Probabilistic evaluation of integrating resource recovery into wastewater treatment to improve environmental sustainability

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Global expectations for wastewater service infrastructure have evolved over time, and the standard treatment methods used by wastewater treatment plants (WWTPs) are facing issues related to problem shifting due to the current emphasis on sustainability. A transition in WWTPs toward reuse of wastewater-derived resources is recognized as a promising solution for overcoming these obstacles. However, it remains uncertain whether this approach can reduce the environmental footprint of WWTPs. To test this hypothesis, we conducted a net environmental benefit calculation for several scenarios for more than 50 individual countries over a 20-y time frame. For developed countries, the resource recovery approach resulted in ~154% net increase in the environmental performance of WWTPs compared with the traditional substance elimination approach, whereas this value decreased to ~60% for developing countries. Subsequently, we conducted a probabilistic analysis integrating these estimates with national values and determined that, if this transition was attempted for WWTPs in developed countries, it would have a ~65% probability of attaining net environmental benefits. However, this estimate decreased greatly to ~10% for developing countries, implying a substantial risk of failure. These results suggest that implementation of this transition for WWTPs should be studied carefully in different temporal and spatial contexts. Developing countries should customize their approach to realizing more sustainable WWTPs, rather than attempting to simply replicate the successful models of developed countries. Results derived from the model forecasting highlight the role of bioenergy generation and reduced use of chemicals in improving the sustainability of WWTPs in developing countries.

wastewater treatment | paradigm shift | resource recovery | sustainability assessment | net environmental benefit

astewater treatment plants (WWTPs) are critical infra-structure for modern urban societies and provide essential protection for both the aquatic environment and human health. Long-standing practice in WWTPs involves eliminating a variety of substances from the wastewater and producing wasteactivated sludge (WAS) that requires further disposal, typically at a landfill (Fig. 1A). However, the traditional approach to WWTPs, which emphasizes what must be removed from wastewater, has resulted in problem shifting, such as energy reserve depletion, production of WAS, and greenhouse gas (GHG) generation. WWTPs use increasing amounts of energy with more stringent effluent standards. For example, treatment of organicrich wastewater in the United States currently consumes ~15 GW/v (1); about 4% of the electricity consumption in the United States is used to transport and treat water (2), and in certain states the proportion is greater (3). Without carbon sequestration, this energy use would also result in $\sim 1.2 \times 10^8$ t/y CO₂ emissions (4, 5). Biological nitrogen removal in WWTPs is a significant anthropogenic

source of N₂O that accounts for $\sim 10\%$ of total N₂O emissions (6, 7), a powerful GHG with global warming potential ~300 times that of CO_2 (8). Additionally, large volumes of WAS generated by WWTPs can undergo uncontrolled biodegradation without proper disposal, resulting in GHGs such as CH_4 and N_2O escaping to the atmosphere (9). Hence, wastewater must be recognized as a valuable resource from which organics, nitrogen, and phosphorus can be harvested to produce energy and raw materials (1, 10–12) (Fig. 1B). Despite considerable interest in the planning, design, and implementation of this emerging approach (13–15), little attention has been paid to whether conventional WWTPs can actually undergo such a transition in a given time frame or geographic context. Such an assessment, performed at an early stage of any substantial change, can help identify promising approaches to operation of WWTPs and direct efforts to make infrastructure investments that are appropriate for future conditions.

Numerous studies have used environmental performance metrics (EPMs), such as the carbon footprint and depletion of both renewable and nonrenewable resources, to evaluate human

Significance

Conventional methods used in wastewater treatment plants (WWTPs) emphasizing removal of detrimental substances from wastewater are essential for protection of the aquatic environment and public health. However, they are associated with costs in terms of environmental problem shifting, such as energy consumption, solid waste production, and greenhouse gas emissions. An improved approach involving wastewater-derived resource recovery in WWTPs is recognized as one potential solution. However, the environmental impacts and benefits of such a substantial change remain uncertain. We conducted an integrated assessment of the net environmental benefits of this transition in WWTPs for more than 50 individual countries to determine how best to update current methods of wastewater treatment and facilitate sustainable WWTPs in various parts of the world.

