
250 Protocol 1 is characterised by a rigid setting, such that the researchers are required to strictly follow  
pre-defined rules for model calibration and validation, as specified in the distributed R script. By  
following Protocol 1, all research groups are expected to obtain the same results in terms of com-  
parable model performance. The alternative Protocol 2 allows researchers more flexibility in order  
to explore and compare several different model calibration options. In this case, research groups  
255 have the opportunity to add their personal experience to assess model performance. This will likely  
provide less comparable results among research groups, but the expected added value of Protocol 2  
would be a more extended exploration of different modelling options, which could be synthesized  
and used for future hydrological experiments in the VWSL. In both protocols the observation pe-  
riod (n years) is divided into two equal-length sub-periods (n/2 years): the first period is used for  
260 calibration, and the second for validation as in a classical split-sample test. In Protocol 1, we also  
switched the two periods (i.e., first period for validation and second period for calibration). Detailed  
model ~~specification~~ [specifications](#) for the two protocols are described in what follows and their main  
settings are summarised in Tables 2 and 3.

### 3.3.1 Protocol 1

265 For Protocol 1, the calibration of the TUWmodel is based on the Differential Evolution optimisation  
algorithm (DEoptim, Mullen et al., 2011). This global optimisation tool with differential evolution is  
readily embedded in the R package that was used to run the entire experiment. Protocol 1 pre-defines  
the uniform prior model parameter distributions (Table 2). 10 calibration runs, each of them based  
on different random seeds, are performed in order to identify the best calibration run. The objective  
270 function used to determine the optimal model parameters is the mean square error (MSE). Model  
parameters estimated during the calibration phase are then used to test the TUWmodel in the valida-  
tion period. For the validation period, Protocol 1 further requires the computation of MSE; root mean  
square error, RMSE; Nash-Sutcliffe efficiency, NSE; NSE of logarithmic discharges, log(NSE); bias;  
mean absolute error, MAE; MAE of logarithmic discharges, MALE; and volume error, VE. A model  
275 warm-up period of 1 year for both calibration and validation (i.e., model calibration and validation  
are applied on  $n/2-1$  years), was adopted in order to minimise the influence of initial conditions. The  
model realisations of the individual research groups were then compared based on the performance  
metrics and the obtained optimal parameter values. The R-script describing Protocol 1 is presented  
as Supplementary Material.

### 280 3.3.2 Protocol 2

In Protocol 2, the different research groups could make individual choices in an attempt to improve  
model performances. More specifically, during model calibration on the first half of the observation  
period, users could (i) shorten the calibration period by excluding what they believe are potentially  
unreliable pieces of data and providing detailed justifications, (ii) modify the prior parameter dis-  
285 tributions, (iii) change the optimisation algorithm and its settings, (iv) select alternative objective  
functions, and (v) freely choose the model warm-up period (see Table 3 and Supplementary Ma-  
terial for a detailed description). Similarly to Protocol 1, the calibrated parameter values are used  
as inputs for the evaluation of the simulated discharge during the validation period, and the same  
goodness-of-fit statistics evaluated in Protocol 1 are also computed.

## 290 4 Results

A web-based discussion ([STAGES 6, 7](#)) was engaged among the researchers to collectively assess  
the results, by comparing the experiment outcomes and benefiting from their personal knowledge  
and experience. The results revealed that reproducibility is ensured when:

- experiment and modelling purpose are outlined in detail, which requires a preliminary agree-  
295 ment on semantics and definitions,

- a standardised format of input data (e.g., file format, data presentation, and units of measurement) and pre-defined variable names are proposed,
- the same model tools (i.e., code and software) are used.

300 Within a collaborative context, this can be achieved only if the involved research groups completely agreed on the detailed protocol of the experiment. In what follows we report the experiences gained from the experiment, and we finally suggest a process that enables research groups to improve the set-up of protocols.

#### 4.1 Protocol 1

The variability in the optimal calibration performance obtained from all research groups for Protocol 1, ordered by catchments, is shown in Fig. 2. For some catchments, notably the Gadera (ITA) and Großarler Ache (AUT), optimal calibration performance is very similar between groups, indicating that the Protocol has been executed properly by each research group. However, for some other catchments including the Vils (AUT), Broye (SUI), Hoan (SWE) and Juktån (SWE), more variability in optimal performance between groups was obtained. Given that Protocol 1 is not deterministic, as the optimisation algorithm contains a random component, variability in optimal performance will be expected even if the protocol were repeated by a given research group. Thus, in order to make proper comparison between research groups – e.g., assess the reproducibility of an experiment – an understanding of this within-group variability, or repeatability, is required. The range in optimal performance obtained by one research group (BRISTOL) when the optimisation algorithm was run 100 times, instead of 10 times as per Protocol 1, is also plotted in Fig. 2 to give an indication of the within-group variability. With the exception of the second calibration period for the Vils (AUT) catchment, where UNIBO found a lower RMSE, the between-group variability in calibration performance falls within the bounds of the within-group variability, which indicates a successful execution of the Protocol across all catchments. Of the 100 optimisation runs conducted for the Vils (AUT) catchment during the second calibration, 99 were at the upper end of the range in Fig. 2, alongside the results of all groups except UNIBO, and only one result at the lower end of the range. In this case, and in the case of the poorer performance of the BRISTOL calibration for the Broye (SUI), where early stopping of the optimisation algorithm consistently occurred, the results suggest the algorithm became trapped in a local minimum and struggled to converge to a global minimum – or at least to an improved solution, as identified by other groups/runs. In addition to convergence issues causing differences in the results of each group, differences in the identified optimal parameter sets suggest that divergence in performance may also result from parameter insensitivity and equifinality (Fig. 3). Furthermore, performance is also affected by the presence of more complex catchment processes which are not fully captured by the chosen hydrological model (e.g., snowmelt or soil moisture routines in catchments with large altitude range or diverse land covers). Thus, from

a hydrological viewpoint, the results were not completely satisfactory, and detailed analysis at each location is required. However, given that in the majority of cases the between-group variability in performance (reproducibility) was within the range of within-group variability (repeatability) identified, it can be concluded that Protocol 1 ensured reproducibility between groups for the proposed  
335 model calibration.

