Supplementary Materials

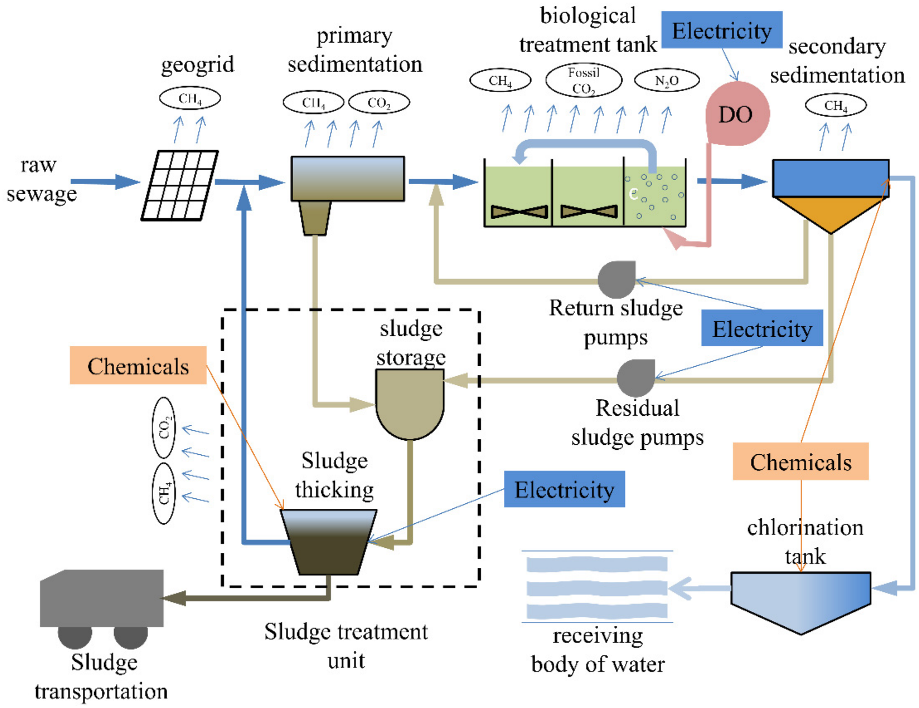

Fig. S1. GHG accounting boundary for wastewater treatment plants.

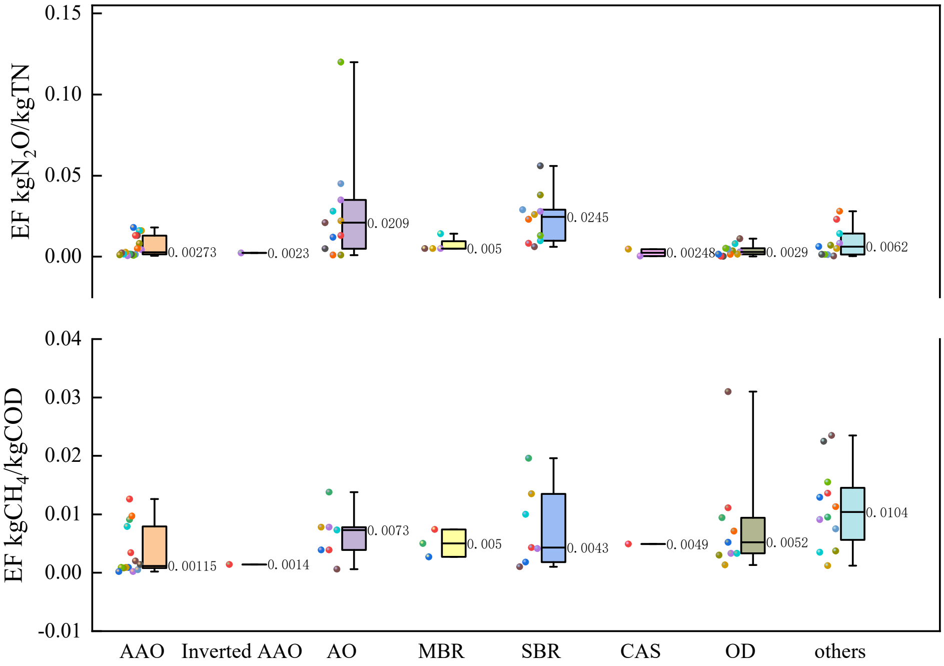

Fig. S2. Carbon emission factors for different wastewater treatment processes.