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Data deposition: A description of the raw data used to determine metric interactions is provided in *Methods*, *Algorithm for Determining Metric Interactions*, and the sources of the datasets are described in detail in *SI Text, Data Sources for Determining Metric Interactions*.

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Fig. 1. Frameworks for WWTPs: (A) conventional approach and (B) emerging resource recovery approach.

impacts on the environment (16–19). However, there is increasing recognition that EPMs alone are insufficient. It is important to incorporate interactions between EPMs and aggregate estimates of anthropogenic activity, because global environmental challenges are complex and numerous issues (e.g., energy conservation, climate change, and resource scarcity) are inextricably related (20–22). Left unaddressed, synergistic effects between EPMs will result in high levels of uncertainty in environmental impact and benefit assessments, complicating integrated analysis of environmental sustainability.

Net environmental benefit (NEB)-the total gains from integration of resource capture and improved wastewater treatment practices minus the adverse environmental effects of these actions-was adopted in the present work to represent the aggregate environmental effect of a transition in WWTP operation. To consider temporal and spatial factors, NEBs were estimated at the individual country level over a 20-y time frame and compared between developed and developing countries. First, we developed a data-driven approach for modeling potential interactions among EPMs and used it to determine NEB scores. We then used a probabilistic approach to better understand the dynamics and distributional effects of metric interactions on the expected NEB values. Throughout this assessment, we incorporated what is known and can be anticipated with respect to the sustainability of introducing multiple resource capture practices in conventional WWTPs in various global contexts.

Results and Discussion

Interactions Between the Metrics: Trends over Time. In the NEB model (Eq. 1), the weighting coefficients determine the strengths of the metrics and affect the aggregate outcomes; thus, various weighting sets are needed to draw robust conclusions. To this end, a data-driven approach taking into account temporal and geographic factors was developed for determining the metric weights and their interactions. The weighting coefficients for all metrics were assumed to satisfy a "linear weighted sum" rule (Eq. 2), allowing all of the metrics to be dynamically weighted against one another and used to quantify NEB ranges. The results depicted in Fig. 2 are sampled totals for both developed and developing countries; the weighting scores among the EPMs varied geographically and temporally and exhibited mutually reinforcing or offsetting effects in varying contexts, often with nonlinear and unexpected effects. Interestingly, the weight of the GHG emissions metric continuously declined during the study period (developed countries: $0.15 \rightarrow 0.05$; developing countries: $0.16 \rightarrow 0.06$), revealing that the GHG emissions metric had a lower value than the other EPMs considered. This trend appears to contradict the recent substantial increases in global GHG emissions (23), implying potential trade-offs between the GHG emissions metric and other EPMs. For example, much attention has been given to development of GHG mitigation strategies such as generation of bioenergy as an alternative fuel, which increased the weight of the bioenergy recovery metric over the same time period (developed countries: $0.17 \rightarrow 0.53$; developing countries: $0.18 \rightarrow 0.37$).

The uncertainties contributed by weighting in the NEB model were evaluated before the scenario analysis. Table 1 shows the results of this evaluation in terms of Spearman's rank-order correlation coefficient (ROCC) and contribution to variance (CTV). The weight for the bioenergy recovery metric contributed most to the variance in NEB for both developed (37.3-49.6%) and developing (35.2–48.8%) countries. The GHG emissions metric contributed approximately one-third of the uncertainty in the NEB for developing countries (35.6–49.3%), but slightly less for developed countries (24.8–26.6%). Use of chemicals (<4%) and sludge recycling (<1.8%) did not contribute substantially to the overall uncertainty in NEB. For developed countries, the total contribution of the environmental cost metrics to the variance in NEB was 38.5-48.4%, whereas the contribution of the environmental benefit metrics was 51.6-61.5%. For developing countries, the contributions of the environmental cost and benefit metrics to NEB variance were 44.3-60.2% and 39.8-55.7%, respectively. Thus, the NEB for developed countries was substantially dominated by environmental benefits rather than environmental costs, which may explain why higher NEB scores were obtained for these countries. SI Text (Fig. S1) presents tornado charts showing additional results of the sensitivity analysis.

