**Supplementary materials**

A causal physics-informed deep learning formulation for groundwater flow modeling and climate change effect analysis

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4. **Clustering**



**Fig. 1** Algorithm for clustering observation wells in the Quebec groundwater monitoring network using the time series clustering method. The minimum number of wells in a cluster has been set at 6 in order to obtain the best trade-off between complexity and speed of the multi-input/multi-output models that will be built from these clusters.

1. **Equations of the HBV model**

The schematic structure of the HBV model used (Schellekens, 2018) is represented in **Fig. 2**. The equations for each reservoir are shown below.

* 1. **Soil moisture reservoir**

The soil routine, characterized by three calibration parameters, allows the simulation of soil moisture storage , actual evaporation , net inflow , infiltration and capillary flow . The temporal variation of soil moisture is given byEquation **1**.

|  |  |
| --- | --- |
|  | 1 |

Actual evaporation , net inflow , infiltration and capillary flow are computed as below (Equations **2** to **5**):

|  |  |
| --- | --- |
|  | 2 |
|  | 3 |
|  | 4 |
|  | 5 |
|  | 6 |

where , and are respectively vertical inflow, potential evapotranspiration and direct runoff; , and are the field capacity (mm), limit above which reaches its potential value, parameter of power that define the degree of non-linearity of respectively.

* 1. **Upper reservoir**

The upper reservoir, characterized by four calibration parameters, simulates quick groundwater storage , quick runoff and percolation . The temporal variation of quick groundwater storage is given byEquation **7**.

|  |  |
| --- | --- |
|  | 7 |

Quick runoff and percolation are computed as below (Equations **8** and **9**):

|  |  |
| --- | --- |
|  | 8 |
|  | 9 |

where and , are the recession coefficients of the upper reservoir (1/day); is a limit for quick runoff to occur and is the percolation rate which is analogous to the hydraulic conductivity of an intermediate layer between the upper and lower reservoir. This way, the HBV model can be used to model groundwater dynamics in (semi)-confined aquifers.

* 1. **Lower reservoir**

The lower reservoir, characterized by two parameters to be calibrated, simulates slow groundwater storage and slow runoff . The temporal variation of slow groundwater storage is given byEquation **10**.

|  |  |
| --- | --- |
|  | 10 |

Slow runoff is computed as below (Equations **11**):

|  |  |
| --- | --- |
|  | 11 |

where is the recession coefficients of the lower reservoir (1/day) and the exchange flux coefficient between the slow and deep groundwater reservoirs.



**Fig. 2** Schematic structure of the HBV model.

1. **Algorithm structures and CMIP ensemble models**



**Fig. 3** Schematic structure of a simple traditional recurrent neural network.



**Fig. 4** Schematic structure of the 1D-CNN used in this study.



**Fig. 5** Schematic structure of the traditional physics-based hybrid model used in this study.

Une image contenant texte, capture d’écran, Police, diagramme

Description générée automatiquement

**Fig. 6** A schematic structure of the proposed formulation of hybrid algorithms. CRC stands for “Causal Relationship Constraints” and represents the novelty of the proposed formulation.



**Fig. 7** Illustration of the multi-input, multi-output modeling approach used in this study.

**Table 1** Climate projections used in this study

|  |  |  |
| --- | --- | --- |
| Emission scenario | Climate model | Number of simulations per emission scenario |
| RCP4.5 | ACCESS1-0\_rcp45\_r1i1p1 | 1 |
| ACCESS1-3\_rcp45\_r1i1p1 | 1 |
| BCC-CSM1-1\_rcp45\_r1i1p1 | 1 |
| BCC-CSM1-1-m\_rcp45\_r1i1p1 | 1 |
| CanESM2\_rcp45\_r1i1p1 | 1 |
| CSIRO-Mk3-6-0\_rcp45\_r1i1p1 | 1 |
| GFDL-CM3\_rcp45\_r1i1p1 | 1 |
| IPSL-CM5A-LR\_rcp45\_r1i1p1 | 1 |
| MIROC5\_rcp45\_r1i1p1 | 1 |
| MPI-ESM-LR\_rcp45\_r1i1p1 | 1 |
| MPI-ESM-MR\_rcp45\_r1i1p1 | 1 |
| RCP8.5 | ACCESS1-0\_rcp85\_r1i1p1 | 1 |
| ACCESS1-3\_rcp85\_r1i1p1 | 1 |
| CanESM2\_rcp85\_r1i1p1 | 1 |
| CSIRO-Mk3-6-0\_rcp85\_r1i1p1 | 1 |
| GFDL-ESM2G\_rcp85\_r1i1p1 | 1 |
| GFDL-ESM2M\_rcp85\_r1i1p1 | 1 |
| IPSL-CM5A-LR\_rcp85\_r1i1p1 | 1 |
| MIROC5\_rcp85\_r1i1p1 | 1 |
| MPI-ESM-LR\_rcp85\_r1i1p1 | 1 |
| SSP2-4.5 / SSP5-8.5 | CAS-FGOALS-g3 | 3 |
| CCCma-CanESM5 | 3 |
| CSIRO-ACCESS-ESM1-5 | 3 |
| EC-Earth-Consortium-EC-Earth3 | 3 |
| IPSL-IPSL-CM6A-LR | 3 |
| MIROC-MIROC6 | 3 |
| MRI-MRI-ESVM2-0 | 3 |
| NIMS-KMA-KACE-1-0-G | 3 |

**Reference**

Schellekens, J., 2018. wflow Documentation. Detares, Delft.