## 4.2 Protocol 2

To overcome the problems arising from Protocol 1 and possibly improve model performances, the effects of personal knowledge and experience of research groups were explored in Protocol 2. Here, researchers were allowed to more flexibly change model settings, which may introduce a more pronounced variability in the results among the individual research groups, due to different decisions  
340 in the modelling processes. Given that flexibility allows a more proficient use of expert knowledge and experience, one may expect an improvement of model performances. Flexibility indeed enables modellers to introduce new choices in order to improve model performance in terms of process representation and consequently correct automatic calibration artefacts for model parameter value selection (as in Protocol 1), which could lead to unexpected model behaviour. The increase in flexibility  
345 in Protocol 2 led to a significant divergence in model performance between groups, as exemplified in Fig. 4 for the NSE performance metric. Such changes reflect the different approaches taken in an attempt to improve model performance in terms of process representation, and to correct problems from Protocol 1. In turn, these changes delineate the effects of different personal knowledge and experience of the different research groups. More specifically, BRISTOL and UNIBO both chose to exclude potentially unreliable data from the calibration data. In the case of BRISTOL, following visual inspection of the data, it was felt that a more thorough data evaluation procedure prior to calibration was required. Based on the calculation of event runoff coefficients, ~~data~~ a subset of the time-series in 9 catchments ~~were~~ was excluded. Researchers from UNIBO decided to exclude  
350 nearly one quarter of available data for each study watershed. Data were removed by looking for the highest MSE for each separate year by using the parameter set that allowed the best results on the calibration set in the Protocol 1 experiment. Data removal appeared to lead to improved calibration performance, and to a lesser extent, improved validation performance. As per Protocol 2, data were not removed from the validation period. Conversely, researchers from TUW and TUD decided not  
360 to remove any data in the calibration period but to adopt alternative optimisation procedures to enhance the robustness of the calibration (see Table 3). The discussion among modellers pointed out that changing the objective function from MSE to different formulations did not lead to an actual decay of the model performances, but only to lower values of the NSE, due to assigning lower priority to the simulation of the peak flows, while other features of the hydrograph were better simulated. For instance, the Kling-Gupta efficiency was used by TUD as it provides a more equally weighted combination of bias, correlation coefficient and relative variation compared to NSE. This led to reduced

bias and volume error compared to the results of the other groups, but in a trade-off, it worsened the performances in terms of the NSE. Similarly, the use of MSE by BRISTOL led to improvements in log(NSE), MAE and MALE for nearly all catchments in calibration and validation, but  
370 increased bias and volume errors in some cases. As there was no uniquely defined objective of Protocol 2, such choices reflected attempts by the groups to achieve an appropriate compromise across performance metrics. SMHI adopted a hydrological process-based approach, where the modellers accepted small performance penalties in terms of NSE if the conceptual behaviour of the model variables looked more appropriate during the calibration procedure. This was done to get a good  
375 model for the right reasons, and expert knowledge on hydrological processes and model behaviour was then included along with the statistical criteria. The evaluation of the goodness-of-fit by SMHI was performed by visual comparison and an analysis of several (internal) model variables, e.g., soil moisture, evapotranspiration rates, and snow water equivalents, instead of simply using a different objective function. These analyses pointed to conceptual model failures in several catchments (e.g.,  
380 Loisach (GER) catchment, Fig. 4), leading to the adoption of a calibration approach which considered the structural limitations of the TUWmodel and their implications for model performance (see also Supplementary Material).

### **4.3 Identified issues in a collaborative experiment**

Collaboration implies communication between scientists. During this first experiment, researchers  
385 engaged in a frequent and close communication both via e-mail and through the VWSL forum in order to highlight encountered problems, discuss about model results and their interpretation, and also identify challenges for future improvement of the VWSL itself. In particular, during this experiment several incidents showed the importance of well-defined terms to be able to cope with reproducibility between the research groups. These problems pointed out that communication between different  
390 groups through the web may be problematic. Indeed, the hydrological community is not well acquainted with inter-group cooperation. Detailed guidelines, including a preliminary rigorous setting of definitions and terminology, are needed to make a virtual laboratory properly working.

### **4.4 Suggested procedure to establish protocols for collaborative experiments**

Based on the experiment results, we were able to identify a recommended workflow sequence for  
395 collaborative experiments, to streamline the work among largely disjoint and independent working partners. The workflow covers three distinct phases: Preparation, Execution, and Analysis (Fig. 5). The Preparation phase contains the bulk of processes specific to collaboration between independent partner groups. Starting from an initial experiment idea, partners are brought together and a coordination structure is chosen. A lead partner, who is responsible for coordination of the experiment  
400 preparation, needs to be identified. There are two main tasks in the Preparation phase: establishment and clear communication of the experiment protocol as well as the compilation of a project database.