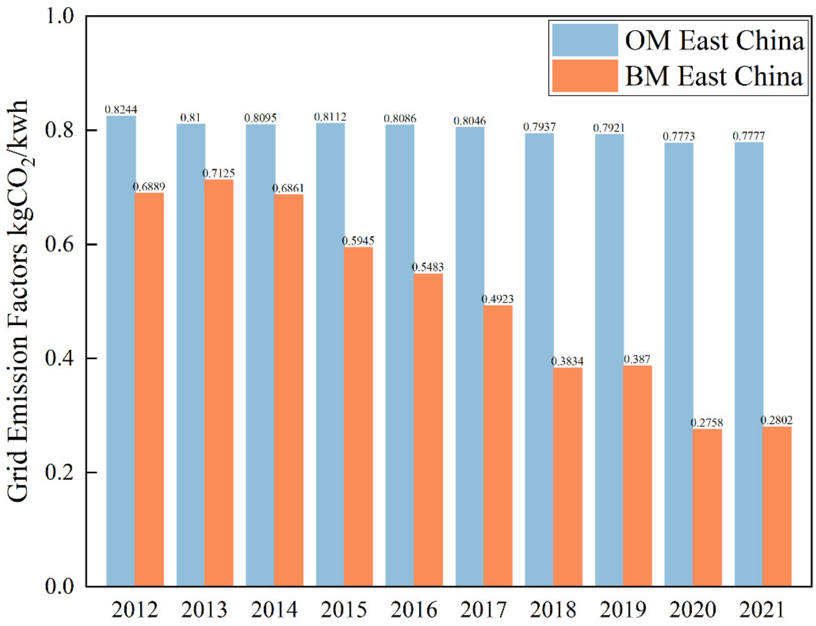

Fig. S3. Carbon emission factor of power grid in East China region.

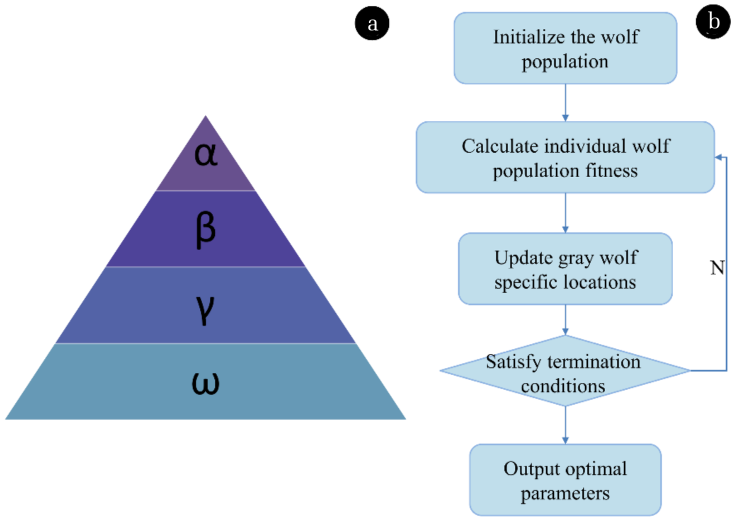

Fig. S4. (a)Top-to-bottom hierarchy of gray wolves. (b) Schematic diagram of the gray wolf optimization algorithm.

Text S1. Explanation of the SVR model.

As shown in Fig. S3, $\omega x + b = 0$ is the separating hyperplane, and 1 and -1 in $\omega x + b = 1$ and $\omega x + b = -1$ are the binary labeling values, in order to ensure that $y_i(\omega x_i + b)$ is always greater than 0. SVR mainly solves the nonlinear regression problem by mapping the nonlinearly mapped data x to the high-dimensional feature space.