Handling uncertainty is a critical challenge in NEB calculations, as it can supply vital information for judging the significance of model-based results. However, dealing with uncertainty is not yet a common practice in such assessments, particularly with respect to weighting issues. We further note that uncertainties are case dependent; the same model option can lead to different results in



Fig. 2. Time trends for weighting coefficients for all assessment metrics during the studied time period for (A) developed countries and (B) developing countries.

Table 1. Uncertainty analysis for NEBs associated with the resource recovery approach for WWTPs

	Developed countries								Developing countries								
5		Scenario 1		Scenario 2		Scenario 3		Scenario 4		Scenario 1		Scenario 2		Scenario 3		Scenario 4	
Weighting coefficient	ROCC	CTV, %	ROCC	CTV, %	ROCC	CTV, %	ROCC	CTV, %	ROCC	CTV, %	ROCC	CTV, %	ROCC	CTV, %	ROCC	CTV, %	
GHG emissions	-0.62	24.8	-0.69	25.6	-0.70	26.3	-0.70	26.6	-0.71	38.3	-0.76	35.6	-0.75	39.4	-0.89	49.3	
Energy consumption	-0.46	13.7	-0.63	21.4	-0.64	22.0	-0.63	21.6	-0.20	3.0	-0.44	11.9	-0.34	8.1	-0.35	7.6	
Chemical use	0.01	0.0	0.07	0.3	0.04	0.1	-0.01	0.0	-0.20	3.0	-0.02	0.0	-0.18	2.3	-0.23	3.3	
Bioenergy recovery	0.76	37.3	0.96	49.6	0.96	49.5	0.95	49.0	0.68	35.2	0.89	48.8	0.82	47.1	0.80	39.8	
Sludge recycling	0.06	0.2	0.10	0.5	0.10	0.5	0.12	0.8	0.09	0.6	0.15	1.4	0.16	1.8	0.00	0.0	
Struvite capture	0.61	24.0	0.22	2.6	0.17	1.6	0.19	2.0	0.51	19.8	0.19	2.2	0.14	1.4	0.00	0.0	

CTV, contribution to variance; ROCC, Spearman's rank-order correlation coefficient.

varying studies. The present findings suggest that dynamically quantifying the weighting coefficients for the assessment metrics provides useful information for drawing robust conclusions and reducing uncertainties in assessment outcomes.

Comparison of Approaches: Emerging vs. Conventional. Weighting coefficients for all assessment metrics for the period 1991-2009 were used in the model (Eq. 1) to estimate the range of NEBs using a Monte Carlo (MC) simulation. Four scenarios representing increasingly stringent effluent limits were modeled for both the conventional and the resource recovery approach. In Fig. 3, the distributions of the NEBs for each scenario incorporating the emerging WWTP approach in developed and developing nations are compared with those for the control. The 5th, 25th, 50th (median), 75th, and 95th percentiles of the distributions obtained from 100,000 MC simulations are shown. All four scenarios under the control had negative NEBs for the metrics assessed, demonstrating that adding resource recovery is critical to mitigating the adverse environmental consequences caused by conventional WWTPs. The emerging approach considered herein may be superior to the control, as evidenced by an improvement of $\sim 154\%$ at each percentile for the developed countries and an improvement of ~60% for the developing countries. Additionally, ~65% of the MC simulations under the emerging approach for WWTPs yielded positive NEBs for the developed countries (Fig. 3), indicating likely improvement in environmental performance. However, only ~10% of the MC simulations yielded positive NEBs for the developing countries. Accordingly, whether the emerging approach will achieve a positive NEB for developing countries is not easily determined. However, a change in WWTP operation has the potential to provide net environmental gains rather than merely mitigating existing environmental impacts. Therefore, we conducted further analysis of the emerging approach in greater detail.