The definition of protocol specifications can be chosen by the partners, but they must provide detailed and exhaustive instructions regarding (i) driving principles of the protocol, which include and reflect the purpose of the experiment; (ii) data requirements and formatting, (iii) experiment execution  
405 steps, and (iv) result reporting and formatting. An initial protocol version is prepared and then evaluated by single partners and returned for improvement if ambiguities are found. Personal choices, independently made by partner groups during a test execution of the experiment, might be included. Such choices need to be well defined, and a comparability of results must be ensured through requirements in the protocol. Once the experiment protocol is agreed, partners collect, compile and  
410 publish the data necessary for the experiment using formal version-control criteria, following again a release and evaluation cycle. The Execution phase starts immediately after the completion of these tasks, and the protocol is released to all partners, who perform the experiment independently. The protocol execution can include further interaction between partners, which must be well defined in the protocol. During this phase, there should be a formal mechanism to notify partners of unexpected  
415 errors that lead to an experiment abort and return to the protocol definition. Errors can then be corrected in a condensed iteration of the Preparation phase. All partners report experiment results to the coordinating partner, who then compiles and releases the overall outcomes to all partners. The Analysis phase requires partners to analyse experiment results with respect to the proposed goals of the experiment. Partners communicate their analyses, leading to (i) rejection of experiment results  
420 as inconclusive regarding the original hypothesis, or (ii) publication of the experiment to a wider research community. This formalized workflow can then be filled by the experiment partners with more specific agreements on the infrastructure for a specific experiment. These may include:

- technical agreements, as data documentation standards to adhere to or computational platforms to be used by the partners;
- 425 – means of communication between partners, which could range from simple solutions as the establishment of an e-mail group to more complex forms, as an online communication platform with threaded public and private forums as well as online conferencing facilities;
- file exchange between partners, including data, metadata, instructions, and experiment result content. This could be implemented through informal agreements as a deadline-based  
430 collection-compilation-release system, or formal solutions as the use of version-controlled file servers with well-defined release cycles.

## 5 Discussion and Conclusions

Hydrology has always been hindered by the large variability of our environment. This variability makes it difficult for us to derive generalisable knowledge given that no single group can assess  
435 many locations in great detail or build up knowledge about a wide range of different systems. Open

environmental data and the possibilities of a connected world offer new ways in which we might overcome these problems.

In this paper, we present an approach for collaborative numerical experiments using a virtual laboratory. The first experiment that was carried out in the SWITCH-ON VWSL suggests that the value  
440 of comparative experiments can be improved by specifying detailed protocols. Indeed, in the context of collaborative experiments, we may recognise two alternative experimental conditions: (i) experimenters want to do exactly the same things (i.e., same model with same data) or (ii) researchers decide to accomplish different model implementations and assumptions based on their personal experience. In the first case, the protocol agreed upon by project participants needs to be accurately  
445 defined in order to eliminate personal choices from experiment execution. Under this experimental condition, reproducibility of experimental results among different research groups should be consistent with repeatability within a single research group. The experience from using Protocol 1 showed the importance of an accurate definition of experiment design and a detailed selection of appropriate tools, which helped to overcome several incidents during experimental set-up and execution. Problems related to insensitive parameters, local optima, and inappropriate model structure for the study  
450 catchments led to variability in performance across research groups. Our experience revealed that quantifying the within-group variability (i.e., repeatability) is necessary to adequately assess reproducibility between-groups. In turn, residual variability may indicate a lack of reproducibility, and aid in the identification of specific issues, as considered above. In the second case, the experiment is similar to traditional model ~~intercomparison~~ intercomparison projects (e.g., WMO, 1986, 1992; Duan et al., 2006; Breuer et al., 2009; Parajka et al., 2013), where each group is allowed to perform the experiment by making personal choices and using their own model concept. These choices may lead to major differences in the model setup and parameters (Holländer et al., 2009, 2014). Under these more flexible experimental conditions, the main goal of the experiment should be clearly defined.  
460 In Protocol 2, all research groups aimed at improving model performances, even though we did not deliberately specify what 'model improvement' meant a priori: this could be either reaching a higher statistical metric, less equifinality among parameter values or a more reliable model in terms of realistic internal variables. In this case, the main goal of the experiment was to profit from researchers personal experience in order to improve model performances. Indeed, each interpretation could be justified and different considerations could be normally taken by the modeller depending on the purpose of the experiment. Through this process, the modellers were able to engage in a collective discussion that pointed out the model limitations and the sensitivity of the results to different modelling options. ~~The~~ Even though results from Protocol 2 are less comparable than the outcomes from Protocol 1, the collective numerical experiment allowed comparison between  
470 different approaches suggested by individual experience and knowledge.

Multi-basin applications of hydrological models allowed the experimenters to identify links between physical catchment behaviours, efficient model structures and reliable priors for model param-

