Bridging Time-Scale Mismatch in WWTPs: Long-Term Influent Forecasting via Decomposition and Heterogeneous Temporal Attention

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Supplementary Materials S1

S1.1. Principle and Explanation of the Maximal Information Coefficient

Mutual information is a fundamental concept in information theory, utilized to quantify the degree of dependence between two variables. Intuitively, it measures "the amount of information obtained about one variable (e.g., Chemical Oxygen Demand, COD) given knowledge of another variable (e.g., Ammonia Nitrogen)." It is capable of capturing dependency relationships of arbitrary types, including characteristics of highly non-linear dynamic coupling. Provided an association exists between two variables, mutual information can detect it regardless of the complexity of the relationship.

The mutual information $I(X;Y)$ is equivalent to the "total information content of variable Y" minus the "remaining uncertainty of Y given that X is known."

$$I(X;Y) = \int_Y \int_X p(x,y) \log\left(\frac{p(x,y)}{p(x)p(y)}\right) dx\, dy$$

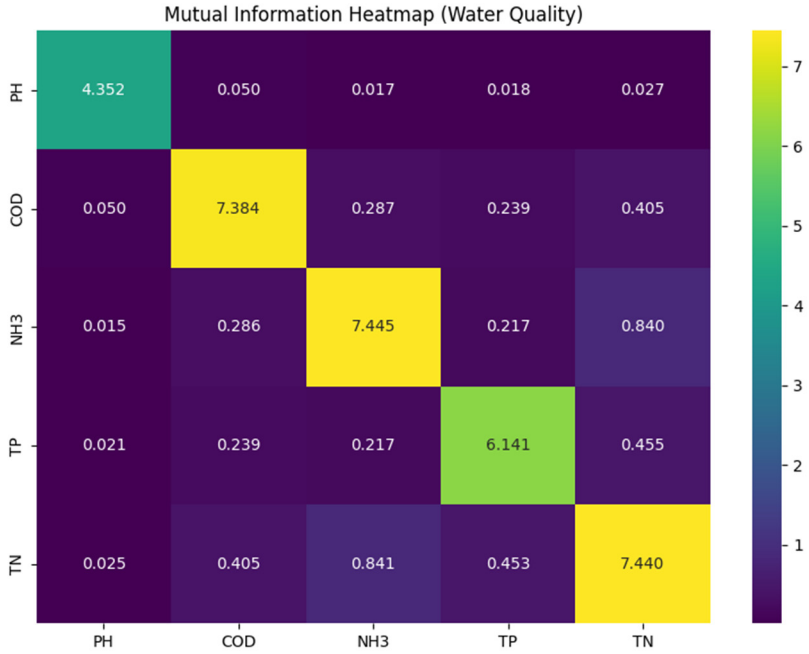


Figure S1. Mutual Information Heatmap.

S1.2. Determination and Calculation of Specific Parameters for the STL Algorithm

To objectively determine the optimal seasonal window size (n_s) for STL decomposition, we introduced two quantitative metrics aimed at evaluating the trade-off between signal smoothness and decomposition completeness.

Seasonal Roughness (SR) is used to quantify the local volatility of the extracted seasonal component. In wastewater treatment processes, underlying diurnal patterns driven by human activities and industrial production cycles should, according to physical laws, manifest as gradual changes rather than abrupt mutations. A higher roughness value indicates that the decomposition process has overfitted high-frequency

noise into the seasonal component.

Mathematically, this metric is defined as the standard deviation of the first-order difference of the seasonal series S_t:

$$SR = \sqrt{\frac{1}{N-1}\sum_{t=2}^{N}\left(\Delta S_t - \overline{\Delta S}\right)^2}$$

Residual Periodicity (RP) is utilized to assess whether periodic signals have been fully extracted from the raw data. In an ideal STL decomposition result, the residual component R_t should approximate white noise and should not contain significant residual periodic correlations. If high autocorrelation exists at the dominant period (24 hours), it indicates underfitting or "periodicity leakage." This implies that the fixed seasonal window failed to effectively capture dynamic cyclic variations, resulting in the leakage of some seasonal patterns into the residuals.

