Supplementary material

1. **The calculation method of grid coefficients described in section 3.2**

$$coef_{jr} = \frac{ra_{ij}}{ga} \quad \text{(S1)}$$

$$coef_{ju} = \frac{ua_{ij}}{ga} \quad \text{(S2)}$$

$$ucoef_j = coef_{ju} = \frac{ua_{ij}}{ga} \quad \text{(S3)}$$

$$coef1_j = pfa_i \frac{fa_{ij}}{ga} + pfo_i \frac{fo_{ij}}{ga} + pgr_i \frac{gr_{ij}}{ga} \quad \text{(S4)}$$

$$coef2_j = coef_{ju} = \frac{ua_{ij}}{ga} \quad \text{(S5)}$$

$$facoef_j = \frac{fa_{ij}}{ga} \quad \text{(S6)}$$

$$rcoef_j = \frac{ra_{ij}}{ga} \quad \text{(S7)}$$

$$coef3_{jr} = pua_i \frac{ua_{ij}}{ga} \quad \text{(S8)}$$

$$coef3_{ju} = pra_i \frac{ra_{ij}}{ga} \quad \text{(S9)}$$

where ra_{ij} is the rural area of *j* grid of district *i*, ua_{ij} is the urban area of *j* grid of district *i*.

pua_i is the proportion of output value of tertiary industries from the urban areas in the total tertiary industry of district *i*.

pra_i is the proportion of output value of tertiary industries from the rural areas in the total tertiary industry of district *i*.

fa_{ij} is the farmland area of *j* grid of district *i*.

pfa_i is the proportion of output value of planting in the primary industry of district *i*.

pfo_i is the proportion of output value of forestry industry in the primary of district *i*, and pgr_i is the animal husbandry accounted for the proportion of the primary industry of district *i*, fo_{ij} and gr_{ij} are the forest land and grassland area of *j* grid of district *i*, respectively.

The gird area of ga is 450 m × 450 m.

2. **The calculation method of grided population and GDP**

(1) Population:

Referring to the existing grid data processing method (Zhou et al., 2017), in this study, we assumed that the urban population was distributed in urban land and the rural population was distributed in rural land. The calculation of population distribution based on land use data was based on the following equation:

$$POP_{ij} = pop_{ir} \times {coef_{jr}}\Big/{\sum_{j=1}^{n} coef_{jr}} + pop_{iu} \times {coef_{ju}}\Big/{\sum_{j=1}^{n} coef_{ju}} \quad \text{(S10)}$$

where POP_{ij} is the population of *j* grid of district *i*, pop_{ir} is the rural population of district *i*, pop_{iu} is the urban population of district *i*, *n* is the number of grids of the district *i*, and $coef_{jr}$ and $coef_{ju}$ are the rural population and urban population coefficients, respectively, of grid *j*. The detailed calculation process of $coef_{jr}$ and $coef_{ju}$ is shown in equations S1 and S2.

(2) GDP:

Similarly, the gridded output value data of different sectors were also calculated and allocated based on the land use type. According to the statistical data of the social and economic yearbook of the study area, the grid calculation formula of the output value of different sectors was performed based on the following equation:

1) primary industry:

$$ECON1_{ij} = Econ_{1i} \times {coef1_j}\Big/{\sum_{j=1}^{n} coef1_j} \quad \text{(S11)}$$

where, $ECON1_{ij}$ is the added value of the primary industry of grid *j* in district *i*, 10^4 CNY; $Econ_{1i}$ is the added value of the primary industry of district *i*, 10^4 CNY; $coef1_j$ is the coefficient of the primary industry-added value of grid *j*. The detailed calculation process of $coef1_j$ is shown in equation S4 According to the structure and proportion of the primary industry in each district, the primary industry

was mainly related to arable land, forestland, and grassland.