eters – all based on expertise with different systems by different groups. Even though we engaged in a relatively simple collaborative hydrological exercise, the results discussed here show that it is  
475 important to revisit experiments that are seemingly simpler than existing inter-group model comparisons  
to understand how small differences affect model performance. What is clear is that it is fundamental  
to control for different factors that may affect the outcomes of more complex experiments, such as  
modeller choice and calibration strategy. In more complex situations the virtual experiments could  
be conducted through comparisons at different levels of detail. For example, if models with different  
480 structures were to be compared there will be no one-to-one mapping of the state variables and model  
parameters and the comparison would be applied to a higher level of conceptualizations. There are  
a number of examples in the literature where comparisons at different levels of conceptualization  
have been demonstrated to provide useful results. One such example is Chicken Creek model inter  
comparison (Holländer et al., 2009, 2014) where the modellers were given an increasing amount  
485 of information about the catchment in steps, and in each step the model outputs in terms of water  
fluxes were compared. The Chicken Creek inter comparison involved models of vastly different  
complexities, yet provided interesting insights in the way models made assumptions about the hydrological  
processes in the catchment and the associated model parameters. Another example is the Predictions  
in Ungauged Basins (PUB) comparative assessment (Blöschl et al., 2013) where a two step process  
490 was adopted. In a first step (Level 1 assessment), a literature survey was performed and publications  
in the international refereed literature were scrutinised for results of the predictive performance of  
runoff, i.e. a meta-analysis of prior studies performed by the hydrological community. In a second  
step (Level 2 assessment) some of the authors of the publications from Level 1 were approached with  
a request to provide data on their runoff predictions for individual ungauged basins. At Level 2 the  
495 overall number of catchments involved was smaller than in the Level 1 assessment but much more  
detailed information on individual catchments was available. Level 1 and Level 2 were therefore  
complementary steps. In a similar fashion, virtual experiments could be conducted using the protocol  
proposed in this paper at different, complementary levels of complexity. The procedure for protocol  
development (Figure 5), which notably checks on independent model choices between partners and  
500 feedback to earlier stages in protocol development, will help in developing protocols for more  
complex collaborative experiments, addressing real science questions on floods, droughts, water  
quality and changing environments. More elaborated experiments are part of ongoing work in the  
SWITCH-ON project, and the adequacy of the protocol development procedure itself will be evaluated  
during these experiments. The modelling study presented in this paper therefore represents a relatively  
505 simple, yet no less important first step towards collaborative research in the Virtual Water-Science  
Laboratory.

To sum up, in this study we set out to answer to the following specific scientific questions related to the concepts of reproducibility of experiments in computational hydrology, previously outlined in the Introduction.

510 1. *What factors control reproducibility in computational scientific experiments in hydrology?*

The reproducibility is preliminarily governed by [shared data and models along with](#) experiment protocols, which define data requirements (metadata, also indicating versions of datasets) and format (for example, units of measurement, identification of no data, significant observation period), experiment execution (e.g., selection of a well-documented hydrological model  
515 code), and result analysis (e.g., criteria for judging model performances). These protocols aim at providing a common agreement and understanding among the involved research groups about data and experiment purpose. Human errors (e.g., ambiguity in variable names, small oversights during model execution) and unclear file-exchange procedures can be considered the main cause of a reduced reproducibility in the case researchers want to do the same thing.  
520 Conversely, if different model implementations are allowed, reduced reproducibility may depend on the lack of means of communication and clarity of the purpose of the modelling exercise or on the condition of multiple choices at once.

2. *What is the way forward to ensure reproducibility in hydrology?*

In the case different research groups use the same data input and model code, an essential  
525 prerequisite to set up a reliable experiment is to formalise a rigorous protocol that has to be based on an agreed taxonomy along with a technical environment to avoid human mistakes. If, on the other hand, researchers are allowed to perform different model implementations, the main purpose of the modelling exercise needs to be clearly defined. [For instance, in Protocol 2, the added value of researchers scientific knowledge was capable of extensively exploring alternative modelling options, which can be helpful for future hydrological experiments in the VWSL.](#)  
530 Furthermore, the experiment should be designed such that the relationship between experimental choices (e.g., cause) and the experimental results (e.g., the effects of these choices) can be clearly determined. This is required to avoid a form of equifinality that results from experimental set-up, where the relative benefits of different choices made between  
535 research groups cannot be established. Also in this second case, a controlled technical environment will help to produce reproducible experiments. Therefore, version management of databases, code documentation, metadata, preparation of protocols, and feedback mechanisms among the involved partners are all issues that need to be considered in order to establish a virtual laboratory in hydrology. Virtual laboratories provide the opportunity to share data,  
540 knowledge and facilitate scientific reproducibility. Therefore they will also open the doors for the synthesis of individual results. This perspective is particularly important to create and disseminate knowledge and data on water science and open the way to more coherence of hydrological research.

