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Supplementary Material: ODD Protocoll

The Overview, Design Concept, Details (ODD) protocol is a suitable framework for describing social simulation models (Grimm, Berger et al. 2010). The following subsections describe the proposed model in detail using the ODD protocol.

1. Purpose

Six types of agents are designed, namely, the nature and ecology department, the life department, the food department, the energy department, the nature and ecology department and the water administration authority, which all have their own and competing demands for WEF (water, energy and food). The complex dynamic interactions in the supply and demand processes of WEF of these six types of agents are explored, considering the quantitative behavior rules of the six types of agents, and how these processes are conceptualized in the model is described and analyzed, as well as various scenarios and their outputs.

2. Entities, state variables, and scales

The upper-level entities of the agent are resources, managers, and users. Resources represent discrete amounts of water, energy and food resources; users consume resources, while managers regulate and manage the flow of resources to users. To represent the characteristics of the Ningdong Base, the following lower-level entities are implemented (Table S1).

Table S1. Entities in the Ningdong Energy Chemical Industry Base.

Higher-level entities	Lower-level entities
Resources	Water
	Energy
	Food
Managers	Nature and Ecology Department
	Life Department
	Food Department
Users	Energy Department
	Nature and Ecology Department
	Water Administration Department

There are six types of agents represented in this model and their parameters are listed as follows:

(1) Nature and ecology department—population growth rate, planting structure, irrigation water utilization coefficient, energy structure, water source;

(2) Life department—resource demand, population, population growth rate;

(3) Food departments—resource demand, irrigation system, planted area, unit energy consumption, irrigation water use coefficient;

(4) Energy department—resource demand, energy reserves, energy consumption quotas, coal, coal products, new energy sources, industrial water quotas, water treatment energy consumption, drainage energy consumption;

(5) Nature and ecology department—urban green space coverage, ecological water quotas, ecological energy quotas;

(6) Water administration department—total water supply.

The spatial scale of the model is Ningdong Base, the time span is from 2016 to 2025.

3. Process Overview and scheduling

Process overview. In the model, resources are created in each step, the manager allocates the resources according to the needs of each stakeholder and then calculates each user's allocation accordingly to the situation. Unlike users, managers do not consume resources themselves, but redirect all or part of them to associated users; i.e., development and reform authorities reallocate water, energy, and food to life department authorities, food administration

authorities, energy administration authorities, water administration authorities, and nature and ecology authorities. In this paper, our analysis considers alternative water, such as scenario with additional reservoirs.

Scheduling. The model is set up once at the beginning. The model receives information on historical water, energy and economic data as inputs, which can be considered as boundary conditions for the ABM environment, and these inputs are updated at the beginning of each year by traversing the inputs directly as a dictionary in the developed model code. The Ministry of Nature and Ecology receives "demands" from each stakeholder sector every year and determines the amount of resources to be allocated to each sector based on the amount of water available, the behavioral rules set by the subject's behavior (e.g., recycled water cannot be used for domestic water use, agricultural savings are allocated to industry, etc.), and the allocation process needs to take into account the prioritization of the resources to be allocated, and then they repeat all of these processes starting in the following year.

4. Design Concepts

(1) Basic principles: All users and managers have a variable "demand" that represents the agent's demand for water, energy and food resources at the current time step. According to their demand, users and managers use water, energy and food resources, i.e., they reduce the "amount" of water, energy and food resources.

(2) Emergence: The water supply variables and the "demand" variables of managers and users are adaptive features that change when specific characteristics or behaviors of water, energy, and food managers and/or users occur; exploring this unexpectedly complex system behavior is the focus of this paper.

(3) Objectives: Simulating the dynamic evolution of the water–energy–food complex system in Ningdong Base over time.

(4) Adaptation: The rules for "allocation" adaptation are based on experience and assumptions. The 'allocation' is adjusted based on predefined trends, and the decision-making process is influenced by other agent resources. Note that the reference to allocation refers to water allocation.

