Full Description of the System-Wide Economic-Water-Energy Model (SEWEM)

1. Model Objective Function: Costs and Benefits

1.1. The Overarching Objective Function and the Calculation of Sectoral Gross Margins

The sum of the benefits (Z^{OBJ}) across the production sites d and sectors s is formulated as:

$$Z^{OBJ} = \sum_{d}\sum_{s} Z_{d,s}^{PRD} + \sum_{n} Z_{n}^{ENV} , \tag{S1}$$

where $Z_{d,s}^{PRD}$ represents the benefit in each of the three production sectors considered (energy production, industry, and agriculture) at production site d. The Z_{n}^{ENV} is the benefit from the environmental flow.

The sector-specific gross margins ($Z_{d,s}^{PRD}$) are calculated as the difference between economic wealth (or revenue) ($W_{d,s}^{PRD}$) and costs:

$$\begin{aligned} Z_{d,s}^{PRD} = W_{d,s}^{PRD} - X_{d,s}^{PRD} - X_{d,s}^{ENS} - X_{d,s}^{CNV} - X_{d,s}^{GWP} - X_{d,s}^{RU} - X_{d,s}^{ENEF} - X_{d,s}^{E\_EXP} - X_{d,s}^{CNE} \\ - X_{d,s}^{WAE} - X_{d,s}^{SPMXP} - X_{d,s}^{GPMXP} - X_{d,s}^{RPMXP} , \end{aligned} \tag{S2}$$

where

$X_{d,s}^{PRD}$ is the cost of production (other than energy and water supply costs, e.g., the sum of the costs of fertilizer, labor, machinery, *etc.*);

$X_{d,s}^{ENS}$ is the cost of energy commodities delivered to the production site;

$X_{d,s}^{CNV}$ is the cost of delivering surface water to the production sectors;

$X_{d,s}^{GWP}$ is the cost of groundwater pumping used for industrial production;

$X_{d,s}^{RU}$ is the cost of the re-use of return water;

$X_{d,s}^{ENEF}$ is the cost of improving the energy use efficiency;

$X_{d,s}^{E\_EXP}$ is the cost of expanding the power production capacity;

$X_{d,s}^{CNE}$ is the cost of improving the conveyance efficiency;

$X_{d,s}^{WAE}$ is the cost of improving the water use efficiency in the production sector s;

$X_{d,s}^{SPMXP}$ is the cost of expanding surface water supply;

$X_{d,s}^{GPMXP}$ is the cost of expanding the groundwater pumping capacity;

$X_{d,s}^{RPMXP}$ is the cost of expanding the drainage water pumping capacity.

1.2. Sector-Specific Wealth or Revenues

Wealth, expressed as total revenues, in the energy production sector is calculated considering energy commodity prices ($P_{d,o,t}^{E}$) and outputs ($T_{d,k,o,t}^{PRD}$):

$$W_{d,'enr'}^{PRD} = \sum_{k}\sum_{o \in KOLINK}\sum_{t}\left(P_{d,o,t}^{E}\, T_{d,k,o,t}^{PRD}\right) . \tag{S3}$$

Wealth in the industrial production sector ($W_{d,'ind'}^{PRD}$) is considered as equal to the industrial value added (VA_{d}^{IND}):

$$W_{d,'ind'}^{PRD} = VA_{d}^{IND} . \tag{S4}$$

Total revenues in the agricultural sector is calculated considering crop prices (P_{c}^{A}) and production outputs ($O_{d,c}^{A}$):

$$W_{d,'agr'}^{PRD} = \sum_{c} \left(P_c^A O_{d,c}^A \right). \quad \text{(S5)}$$

1.3. Production Costs

The production costs in the energy sector are estimated as

$$X_{d,'ENR'}^{PRD} = \sum_{k} \sum_{o \in KOLINK} \sum_{t} \left(T_{d,k,o,t}^{PRD} \ v_{d,k,o,t}^{EPRD} \right), \quad \text{(S6)}$$

where $v_{d,k,o,t}^{EPRD}$ is the variable cost (labor costs, raw materials, etc.) in the energy production sector per unit of energy commodity o.

The value added of the industrial output is the equivalent of the difference between total industrial revenue and variable production costs (except energy and water related costs). Thus, for calculation purposes, $X_{d,'ind'}^{PRD}$ is considered to be equal to 0.

The production cost at the irrigation sites (here considered at a field) is the cost other than for water and energy supply (e.g., fertilizer, chemicals, seed, wages, *etc.*) per unit of cropped land plus the costs for harvesting and transportation per unit of crop output:

$$X_{d,'agr'}^{PRD} = \sum_{c} \left[v_{d,c}^{A\_PRD} A_{d,c}^{CROP} + v_{d,c}^{A\_HRV} O_{d,c}^{A} \right], \quad \text{(S7)}$$

where

$A_{d,c}^{CROP}$ is cropped land area;

$O_{d,c}^{A}$ is agricultural output;

$v_{d,c}^{A\_PRD}$ is the other production cost per unit of cropped land (fertilizer, labor, capital, chemical protection, seeds, *etc.*);

$v_{d,c}^{A\_HRV}$ is the harvesting and post-harvesting costs per unit of crop output (harvesting, transportation, storage, marketing, *etc.*).

1.4. Costs of Energy Use

The energy supply costs for production is calculated as

$$X_{d,s}^{ENS} = \sum_{t} \left(\sum_{o} P_{d,o,t}^{E} \, T_{d,s,o,t}^{PRDU} \right), \quad \text{(S8)}$$

where $P_{d,o,t}^{E}$ is the price of an energy commodity, and $T_{d,s,o,t}^{PRDU}$ is energy use for production operations in sector s.

1.5. Water Supply Costs

The surface water conveyance costs ($X_{d,s}^{CNV}$) are estimated as the sum of the energy and diesel costs to pump water, plus the costs of the keeping gravitation for supplying water from the river node:

$$X_{d,s}^{CNV} = \sum_{t} \left(v_{d,s,t}^{GRV} Q_{d,s,t}^{GRV} + \sum_{o} \left(P_{d,o,t}^{E} \, T_{d,s,o,t}^{SPMP} + v_{d,s,o,t}^{SPMP} \right) Q_{d,s,o,t}^{SPMP} \right), \quad \text{(S9)}$$

where

$v_{d,s,t}^{GRV}$ is the fixed cost per unit of surface water delivered using gravity;

$v_{d,s,o,t}^{SPMP}$ is the cost per unit of pumped surface water (labor, maintenance, *etc.*);

$T_{d,s,o,t}^{SPMP}$ is the energy requirement per unit of surface water pumped;

$Q_{d,s,o,t}^{SPMP}$ is the amount of surface water pumped.

