Appendix A. Soil Layers and Their Interactions in the JRB Model

In the JRB model, the soil layers are classified into:

- **Land surface layer (layer 1a)**. This layer is characterized by inflows from outside the research region (e.g., rainfall, water transfer), and outflows leaving the region (e.g., immediate evaporation, water transfer). Within the system, water flows include runoff to rivers, percolation to the root zone, and transfer of water to the anthropogenic activities (e.g., water harvesting).
- **River layer (layer 1a)**. This layer is characterized by inflows from upstream river segments and rain and outflows to downstream river segments, with water exiting rivers through evaporation. Within this layer, the runoff from the land surface layer flows into the rivers, and water can flow out to anthropogenic activities.
- **Anthropogenic activity layer (layer 1b)**. This layer encompasses all human-induced alterations to water flows, such as dams, irrigation water pumping from groundwater, wastewater treatment, drinking water treatment, return flows from consumption and water transfer (import and export).
- **Root zone layer (layer 2)**. This layer receives water from anthropogenic activity layer through irrigation and leakages, while percolation from the surface layer also adds to the water availability in this layer. Water can leave the system by evaporation and crop evapotranspiration, as well as through leakages and percolation into the aquifer layer.
- **Aquifer zone layer (layer 3)**. This layer receives water from percolation and leakages from the root zone. Groundwater pumping transfers water from the aquifer zone to the anthropogenic activity layer, while natural springs transfers water to the land surface layer. In addition, lateral flows within aquifers are possible, although these typically will be very limited.

These soil layers collectively capture the complex interplay between natural hydrological processes and human activities, thereby facilitating a comprehensive understanding of water dynamics. Fig. A1. presents the schematic overview of water flows within the JRB basin, including water flows across five soil layers as well as water flows entering the basin as whole (rainfall and lateral flows from outside the basin) and leaving the basin (evaporation, lateral flows leaving the basin).

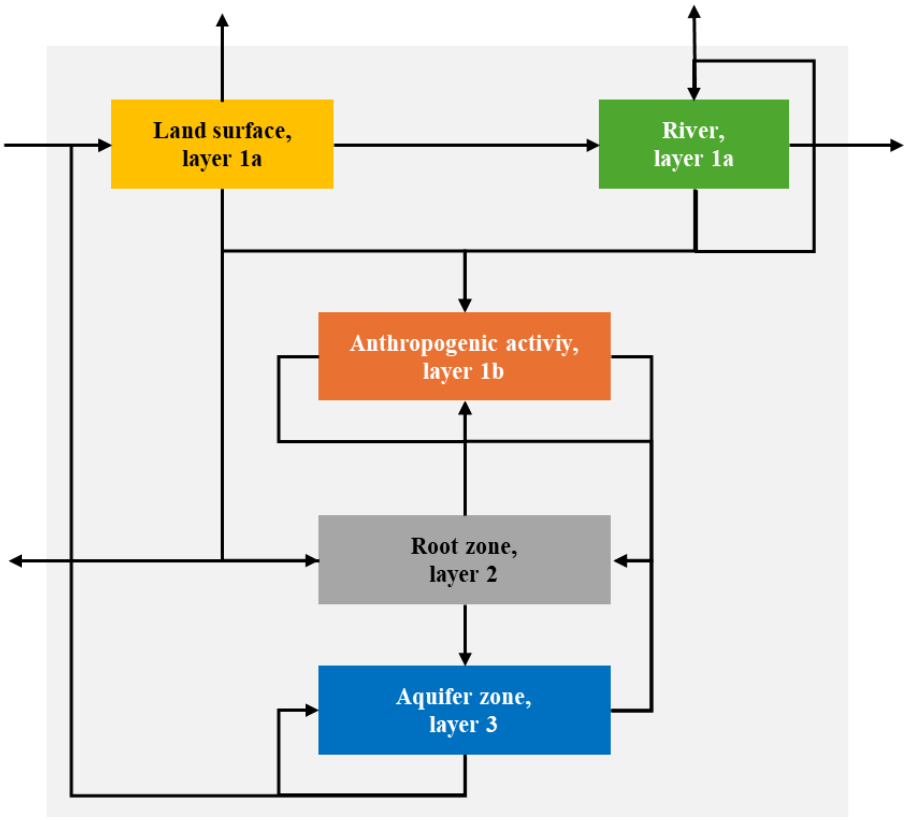

Fig. A1. Schematic overview of water flows within the JRB basin.[1]

Appendix B. Additional Constraints to Incorporate Carbon Emissions

As discussed in Subsection 2.2, the baseline WEF nexus model treats carbon emissions as external to the nexus and does not directly account for them. However, the model's flexible structure allows for the integration of carbon emissions through two distinct approaches, enabling a more comprehensive analysis of environmental impacts of the WEF nexus.