(5) Sensing: In most of the sub-models of this study, managers or users clearly understand their "amount of resources" or the "amount of demand" of other agents, and take this into account in their water, energy and food resource decisions.

(6) Interaction: Interaction is between the managers and the users through the allocation and demand.

(7) Stochasticity: Several sub-models are driven by randomly generated numbers. Here, randomness is used to cover a variety of external trends that are not fully predictable, for example, changes in the irrigation water use coefficient (0.68 to 0.88).

(8) Observation: The water–energy–food resource requirements for each department were calculated and analyzed, and the actual resource allocations for each department under different scenarios were simulated.

5. Input and initialization

The developed model involves six categories of sectoral agents, using data related to each agent variable based on the formulated scenarios. The data used mainly relate to the economy and the amount of resources used to represent the attributes of the agent, or to define the rules of behavior. The data set used in the simulation was calculated using the exponential smoothing method, which is based on historical time data to predict data in any future time period, with a default confidence interval of 95%. The specific variables used in this study using this method are: Yellow River water volume, groundwater volume, unconventional water volume, irrigation water utilization coefficient, per capita daily domestic water demand, crop price, crop area and urban green space. The details are shown in Figure A1 to Figure A8 below, from which we can see that the values of the variables show an almost fluctuating upward trend in the actual measurement stage, and an almost linear upward trend in the prediction stage. The predicted values of coal and coal chemical products in the paper are designed using the recursive formula with the main indicators of the "14th Five-Year Plan" of Ningdong Base as the target. The resource inputs are either externally generated, i.e., read from one or more data files in csv format, or directly traversed in the developed model code as a dictionary, and in this paper we use the latter input method.

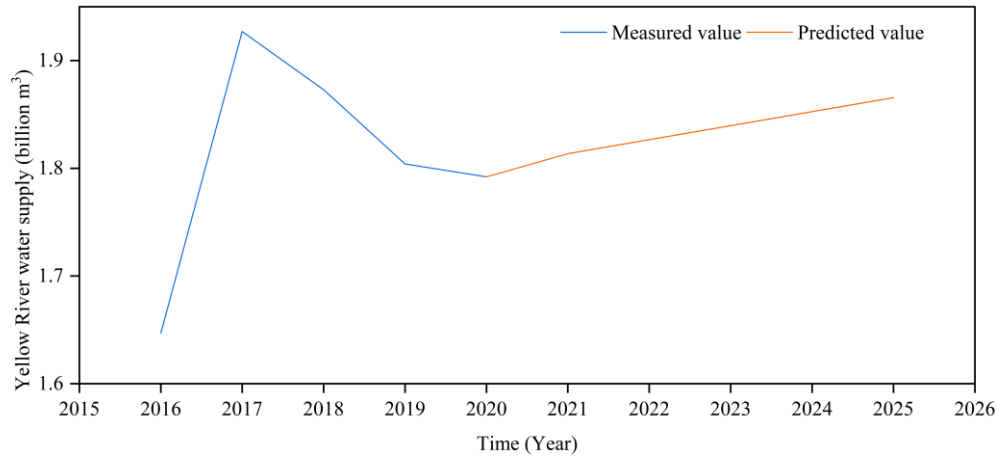

Figure S1. Measured and predicted water supply from the Yellow River at Ningdong Base.