The energy costs for groundwater supply are calculated as the sum of the electricity and diesel costs for extracting groundwater for the irrigation of crops:

$$X_{d,s}^{GWP} = \sum_t \left(\sum_o \left(P_{d,o,t}^{E} \, T_{d,s,o,t}^{GPMP} + v_{d,o,t}^{GPMP} \right) Q_{d,s,o,t}^{GPMP} \right), \tag{S10}$$

where

$v_{d,o,t}^{GPMP}$ is the non-energy-related costs (labor, maintenance, etc.) of pumping per unit of pumped groundwater;

$T_{d,s,o,t}^{GPMP}$ is the amount of energy per unit of groundwater extracted through pumping;

$Q_{d,s,o,t}^{GPMP}$ is the amount of groundwater pumped.

The cost of using the return water in the demand sites is calculated as the sum of the operation costs and the electricity and diesel costs for extracting the groundwater:

$$X_{d,s}^{RU} = \sum_t \left(\sum_o \left(P_{d,o,t}^{E} \, T_{d,s,o,t}^{RPMP} + v_{d,s,o,t}^{RPMP} \right) Q_{d,s,o,t}^{RPMP} \right), \tag{S11}$$

where

$v_{d,s,o,t}^{RPMP}$ are the non-energy-related costs (labor, maintenance, etc.) per unit of drainage water pumped for re-use;

$T_{d,s,o,t}^{RPMP}$ is the energy requirement per unit of return water re-use;

$Q_{d,s,o,t}^{RPMP}$ is the amount of return water re-use.

1.6. Costs of Energy Use Efficiency Improvement and Energy Production Capacity Expansion

The cost of improving energy use efficiency is estimated as

$$\begin{aligned} X_{d,s}^{ENEF} = \Big[& v_{d,s,o}^{NEFSP} \left(\bar{T}_{d,s,o}^{SPMP} - T_{d,s,o}^{SPMP} \right) Q_{d,s,o,t}^{SPMP} + v_{d,s,o}^{NEFGP} \left(\bar{T}_{d,s,o}^{GPMP} - T_{d,s,o,t}^{GPMP} \right) Q_{d,s,o,t}^{GPM} \\ & + v_{d,s,o}^{NEFRP} \left(\bar{T}_{d,s,o}^{RPMP} - T_{d,s,o}^{RPMP} \right) Q_{d,s,o,t}^{RPMP} + v_{d,s,o}^{NEFPR} \left(\bar{T}_{d,s,o,t}^{PRDU} - T_{d,s,o,t}^{PRDU} \right) \Big], \end{aligned} \tag{S12}$$

where

$\bar{T}_{d,s,o}^{SPMP}$ and $T_{d,s,o}^{SPMP}$ are the base and estimated levels of energy requirement to deliver a unit of surface water to an irrigation site;

$\bar{T}_{d,s,o,t}^{GPMP}$ and $T_{d,s,o,t}^{GPMP}$ are the base and estimated levels of energy required for pumping a unit of groundwater (depending on groundwater depth);

$\bar{T}_{d,s,o}^{RPMP}$ and $T_{d,s,o}^{RPMP}$ are the base and estimated levels of energy needed to pump water from the drainage-collector system;

$\bar{T}_{d,s,o,t}^{PRDU}$ and $T_{d,s,o,t}^{PRDU}$ are the base and estimated levels of total energy use for the production activity by sector s;

$v_{d,s,o}^{NEFSP}$, $v_{d,s,o}^{NEFGP}$, $v_{d,s,o}^{NEFRP}$, and $v_{d,s,o}^{NEFPR}$ are investment costs per unit of energy conserved in surface, ground, drainage water pumping, and production operations, respectively.

Increasing the energy production capacity comes at a higher investment cost. It is assumed that these costs grow exponentially with the increase in capacity:

$$X_{d,'enr'}^{E\_EXP} = \sum_k \sum_{o \epsilon KOLINK} \alpha_{d,k,o}^{E\_EXP} \left(C_{d,k,o}^{E\_PRD} - \bar{C}_{d,k,o}^{E\_PRD} \right)^{\beta_{d,k,o}^{E\_EXP}}, \tag{S13}$$

where $\bar{C}_{d,k,o}^{E\_PRD}$ and $C_{d,k,o}^{E\_PRD}$ are the base and estimated levels of power production capacity; $\alpha_{d,k,o}^{E\_EXP}$ and $\beta_{d,k,o}^{E\_EXP}$ are the parameters of the power production capacity expansion function.

The total cost of expanding the energy production capacity is considered only for the energy production sector but not for the other two sectors (industry and agriculture). Thus, $X_{d,'agr'}^{E\_EXP} = 0$ and $X_{d,'ind'}^{E\_EXP} = 0$.

1.7. Water Use Efficiency Improvement Costs

The cost of improving the conveyance efficiency is calculated as

$$X_{d,s}^{CNE} = v_{d,s}^{CNEF}\left(E_{d,s}^{CNV} - \bar{E}_{d,s}^{CNV}\right)\left(\sum_t Q_{d,s,t}^{DIV}\right), \tag{S14}$$

where

$v_{d,s}^{CNEF}$ is the cost of improving the conveyance efficiency per unit of water withdrawn from the surface water system ($Q_{d,s,t}^{DIV}$);

$\bar{E}_{d,s}^{CNV}$ and $E_{d,s}^{CNV}$ are the base and estimated levels of conveyance efficiency.

The cost of improving the water application efficiency ($X_{d,'enr'}^{WAE}$) in the energy sector is calculated by considering the amount of water savings achieved and the cost per unit of saved water:

$$X_{d,'enr'}^{WAE} = v_d^{E\_WUE}(E_d^{E\_APL} - \bar{E}_d^{E\_APL})\sum_t(Q_{d,'ind',t}^{USE}) , \tag{S15}$$

where

$v_d^{E\_WUE}$ is the cost of improving the water use efficiency per unit of saved water;

$\bar{E}_d^{E\_APL}$ and $E_d^{E\_APL}$ are the base and estimated levels of water use efficiency in the energy production sector respectively;

$Q_{d,'ind',t}^{USE}$ is the total water used by industry sector.