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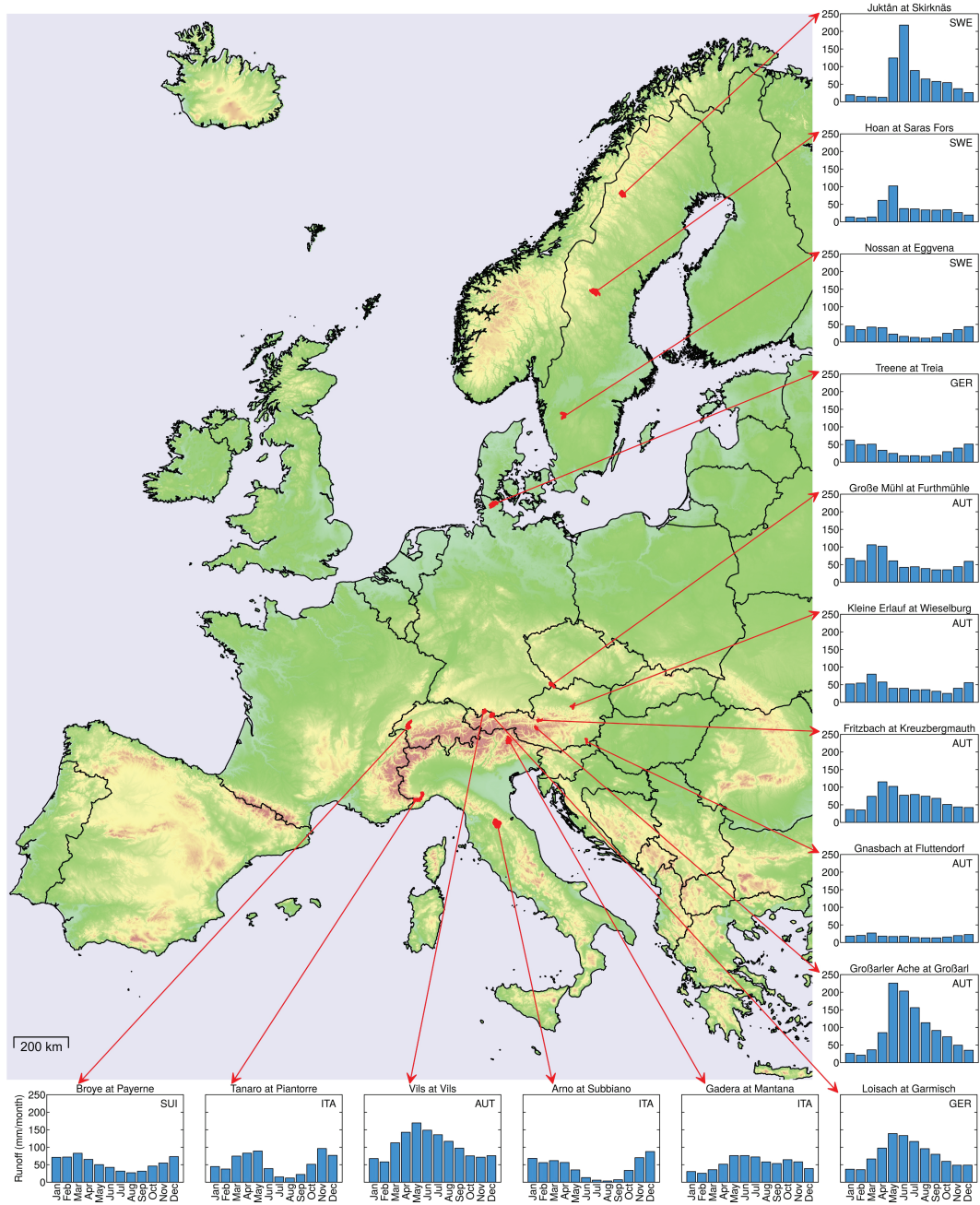
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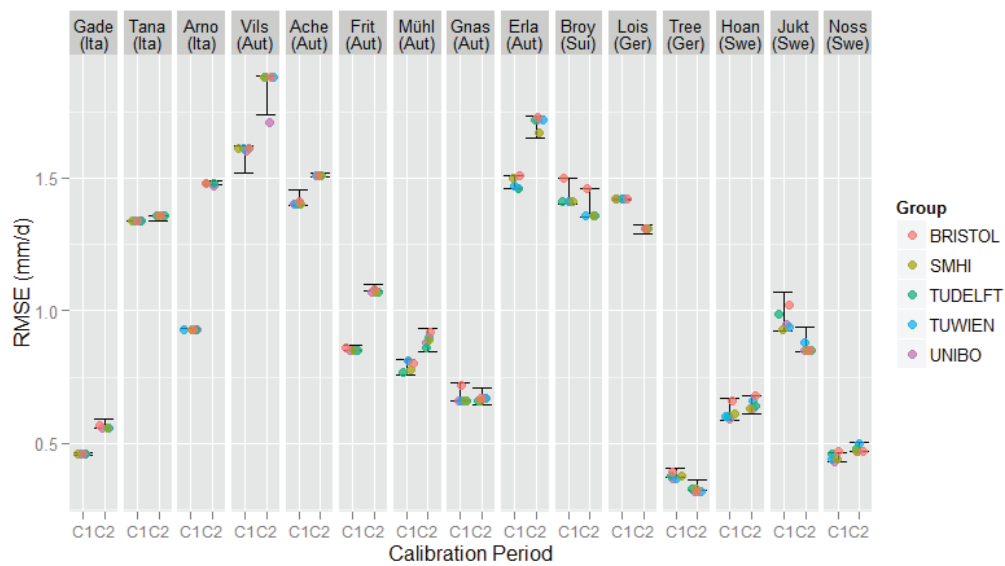