This metric is quantified using the autocorrelation function (ACF) with a lag of k=24 hours:

$$RP = \frac{\sum_{t=1}^{N-k}\left(R_t - \overline{R}\right)\left(R_{t+k} - \overline{R}\right)}{\sum_{t=1}^{N}\left(R_t - \overline{R}\right)^2}$$

The seasonal roughness and residual periodicity of the water quality indicators are shown in S2–S10.

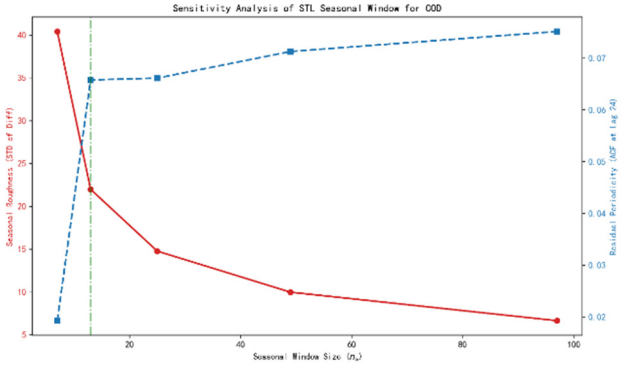


Figure S2. Sensitivity Analysis of STL Seasonal Window for COD.

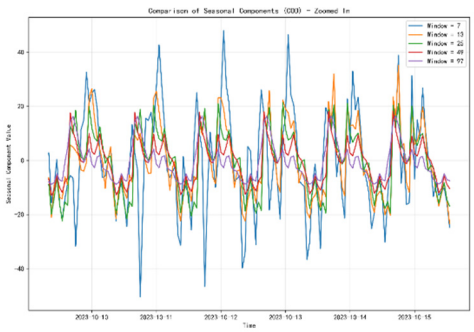


Figure S3. Comparison of Seasonal Components (COD).

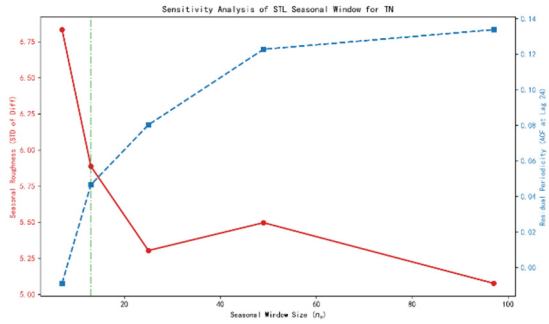


Figure S4. Sensitivity Analysis of STL Seasonal Window for TN.

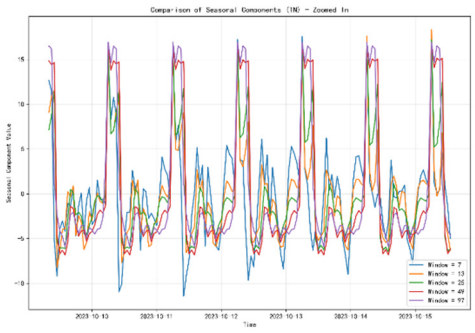


Figure S5. Comparison of Seasonal Components (TN).

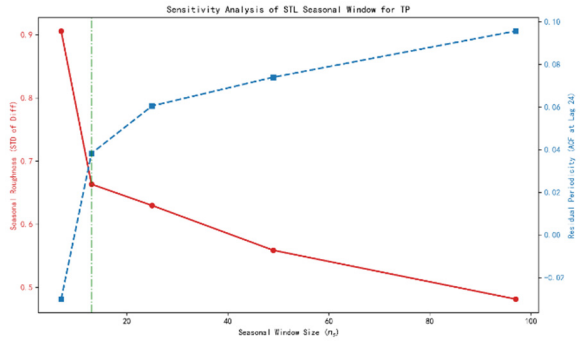


Figure S6. Sensitivity Analysis of STL Seasonal Window for TP.