The first approach is a post-analysis calculation of carbon emissions based on energy consumption associated with key carbon-emitting activities, including human energy use (e.g., household electricity and heating), industrial processes (e.g., food processing), and agricultural activities (e.g., livestock farming). Emissions are estimated by multiplying the energy consumption of each activity by the carbon dioxide emission factor[2] (denoted as C_m) for the

[1] This figure was redrawn by the authors, based on the original figure from "Optimal calibration and control in a regional water economy model for the Jordan River Basin" by M.A. Keyzer in 2015.
[2] For more information, please refer to "Carbon dioxide emissions factors", Our World in Data, https://ourworldindata.org/grapher/carbon-dioxide-emissions-factor, accessed April 16, 2025.

energy commodity used (e.g., natural gas: 202 kg CO_2/MWh, diesel oil: 267 kg CO_2/MWh) (Willaarts et al. 2020).

The second approach integrates carbon emissions directly into the optimization model by introducing emission constraints. Total emissions are constrained by an upper limit $\overline{Carbon}$, ensuring compliance with climate goals: $\sum_t \sum_s \sum_m (\sum_i d_{stm}^i + \sum_j e_{stm}^j) C_m \leq \overline{Carbon}$. The threshold $\overline{Carbon}$ can be set according to policy guidelines, such as the EU's Fit for 55 package (targeting a 55% GHG reduction by 2030 from 1990 levels) or the U.S. Inflation Reduction Act (aiming for a 40% cut by 2030 from 2005 levels).

The model also accounts for the energy mix through the energy production, $B^j e^j$, which captures contributions from multiple sources, including fossil fuels, hydropower, solar energy, and wind power. Policy-driven targets—such as the EU's goal of 42.5% renewable energy by 2030 (Specifically, Germany's coal phase-out by 2038) or projected a 50% reduction in coal-based electricity by 2030—can inform constraints on energy mix in the model.

Appendix C. Visual Illustrations of Resource Interactions for the Beijing-Tianjin-Hebei Region, China

To better illustrate how our theoretical model bridges the gap between schematic representations and mathematical models of the WEF nexus, this subsection presents the nexus in a more transparent manner. First, it formulates the schematic representation of the WEF nexus for the Beijing-Tianjin-Hebei (abbreviated as BTH) region in China. Then, it demonstrates how the resource balance model identifies and quantifies resource interactions within the depicted WEF nexus.

The BTH region comprises Beijing, Tianjin, and Hebei Province, covering a total area of 217,000 km², which accounts for 2.25% of China's total land area. Bordered by the Bohai Sea to the east, the BTH region is located within the Haihe River basin and forms part of the North China Plain, serving as a key urban cluster. Beijing and Tianjin have notably high population densities, reaching 1,332 and 1,144.6 people/km², respectively, in 2023—approximately three times higher than Hebei's population density of 391.6 people/km². Economic disparities among the three regions are also significant. In 2023, the GDP per capita was 200,278 CNY in Beijing, 122,752 CNY in Tianjin, and 59,332 CNY in Hebei (National Bureau of Statistics of China 2024). In 2015, the central government of China proposed the Outline of the Plan for

Coordinated Development of the Beijing-Tianjin-Hebei Region[3], fostering greater cooperation in resource management across the three regions.

For simplicity, we will focus on three resource commodities: water, electricity, and crops. In the context of the BTH region[4], human demand for the three resource commodities i is specified as urban domestic resource use and rural domestic resource use. Firm activities j include river water and groundwater pumping, water transfer (import and export), artificial ecological water replenishment, water harvesting, seawater desalination, wastewater treatment, electricity generation (thermal, hydropower, and biomass), electricity storage, electricity trade (import and export), electricity loss, organic fertilizer production, crop farming, animal farming, crop storage, crop loss, and crop trade (import and export).

