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Editorial

Sustainability Analysis and Environmental Decision-Making Using Simulation, Optimization, and Computational Analytics

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In practice, environmental analytics involves an integration of science, methods, and techniques involving a combination of computers, computational intelligence, information technology, mathematical modelling, and system science to address "real-world" environmental and sustainability problems. Effective environmental decision-making is often challenging and complex where final results often involve inherently subjective political and socio-economic facets. Furthermore, while certain environmental and sustainability decision-making specifications may be self-evident (post hoc analysis always tends to be incredibly accurate), more typical problems possess components that cannot be directly included in the underlying decision process without additional manipulation. Such decision-making is frequently further compounded by additional stochastic uncertainties. Consequently, complex "real world" sustainability problems frequently employ computational decision-making approaches to construct solutions to applications containing numerous quantitative dimensions and considerable sources of uncertainty.

This Special Issue includes a number of applied computational analytics papers that either create new decision-making methods or provide innovative implementations of existing methods for assisting with a wide spectrum of sustainability applications, broadly defined. In line with the aims and scope of this issue, the rich diversity of applications within the papers exemplifies the considerable range of both methodological relevance and practical contributions to research in environmental analysis. The disparate contributions included in the Special Issue all emphasize novel approaches of computational analytics as applied to environmental decision-making and sustainability analysis—be this on the side of optimization, simulation, modelling, computational solution procedures, visual analytics, and/or information technologies.

In the first paper, *A C-Vine Copula-Based Quantile Regression Method for Streamflow Forecasting in Xiangxi River Basin, China*, Li, Huang, Li, Sun, and Gao introduce a C-vine copula-based quantile regression (CVQR) model for forecasting streamflow. The CVQR model integrates techniques for vine copulas and quantile regression into a framework that can effectively establish relationships between the multidimensional response-independent variables with asymmetrical extreme values and apply the model to the Xiangxi River Basin. Multiple linear regression and artificial neural network are also compared to illustrate the applicability of CVQR. Their findings can be directly applied to hydrological process identification and water resource management practices.

In the second paper, *A Factorial Ecological-Extended Physical Input-Output Model for Identifying Optimal Urban Solid Waste Path in Fujian Province, China*, Liu, Li, Huang, Yang, and Wu develop a factorial ecological-extended physical input–output model to identify an optimal urban solid waste path in an urban solid waste system. Such a model is crucial for balancing the tradeoff between economic development and environmental protection. Their model integrates a physical input–output model, ecological network analysis, and fractional factorial analysis into a general framework that is applied to managing the urban waste system of Fujian Province, China.

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In *Analytical Models for Seawater and Boron Removal through Reverse Osmosis*, Binns simultaneously examines the total salt and boron concentrations in the purification process of seawater into safe drinking water. Reverse osmosis modules are designed by computer models to establish energy efficient configurations and operating conditions. A new analytical model is applied to two case studies and, in both cases, the new analytical approach predicts the performance with similar accuracy to existing finite-difference numerical models from the literature.

In *Development of a Cyberinfrastructure for Assessment of the Lower Rio Grande Valley North and Central Watersheds Characteristics*, Navarro, Mahmoud, Ernest, Oubeidillah, Johnstone, Santos Chavez, and Fuller construct a watershed characterization to determine potential pollution sources by developing a cyberinfrastructure to collect a wide inventory of data to identify which waterways contribute the highest concentrations of bacteria and lowest levels of dissolved oxygen. The cyberinfrastructure development employs a Geographic Information System database in which geospatial and non-geospatial data are incorporated from numerous point and nonpoint pollution sources. Their results identify the potential major sources of water quality impairments such as cultivated crops, urbanized areas, on-site sewage facilities, colonias, and wastewater effluents.

In *Eco-Efficiency for the G18: Trends and Future Outlook*, Sadorsky explores eco-efficiency as an important ecological indicator for tracking the progress of how countries' environmental-adjusted economic activity change over time and calculates country-level eco-efficiency for 18 major countries (G18) that are part of the G20. Eco-efficiency leaders include Australia, Brazil, France, Germany, Great Britain, Italy, Japan, Russia, and the United States, while the laggards include Canada, China, India, and Indonesia. The laggard countries recorded negative growth rates in eco-efficiency over the period 1997 to 2019 and 2019 to 2040, where negative growth points to a worsening of environmental sustainability. Large variations in eco-efficiency between countries make it more difficult to negotiate major international environmental/sustainability agreements and it is imperative that the G18 demonstrate leadership by increasing their eco-efficiency.