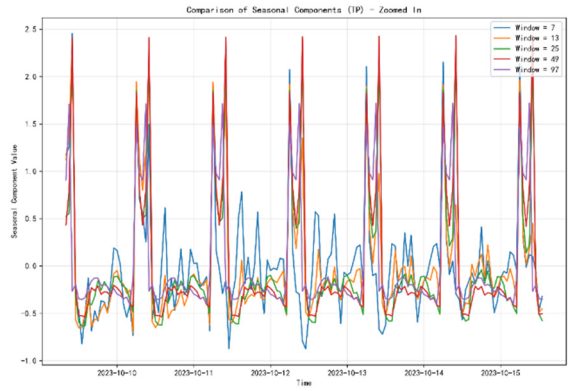


Figure S7. Comparison of Seasonal Components (TP)

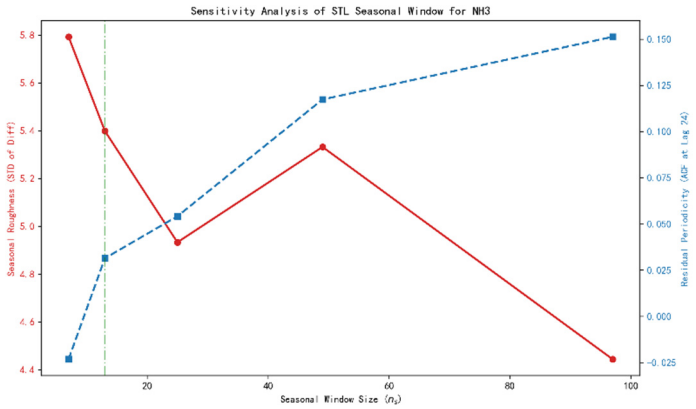


Figure S8. Sensitivity Analysis of STL Seasonal Window for NH3-N.

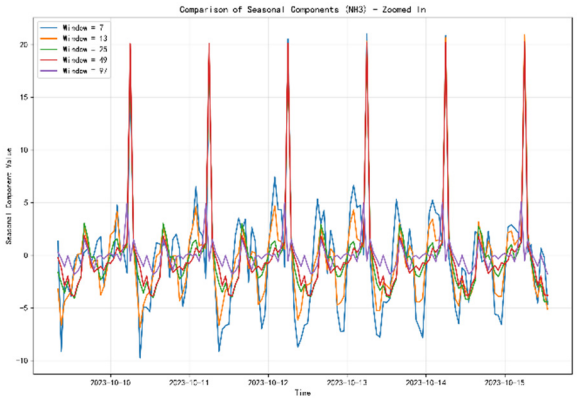


Figure S9. Comparison of Seasonal Components (NH3-N).

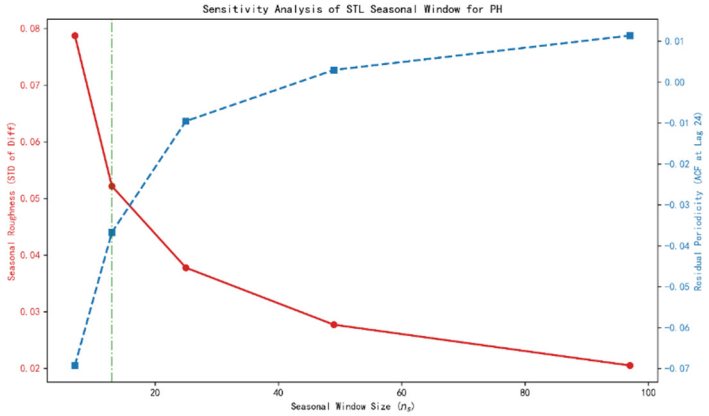


Figure S10. Sensitivity Analysis of STL Seasonal Window for pH.