Let the known training set be $T = \{(x_1, y_1), (x_2, y_2), \cdots, (x_l, y_l)\}$, The function is obtained from SVR training regression, and could be expressed as Eq. (1):

$$f(x) = \omega^T \emptyset(x) + b \tag{1}$$

Where ω and b are the weight coefficients and constant coefficients, respectively. $\emptyset(x)$ is the nonlinear mapping function in the feature space. An insensitive loss function ε is introduced, errors smaller than ε will not be included in the loss function. Regularize the risk function by minimizing the following. Introduce the regularization parameter C to optimize the regression problem could be expressed as Eq. (2):

$$min \frac{1}{2}\|\omega\|^2 + C\frac{1}{l}\sum_{i=1}^{l} L_\varepsilon(y_i, f(x_i)) \tag{2}$$

Where C is the penalty factor and L is the loss function.

Introducing slack variables ξ_i and ξ_i^* can express the optimization objective as Eq. (3), Eq. (4):

$$min \frac{1}{2}\|\omega\|^2 + C\sum_{i=1}^{l}(\xi_i + \xi_i^*) \tag{3}$$

$$s.t. \begin{cases} y_i - \omega \cdot \emptyset(x_i) - b \le \varepsilon + \xi_i \\ \omega \cdot \emptyset(x_i) + b - y_i \le \varepsilon + \xi_i^* \\ \xi_i, \xi_i^* \ge 0 \quad (i = 1, 2, \cdots, l) \end{cases} \tag{4}$$

The dyadic problem of the issue could be expressed as Eq. (5):

$$max - \frac{1}{2}\sum_{i,j=1}^{l}(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)K(x_i \cdot x_j) - \sum_{i,j=1}^{l}\alpha_i^*(\varepsilon - y_i) - \sum_{i,j=1}^{l}\alpha_i^*(\varepsilon + y_i) \tag{5}$$

$$s.t. \begin{cases} \sum_{i,j=1}^{l}(\alpha_i - \alpha_i^*) = 0 \\ 0 \le \alpha_i, \alpha_i^* \le C \quad (i = 1, 2, \cdots, l) \end{cases} \tag{6}$$

By solving the above problem, the decision function for support vector regression can be obtained, the relevant Eq. (7) is as follows:

$$f(x) = \sum_{i=1}^{l}(\alpha_i - \alpha_i^*)K(x_i, x) + b \tag{7}$$

Where $K(x_i \cdot x_j) = \emptyset(x_i)\emptyset(x_j)$ denotes the kernel function, it is crucial to choose a suitable kernel function in the prediction model, and the most commonly used is the RBF (Radial Basis Function) kernel function.

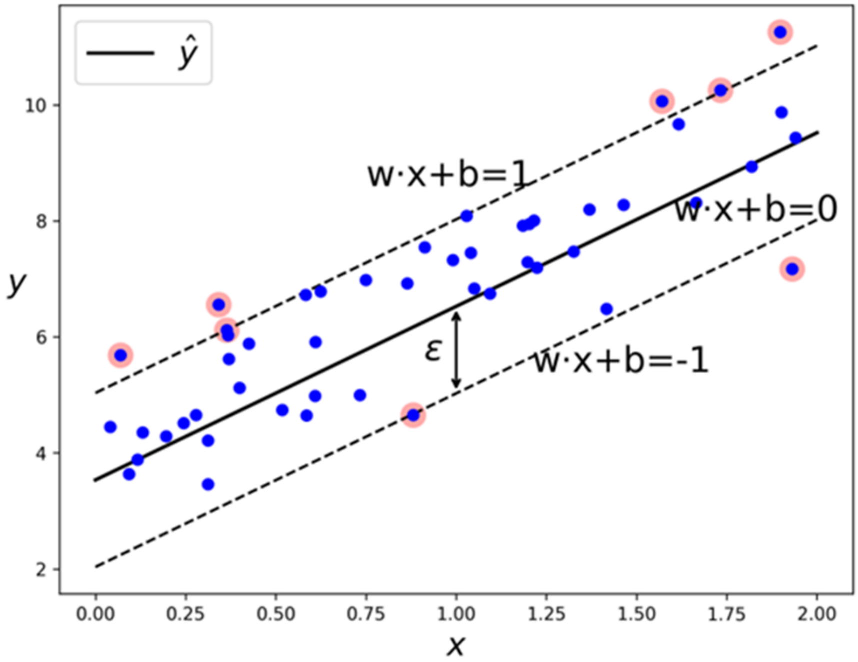

Fig. S5. Schematic diagram of SVR principle.