In the paper *Model Reduction Applied to Empirical Models for Biomass Gasification in Downdraft Gasifiers*, Binns and Ayub use various modeling approaches for the modeling and simulation of gasification processes to predict gasifier performance at different condition levels and use different feedstocks to optimally design efficient gasifiers. Complex models require significant time and effort to develop, and are only be accurate for use with a specific catalyst. Based on linear regression, Binns and Ayub develop linear and quadratic expressions of the gasifier input value parameters. A shrinkage method is applied to identify significant parameters and reduce the complexity of these expressions, thereby revealing significant parameters from which simple models with reasonable accuracy are obtained.

In the paper *Accuracy and Predictive Power of Sell-Side Target Prices for Global Clean Energy Companies*, Lohrmann and Lohrmann focus on mean target prices for stocks on the Standard and Poor's Global Clean Energy Index during the time period from 2009 to 2020. Their analysis shows that for all models, the mean target price is the most relevant variable, whereas the number of target prices appears to be highly relevant as well. Moreover, their results indicate that following the rare positive predictions of a random forest for the highest target return groups may potentially represent attractive investment opportunities.

In *Steering Renewable Energy Investments in Favor of Energy System Reliability: A Call for a Hybrid Model*, Kozlova and Lohrmann examine the volatility of electricity system reliability and the role played by renewable energy sources within these systems. While renewable energy is a key element in debates on future global energy systems, more extensive use of renewable energy sources within these systems implies a higher dependence on intermittent power, which places the reliability of the entire electricity system at risk. However, renewable energy use has often been designed without accounting for system reliability. This paper provides a hybrid model that guides renewable energy investments toward energy system reliability by incorporating reliability-based support for renewable energy

sources. It is shown that this reliability-based support can substantially reduce backup capacity, cut the overall costs, and reduce its environmental footprint.

In *Profitability Determinants of Unlisted Renewable Energy Companies in Germany—A Longitudinal Analysis of Financial Accounts*, Luts, Savolainen, and Collan, identify key profitability determinants of several unlisted, German, electricity-producing, renewable-energy companies. A multi-year analysis based on 783 companies for the years 2010–2018 is used. The results show that both company- and industry-specific profitability determinants are statistically significant, but that company-specific determinants seem to be a more important factor. The results shed new light on what drives the profitability of private German renewable-energy companies. The implications of the study hold wider environmental and economic importance as the performance of the renewable-energy companies is critical for achieving the emission targets of the energy industry and for ensuring more sustainable energy production for the future.

In *Ex-Ante Study of Biofuel Policies—Analyzing Policy-Induced Flexibility*, Ruponen, Kozlova, and Collan examine the appropriate policy selection process to enable various business sectors to optimize their transition toward a low-carbon economy. To accomplish this task efficiently, it is essential to recognize how different mechanisms incentivize the investments in terms profitability, flexibility, and inherent uncertainty. This paper focuses on financial incentive policies for the bio-component of fuel, in combination with penalties and tax-relief, on transportation-biofuel policies. Using the pay-off method and simulation-decomposition, their study shows that a combination of penalties and tax-relief can be employed to efficiently lead fuel-production towards sustainability. Their approach provides important insights to the decision-making process beyond more commonly-used profitability analysis methods.

In *Why Do Companies Need Operational Flexibility to Reduce Waste at Source?*, Elalem, Bicer, and Seifert analyze the environmental benefits of operational flexibility that emerge in the form of less product waste during the sourcing process by reducing overproduction. They employ a multiplicative demand process to model the evolutionary dynamics of demand uncertainty and quantify the impact of key modeling parameters for each operational-flexibility strategy on the waste ratio. Their results indicate that operational-flexibility strategies that rely on the localization of production are key to reducing waste and improving environmental sustainability at source.

In *Technical Advances in Aviation Electrification: Enhancing Strategic R&D Investment Analysis Through Simulation Decomposition*, Kozlova, Nykänen, and Yeomans examine the climate impacts arising from the electrification of aviation using the newly created analytical technique, Simulation-Decomposition (SimDec). It has been estimated that the carbon contributions from aviation contribute between 2–5% of all global emissions, annually. Consequently, decreasing carbon emissions from the aviation industry has become one of the primary initiatives within current global climate policy formulation and represents a significant component of the overall strategy for achieving climate neutrality by 2050. This paper examines the sustainability of aviation electrification by concurrently integrating environmental impacts from the ongoing technological developments of electric motors into the R&D investment analysis. A Monte Carlo model in combination with SimDec is used to model the flying range of an all-electric aircraft based upon improvements to its batteries together with the specific power of its motors. At the strategic level, SimDec enables a visual analytic display of the simultaneous interaction between multiple different factors that affect the flying range of electrical aircraft, thereby more fully portraying the financial and environmental benefits of aviation electrification to the decision-makers. Since SimDec can be run concurrently with any Monte Carlo model with only negligible additional overhead, it can easily be extended into the analysis of any environmental application that employs simulation. This generalizability in conjunction with its straightforward visualizations of complex stochastic uncertainties makes the practical contributions of SimDec very powerful in sustainability analysis and environmental decision-making.