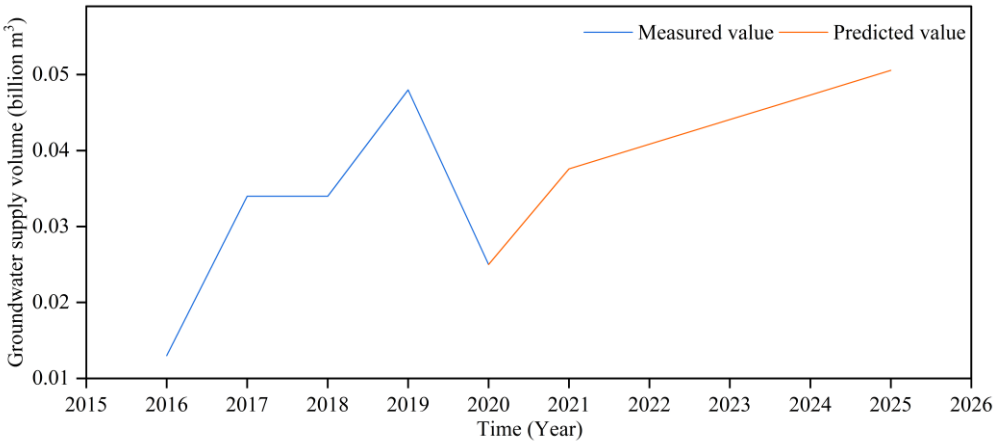

Figure S2. Measured and predicted groundwater supply at Ningdong Base.

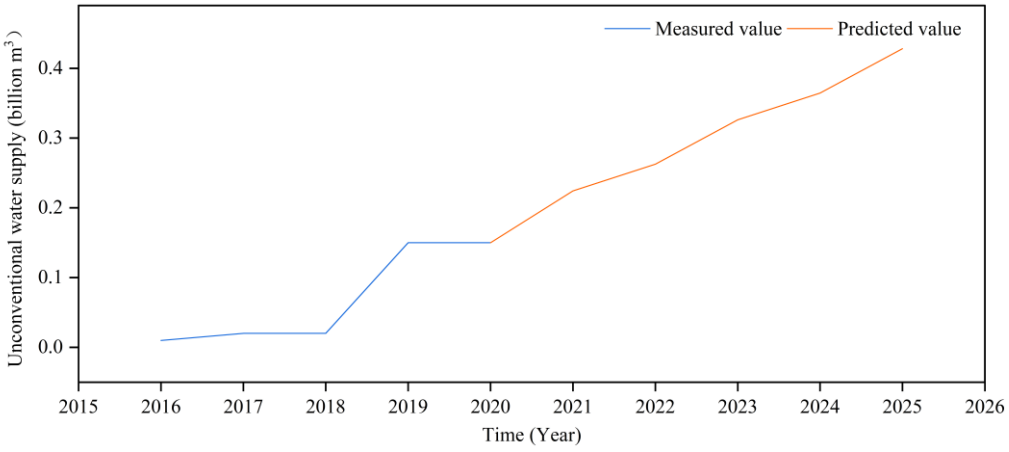

Figure S3. Measured and predicted non-conventional water supply at Ningdong Base.

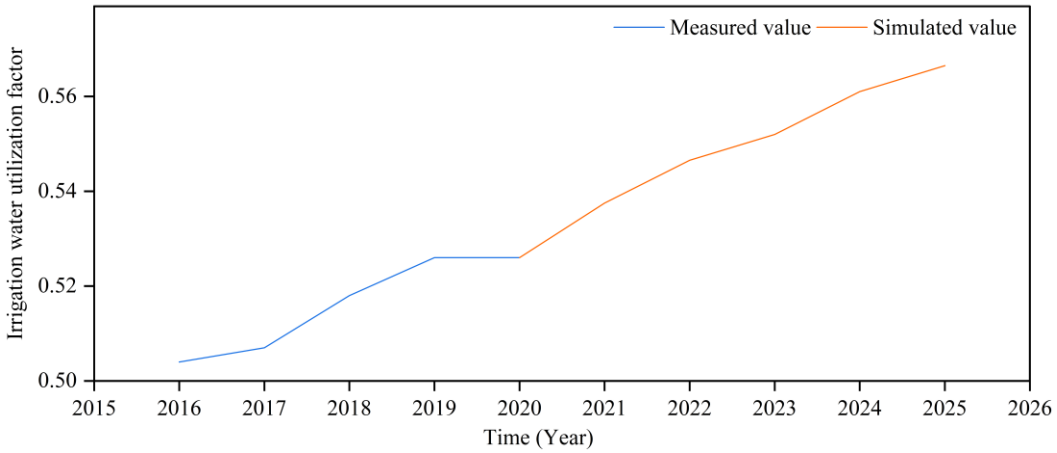

Figure S4. Measured and predicted irrigation water utilization coefficient of Ningdong Base.