Since resource interactions are primarily driven by firm activities, we take the firm activity layer as an example. The origins and uses of water, electricity, and crops within this layer, as well as the resource flows between this layer and other soil layers, are shown in Fig. B1, Fig. B2, and Fig. B3, respectively. [5]

When the resource balance model represents water, the left side of Eq. (5) corresponds to the left side of Fig. B1, which illustrates the water uses, including: (1) human water demand $\sum_i d^i$, which consists of rural domestic water use and urban domestic water use; (2) water uses in firm activities $\sum_j e^j$, which include crop farming water use, artificial ecological water replenishment, hydropower water use, internal water export[6], farm animal water use, thermal power water use, and other uses[7], and; (3) water outflows $\tilde{x}$, which account for leakage and outflow.

The right side of Eq. (5) corresponds to the right side of Fig. B1, showing the origins of water, including: (1) return flows from human demand $\sum_i B^{0i} d^i$, including human urine after

[3] The official document can be accessed on the website: data.beijing.gov.cn, accessed April 16, 2025.
[4] The parameter settings are informed by a three-month field visit and discussions with local village officials in the BTH region from July to September 2023, combined with news reports and statistical data from the region.
[5] Although other soil layers are depicted in B1, Fig. B2, and Fig. B3, we focus on the interactions within the firm activity layer and between this layer and others, while disregarding the detailed interactions within and between the other layers. This simplification aims to ensure the figures remain explicit.
[6] We distinguish between water transfers (import and export) within the BTH region (referred to as "internal water import" and "internal water export") and water transfers between the BTH region and other regions (referred to as "external water import" and "external water export"). Water from external transfers is represented in the exogenous availability b, while internal water transfers are counted as firm activities.
[7] Because our resource balance model is designed for the WEF nexus, we focus on resource uses and origins in firm activities related to resource interactions, aggregating other activities into the term "other uses" or "other origins". This approach applies to all resource balance equations.

rural and urban domestic water use, which appears as a new origin after treatment; (2) flows from firm activities $\sum_j B^j e^j$, including water flows from the river layer (i.e., river water pumping and internal water import), water flows from the aquifer zone layer (i.e., groundwater pumping), water flows from the land surface layer (i.e., water harvesting), treated wastewater deriving from water uses (i.e., rural and urban domestic water use, and thermal power water use), and other origins; (3) natural inflows $A\tilde{x}$, which refer to the inflow from the river layer; and (4) net exogenous availability b, which denotes the net values of external water import, seawater import, minus losses due to evaporation and external water export.