2) industrial sector:

The secondary industry-added value was mainly distributed on the urban land and the grid calculation of the industrial-added value was performed according to the following equation:

$$ECON2_{ij} = Econ_{2i} \times {coef2_j}/{\sum_{j=1}^{n} coef2_j} \quad \text{(S12)}$$

where $ECON2_{ij}$ is the second industrial added value of grid j in district i, 10^4 CNY; $Econ_{2i}$ is the second industrial added value of district i, 10^4 CNY; $coef2_j$ is the coefficient of the second industrial added value of grid j. The detailed calculation process of $coef2_j$ is shown in equation S5.

3) service sector:

$$ECON3_{ij} = Econ3_{ir} \times {coef3_{jr}}/{\sum_{j=1}^{n} coef3_{jr}} + Econ3_{iu} \times {coef3_{ju}}/{\sum_{j=1}^{n} coef3_{ju}} \quad \text{(S13)}$$

where $ECON3_{ij}$ is the added value of the tertiary industry of grid j in district i, 10^4 CNY; $Econ3_{ir}$ is the added value of the rural tertiary industry in district i, 10^4 CNY; $Econ3_{iu}$ is the added value of the urban tertiary industry in district i, 10^4 CNY; $coef3_{jr}$ is the coefficient of the added value of the rural tertiary industry of grid j, $coef3_{ju}$ is the coefficient of the added value of the urban tertiary industry of grid j. The detailed calculation process of $coef3_{jr}$ and $coef3_{ju}$ are shown in equations S8 and S9.

Finally, $GDP_{ij} = ECON1_{ij} + ECON2_{ij} + ECON3_{ij}$ (S14)

where GDP_{ij} is the GDP of grid j in district i, 10^4 CNY.

Table S1. Pollutant production, export loading, and inflow coefficients in the YRB watershed.

Source	Parameter	Production or export load		Pollutant inflow coefficient[1]	
		Value	Unit	Value	Unit
Urban residences	COD	25.5	kg/per person/year	0.8	dimensionless
	NH_4^+	3.0		0.8	
	TP	0.4		0.8	
Rural residences	COD	16.6		0.05	
	NH_4^+	1.2		0.25	
	TP	0.146		0.25	
Crop	COD	2280	kg/km^2/year	0.05	
	NH_4^+	250		0.05	
	TP	51		0.1	
Urban non-point	COD	2993		0.1	
	NH_4^+	12.6		0.1	
	TP	230		0.1	
Large domestic animals	COD	550.8, 375.0 (2035)	kg/per capita/year	0.05	
	NH_4^+	9.3		0.05	
	TP	20.4		0.05	
Small domestic animals	COD	0.5		0.05	
	NH_4^+	0.13		0.05	
	TP	0.06		0.05	
Industrial				0.8	

Note: According to China's discharge standard of pollutants for livestock and poultry breeding (GB 18596-2001), in terms of pollutant productions, two beef cattle are equal to one dairy cow, ten pigs are equal to one dairy cow, 30 sheep are equal to one dairy cow, and two laying hens are equal to one broiler. Therefore, pigs, beef cattle, and sheep were converted into dairy cows as large livestock, and hens were converted into broilers as small livestock for pollutant production calculations. The values of these coefficients are mainly collected from Zhu (2011) and Cheng (2018).

Considering the benchmark year of the second national survey of pollution sources of China is 2017, the spatial distribution pollutants were based on 2017's pollutant load.

[1] The pollutant inflow coefficient determines the final amount of loads that flow into the river.

Table S2. Pollutant treatment efficiency of different wastewater treatment (WWT) capacities, according to the “Overall Plan of Comprehensive Management and Ecological Restoration of Yongding River” policy, in the YRB, by 2035.