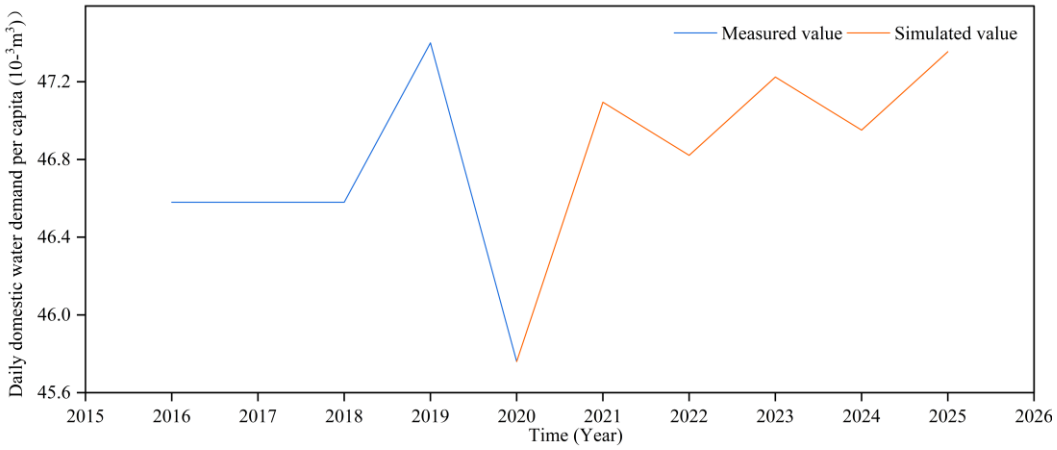

Figure S5. Measured and predicted daily per capita domestic water demand of Ningdong Base.

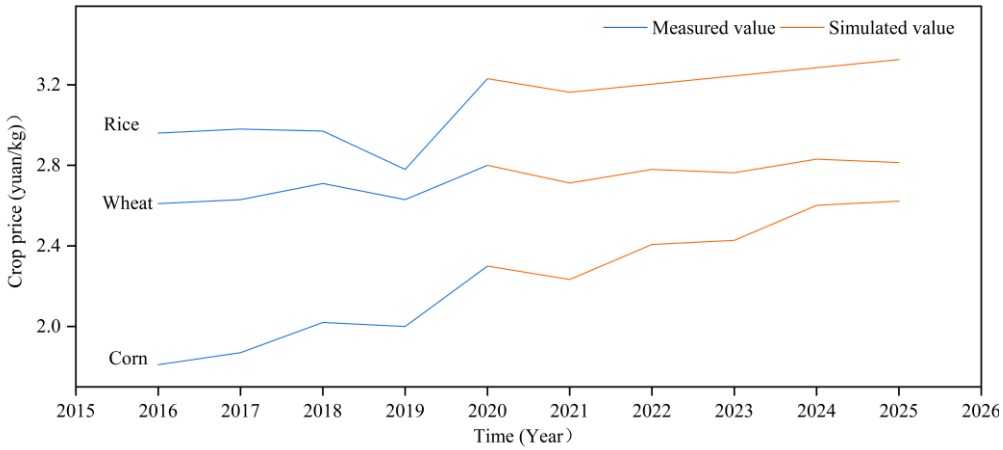

Figure S6.Measured and predicted crop prices at Ningdong base.