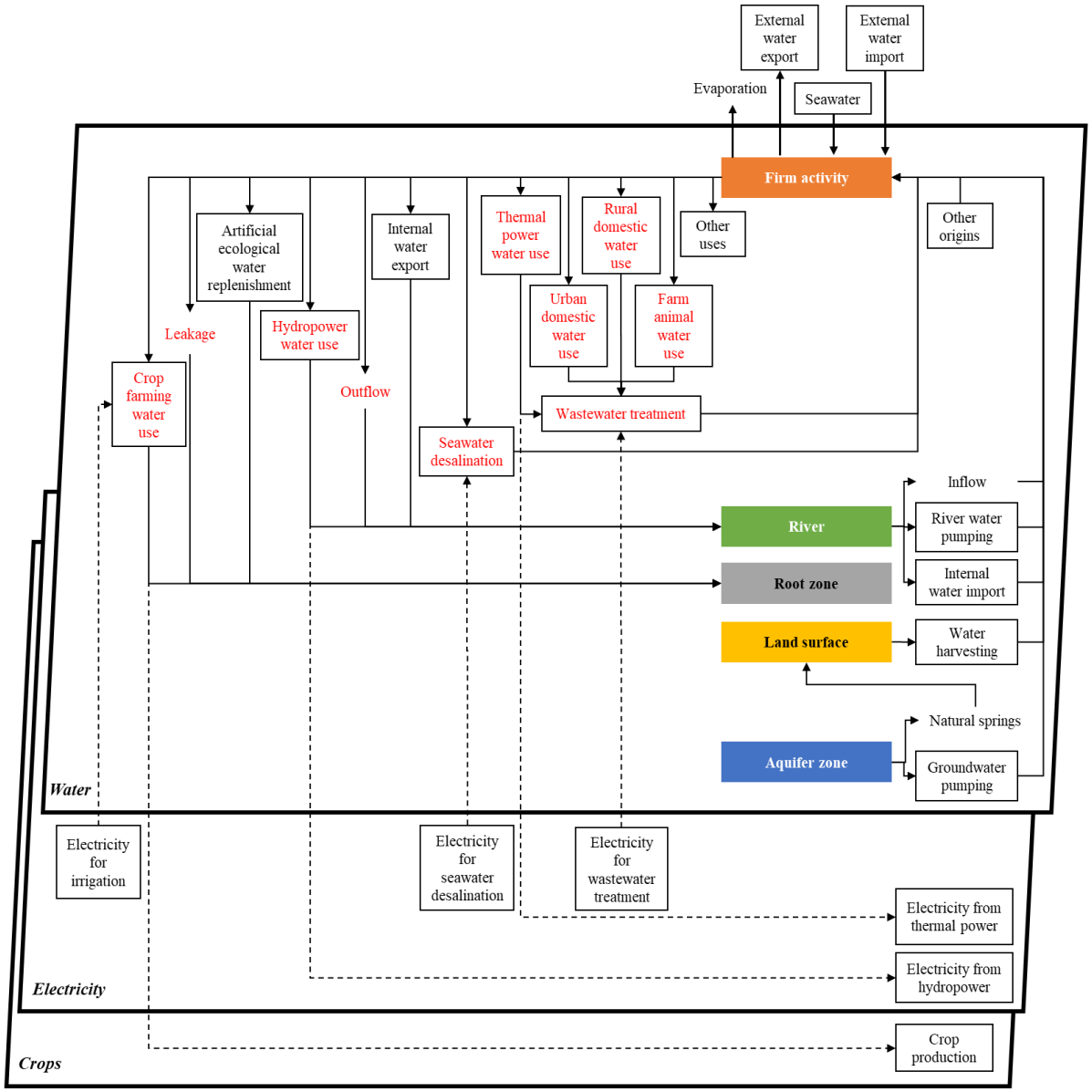

Fig. B1. Water origins and uses within the firm activity layer and water flows across the firm activity layer. The bold parallelogram delineates the boundary of the WEF nexus. Activities

within this boundary are considered endogenous, while those outsides are exogenous. Black rectangular boxes represent firm activities and human resource use, while activities without boxes represent natural flows. Red texts indicate activities where resource quality changes. Annotations here also apply to Fig. B2 and Fig. B3.

When the resource balance model represents the electricity, the left side of Eq. (5) corresponds to the left side of Fig. B2, which illustrates electricity uses, including: (1) human electricity demand $\sum_i d^i$, which consists of rural and urban domestic electricity use; (2) electricity uses in firm activities $\sum_j e^j$, which include electricity for water pumping, electricity for seawater desalination, electricity for wastewater treatment, electricity for crop farming, electricity for animal farming, electricity for crop storage, electricity loss, internal electricity export, electricity storage, and other uses. As discussed in Section 2, energy does not have natural flows, so the resource balance model for electricity excludes nature outflows $\tilde{x}$.