The costs for improving the water application efficiency in the industrial sector ($X_{d,'ind'}^{WAE}$) depend on the difference between the base level and actual water use efficiencies ($\bar{E}_d^{I\_APL}$ and $E_d^{I\_APL}$, respectively), the industrial water uses ($Q_{d,'ind',t}^{USE}$), and the cost per unit of water saving ($v_d^{I\_WUE}$):

$$X_{d,'ind'}^{WAE} = v_d^{I\_WUE}(E_d^{I\_APL} - \bar{E}_d^{I\_APL})\sum_t(Q_{d,'ind',t}^{USE}) . \tag{S16}$$

The cost of improving the water application efficiency at an irrigation site is calculated considering the amount of water savings achieved and the cost per unit of water saved:

$$X_{d,'agr'}^{WAE} = \sum_c\left(v_{d,c}^{IREF}\left(E_{d,c}^{A\_APL} - \bar{E}_{d,c}^{A\_APL}\right)\sum_t Q_{d,c,t}^{A\_CP}\right), \tag{S17}$$

where

$v_{d,c}^{IREF}$ is the cost of adopting an irrigation technology per unit of saved water;

$\bar{E}_{d,c}^{A\_APL}$ and $E_{d,c}^{A\_APL}$ are the base and actual levels of the water application efficiency;

$Q_{d,c,t}^{A\_CP}$ is the water use by crops.

1.8. Diesel and Electricity Pumping Capacity Constraints and Expansion Costs

The extraction of surface water through pumping ($Q_{d,s,o,t}^{SPMP}$) is constrained by the capacity of the installed electricity and diesel pumps ($C_{d,s,o}^{SPMP}$):

$$Q_{d,s,o,t}^{SPMP} \leq 3600 \cdot 24 \cdot \left(\frac{365}{12}\right) \cdot C_{d,s,o}^{SPMP} \tag{S18}$$

The surface water extraction capacity can be expanded through investments:

$$X_{d,s}^{SPMXP} = \sum_{o} \left(\alpha_{d,s,o}^{SPMXP} (C_{d,s,o}^{SPMP} - \bar{C}_{d,s,o}^{SPMP})^{\beta_{d,s,o}^{SPMXP}} \right) , \tag{S19}$$

where

$X_{d,s,o}^{SPMXP}$ is the cost of expanding the capacity of pumps for surface water supply;

$\bar{C}_{d,s,o}^{SPMP}$ and $C_{d,s,o}^{SPMP}$ are the base and actual levels of water pumping capacity (amount of flow per second);

$\alpha_{d,s,o}^{SPMXP}$ and $\beta_{d,s,o}^{SPMXP}$ are the parameters of a non-linear regression function depicting the relationship between the costs and level of capacity expansion of the surface water pumping.

Similarly, groundwater pumping using energy type o ($Q_{d,s,o,t}^{GPMP}$) is constrained by the pumping capacity of the installed pumps ($C_{d,s,o}^{GPMP}$):

$$Q_{d,s,o,t}^{GPMP} \leq 3600 \cdot 24 \cdot \left(\frac{365}{12}\right) \cdot C_{d,s,o}^{GPMP} . \tag{S20}$$

This pumping capacity can be expanded with additional investments:

$$X_{d,s}^{GPMXP} = \sum_{o} \left(\alpha_{d,s,o}^{GPMXP} (C_{d,s,o}^{GPMP} - \bar{C}_{d,s,o}^{GPMP})^{\beta_{d,s,o}^{GPMXP}} \right) , \tag{S21}$$

where

$X_{d,s}^{GPMXP}$ is the cost of expanding the pumping capacity for groundwater extraction;

$\bar{C}_{d,s,o}^{GPMP}$ and $C_{d,s,o}^{GPMP}$ are the base and actual levels of the groundwater pumping capacity (amount of flow per second);

$\alpha_{d,s,o}^{GPMXP}$ and $\beta_{d,s,o}^{GPMXP}$ are the parameters of a non-linear regression function reflecting the relationship between the costs and level of capacity expansion of the groundwater extraction through pumping.

Likewise, the pumping of the drainage water using energy type o ($Q_{d,s,o,t}^{RPMP}$) is constrained by the capacity of the installed pumps ($C_{d,s,o}^{RPMP}$):

$$Q_{d,s,o,t}^{RPMP} \leq 3600 \cdot 24 \cdot \left(\frac{365}{12}\right) \cdot C_{d,s,o}^{RPMP} . \tag{S22}$$

The capacity of extracting the drainage water through pumping can be expanded with additional investments:

$$X_{d,s}^{RPMXP} = \sum_{o} \left(\alpha_{d,s,o}^{RPMXP} (C_{d,s,o}^{RPMP} - \bar{C}_{d,s,o}^{RPMP})^{\beta_{d,s,o}^{RPMXP}} \right), \tag{S23}$$

where

$X_{d,s}^{RPMXP}$ is the cost of expanding the capacity of the electricity and diesel-driven pumps to increase the extraction and use of drainage water;

$\bar{C}_{d,s,o}^{RPMP}$ and $C_{d,s,o}^{RPMP}$ are the base and actual levels of the groundwater pumping capacity (amount of flow per second); and

$\alpha_{d,s,o}^{RPMXP}$ and $\beta_{d,s,o}^{RPMXP}$ are the parameters of a non-linear regression function showing the relationship between the costs and level of capacity expansion to extract drainage water through pumping.

2. Equations Representing the Hydrologial Component

2.1. Node/Reservoir Water Balance

The water balance at the river nodes in the SEWEM is based on the equality of all inflows to the node with all outflows from the node. Thus, following this definition, the water balance in river and reservoir nodes can be formulated as

$$\begin{aligned}
&\bar{Q}_{n,t}^{INF} + (1-\xi_{n,t}^{F})\left[\sum_{nu\in NNLINK}(1-\sigma_{nu}^{RES})Q_{nu,n,t}^{F} + \sum_{nu\in NNLINK}\sigma_{nu}^{RES}(Q_{nu,n,t}^{TUR}+Q_{nu,n,t}^{SP})\right] \\
&\qquad + \sum_{s}\sum_{d\in DNLINK} Q_{d,s,t}^{RFR} \\
&= \sigma_{n}^{RES}\left[\Delta S_{n,t}^{RES} + \frac{\xi_{n,t}^{RES}}{2}\left(A_{n,t-1}^{RES}+A_{n,t}^{RES}\right)\right] + (1-\sigma_{n}^{RES})\sum_{nl\in NNLINK} Q_{n,nl,t}^{F} \\
&+\sigma_{n}^{RES}\sum_{nl\in NNLINK}(Q_{n,nl,t}^{TUR}+Q_{n,nl,t}^{SP}) + \sum_{d\in NDLINK}\left(\sum_{s} Q_{d,s,t}^{DIV} + +\bar{Q}_{d,t}^{M_SP}\right) + \sigma_{n,t}^{G}\, Q_{n,t}^{GWC}\,,
\end{aligned} \tag{S24}$$

where

$\bar{Q}_{n,t}^{INF}$ is the flow from the source node (runoff) at time t;