Source	Parameter	Unit	Year		
			2017	2025	2035
Urban living	COD	%	92	95	98
	NH_4^+		95.9	96.4	98
	TP		91.8	95	98
Rural living	COD		20	70	90
	NH_4^+		20	70	90
	TP		20	70	90
Industrial	COD		0.92	0.94	0.95
	NH4+		0.824	0.9	0.95
	TP		0.824	0.9	0.98

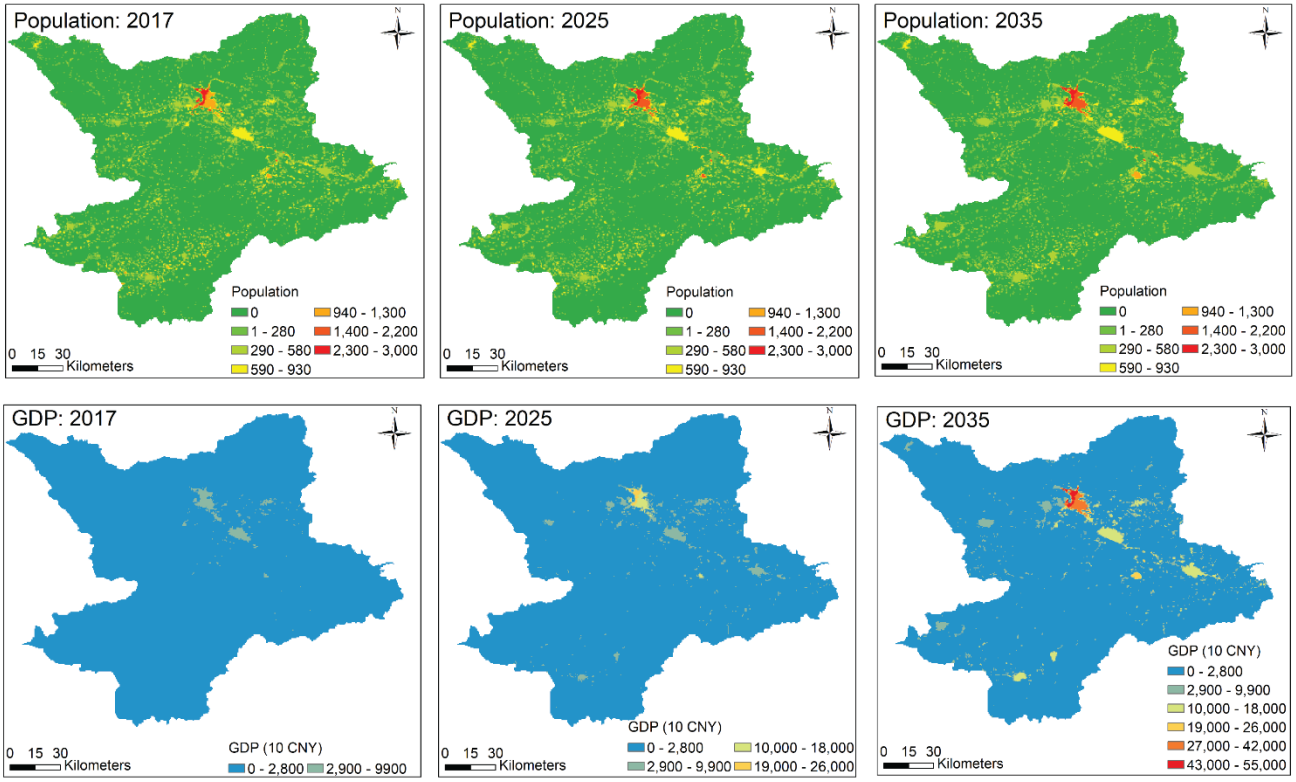

Figure S1. Spatial distribution of the population and GDP of the study area.

According to the economic pattern of Zhangjiakou City, the urban and rural dual system is obvious, thus land use change can directly reflect the distribution characteristics of the population and economy. Considering the research scope and the precision of data, this study takes the district as the smallest administrative unit and takes the number of urban population and rural populations and the added value of each sector in each district as the control variable to calculate the spatial pattern of population and GDP. The details of the calculation processes are shown as mentioned above.

References:

Cheng, P., 2018. Study of typical river water quality target management technique in the North China. Research Center for Eco-Environmental Sciences Chinese Academy of Sciences, Beijing. 148.

Zhou, X., Lei, K., Meng, W., Khu, S.-T., Jian, Z., Wang, M., Yang, J., 2017. Space–time approach to water environment carrying capacity calculation. J. Clean. Prod. 149, 302-312.

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