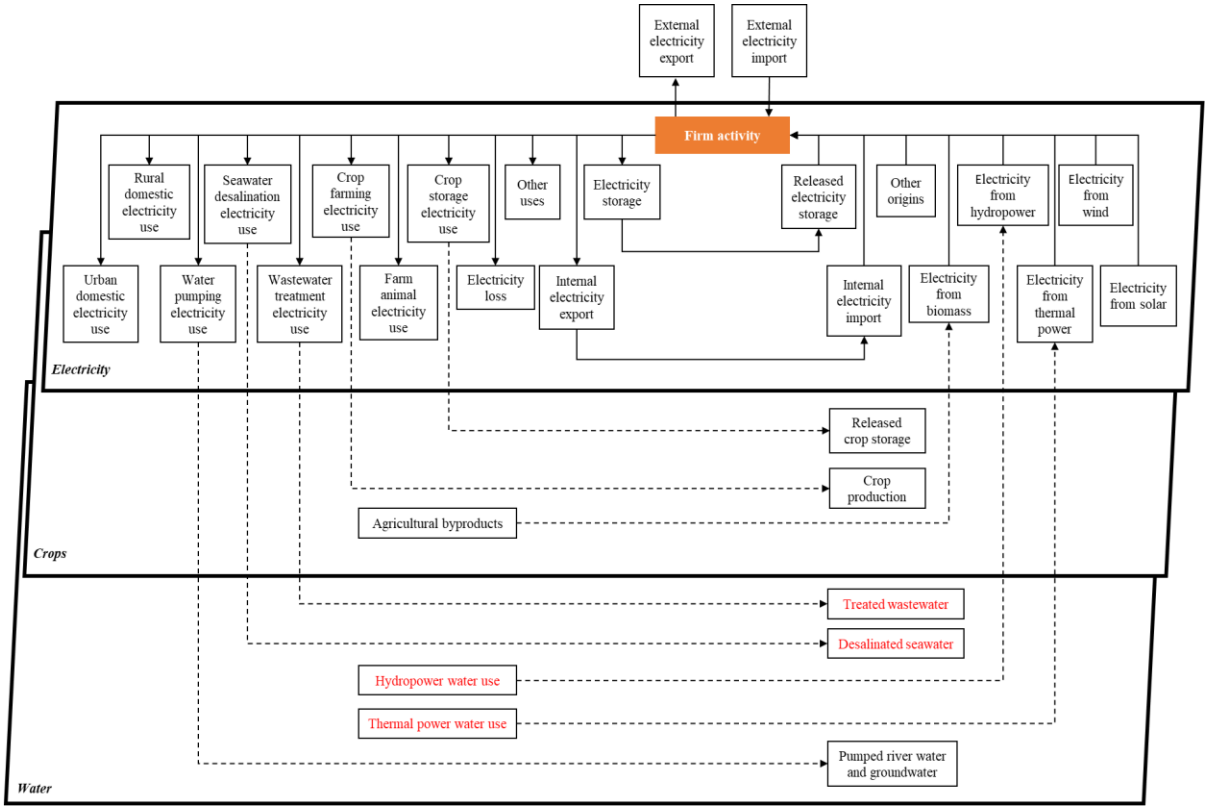

Fig. B2. Electricity origins and uses within the firm activity layer and water flows across the firm activity layer.

The right side of Eq. (5) for electricity corresponds to the right side of Fig. B2, which shows the origins of electricity, including: (1) flows from firm activities $\sum_j B^j e^j$, including released

electricity storage, internal electricity import, electricity from biomass, hydropower, thermal power, wind, solar power, and other origins; (2) net exogenous availability b, which denotes the net values of external electricity import minus the externally exported electricity. As energy does not have natural flows, there are no natural inflows $A\tilde{x}$ in the resource balance model for electricity. Additionally, as discussed in Subsection 2.2, electricity has no return flows from human demand $\sum_i B^{0i} d^i$.

When the resource balance model represents crops, the left side of Eq. (5) corresponds to the left side of Fig. B3, which illustrates crop uses, including: (1) human crop demand $\sum_i d^i$, which consists of rural and urban domestic crop use; (2) crop uses in firm activities $\sum_j e^j$, which include agricultural byproducts for biomass power generation, energy crop for biofuel generation, farm animal feed use, crop loss, crop storage, internal crop export, and other uses. As discussed in Section 2, crops do not have natural flows, so the resource balance model for crops excludes nature outflows $\tilde{x}$.