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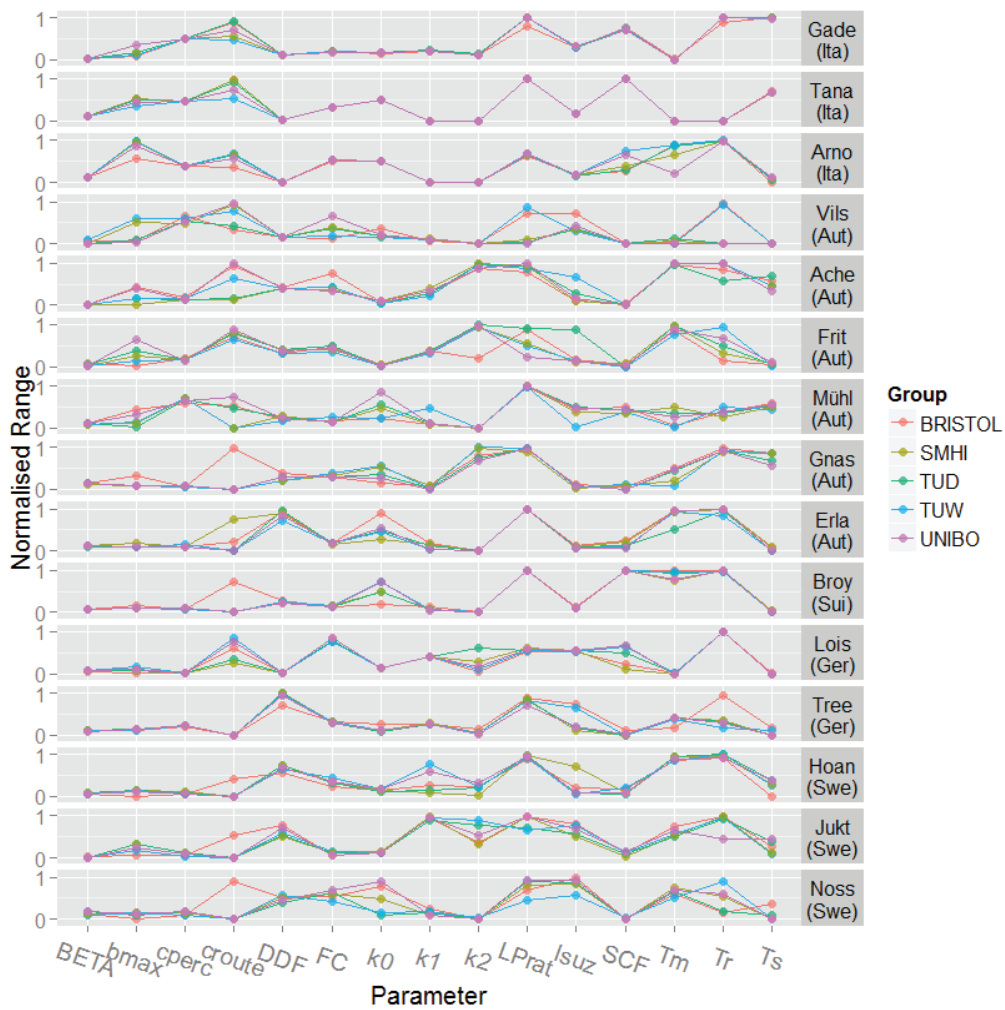
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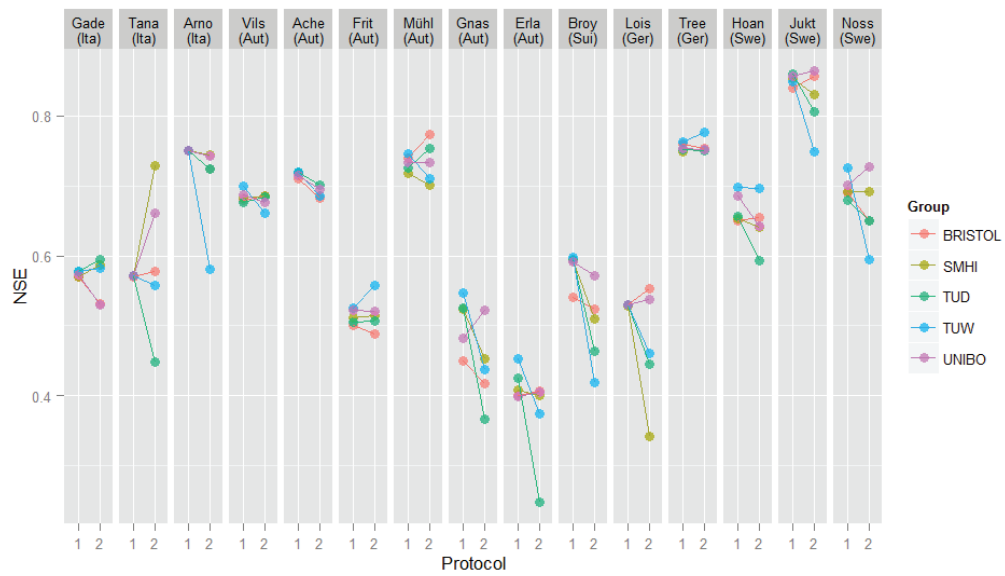
**Figure 1.** Geographical location and runoff seasonality (average among the observation period listed in Table 1) ( $\text{mm month}^{-1}$ ) for the 15 catchments considered in the first collaborative experiment of the SWITCH-ON Virtual Water-Science Laboratory.



**Figure 2.** Optimal Root Mean Square Error of runoff (RMSE; square root of the objective function) obtained for calibration period 1 and calibration period 2 by each research group for the 15 catchments. The black bars show the range in optimal performance obtained by a single research group (BRISTOL) from 100 calibration runs initiated from different random seeds.



**Figure 3.** Parallel co-ordinate plots of the optimal parameter set estimates derived from each participant group in each of the 15 catchments for Protocol 1. Model parameters are shown on the x-axis and catchments on the right hand y-axis. The parameters have been scaled to the ranges shown in Table 2.



**Figure 4.** Nash-Sutcliffe Efficiency (NSE) estimated for model validation, obtained by the five research groups, for the 15 catchments, according to Protocol 1 and 2.