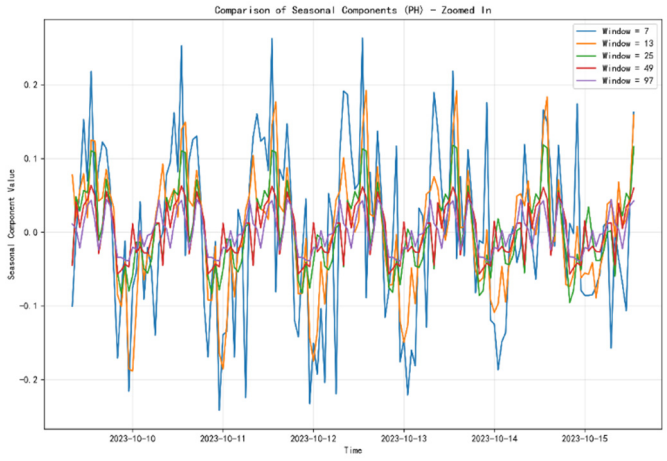


Figure S11. Comparison of Seasonal Components (pH).

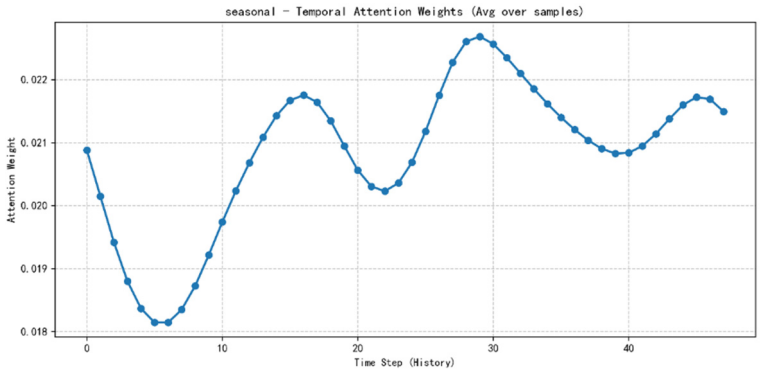


Figure S12. Seasonal-Temporal Attention Weights (Avg over Samples).

Table S1. Parameter Selection for STL Decomposition.

Decomposition Target	Seasonal-Window	Roughness	Residual-ACF
COD	7	40.421	0.020
COD	13	21.986	0.065
COD	25	14.770	0.069
COD	49	9.973	0.071
COD	97	6.641	0.075
TN	7	6.833	-0.09
TN	13	5.888	0.047
TN	25	5.304	0.081
TN	49	5.497	0.123
TN	97	5.077	0.134
TP	7	0.906	-0.03
TP	13	0.663	0.038
TP	25	0.630	0.061
TP	49	0.559	0.074

TP	97	0.481	0.957
NH3-N	7	0.906	-0.031
NH3-N	13	0.663	0.383
NH3-N	25	0.630	0.605
NH3-N	49	0.559	0.074
NH3-N	97	0.481	0.957
pH	7	0.078	-0.069
pH	13	0.052	-0.010
pH	25	0.038	-0.010
pH	49	0.028	0.003
pH	97	0.021	0.011

Supplementary Materials S2

Table S2. Attention Weight Parameters During Model Training.

Time Step-Index	pH	COD	NH3-H	TP	TN
0	0.046300106	0.802184224	0.052246191	0.057380736	0.041888766
1	0.046318695	0.802114129	0.0522625	0.05740096	0.041903753
2	0.046339978	0.802040279	0.0522823	0.057421483	0.04191602
3	0.046342611	0.802029371	0.052284688	0.05742494	0.041918416
4	0.046349872	0.802002192	0.052288558	0.05743378	0.041925572
5	0.04636142	0.801956117	0.052298762	0.057447843	0.041935835
6	0.046373054	0.801898599	0.052312423	0.057465106	0.041950792
7	0.046386	0.801839828	0.052326012	0.057482556	0.041965581
8	0.046394687	0.801797926	0.052334793	0.057495233	0.041977335
9	0.046418786	0.801714003	0.05235149	0.057521764	0.041993935
10	0.046428122	0.801679373	0.052355938	0.057532873	0.042003736
11	0.046409741	0.801738679	0.052339587	0.057516761	0.041995291
12	0.0463947	0.8017914	0.0523258	0.0575009	0.0419869