$\xi_{n,t}^{F}$ is the rate (in %) of evaporative loss of flows to node n;

$Q_{nu,n,t}^{F}$ is the river flow from the upstream node nu to node n (given a link $(nu,n) \in NNLINK$ between these nodes);

σ_{n}^{RES} is a binary parameter that equals to 1 if the node n is a reservoir, or 0 otherwise;

$Q_{nu,n,t}^{TUR}$ and $Q_{nu,n,t}^{SP}$ are flows through the turbines and spillway flowing to node n from the upstream reservoir node nu, respectively;

$Q_{d,s,t}^{RFR}$ is the return flow to the river node from production site d and sector s, e.g., from irrigated production, of from municipal and industrial, or energy production (given a link $(d,n) \in DNLINK$ between the demand site and river node);

$Q_{n,t}^{GWC}$ is the aquifer recharge with water stemming from the river node n;

$S_{n,t}^{RES}$ is the reservoir storage volume at node n;

$\xi_{n,t}^{RES}$ is the evaporative loss (in depth per unit time) from the surface of the reservoir;

$A_{n,t}^{RES}$ is the surface area of the reservoir;

$Q_{d,s,t}^{DIV}$ is the surface water withdrawal from the river node to the production site d and sector s, e.g., irrigation, municipal and industrial, power production sector (given a link $(n,d) \in NDLINK$ between the node and demand site);

$\sigma_{n,t}^{G}$ is the binary parameter that takes a value of either -1, 0, or 1 depending on the direction of the flow between the groundwater aquifer and the river system, which thus may vary over time and in space (if $\sigma_{n,t}^{G} = 1$, then groundwater recharge occurs; if $\sigma_{n,t}^{G} = -1$, then groundwater seepage to the river node occurs; if $\sigma_{n,t}^{G} = 0$, then there is no water flow between river node and groundwater aquifer);

$\bar{Q}_{d,t}^{M\_SP}$ is the surface water use by municipality.

2.2. Morphological Relationships of the Surface Water Reservoir

A polynomial function formulates the relationship between the storage volume and surface area of the reservoir (if $\sigma_{n}^{RES} = 1$):

$$A_{n,t}^{RES} = \alpha_{n}^{RV} + \beta_{n}^{RV}\, S_{n,t}^{RES} + \gamma_{n}^{RV}\,[S_{n,t}^{RES}]^{2} + \tau_{n}^{RV}\,[S_{n,t}^{RES}]^{3}\,, \tag{S25}$$

where α_n^{RV}, β_n^{RV}, γ_n^{RV} , and τ_n^{RV} are the parameters of the polynomial function and which are statistically estimated.

The reservoir net head depends on the reservoir storage volume:

$$H_{n,t}^{RES} - tw_n = \alpha_n^{RH} + \beta_n^{RH}\, S_{n,t}^{RES} + \gamma_n^{RH}\, [S_{n,t}^{RES}]^2\, , \tag{S26}$$

where α_n^{RH}, β_n^{RH}, and γ_n^{RH} are parameters of a function to be estimated using regression methods, and $H_{n,t}^{RES}$ is the water level at the reservoir and tw_n is the tailwater level.

The maximum and minimum water levels as well as the total storage volume in reservoirs are imposed based on their capacity and minimum operating levels:

$$\underline{H}_{n,t}^{RES} \le H_{n,t}^{RES} \le \overline{H}_{n,t}^{RES}\, , \text{ and} \tag{S27}$$

$$\underline{S}_{n,t}^{RES} \le S_{n,t}^{RES} \le \overline{S}_{n,t}^{RES}\, . \tag{S28}$$

2.3. Groundwater Balance

Like the surface water balance in the nodes, the groundwater balance considers an equity of total inflows and outflows plus water volume changes in the aquifer. Thus, the water balance relationship in groundwater aquifers is

$$\bar{Q}_{n,t}^{CHG} + \sigma_{n,t}^{G} Q_{n,t}^{GWC} + \sum_{d \in NDLINK} \sum_{s} Q_{d,s,t}^{DP} = \Delta S_{n,t}^{GW} + \sum_{d \in NDLINK} \left(\sum_{s} Q_{d,s,t}^{GP} + \bar{Q}_{d,t}^{M\_GP} \right), \tag{S29}$$

where

$\bar{Q}_{n,t}^{CHG}$ is the monthly groundwater aquifer charge;

$Q_{d,s,t}^{DP}$ is the deep percolation (during conveyance and water application (use) at production site);

$S_{n,t}^{GW}$ is the water volume in the aquifer attached to node n;

$Q_{d,s,t}^{GP}$ is the use of groundwater by sector s at at production site d; and

$\bar{Q}_{d,t}^{M\_GP}$ is the groundwater use by the municipal sector (municipal water use is assumed fixed and separate from industrial water use).

The changes in groundwater volumes depend on the water level in the aquifer, which in turn is determined by water percolation from production sites, fields, and irrigation canals, groundwater use and water seepage to (and from) the river:

$$S_{n,t}^{GW} = \bar{G}_n^{YGW}\, \bar{A}_n^{GWA}\, H_{n,t}^{GWA}\, , \tag{S30}$$

where

$\bar{G}_n^{YGW}$ is a specific yield of groundwater aquifer (unitless) to indicate the amount of water out of entire mass in the aquifer;

$\bar{A}_n^{GWA}$ is the size (area) of the groundwater aquifer attached to node n;

$H_{n,t}^{GWA}$ is the groundwater level (head) in the aquifer attached to node n.

Groundwater seepage into the river depends on the water volume in the groundwater aquifer and the transitivity coefficient ($\varphi_{n,t}$):

$$\sigma_{n,t}^{G} Q_{n,t}^{GWC} = \varphi_{n,t}\, \bar{G}_n^{YGW}\, \bar{A}_n^{GWA} \left(\frac{H_{n,t}^{GWA} + H_{n,t-1}^{GWA}}{2} \right). \tag{S31}$$

Maximum groundwater level ($\overline{H}_{n,t}^{GWA}$) constraints are considered to take into account physical limits to aquifer levels:

$$H_{n,t}^{GWA} \leq \overline{H}_{n,t}^{GWA}. \quad (S32)$$

2.4. Water Balance at Production Sites

The water balance at any production node considers water conveyance, effective consumption, deep percolation, and return-flow relationships. Total water delivered to the production site ($Q_{d,s,t}^{DEL}$) was estimated while considering a conveyance efficiency ($E_{d,s}^{CNV}$), evaporation losses ($\xi_{d,s}^{CNV}$), and water withdrawals ($Q_{d,s,t}^{DIV}$) for the production purposes:

$$Q_{d,s,t}^{DEL} = \left(1 - \xi_{d,s}^{CNV}\right) Q_{d,s,t}^{DIV} E_{d,s}^{CNV}. \quad (S33)$$

The water balance at any production site can next be formulated as

$$Q_{d,s,t}^{DEL} + Q_{d,s,t}^{GP} + Q_{d,s,t}^{RU} = (Q_{d,s,t}^{ECM} - Q_{d,s,t}^{RAIN}) + Q_{d,s,t}^{ALS}, \quad (S34)$$

where $Q_{d,s,t}^{RU}$ is the re-use of the return flow, $Q_{d,s,t}^{RAIN}$ is the effective rainfall, $Q_{d,s,t}^{ECM}$ is the effective water consumption, and $Q_{d,s,t}^{ALS}$ is the loss of water during application.