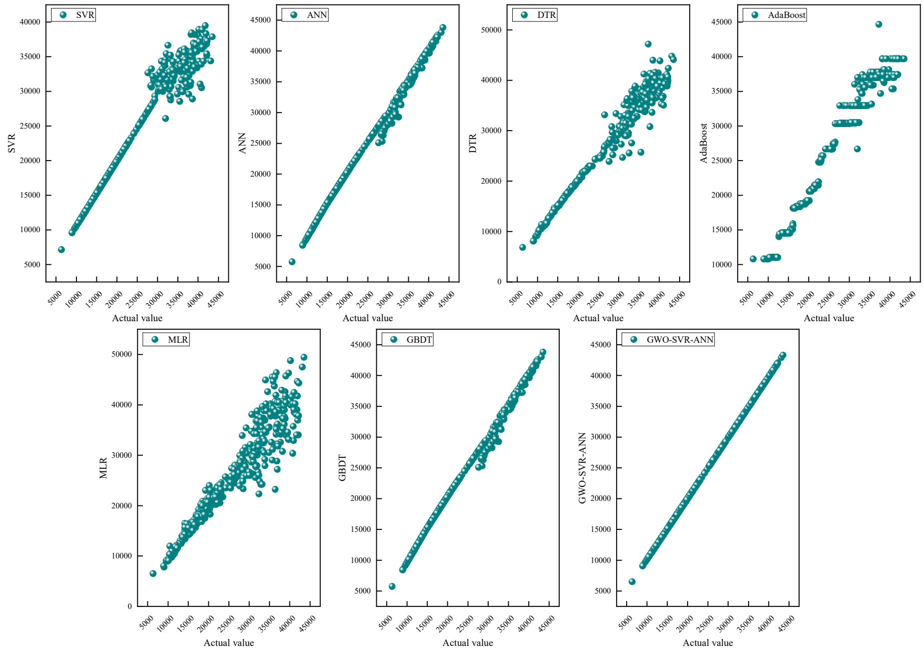

Fig. S6. Model test set prediction results.

Table S1. Emission factors of N_2O and CH_4 for various WWTPs process by plenty of literatures.