In *Effects of Weather on Iowa Nitrogen Export Estimated by Simulation-Based Decomposition*, Raul, Liu, Leifsson, and Kaleita examine the impacts of weather variability on the State of Iowa's food–energy–water system and the resulting agricultural nitrogen that is exported from Iowa. The delivery of nutrients, especially nitrogen, from the upper Mississippi River Basin, is a function not only of agricultural activity but also of hydrology and the hypoxic zone in the Gulf of Mexico is a direct consequence of the nutrient-rich water it receives from the Mississippi River. Extreme weather conditions, such as drought and flooding, not only have a significant impact on the agriculture system, but also directly affect the nitrogen loading that enters the Mississippi River. A SimDec approach is implemented using a combined IFEW/crop-weather simulation model to better understand the impacts of weather on the nitrogen exported from the agricultural industry in Iowa. The SimDec analysis of the IFEW simulation model provides an enhanced understanding of weather variability on the environmental impacts from the soil nitrogen surplus.

In *A Fuzzy-Interval Dynamic Optimization Model for Regional Water Resources Allocation under Uncertainty*, Suo, Xia, and Fan propose a fuzzy-interval dynamic programming model for regional water management under uncertainty by combining fuzzy-interval linear programming with dynamic programming. Their model treats inherent uncertainties expressed as intervals while simultaneously considering the dynamic characteristics in the optimal allocation of water resources. The benefits of this modelling approach are demonstrated on the case study of optimal allocation of water resources under uncertainty in Handan, Hebei Province, China.

We trust that the number and quality of the papers will prove to be of significant value to the many different researchers and practitioners who actively engage in applying disparate computational methodologies to sustainability analysis and environmental decision-making using simulation, optimization, and analytics. It is our sincere hope that this issue will not only enlighten readers on the current state-of-the-art applications in computational sustainability, but will also serve to inspire further collaboration and cooperation on extensions to these topics. Continuing advancement on these topics is always necessary as "It is difficult to predict, especially the future" (Danish proverb often attributed to Niels Bohr) but, more to the point and borrowing from the deeply philosophical characters in the cartoon Calvin and Hobbes, "The trouble with the future is that it keeps turning into the present".

List of Contributions

1. Li, H.; Huang, G.; Li, Y.; Sun, J.; Gao, P. A C-Vine Copula-Based Quantile Regression Method for Streamflow Forecasting in Xiangxi River Basin.
2. Liu, J.; Li, Y.; Huang, G.; Yang, Y.; Wu, X. A Factorial Ecological-Extended Physical Input-Output Model for Identifying Optimal Urban Solid Waste Path in Fujian Province, China.
3. Binns, M. Analytical Models for Seawater and Boron Removal through Reverse Osmosis.
4. Navarro, L.; Mahmoud, A.; Ernest, A.; Oubeidillah, A.; Johnstone, J.; Chavez, I.R.S.; Fuller, C. Development of a Cyberinfrastructure for Assessment of the Lower Rio Grande Valley North and Central Watersheds Characteristics Osmosis.
5. Sadorsky, P. Eco-Efficiency for the G18: Trends and Future Outlook.
6. Binns, M.; Ayub, H.M.U. Model Reduction Applied to Empirical Models for Biomass Gasification in Downdraft Gasifiers.
7. Lohrmann, C.; Lohrmann, A. Accuracy and Predictive Power of Sell-Side Target Prices for Global Clean Energy Companies.
8. Kozlova, M.; Lohrmann, A. Steering Renewable Energy Investments in Favor of Energy System Reliability: A Call for a Hybrid Model.
9. Luts, M-K.; Savolainen, J.; Collan, M. Profitability Determinants of Unlisted Renewable Energy Companies in Germany—A Longitudinal Analysis of Financial Accounts.
10. Ruponen, I.; Savolainen, J.; Collan, M. Ex-Ante Study of Biofuel Policies—Analyzing Policy-Induced Flexibility.

11. Elalem, Y.K.; Bicer, I.; Seifert, R. Why Do Companies Need Operational Flexibility to Reduce Waste at Source?
12. Kozlova, M.; Nykänen, T.; Yeomans, J.S. Advances in Aviation Electrification: Enhancing Strategic R&D Investment Analysis Through Simulation Decomposition.
13. Raul, V.; Liu, Y-C.; Leifsson, L.; Kaleita, A. Effects of Weather on Iowa Nitrogen Export Estimated by Simulation-Based Decomposition.
14. Suo, M.; Xia, F.; Fan, Y. A Fuzzy-Interval Dynamic Optimization Model for Regional Water Resources Allocation under Uncertainty.

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