Total water use ($Q_{d,s,t}^{USE}$) originates from surface, aquifer, and drainage water sources:

$$Q_{d,s,t}^{USE} = Q_{d,s,t}^{DEL} + Q_{d,s,t}^{GP} + Q_{d,s,t}^{RU}. \quad (S35)$$

Water losses during conveyance is estimated as

$$Q_{d,s,t}^{CLS} = \left(1 - \xi_{d,s}^{CNV}\right) Q_{d,s,t}^{DIV}\left(1 - E_{d,s}^{CNV}\right), \quad (S36)$$

where $\xi_{d,s}^{CNV}$ is the coefficient indicating evaporation losses.

The drainage waters ($Q_{d,s,t}^{DRN}$) are composed of shares of water losses during conveyance and water applications:

$$Q_{d,s,t}^{DRN} = Q_{d,s,t}^{CLS} f_{d,s}^{DRNC} + Q_{d,s,t}^{ALS} f_{d,s}^{DRNP}. \quad (S37)$$

$f_{d,s}^{DRNP}$ and $f_{d,s}^{DRNC}$ are fractions of water losses during water applications and conveyance, respectively, and end up as drainage water.

Part of the losses during conveyance and water applications seep to the groundwater aquifer ($Q_{d,s,t}^{DP}$) through percolation:

$$Q_{d,s,t}^{DP} = Q_{d,s,t}^{CLS}\left(1 - f_{d,s}^{DRNC}\right) + Q_{d,s,t}^{ALS}\left(1 - f_{d,s}^{DRNP}\right). \quad (S38)$$

The return flow to the river from any production site ($Q_{d,s,t}^{RFR}$) is calculated as the remaining drainage water after subtracting the amounts of flows to the tail-end depressions, losses to evaporation, and re-uses:

$$Q_{d,s,t}^{RFR} = Q_{d,s,t}^{DRN} - Q_{d,s,t}^{RFL} - Q_{d,s,t}^{DREP} - Q_{d,s,t}^{RU}, \quad (S39)$$

where $Q_{d,s,t}^{RU}$ is the amount of water re-use, $Q_{d,s,t}^{RFL}$ is the flow to the tail-end sinks, and $Q_{d,s,t}^{DREP}$ is the evaporative losses from the drainage systems.

The evaporation losses from the drainage system ($Q_{d,s,t}^{DREP}$) is calculated as a fraction of the evaporative loss ($f_{d,s}^{DREP}$) multiplied by the total drainage water:

$$Q_{d,s,t}^{DREP} = Q_{d,s,t}^{DRN} f_{d,s}^{DREP}. \quad (S40)$$

The drainage flow to the tail-end sinks that can be further evaporated ($Q_{d,s,t}^{RFL}$) is also estimated as fixed share of total drainage water ($r_{d,s}^{DRL}$):

$$Q_{d,s,t}^{RFL} = Q_{d,s,t}^{DRN} r_{d,s}^{DRL}. \quad (S41)$$

The re-use of return flows is constrained due to the low quality of return flows:

$$Q_{d,s,t}^{RU} \leq Q_{d,s,t}^{DRN}\, r_{d,s}^{DRU}\,, \tag{S42}$$

where $r_{d,s}^{DRU}$ is the rate of return flow re-use.

It is assumed that the return flow discharged into the river ($Q_{d,s,t}^{RFR}$) is less than the predetermined share of the water withdrawal ($Q_{d,s,t}^{DIV}$):

$$Q_{d,s,t}^{RFR} \leq\; Q_{d,s,t}^{DIV}\, r_{d,s}^{DIVRF}\,, \tag{S43}$$

where $r_{d,s}^{DIVRF}$ is the maximum ratio of return flows discharged into the river to the regional water withdrawal.

2.5. Water Pumping Balance

Surface water can be supplied to any production site and sector either by the use of electric and/or diesel pumps or through gravity:

$$Q_{d,s,t}^{DIV} = \sum_{o} Q_{d,s,o,t}^{SPMP} + Q_{d,s,t}^{GRV}\,, \tag{S44}$$

where $Q_{d,s,o,t}^{SPMP}$ and $Q_{d,s,t}^{GRV}$ are surface water supplied using electric and diesel pumps or delivered through gravity, respectively.

Groundwater can be supplied through the use of electricity or diesel pumps ($Q_{d,s,o,t}^{GPMP}$):

$$Q_{d,s,t}^{GP} = \sum_{o} Q_{d,s,o,t}^{GPMP}\,. \tag{S45}$$

The return water re-use is the sum of return water delivered by using electricity and diesel pumps ($Q_{d,s,o,t}^{RFPM}$):

$$Q_{d,s,t}^{RU} = \sum_{o} Q_{d,s,o,t}^{RPMP}\,. \tag{S46}$$

2.6. Water Allocation to Power Production Activities and Industrial Production

Total surface water use by the power production sector is calculated by considering water requirements per unit of energy commodity output:

$$Q_{d,\prime enr\prime,t}^{ECM} = \sum_{k} \sum_{o \epsilon KOLINK} (q_{d,k,o}^{E\_REQ}\; T_{d,k,o,t}^{PRD})\,, \tag{S47}$$

where $q_{e,k,o}^{E\_REQ}$ is the net water requirement per unit of energy production; $T_{d,k,o,t}^{PRD}$ is the amount of energy commodity o produced by the power plant using technology k at production site d in period t.

Water application losses at the energy production sites ($Q_{d,\prime enr\prime,t}^{ALS}$) are calculated as

$$Q_{d,\prime enr\prime,t}^{ALS} = Q_{d,\prime enr\prime,t}^{USE}\left(1 - E_{d}^{E\_APL}\right), \tag{S48}$$

where $E_{d}^{E\_APL}$ is the average water use efficiency in the energy production sector.