NEB Ranges for the Emerging Approach: Probabilistic Analysis. The 95% confidence intervals for the NEBs associated with all of the scenarios under the emerging WWTP paradigm for the developed and developing countries are presented in Table S1. Specifically, the normal distribution most closely fit the sample outputs and the parameters for the distribution function, as summarized in SI Text. Fig. 4 shows the probability distribution functions (PDFs) and cumulative probability distribution curves (CPDCs) for the NEB outcomes associated with the emerging paradigm for developed and developing countries. Marked differences between the mean values and shapes of the PDFs between the developed and developing countries were observed. Specifically, scenario 2 was associated with better average performance than scenario 1 (with 6% and 30% higher NEBs for developed and developing countries, respectively), scenario 3 (with 350% and 70% higher NEBs for developed and developing countries, respectively), or scenario 4 (with 284% and 84% higher NEBs for developed and developing countries, respectively), although the distributions significantly overlapped. Furthermore, marked differences between the shapes of the PDFs between scenario 1 and each of the other scenarios were observed for the developed and developing countries, but only minor differences were observed between the shapes of the PDFs among scenarios 2, 3, and 4. In other words, if the effluent limit were strengthened to a moderate limit (scenario 2) from a lenient limit (scenario 1), the differences in the discharge requirements



Fig. 3. Ranges of potential NEB scores for all estimated scenarios for the conventional (orange) and resource recovery (blue) WWTP approaches for (*A*) developed and (*B*) developing countries. The center lines represent median values, boxes represent 25th to 75th percentiles, and bars represent 5th to 95th percentiles of the distributions resulting from 100,000 MC simulations.



Fig. 4. PDFs (Left) and CPDCs (Right) for NEBs associated with the resource recovery approach for all estimated scenarios for (A) developed countries and (B) developing countries. The 95% confidence interval for scenario 1 is represented by black vertical lines in the PDF charts.

would increase the variability and uncertainty in the results, but would not greatly alter the general trends in the NEBs. However, more stringent effluent limits (scenarios 3 and 4) had greater influence on the NEBs. Overall, the results indicate that uncertainties in the NEB will always exist under varying conditions.

Fig. 4 displays the ranges of NEBs and the corresponding probabilities of realizing the desired performance. A "breakeven" score of zero at which the environmental benefits gained from resource recovery practices (RRPs) just offset the environmental costs of the WWTPs is indicated by the black vertical line through the x axis. Following the black line to the curve for each scenario for the developed countries yields the probability that a positive NEB can be achieved by using the emerging approach; these probabilities were about 95%, 85%, 55%, and 25% for scenarios 1, 2, 3, and 4, respectively. Similarly, the probabilities of achieving positive NEBs for the developing countries for the four scenarios were around 10%, 30%, 5%, and 0%, respectively, implying that the emerging approach has on average only a 10% probability of yielding a positive NEB in developing countries. Such low probabilities of achieving a desirable NEB indicate a considerable risk of failure of the emerging approach in developing countries. Furthermore, a markedly higher probability of obtaining a satisfactory NEB was observed for scenario 1 for developed countries, whereas scenario 2 had a higher probability for developing countries. Comprehensively, these results illustrate that effluent standards significantly affect the NEB for implementing an emerging technology. Specifically, the greatest benefits from resource recovery in developed countries may be realized when less stringent discharge limits are being used (scenario 1), balancing environmental impacts and benefits through resource harvesting and basic wastewater treatment. In contrast, greater benefits for developing countries may be achieved through resource recovery at a somewhat more stringent discharge limit (scenario 2). Although further research is needed to clarify these interesting implications, they imply that multiple goals and

perspectives on sustainability should be kept in mind in addition to protection of ecosystems and public health when evaluating the relationship between new WWTP technologies and discharge limits.