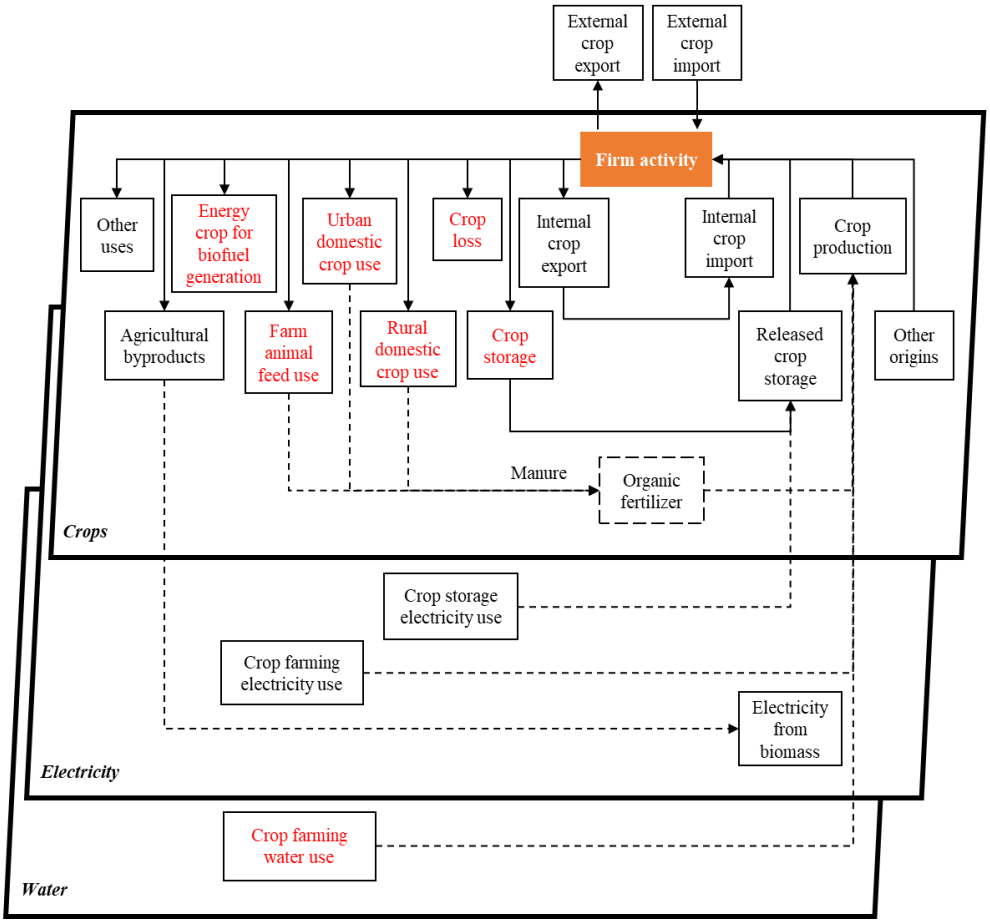

Fig. B3. Crop origins and uses within the firm activity layer and water flows across the firm activity layer.

The right side of Eq. (5) for crops corresponds to the right side of Fig. B3, which shows the origins of crops, including: (1) return flows from human demand $\sum_i B^{0i} d^i$, including human manure after rural and urban domestic crop use, which serves as organic fertilizer after treatment; (2) flows from firm activities $\sum_j B^j e^j$, including internal crop import, released crop storage, crop production, organic fertilizer production from animal manure, and other origins; (3) net exogenous availability b, which denotes the net values of external crop import minus the externally exported crop. As crop does not have natural flows, there are no natural inflows $A\tilde{x}$.

Since Fig. B1, Fig. B2, and Fig. B3 focus on the three commodities, not all cross-commodity interactions are depicted. For example, in Fig. B3, the interactions between crop and commodities other than electricity and water are not fully illustrated. Energy crops used for biofuel generation are converted into biofuel, which then enters the resource balance equation for biofuel as an origin. Similarly, crops used for feeding farm animals contribute to farm animal production and are accounted for in the resource balance equation for farm animals as an origin. While these interactions are captured by the resource balance model, they are not explicitly shown here, as the focus remains on crop-related interactions within the firm activity layer and its interactions with electricity and water.

Despite the simplified depiction in Fig. B1, Fig. B2, and Fig. B3, these figures capture various in-balance and cross-balance interactions across the six dimensions. Take Fig. B1 for example, in the water dimension, in-balance interactions include urban and rural domestic water use, and farm animal water use. Cross-balance interactions occur across locations (e.g., internal imports and exports), time (all firm activities take time, and whether they span across time depends on the chosen temporal resolution), quality (e.g., firm activities affecting water quality, marked in red), soil layers (e.g., water flows across soil layers), and temperatures (e.g., cooling water use in thermal power generation). Moreover, water flows to the crops and electricity dimensions, inducing cross-balance interactions between commodities.

All the resource interactions depicted are captured by the resource balance model, which consists of $H * S * T * L * M * C$ resource balance equations. Each equation is a combination of six dimensions: location, time, soil layer, quality, commodity, and water temperature. These equations are interconnected, with resource flows spanning all six dimensions. Together, Fig. B1, Fig. B2, and Fig. B3 provide a holistic representation of resource flows within the nexus.

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