Water application losses (unused water) from any industrial production process ($Q_{d,\prime ind\prime,t}^{ALS}$) are estimated as

$$Q_{d,\prime ind\prime,t}^{ALS} = Q_{d,\prime ind\prime,t}^{USE}\left(1 - E_{d}^{I\_APL}\right), \tag{S49}$$

where $E_{d}^{I\_APL}$ is the water use efficiency.

It is assumed that the monthly industrial water uses are fixed shares of the annual water use in the industrial production sectors:

$$Q^{USE}_{d,\prime ind\prime,t} = r^{I\_SEAS}_{d,t}\, Q^{I\_USE\_ANN}_{d}\ , \tag{S50}$$

where $Q^{I\_USE\_ANN}_{d}$ is annual industrial water use; $r^{I\_SEAS}_{d,t}$ is a fixed monthly share of the annual water use.

2.7. Crop Water Allocation

Additional constraints concerning water uses at the irrigation demand sites also considered. Water delivered to any agricultural production site ($Q^{DEL}_{d,\prime agr\prime,t}$) was assumed to be distributed among crops:

$$Q^{DEL}_{d,\prime agr\prime,t} = \sum_{c} Q^{A\_SCP}_{d,c,t}\ . \tag{S51}$$

$Q^{A\_SCP}_{d,c,t}$ is the surface water used by crops.

The total amount of water applied to each crop ($Q^{A\_CP}_{d,c,t}$) is composed by the amount of surface water used for crops ($Q^{A\_SCP}_{d,c,t}$), water stemming from the groundwater aquifers ($Q^{A\_GCP}_{d,c,t}$), and the re-use of water originating from return flows ($Q^{A\_RUCP}_{d,c,t}$):

$$Q^{A\_CP}_{d,c,t} = Q^{A\_SCP}_{d,c,t} + Q^{A\_GCP}_{d,c,t} + Q^{A\_RUCP}_{d,c,t}\ . \tag{S52}$$

The crop-specific pumped groundwater ($Q^{A\_GCP}_{d,c,t}$) adds up as the total of groundwater pumped to crops at agricultural sites ($Q^{GP}_{d,\prime agr\prime,t}$):

$$Q^{GP}_{d,\prime agr\prime,t} = \sum_{c} Q^{A\_GCP}_{d,c,t}\ . \tag{S53}$$

Similarly, crop-specific water re-use ($Q^{A\_RUCP}_{d,c,t}$) adds up as the total water re-use at the agricultural production sites ($Q^{RU}_{d,\prime agr\prime,t}$):

$$Q^{RU}_{d,\prime agr\prime,t} = \sum_{c} Q^{A\_RUCP}_{d,c,t}\ . \tag{S54}$$

Percolation by crops ($Q^{A\_PERC}_{d,c,t}$) depends on the water application (irrigation) efficiency ($E^{A\_APL}_{d,c}$) and the total water supplied to the field and for each crop ($Q^{A\_CP}_{d,c,t}$):

$$Q^{A\_PERC}_{d,c,t} = Q^{A\_CP}_{d,c,t}\left(1 - E^{A\_APL}_{d,c}\right). \tag{S55}$$

The water application loss at agricultural sites for each month ($Q^{APL}_{d,\prime agr\prime,t}$) is based on the sum of the water percolations by crops ($Q^{A\_PERC}_{d,c,t}$):

$$Q^{APL}_{d,\prime agr\prime,t} = \sum_{c} Q^{A\_PERC}_{d,c,t}\ . \tag{S56}$$

Total effective water use or actual crop evapotranspiration for the entire irrigation site ($ET^{ACT}_{d,c,t}$) equals the sum of non-precipitation water effectively used by crops ($E^{A\_APL}_{d,c}\, Q^{A\_CP}_{d,c,t}$) and the total effective rainfall ($R^{EFF}_{d,c,t}$):

$$ET^{ACT}_{d,c,t} = E^{A\_APL}_{d,c}\, Q^{A\_CP}_{d,c,t} + R^{EF}_{d,c,t}\ . \tag{S57}$$

The effective water consumption at agricultural sites ($Q^{ECM}_{d,\prime agr\prime,t}$) is the sum of the actual evapotranspiration by crops ($ET^{ACT}_{d,c,t}$):

$$Q^{ECM}_{d,\prime agr\prime,t} = \sum_{c} ET^{ACT}_{d,c,t}\ . \tag{S58}$$

The actual crop evapotranspiration at time t ($ET^{ACT}_{d,c,t}$) should be less than the total crop reference evapotranspiration ($ET^{POT}_{d,c,t}$):

$$ET^{ACT}_{d,c,t} \leq ET^{POT}_{d,c,t}\,. \tag{S59}$$

The total reference crop evapotranspiration ($ET^{POT}_{d,c,t}$) is calculated as the multiplication of the agricultural cropland area with the reference (potential) crop evapotranspiration ($\xi^{PET}_{d,c,t}$):

$$ET^{POT}_{d,c,t} = A^{AGR}_{d,c}\,\xi^{PET}_{d,c,t}\,. \tag{S60}$$

The total effective rainfall ($R^{EFF}_{d,c,t}$) is estimated as the multiplication of the total agricultural area with the effective rainfall ($\zeta^{EFFR}_{d,c,t}$):

$$R^{EF}_{d,c,t} = A^{AGR}_{d,c}\,\zeta^{EFFR}_{d,c,t}\,. \tag{S61}$$

Summing up the crop-specific effective rainfall ($R^{EFF}_{n,c,t}$), total water consumption through precipitation is estimated as

$$Q^{RAIN}_{n,'agr',t} = \sum_{c} R^{EF}_{n,c,t}\,. \tag{S62}$$

3. Relationships and Equations Representing the Energy Sub-System

3.1. Scheme and Balance of Energy Production and Use

The energy generation is assumed to be based on the different energy production technologies while the energy use is considered for different production. The total energy supplied to the energy market m is assumed to be distributed among the production sites d connected to the regional energy market ($(m,d) \in MDLINK$):

$$T^{SUP}_{m,o,t} = \bar{T}^{TBAL}_{m,o,t} + \sum_{n \in MNLINK} \sum_{s} \left[\left(1 + r^{ELOSS}_{d,s,o,t}\right)\left(T^{USE}_{d,s,o,t} + \bar{T}^{M\_USE}_{d,o,t}\right)\right] \tag{S63}$$

where

$T^{SUP}_{m,o,t}$ is the supply of energy (electricity or diesel) to the regional energy market m;

$T^{USE}_{d,s,o,t}$ is energy use by the production sectors (agriculture, energy, industry);

$\bar{T}^{M\_USE}_{d,o,t}$ is energy use by the municipal sector (without the use by the industry);

$\bar{T}^{TBAL}_{m,o,t}$ is the energy trade balance. This takes a positive value when energy is exported out of the regional market, but a negative value when energy is imported to the regional market);

$r^{ELOSS}_{d,s,o,t}$ is a discount coefficient that takes into account the energy losses during transportation (transmission) and distribution.