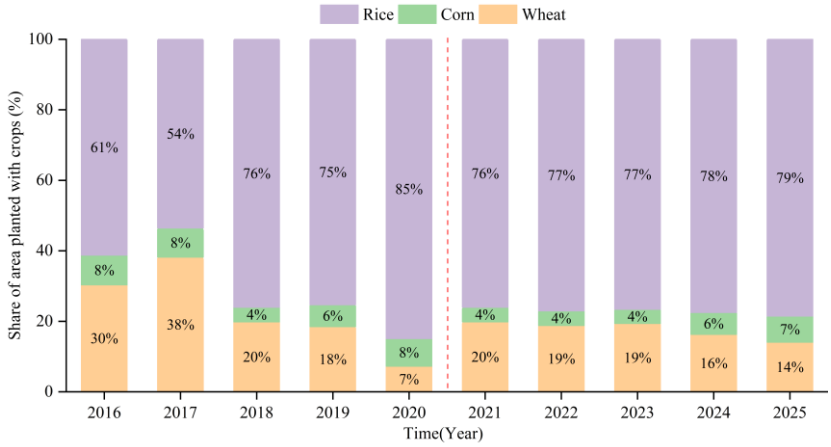

Figure S7. Measured and predicted crop area in Ningdong Base.

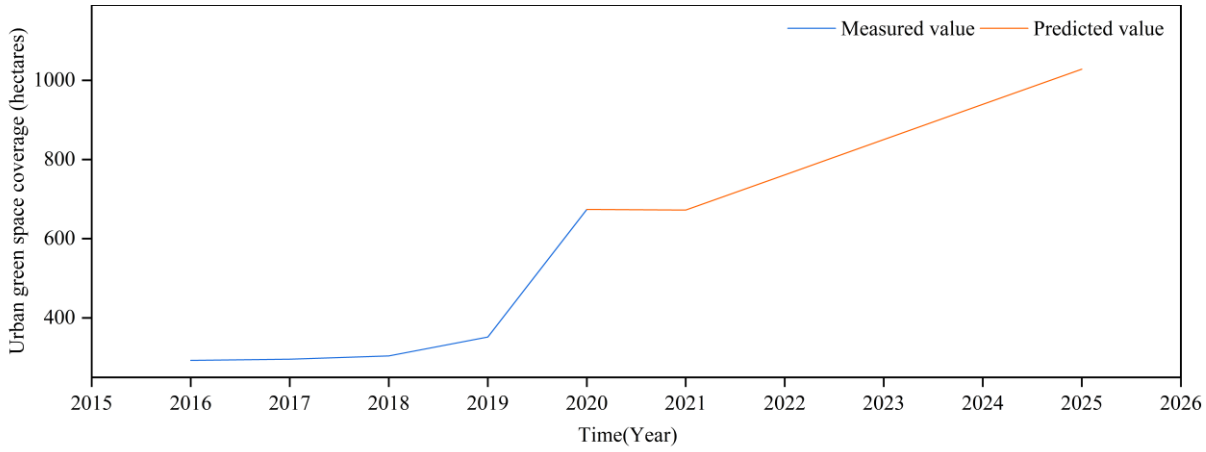

Figure S8. Measured and predicted urban green space area in Ningdong Base.

6. Submodels

(1) Development and Reform Department Agent

The development and reform department agent was designed as the coordinating and management department of Ningdong Base, which has a crucial role in the future development of Ningdong Base and is responsible for allocating the limited resources to meet the demand from each sector. In this model, we consider the competing demands for resources within a step for the living sector, food sector, energy sector, water administration and ecological sector. The amount of resources rationed among these sectors is allocated by the development and reform sector.

Objective module: The development and reform department acts as a management coordinator to achieve the objectives of the Ningdong base, such as rapid economic development, environmental friendliness, and national stability.

Attribute module: The main ones are population growth rate, planting structure, irrigation water utilization coefficient, energy structure, water source, etc.