NEB Forecasting for the Emerging Approach to Wastewater Treatment. Based on the verified model (*SI Text*), updated weights for all assessment metrics for 2020 were simulated and substituted into the NEB model (Eq. 1), and the future NEB outcomes for the emerging approach to WWTPs were then calculated (Fig. 5). As predicted, all four scenarios for the approach produced increases in the NEB. However, the NEBs for developed countries (0.20–0.45) under the emerging approach were markedly higher than those for developing countries (0.00–0.20). Additionally, Fig. 6 displays the balance between the environmental costs and benefits for each scenario under the emerging WWTP approach. The bioenergy recovery metric had greater weight than the other EPMs, suggesting that incorporation of bioenergy recovery into WWTPs is critical to obtaining a favorable NEB. This analysis also indicates that developing countries should reduce the use of chemicals in WWTPs to improve sustainability.

Implications of This Work. Many urban areas will need to optimize their wastewater service infrastructure over the next 10–15 y, and an approach incorporating reuse of wastewater-derived resources is a promising option. We developed a detailed approach for weighting the dynamic components of environmental impact and benefit assessments, highlighting the significance of various EPMs and their interactions for WWTPs. The results revealed that, overall, the environmental sustainability of WWTPs can be increased through adoption of resource recovery. Despite increasingly positive expectations for reaping multiple wastewater-derived resources, substantial uncertainty still exists in the effectiveness of RRPs when used on an industrial scale. For example, recapture of wastewater-derived phosphorus to industry seems

a clear solution for closing the phosphorus cycle. However, it may be desirable in future research to investigate the potential contribution of wastewater-recovered phosphorus in the anthropogenic phosphorus cycle using different assumptions for the potential value of phosphorus in economic markets. Anticipated changes in WWTP operations should be considered very carefully, taking into account the temporal and geographic context, because the benefits will vary substantially due to complex interactions among environmental issues. These results also imply that developing nations should pursue customized approaches toward greater environmental sustainability for WWTPs, rather than simply replicating the successful models of developed countries. Additionally, the forward-looking modeling results suggest two specific management strategies, i.e., enhanced capture of wastewater-derived bioenergy and reduced use of chemicals, to improve the sustainability of WWTPs in developing countries.

Our results also show that there are substantial interactions between technical approaches and effluent standards in the wastewater sector, although further research is still needed. These two areas are often considered separately and optimized to generate maximum benefits for each aspect without taking into account interactions between them. Our findings imply that a disconnected management strategy can significantly affect the sustainability of this emerging approach. Hence, technological breakthroughs and best practices alone cannot ensure a sustainable future. Multidisciplinary research in technology development, environmental and ecological impacts, societal adaptation, economic markets, and policy frameworks is needed to reap the greatest benefits in the wastewater service infrastructure through integration of wastewater-derived resources capture.

Methods

Approaches and Scenarios for WWTPs. Based on currently available technologies (24), an emerging approach was selected that integrates multiple wastewater-derived RRPs into WWTP operation (Fig. 1*B*). Briefly, CH₄ gas is harvested in a WAS digester and then burned to produce electricity, struvite (NH₄MgPO₄·6H₂O) is reaped from the supernatant of the digester for use as a slow-release fertilizer, and dewatered digested sludge is recycled through composting on agricultural fields. A traditional approach that does not involve RRPs served as a control for the comparative evaluation (Fig. 1*A*).

As previously reported, WWTPs have varied performance at different treatment levels with varying effects on the natural environment (25, 26). To this end, the WWTPs (Table S2) considered under the improved and conventional approaches were each hypothesized to treat municipal wastewater to several different sets of effluent standards for comparative investigation of the potential environmental impacts and benefits of the resource recovery approach for WWTPs. Three increasingly stringent discharge limits from Chinese discharge regulations (class 2, class 1B, and class 1A) (27) were selected as representative of developing countries; in addition, a set of more stringent effluent limits representative of developed countries was also included according to a previous literature (26). Briefly, class 2 limits effluent chemical oxygen demand (COD) to <100 mg/L, NH₃-N to <25 mg N/L, and total phosphorus (TP) to <3 mg P/L, but no limit is imposed on total nitrogen (TN); this is referred to as scenario 1. Class 1B limits the effluent COD to <60 mg/L, TN



Fig. 5. Predicted NEBs for 2020 associated with the resource recovery WWTP approach for all estimated scenarios for developed and developing countries.