The energy supply to the regional market m is the sum of the energy production ($T^{PRD}_{m,k,o,t}$) using different technologies k at each of the production site (k) that is connected to this market:

$$T^{SUP}_{m,o,t} = \sum_{d \in MDLINK} \sum_{k \in KOLINK} T^{PRD}_{m,k,o,t}\,. \tag{S64}$$

3.2. Energy Price and Demand Relationships

Depending on the price of the energy commodity (o), the energy supply to the market m varies according to

$$T^{SUP}_{m,o,t} = \alpha^{END}_{m,o,t}\left[P^{E\_M}_{m,o,t}\right]^{\beta^{END}_{m,o,t}}, \tag{S65}$$

where

$\alpha_{m,o,t}^{END}$ and $\beta_{m,o,t}^{END}$ are the parameters of the energy demand function;

$P_{m,o,t}^{E\_M}$ is price of the energy commodity o in market m.

The energy prices for commodity o at the production sites attached to a particular regional energy market (m) are considered the same:

$$P_{d,o,t}^{E} = \sum_{m \in MNLINK} P_{m,o,t}^{E\_M} \,. \tag{S66}$$

3.3. Power Production and Capacity Constraints

The energy production at node n in month t is constrained by the production capacity ($C_{d,k,o}^{E\_PRD}$):

$$T_{d,k,o,t}^{PRD} \leq \frac{1}{1000} \cdot 24 \cdot \frac{365}{12} \cdot C_{d,k,o}^{E\_PRD} \,. \tag{S67}$$

Similarly, it is assumed that biofuel production is determined by the availability and amount of biomass ($O_{d,'bio'}^{A}$):

$$\sum_{t} T_{d,'bio','oil',t}^{PRD} \leq \bar{G}_{d}^{B\_YLD} O_{n,'bio'}^{A} \,, \tag{S68}$$

where $\bar{G}_{e}^{B\_YLD}$ is a coefficient indicating the amount of energy that can potentially be produced per unit of raw biomass.

Hydropower production ($T_{d,'hp','elec',t}^{PRD}$) depends on the water flow through turbines and water level at the storage reservoirs of the related nodes ($(n,d) \in HPDLINK$):

$$\begin{aligned} T_{d,'hp','elec',t}^{PRD} = \sum_{n} \Bigg[g \Bigg[\Bigg(\sigma_{n}^{RES} \bar{E}_{n}^{HP} \sum_{nl \in NNLINK} Q_{n,nl,t}^{TUR} \left(0.5 \;\, H_{n,t}^{RES} + \; 0.5 \;\, H_{n,t-1}^{RES} - tw_{n} \right) \Bigg) \\ + \Bigg(\sigma_{n}^{RRS} \bar{E}_{n}^{HP} \bar{G}_{n}^{HP} \sum_{nl \in NNLINK} Q_{n,nl}^{F} \Bigg) \Bigg] \Bigg] , \end{aligned} \tag{S69}$$

where

$\bar{E}_{n}^{HP}$ is the production efficiency of the hydropower station at river node n;

g is the gravitational constant;

$Q_{n,nl,t}^{TUR}$ is the amount of water flow through the turbines;

$H_{n,t}^{RES}$ is the water level in the reservoir;

tw_{n} is the tail-end water level of the reservoir;

σ_{n}^{RRS} is a binary parameter that indicates the existence of a run-of-the-river hydropower facility at river node n (equal to 1 if yes otherwise 0);

$Q_{n,nl}^{F}$ is the river flow from the river node n to the lower node nl; and

$\bar{G}_{n}^{HP}$ is a coefficient showing the amount of electricity generated by run-of-the-river facilities per unit of river water flow.

3.4. Energy Demand

The total energy demand by production sector s ($T_{d,s,o,t}^{USE}$) in period t is accumulated as the sum of the energy uses for pumping surface water, groundwater, re-use of return flow, and for running production activities ($T_{d,s,o,t}^{PRDU}$):

$$T^{USE}_{d,s,o,t} = T^{SPMP}_{d,s,o} Q^{SPMP}_{d,s,o,t} + T^{GPMP}_{d,s,o,t} Q^{GPM}_{d,s,o,t} + T^{RPMP}_{d,s,o} Q^{RPMP}_{d,s,o,t} + T^{PRDU}_{d,s,o,t} , \quad \text{(S70)}$$

where

$T^{SPMP}_{d,s,o}$ is the energy demand to deliver a unit of surface water to an irrigation site;

$T^{GPMP}_{d,s,o,t}$ is the energy demand to pump a unit of groundwater (varies depending on groundwater depth);

and $T^{RPMP}_{d,s,o}$ is the energy requirement to pump water from drainage-collector system.

The total energy use for running agricultural activities ($T^{PRDU}_{d,\prime agr\prime,o,t}$) is estimated as the sum of crop-specific energy uses:

$$T^{PRDU}_{d,\prime agr\prime,o,t} = \sum_{c} \left(t^{APRD}_{d,c,o,t} A^{CROP}_{d,c} \right) , \quad \text{(S71)}$$

where $t^{APRD}_{d,c,o,t}$ is the energy demand per unit of cropped land.

Total energy use for an industrial activity ($T^{PRDU}_{d,\prime ind\prime,o,t}$) depends on the industrial value added (VA^{IND}_{d}), energy requirement per unit of industrial value added ($l^{I\_PRD}_{n,o}$), and a coefficient dealing with the seasonality of the energy consumption ($r^{I\_ENS}_{d,o,t}$):

$$T^{PRDU}_{d,\prime ind\prime,o,t} = r^{I\_ENS}_{d,o,t} \; t^{I\_PRD}_{d,o} \; VA^{IND}_{d} . \quad \text{(S72)}$$

Similarly, the total use of energy type o for energy production activity ($T^{PRDU}_{d,\prime enr\prime,o,t}$) depends on the produced amount of energy type o' using technology k ($T^{PRD}_{d,k,o\prime,t}$) and energy demand per unit of this produced energy ($t^{E\_PRD}_{d,o,k,o\prime}$):

$$T^{PRDU}_{d,\prime enr\prime,o,t} = \sum_{o\prime} \sum_{k \in KOLINK} \left(t^{E\_PRD}_{d,o,k,o\prime} T^{PRD}_{d,k,o\prime,t} \right) . \quad \text{(S73)}$$

It is assumed that energy requirements for groundwater pumping depend on the groundwater levels only:

$$L^{GPMP}_{d,s,o,t} = \sum_{n \in NDLINK} \left(\bar{G}^{GWP}_{n,s,t} \left(\bar{H}^{GWA}_{n} - H^{GWA}_{n,t} + \bar{H}^{DD}_{n} \right) \right) , \quad \text{(S74)}$$

where $\bar{H}^{GWA}_{n}$ is the height at the top of the groundwater aquifer, $H^{GWA}_{n,t}$ is head of the aquifer in month t, $\bar{H}^{DD}_{n}$ is pump draw-down, and $\bar{G}^{GWP}_{n,s,t}$ is a coefficient for indicating the energy requirement, which depends on the groundwater aquifer depth.