Behavior module: coordinate planning, make policies, and coordinate and manage the other five major departments except the development and reform department.

(2) Life Sector Agent

In the life sector agent, the per capita urban living water use is calculated based on the monthly average of urban water use from 2016 to 2020. In all policy scenarios, the annual domestic sector allocation is calculated by the development and reform department based on the domestic sector demand.

Objective module: Meeting water demand, energy consumption and food consumption in the domestic sector.

Attribute module: Population growth rate, domestic water quota, and domestic energy consumption

Behavior module: Population consumes water, consumes energy, and consumes food.

(3) Food sector agent

In the food sector agent, the farmer's "demand" is calculated based on the determined cropping structure, irrigated area, and specific water requirements per unit area, among other auxiliary variables. In economically oriented ABM, farmers are assumed to have full foresight and knowledge, and they are rational maximizers of self-interest. In this case, farmers only want to make as much profit as possible with the size of their available farmland. Assuming that the main crop types in the Ningdong base are wheat, corn and rice, the sales prices of the main crop types in the study area are queried through the Chinese economic and social big data platform, and the irrigated area of the crop is calculated using the genetic algorithm with the goal of maximizing the profit obtained. Based on the water demand of the selected crop type and the planting area of the agent, the farmers' irrigation water demand was estimated. In general, the water needed for grain irrigation comes mainly from the Yellow River. If the local surface water cannot meet the irrigation water demand, farmers can extract their unmet demand from groundwater resources through legal or illegal wells and use groundwater as a supplementary water source for irrigation. It is worth noting that in the agricultural decision-making process, the lower line of water for food irrigation should be ensured even under severe drought conditions to prevent the occurrence of fallow farmland.

Objective module: Determine the number of crop types and irrigated area of crops, and the water requirement for agricultural irrigation

Attribute module: Agricultural water quotas, acreage, unit energy consumption, irrigation water use coefficient.

Behavior module: Irrigation water use, irrigation energy consumption and food production.

(4) Energy sector Agent

The core function of the energy sector agent in Ningdong Base is the supply of energy and the consumption of water resources. Consider the water consumption of coal and coal products (raw coal, oil, olefin, glycol, methanol and thermal power) and the amount of energy that can be delivered outward after meeting the energy demand of Ningdong base.

Objective module: The energy sector agent is the energy supplier of the whole Ningdong Base and the largest consumer of water resources.

Attribute module: Coal, coal products, new energy, industrial water quota, water supply and treatment energy consumption, energy consumption quota, drainage energy consumption.

Behavior attributes: living energy consumption, food energy consumption, energy industry water consumption, ecological energy consumption, energy industry water supply and treatment energy consumption, drainage energy consumption.

(5) Water administration authority agent

The main function of the water administration department agent in Ningdong Base is the supply of water to meet the demand from other departmental agents. In the water administration department agent, water sources such as Yellow River water, groundwater and other water are allocated to each water user agent, mainly for domestic, industrial, ecological and agricultural purposes, and energy consumption is considered from the perspective of water supply, water use, consumption and discharge, and auxiliary variables such as water treatment energy consumption and drainage energy consumption are used.

Objective module: The agent of the water administration authority is the supplier of all water demand units in Ningdong Base.

Attribute module: Yellow River water, groundwater, others.

Behavioral attributes: Domestic water supply, industrial water supply, agricultural water supply, ecological water supply.

(6) Ecological sector Agent

The ecological sector agent considers the Ningdong base from the environmental point of view, mainly including the water consumption for watering roads, greening and other uses, and the energy consumption in the water consumption process.

Objective module: The calculation of ecological energy consumption and ecological water consumption using auxiliary variables such as urban green space coverage, ecological water quota and ecological energy consumption quota is considered.

Attribute module: urban green area coverage, ecological water consumption quota, ecological energy consumption quota.

Behavioral attributes: Ecological greenery water consumption, ecological greenery energy consumption