	17	3	75	96	53
13	0.0463658 12	0.8018968 7	0.0523063 21	0.0574687 01	0.0419622 4
14	0.0463317 52	0.8020191 19	0.0522811 11	0.0574312 1	0.0419367 25
15	0.0462888 96	0.8021629 45	0.0522538 09	0.0573875 46	0.0419067 74
16	0.0462246 72	0.8023842 57	0.0522031 52	0.0573229 34	0.0418648 98
17	0.0461932 38	0.8024844 53	0.0521837 25	0.0572937 73	0.0418447 37
18	0.0461607 87	0.8025935 29	0.0521606 21	0.0572624 17	0.0418226 05
19	0.0461484 38	0.8026354 91	0.0521533 45	0.0572499 71	0.0418127 63
20	0.0461334 51	0.8026903 27	0.0521435 18	0.0572335 94	0.0417990 8
21	0.0461453 98	0.8026465 18	0.0521556 4	0.0572462 12	0.0418062 1
22	0.0461622 33	0.8025826 81	0.0521720 01	0.0572650 54	0.041818
23	0.0461773 05	0.8025239 11	0.0521860 61	0.0572827 38	0.0418300 11
24	0.0461918 3	0.8024688 36	0.0521983 58	0.0572990 4	0.0418419 5
25	0.0462087 58	0.8024047 02	0.0522130 21	0.0573175 59	0.0418559 8
26	0.0462277 61	0.8023391 37	0.0522307 01	0.0573356 9	0.0418667 01
27	0.0462286 55	0.8023356 2	0.0522312 93	0.0573370 05	0.0418675 32
28	0.0462373 05	0.8023027 78	0.0522368 36	0.0573474 39	0.0418757 46
29	0.0462507 53	0.8022492 53	0.0522491 04	0.0573635 59	0.0418873 58
30	0.0462637 21	0.8021873 83	0.0522640 01	0.0573819 8	0.0419029 85
31	0.0462769 64	0.8021286 73	0.0522777 1	0.0573992 65	0.0419174 36
32	0.0462818 93	0.8020995 26	0.0522838 12	0.0574081 61	0.0419266 34
33	0.0463062 3	0.8020150 07	0.0523008 03	0.0574349 28	0.0419431 37
34	0.0463171	0.8019741	0.0523073	0.0574476	0.0419538

	82	18	04	09	58
35	0.0463025 83	0.8020219 8	0.0522938 59	0.0574345 59	0.0419471 3
36	0.0462932 07	0.8020560 15	0.0522847 55	0.0574241 02	0.0419419 89
37	0.0462656 51	0.8021568 06	0.0522655 32	0.0573933 46	0.0419187 92
38	0.0462328 23	0.8022754 19	0.0522412 25	0.0573569 61	0.0418936 42
39	0.0461913 31	0.8024133 44	0.0522147 12	0.0573153 12	0.0418653 19
40	0.0461325 46	0.8026177 88	0.0521669 13	0.0572557 3	0.0418270 9
41	0.0461083 17	0.8026964 66	0.0521519	0.0572326 48	0.0418107 62
42	0.0460811 85	0.8027884 96	0.0521323 23	0.0572060 57	0.0417919 27
43	0.0460666 38	0.8028369 55	0.0521230 33	0.0571919 61	0.0417814 37
44	0.0460508 65	0.8028928 04	0.0521124 27	0.0571754 72	0.0417683 12
45	0.0460615 75	0.8028535 25	0.0521231 37	0.0571868 79	0.0417748 35
46	0.0460766 33	0.8027974 37	0.0521374 31	0.0572034 49	0.0417849 61
47	0.0460886 77	0.8027524 35	0.0521479 85	0.0572171 25	0.0417937 52