Fig. 6. Deterministic balance of environmental costs and benefits under the resource recovery approach for all estimated scenarios for (*A*) developed and (*B*) developing countries.

to <20 mg N/L, NH₃-N to <8 mg N/L, and TP to <1 mg P/L, and is referred to as scenario 2. Class 1A limits the effluent COD to <50 mg/L, TN to <15 mg N/L, NH₃-N to <5 mg N/L, and TP to <0.5 mg P/L and is referred to as scenario 3. The most stringent set limits the effluent COD to <30 mg/L, TN to <3 mg N/L, NH₃-N to <1 mg N/L, and TP to <0.3 mg P/L and is referred to as scenario 4.

NEB Method for Assessing WWTPs. We used a tailored approach (28) involving three simplified indicators as environmental cost metrics: energy consumption (NF_{ener}) , GHG emissions (NF_{gree}) , and chemical use (NF_{chem}) . Three additional indices, bioenergy recovery performance (PF_{bioe}) , recycling capacity of sludge on agricultural fields (PF_{slud}) , and struvite capture potential (PF_{stru}) , were used to evaluate the benefits generated by the RRPs. Consequently, the NEB for scenario *a* is the total environmental benefits gained by the incorporation of RRPs minus the total environmental costs of implementation (Eq. 1):

$$\mathsf{NEB}(a) = \sum_{i}^{n} w_i \times \mathsf{PF}_i(a) - \sum_{j}^{m} w_j \times \mathsf{NF}_j(a), \tag{1}$$

where *PF*(a) is the environmental benefit for scenario a, *NF*(a) is the environmental cost for scenario a, w is a weighting coefficient quantifying the relative importance of each EPM, the subscript *i* specifies the environmental gain metric, and the subscript *j* specifies the environmental cost metric. A detailed description of the calculations for *PF* and *NF* can be found in *SI Text*. Moreover, Table S3 presents the calculated values for each metric for each scenario (scenarios 1, 2, 3, and 4).

Algorithm for Determining Metric Interactions. Following quantitative assessment of each environmental cost and gain metric for all scenarios, interactions between the metrics were determined before the NEB scores were quantified. A data-driven method for quantifying the interactions among metrics in a broader context was developed and expressed using weighting coefficients and linked to the NEB algorithm. The weighting coefficients for all indices were assumed to satisfy the following "linear weighted sum" rule:

$$\sum_{i}^{n} w_{i} + \sum_{j}^{m} w_{j} = 1.$$
 [2]

Thus, the assessment metrics can be weighted against each other in a given context and then used in Eq. 1 to determine the NEB scores.

The algorithm for generating the weighting coefficient (w) of assessment metric i or j is as follows:

$$w_{i(j)} = \frac{w_{i(j)}^{\langle absolute \rangle}}{\sum_{i}^{n} w_{i}^{\langle absolute \rangle} + \sum_{j}^{m} w_{i}^{\langle absolute \rangle'}}$$
[3]

where *n* and *m* are the number of environmental gain and cost metrics, respectively, and the operator $w_{i(l)}^{sabolute>}$ converts the data subjected to the

assessment metric [D^{<target>}] to a dimensionless score using the corresponding baseline data $D_{i(j)}^{
baseline>}$]. The operator $w_{i(j)}^{
baseline>}$ is defined as follows:

$$w_{i(j)}^{\langle \text{absolute} \rangle} = \frac{D_{i(j)}^{\langle \text{target} \rangle}}{D_{i(j)}^{\langle \text{baseline} \rangle}}.$$
[4]

A greater value of w indicates that the corresponding metric is more important in aggregation of an NEB score.