Process	EF(N2O) kgN2O-N/kgTN	EF(CH4) kgCH4/kgCOD	Number of EFs references (CH4 and N2O)	Median Value	Reference
AAO	0.0043,0.016, 0.016,0.013,0.0081, 0.005,0.0014,0.0008, 0.0014,0.013,0.018, 0.0016,0.0005,0.0027, 0.00161,0.0023,0.0011	-	17	0.00273	[1] [2] [3] [4] [5] [6] [7] [8] [9] [10] [11] [12] [13] [14] [15]
AAO	-	0.0034,0.0009,0.0091, 0.0002,0.0009,0.0079, 0.002,0.0008,0.0097, 0.0005,0.0009,0.0014, 0.0126,0.0002	14	0.00115	[2] [4] [6] [8] [9] [10] [13] [14]
Inverted AAO	0.0023		1	0.0023	[9]
Inverted AAO		0.0014	1	0.0014	[9]
OD	0.0029,0.0015,0.008, 0.0111,0.0036,0.0014, 0.0046,0.0052,0.0002, 0.0003,0.0015	-	11	0.0029	[2] [4] [5] [6] [9] [10] [12] [16] [17] [18] [19]
OD	-	0.0111,0.0052,0.0094, 0.0033,0.00133,0.0033, 0.031,0.003,0.0071	9	0.0052	[2] [4] [6] [9] [10] [19]
SBR	0.0279,0.026,0.0098, 0.0061,0.038,0.023, 0.029,0.013,0.056, 0.0082	-	10	0.0245	[2] [4] [6] [10] [12] [19] [20] [21] [22] [23] [24]
SBR	-	0.0043,0.0018,0.0196, 0.00414,0.0135,0.01, 0.001	7	0.0043	[2] [4] [10] [14] [24]
AO	0.035,0.0221,0.028, 0.0209,0.001,0.001, 0.045,0.12,0.0049, 0.013,0.012	-	11	0.0209	[2] [4] [5] [6] [8] [10] [12] [19] [20] [21] [25] [26] [27]
AO	-	0.0039,0.0039,0.0138, 0.0078,0.0078,0.0073, 0.0006	7	0.0073	[2] [4] [6] [8] [10] [19] [21]
MBR	0.005,0.005,0.0141, 0.005	-	4	0.0050	[2] [4] [6] [10]
MBR	-	0.0074,0.0027,0.005	3	0.0050	[2] [4] [6] [10]
CAS	0.00036,0.0046	-	2	0.00248	[5] [10]
CAS	-	0.0049	1	0.0049	[10]
Others	0.0082,0.005,0.0142, 0.0004,0.007,0.028, 0.00128,0.0013,0.023,0.0014, 0.0062	-	11	0.0062	[2] [4] [6] [19] [28] [29] [30] [31] [32] [33] [34]
Others	-	0.0136,0.0129,0.0095, 0.0091,0.0012,0.0035, 0.0235,0.003734, 0.0113,0.0075,0.0155, 0.0225	12	0.0014	[2] [4] [6] [19] [24] [29] [35] [36] [37]

Table S2. chemicals carbon emission factors

	Emission Factors	Source
PAM	0.851 kgCO2/kg	[38]
Aluminum sulfate	0.5 kgCO2/kg	Technical specification for low-carbon operation evaluation of sewage treatment plant
Sodium hypochlorite	0.92 kgCO2/kg	Technical specification for low-carbon operation evaluation of sewage treatment plant
Sodium acetate	0.623 kgCO2/kg	[39]
Tap water	0.168 kgCO2/t	CPCD, China Products Carbon Footprint Factors Database
Other pharmaceuticals	1.6 kgCO2/kg	[40]

Table S3. Rate of change of indicators for different scenarios (%)

Indicator name	Scenario	2023-2025	2026-2030	2031-2035	2035-2040
Amount of treated water (A)	L	4.8	3.6	2.4	1.2
	M	5.3	4.1	2.9	1.7
	H	6	4.8	3.6	2.4
Pollutant concentration (B)	L	-6.6	-6.2	-5.7	-5.3
	M	-9.3	-8.4	-7.9	-7.4
	H	-10.2	-9.2	-8.6	-8.2
Energy consumption (C)	L	3.8	2.8	1.9	1.3
	M	4.2	3.2	2.3	1.7
	H	4.6	3.6	2.7	2.1
chemicals consumption (D)	L	4.8	3.6	2.4	1.2
	M	5.3	4.1	2.9	1.7
	H	6	4.8	3.6	2.4
clean energy substitution rate (E)	L	4	6	8	10
	M	5	8	11	14
	H	8	14	20	26
Methane recovery power generation rate (F)	L	4	6	8	10
	M	5	7	10	12
	H	6	10	14	18
Biological carbon sequestration rate (G)	L	4	6	8	10
	M	6	10	14	18
	H	8	14	20	26

Table S4. Scenario settings

Scenario	A	B	C	D	E	F	G
Baseline Scenario	M	M	M	M	M	M	M
No Emission Reduction Measures Scenario	M	M	M	M	-	-	-
Technological Innovation Scenario	M	M	L	L	H	M	H
Energy Saving and Consumption Reduction Scenario	L	L	L	M	M	M	M
Sustainable Development Scenario	L	H	L	L	H	H	H
Low Development Scenario	H	H	H	H	L	L	L

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