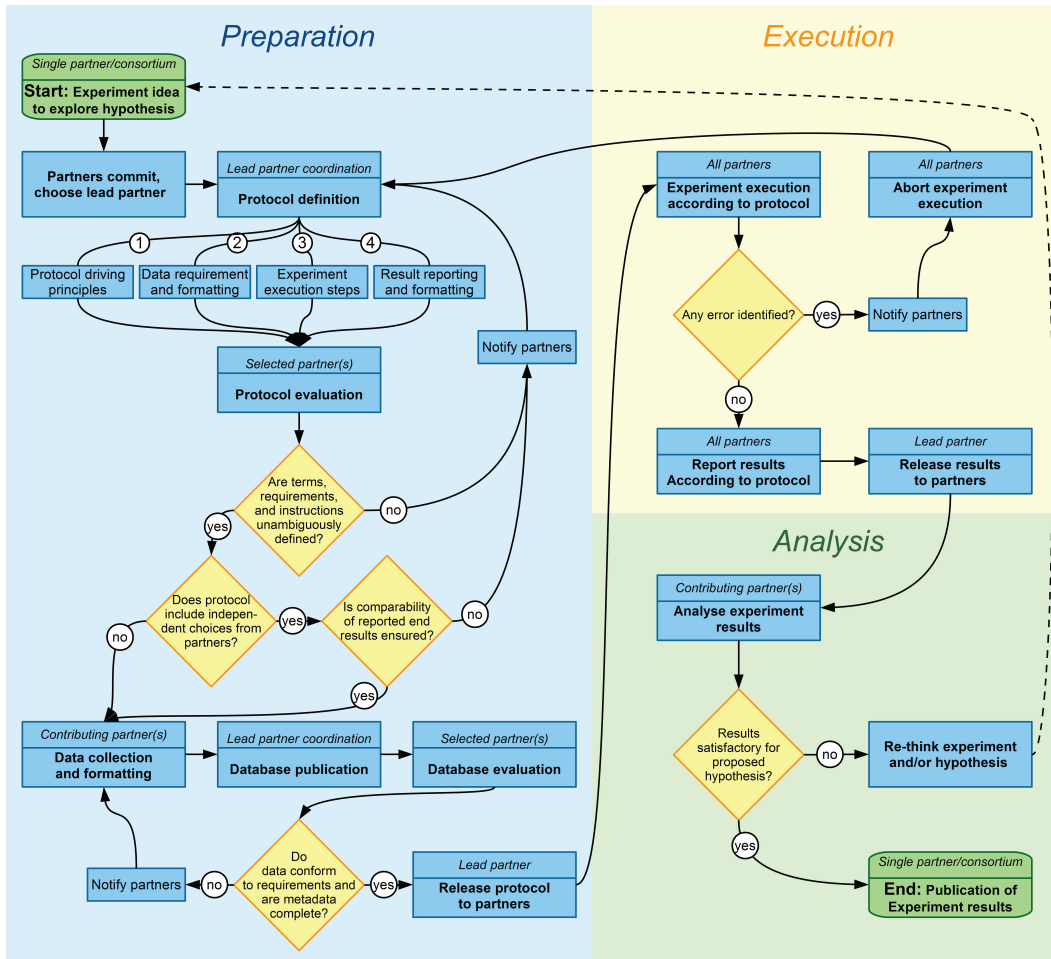


Figure 5. Flowchart of the suggested procedure to establish protocols for collaborative experiments.

**Table 1.** Summary of the key geographical and hydrological features for the 15 catchments considered in the first collaborative experiment of the SWITCH-ON Virtual Water-Science Laboratory.

| <b>Catchment</b>                      | <b>Area (km<sup>2</sup>)</b> | <b>Mean (min, max) elevation (m a.s.l.)</b> | <b>Observation period start - end</b> | <b>Mean catchment rainfall (mm year<sup>-1</sup>)</b> | <b>Mean catchment temperature (° C)</b> | <b>Mean observed streamflow per unit area (mm year<sup>-1</sup>)</b> |
|---------------------------------------|------------------------------|---|---------------------------------------|---|---|--|
| Gadera at Mantana (Italy)             | 394                          | 1844 (811, 3053)                            | 1.1.1990 - 31.12.2009                 | 842   | 5.2                                     | 640  |
| Tanaro at Piantorre (Italy)           | 500                          | 1067 (340, 2622)                            | 1.1.2000 - 31.12.2012                 | 1022  | 8.6                                     | 692  |
| Arno at Subbiano (Italy)              | 751                          | 750 (250, 1657)                             | 1.1.1992 - 31.12.2013                 | 1213  | 11.5                                    | 498  |
| Vils at Vils (Austria)                | 198                          | 1287 (811, 2146)                            | 1.1.1976 - 31.12.2010                 | 1768  | 5.5                                     | 1271   |
| Großarler Ache at Großarl (Austria)   | 145                          | 1694 (859, 2660)                            | 1.1.1976 - 31.12.2010                 | 1314  | 3.5                                     | 1113   |
| Fritzbach at Kreuzbergmauth (Austria) | 155                          | 1169 (615, 2205)                            | 1.1.1976 - 31.12.2010                 | 1263  | 5.7                                     | 799  |
| Große Mühl at Furtmühle (Austria)     | 253                          | 723 (252, 1099)                             | 1.1.1976 - 31.12.2010                 | 1075  | 7.2                                     | 696  |
| Gnasbach at Flutten-dorf (Austria)    | 119                          | 311 (211, 450)                              | 1.1.1976 - 31.12.2010                 | 746   | 9.8                                     | 218  |
| Kleine Erlauf at Wieselburg (Austria) | 168                          | 514 (499, 1391)                             | 1.1.1976 - 31.12.2010                 | 973   | 8.6                                     | 545  |
| Broye at Payerne (Switzerland)        | 396                          | 714 (391, 1494)                             | 1.1.1965 - 31.12.2009                 | 899   | 9.1                                     | 647  |
| Loisach at Garmisch (Germany)         | 243                          | 1383 (716, 2783)                            | 1.1.1976 - 31.12.2001                 | 2010  | 5.8                                     | 957  |
| Treene at Treia (Germany)             | 481                          | 25 (-1, 80)                                 | 1.1.1974 - 31.12.2004                 | 905   | 8.4                                     | 413  |
| Hoan at Saras Fors (Sweden)           | 616                          | 503 (286, 924)                              | 27.4.1988 - 31.12.2012                | 739   | 2.3                                     | 428  |
| Juktån at Skirknäs (Sweden)           | 418                          | 756 (483, 1247)                             | 19.5.1980 - 31.12.2012                | 941   | -1.4                                    | 739  |
| Nossan at Eggvena (Sweden)            | 332                          | 168 (91, 277)                               | 10.10.1978 - 31.12.2012               | 894   | 6.4                                     | 344  |