To estimate the weight sets $w_{i(j)}$ in Eq. 4 taking into account temporal and geographic factors, historical national data [i.e., energy consumption, MkWh/cap-y (million kilowatts per capita per year); CO2 emissions, t CO2-eq/ cap-y (tons of carbon dioxide equivalents per capita per year); chemical imports, \$1,000/capy (one thousand dollar per capita per year); bioenergy production using wastes as feedstock, kWh/cap-y (kilowatts per capita per year); municipal waste generation, t/cap·y (tons per capita per year); phosphate exploitation, t/cap·y] for 1990-2010 were extracted from multiple global databases. Customized data for more than 50 individual countries were acquired and grouped according to whether the country was considered developed (Australia, Austria, Belgium, Canada, Denmark, Finland, France, Greece, Hungary, Iceland, Ireland, Israel, Italy, Japan, Luxembourg, The Netherlands, Norway, Poland, Portugal, South Korea, Spain, Sweden, Switzerland, Turkey, United Kingdom, and United States) or developing (Algeria, Argentina, Barbados, Benin, Brazil, Cameroon, Chile, China, Columbia, Egypt, Fiji, Gabon, India, Iran, Iraq, Malaysia, Mali, Mexico, Morocco, Oman, Saint Lucia, South Africa, Thailand, Yemen, Zambia, and Zimbabwe). Data for 1990 were used as the baseline data for model calculations, and data for 2010 were used for model verification. A detailed description of all data sources can be found in SI Text.

Prediction of Metric Interactions. To obtain updated weighting coefficients for each estimated category and to forecast the expected NEB scores, an analytical tool for time series, the autoregressive integrated moving average (ARIMA) (p, d, q) model (29, 30), was used to fit the calculated sets of weighting coefficients (w_i or w_i) for the studied time period of 1991–2009 and to forecast updated values for the weights, as follows:

$$\phi(B)(1-B)^{2}X_{t} = \theta(B)Z_{t}, \ \{Z_{t}\} \sim WN(0, \sigma^{2}),$$
[5]

where the parameters p, d, and q are nonnegative integers that represent the order of the autoregressive, integrated, and moving average parts of the model, respectively; ϕ and θ are polynomials of the degree p and q, respectively; and Z_t are error terms that are generally assumed to be

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independent, identically distributed variables sampled from a normal distribution with a zero mean.

The backshift operator B in Eq. 5 can be further expressed as the secondorder difference as follows:

$$X_t'' = X_t' - X_{t-1}'.$$
 [6]

Additionally, the functions $\phi(B)$ and $\theta(B)$ can be written as follows:

$$\phi(B) = 1 - \sum_{k=1}^{p} \varphi_k B^k$$
, [7]

$$\theta(B) = 1 + \sum_{k=1}^{q} \psi_k B^k,$$
[8]

where φ_k and ψ_k are the parameters for the autoregressive and moving average parts of the ARIMA (p, d, q) model, respectively. Model validation was also conducted to evaluate the generated models using observed data for 2010 (Fig. S2).

Probabilistic Analysis Method. The weights for the assessment metrics were input as PDFs to quantitatively represent the inherent variability and uncertainty of each metric weight. Fitted distributions were used based on the datasets estimated as described in Interactions Between the Metrics: Trends over Time (detailed information on the fitted distributions is provided in Table 54). Uncertainties in the metric weights, depicted by the PDFs and CPDCs, were simultaneously propagated through the model using 100,000 MC simulations with IBM SPSS Statistics 21.0 software (SPSS). To assess the distributional influence of each assessment metric on the uncertainties in the NEBs, CTVs (31) were then calculated. The ROCCs for each metric weight in the NFB results were determined for the set of MC iterations, and the CTV was calculated as follows:

$$CTV_{i(j)}(\%) = \frac{ROCC_{i(j)}^2}{\sum_{i}^{n} ROCC_{i}^2 + \sum_{j}^{m} ROCC_{j}^2} \times 100.$$
[9]

We also tested the sensitivity of the final NEB results to the metric weights by pulsing and subtracting a SD of the input from the MC modeling.

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