4. Relationships and Equations Representing the Agricultural Sub-System

4.1. Agricultural Price and Demand Relationships, and Agricultural Production

Crop demand functions are considered at aggregated level for the entire basin. Thus, the crop prices are the same throughout the basin and they determine the total amount of the crop produced in the basin:

$$\sum_{d} O^{A}_{d,c} = \alpha^{AGD}_{c} \left[P^{A}_{c} \right]^{\beta^{AGD}_{c}} , \quad \text{(S75)}$$

where α^{AGD}_{c} and β^{AGD}_{c} are the coefficients of the agricultural commodity demand function that relates crop price to the quantity produced.

Total crop production ($O^{A}_{d,c}$) is calculated as the product of crop yield and cropped area:

$$O^{A}_{d,c} = J_{d,c} A^{CROP}_{d,c} + \bar{J}^{RFED}_{d,c} \bar{A}^{RFED}_{d,c} , \quad \text{(S76)}$$

where $J_{d,c}$ is the crop yield and $A_{d,c}^{CROP}$ is the area of a crop c in a certain production site d; $J_{d,c}^{RFED}$ and $\bar{A}_{d,c}^{RFED}$ are the yield and cropped area for rain-fed crops.

Actual crop yield level is a function of the maximum attainable yield ($\bar{J}_{d,c}^{MAX}$) and the real yield rate that varies between 0.1 and 1 ($F_{d,c}^{YLD}$):

$$J_{d,c} = \bar{J}_{d,c}^{MAX} F_{d,c}^{YLD} . \tag{S77}$$

In other words, the real yield rate is the ratio of the actual yield to potential yield.

4.2. The Impact of Monthly Water Deficits on Crop Yield Reduction Rate

As modeled in other studies [24,35], the real yield rate ($F_{d,c}^{YLD}$) depends on the maximum monthly water deficit ($D_{d,c}^{MAX}$) as follows:

$$F_{d,c}^{YLD} \leq 1 - D_{d,c}^{MAX} . \tag{S78}$$

The maximum monthly water deficit is in turn estimated based on actual monthly water deficits ($D_{d,c,t}$):

$$D_{d,c}^{MAX} = \max_t \{D_{d,c,t}\} , \tag{S79}$$

or

$$D_{d,c}^{MAX} \geq D_{d,c,t} . \tag{S79'}$$

Monthly water deficits are estimated according to the FAO [24,36]:

$$D_{d,c,t} = k_{d,c,t}^{MON} \left(1 - \frac{ET_{d,c,t}^{ACT}}{ET_{d,c,t}^{POT}}\right) , \tag{S80}$$

where $k_{d,c,t}^{MON}$ is a crop coefficient (monthly), and $ET_{d,c,t}^{ACT}$ and $ET_{d,c,t}^{POT}$ are total actual and potential evapotranspiration, respectively.

The real yield rate ($F_{d,c}^{YLD}$) should also be less than the seasonal real yield rate ($F_{d,c}^{SYLD}$):

$$F_{d,c}^{YLD} \leq F_{d,c}^{SYLD} . \tag{S81}$$

Seasonal real yield rate ($F_{d,c}^{SYLD}$) is estimated as [24,36]:

$$F_{d,c}^{SYLD} = 1 - k_{d,c}^{SEA} \left(1 - \frac{\sum_t ET_{d,c,t}^{ACT}}{\sum_t ET_{d,c,t}^{POT}}\right) , \tag{S82}$$

where $k_{d,c}^{SEA}$ is the seasonal crop coefficient.

4.3. Cropland Restriction

The sum of the crop-specific land occupation must be less than the total potentially available cropped area ($\bar{A}_{d}^{CR\_MAX}$) for each irrigation site:

$$\sum_c A_{d,c}^{CROP} \leq \bar{A}_{d}^{CR\_MAX} . \tag{S83}$$

5. Industrial Production Function

The value added by the industrial sector in turn depends on the use of the water and energy resources. This relationship is formulated using a nested Constant Elasticity of Substitution (CES) production function:

$$VA_d^{IND} = CES\left(\sum_t Q_{d,'ind',t}^{ECM}, CES\left(\sum_t T_{d,'ind','elec',t}^{PRDU}, \sum_t T_{d,'ind','dies',t}^{PRDU}\right)\right). \tag{S84}$$

6. Relationships and Equations Representing the Environmental Sub-System

6.1. Environmental Flow Benefits

The economic values of the environmental flows (B_n^{ENV}) are assumed to be dependent on the sum of benefits from the off-stream ecosystems (lakes, ponds, *etc*.), from the instream flows (ecosystems along the river banks) and from the water reservoir releases (recreation, fishery, *etc*.).

$$Z_n^{ENV} = \sigma_n^{LAK} \sum_{d \in NDLINK}\left(f_1\left(\sum_t Q_{d,t}^{DRL}\right)\right) + \sigma_n^{FOR}\ f_2\left(\sum_t \sum_{nl \in NNLINK} Q_{n,nl,t}^{F}\right), \tag{S85}$$

where f_1 and f_2 are the notations for defining the functional relationships; σ_n^{LAK} and σ_n^{FOR} are binary variables showing if a particular type of ecosystem service (e.g., lakes or ponds receiving water from the node (here, tail-end depressions) and forests, lakes, or watersheds along the river (here the Aral Sea)) linked to node n exists.

6.2. Environmental Flow Constraints

A minimal environmental flow requirement ($\bar{Q}_{n,nl,t}^{FMIN}$) is considered for each river node:

$$(1 - \sigma_n^{RES}) \sum_{nl \in NNLINK} Q_{n,nl,t}^{F} + \sigma_n^{RES} \sum_{nl \in NNLINK} \left(Q_{n,nl,t}^{TUR} + Q_{n,nl,t}^{SP}\right) \geq \sum_{nl \in NNLINK} \bar{Q}_{n,nl,t}^{FMIN}. \tag{S86}$$