**Table 2.** Main settings of Protocol 1 of the first collaborative experiment of the SWITCH-ON Virtual Water-Science Laboratory.

| Component  | Description & Link  |   |              |
|--|---|---|--------------|
| Model version  | TUWmodel, <a href="http://cran.r-project.org/web/packages/TUWmodel/index.html">http://cran.r-project.org/web/packages/TUWmodel/index.html</a> |   |              |
| Input data   | Rainfall, temperature and potential evaporation data; catchment area  |   |              |
| Objective function   | Mean square error (MSE)   |   |              |
| Optimisation algorithm   | DEoptim, <a href="http://cran.r-project.org/web/packages/DEoptim/index.html">http://cran.r-project.org/web/packages/DEoptim/index.html</a>    |   |              |
| Parameter values or ranges   |   | Lower limits  | Upper limits |
|  | SCF [-]   | 0.9   | 1.5          |
|  | DDF [ $\text{mm } ^\circ\text{C}^{-1}$<br>$\text{day}^{-1}$ ]   | 0.0   | 5.0          |
|  | Tr [ $^\circ\text{C}$ ]   | 1.0   | 3.0          |
|  | Ts [ $^\circ\text{C}$ ]   | -3.0  | 1.0          |
|  | Tm [ $^\circ\text{C}$ ]   | -2.0  | 2.0          |
|  | LPrat [-]   | 0.0   | 1.0          |
|  | FC [mm]   | 0.0   | 600.0        |
|  | BETA [-]  | 0.0   | 20.0         |
|  | k0 [day]  | 0.0   | 2.0          |
|  | k1 [day]  | 2.0   | 30.0         |
|  | k2 [day]  | 30.0  | 250.0        |
|  | lsuz [mm]   | 1.0   | 100.0        |
|  | cperc [ $\text{mm day}^{-1}$ ]  | 0.0   | 8.0          |
|  | bmax [day]  | 0.0   | 30.0         |
|  | croute [ $\text{day}^2 \text{mm}^{-1}$ ]  | 0.0   | 50.0         |
|  | Calibration and validation periods  | Divide the observation period in two subsequent pieces of equal length. First calibrate on the first period and validate on the second and then invert the calibration and validation periods |              |
| Initial warm-up period   | 365 days for both calibration and validation periods  |   |              |
| Temporal scales of model simulation  | Daily   |   |              |
| Additional data used for validation (state variables, other response data) | None  |   |              |
| Uncertainty analysis (Y/N)   | None  |   |              |
| Method of uncertainty analysis   | None  |   |              |
| Post-calibration evaluation metrics (skills)                               | MSE, RMSE, NSE, log(NSE), bias, MAE, MALE, VE   |   |              |

**Table 3.** Comparison among Protocol 1 and Protocol 2 settings of the first collaborative experiment of the SWITCH-ON Virtual Water-Science Laboratory.

|  | <b>Protocol 1</b>  | <b>Protocol 2</b>   |                                       |  |  |  |
|--|--|---|---------------------------------------|--|--|--|
|  | <b>All research groups</b>   | <b>BRISTOL</b>  | <b>SMHI</b>                           | <b>TUD</b>   | <b>TUW</b>   | <b>UNIBO</b>   |
| <b>Identification of unreliable data</b> | All data are considered  | Runoff coefficient analysis   | All data are considered               | Visual inspection of unexplained hydrograph peaks                | All data are considered                                    | Exclusion of 25% of calibration years with high MSE                      |
| <b>Parameter ranges</b>                  | See Table 2  | See Table 2   | See Table 2                           | See Table 2  | See Table 2 except for Tr, Ts, Bmax, croute (fixed values) | See Table 2  |
| <b>Optimisation algorithm</b>            | Differential Evolution optimisation (DEoptim) – 10 times, 600 iterations | Differential Evolution optimisation (DEoptim) – 10 times, 1000 iterations | Latin hypercube approach              | Dynamically Dimensioned Search (DDS) – 10 times, 1000 iterations | Shuffle Complex Evolution (SCE)                            | Differential Evolution optimisation (DEoptim) – 10 times, 600 iterations |
| <b>Objective function</b>                | Mean Square Error (MSE)  | Mean Absolute Error (MAE)   | Mean Square Error (MSE)               | Kling-Gupta Efficiency (KGE)                                     | Objective function from Merz et al. (2011), Eq. 3          | Mean Square Error (MSE)  |
| <b>Warm-up period</b>                    | 1 year for calibration and validation                                    | 1 year for calibration and validation                                     | 1 year for calibration and validation | 1 year for calibration and validation                            | 1 year for calibration and validation                      | 1 year for calibration and validation                                    |