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Original Article

Applications of Mathematical Modelling in Science, Technology, and Sustainable Development

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Abstract

Mathematical modelling is an interdisciplinary approach for representing, analysing, and predicting the behaviour of complex systems. It supports scientific explanation, engineering design, technological innovation, and sustainable-development planning by translating assumptions about real-world processes into mathematical structures that can be tested against observations. This paper presents a structured review of mathematical modelling approaches, including deterministic and stochastic models, continuous and discrete models, mechanistic and data-driven models, agent-based models, and partial differential equation models. It outlines a modelling workflow encompassing problem formulation, assumption setting, model construction, calibration, validation, sensitivity analysis, interpretation, and communication. A statistical evaluation framework is presented using descriptive statistics and common predictive-performance measures, including mean absolute error (MAE), root mean square error (RMSE), and the coefficient of determination (R^2). A small numerical example is included solely to demonstrate the calculations; its values are simulated and are not empirical findings. The review highlights applications in biological and medical systems, engineering, environmental science, energy planning, climate adaptation, and urban transport. It concludes that transparent assumptions, reliable data, independent validation, uncertainty analysis, and stakeholder engagement are essential if model outputs are to support responsible and equitable decisions.

Keywords: *mathematical modelling; statistical analysis; model validation; simulation; optimisation; sustainable development; uncertainty analysis*

Introduction

Mathematical modelling connects abstract mathematical ideas with observable systems in biology, economics, engineering, environmental science, medicine, and technology. A model simplifies a complex system by identifying relevant variables and describing relationships among them. The resulting equations or computational rules can be used to explain observed behaviour, compare scenarios, and estimate outcomes under stated assumptions. Models differ in structure and purpose. Agent-based models represent the behaviour and interactions of individual entities, whereas partial differential equations often describe aggregate patterns that vary across space and time. Deterministic models produce the same outcome when the same inputs and initial conditions are repeated; stochastic models incorporate random variation and therefore represent a distribution of possible outcomes. Mechanistic models are based on an understanding of the underlying process, while data-driven models infer relationships from observed data.The usefulness of a model depends not only on mathematical sophistication but also on the quality of its assumptions, input data, calibration, and validation. Statistical evaluation is particularly important because a model that fits the data used to construct it may not predict new observations accurately. Accordingly, this paper combines a conceptual review of modelling applications with a practical statistical framework for assessing predictive performance.

Objectives of the Study

1. To explain the main foundations, categories, and stages of mathematical modelling.

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2. To review the role of modelling in scientific research, engineering, technology, and sustainable development.
3. To describe statistical techniques used for model calibration, validation, and performance assessment.
4. To demonstrate the calculation and interpretation of selected error metrics using a clearly labelled simulated example.
5. To identify limitations and good practices for transparent, reproducible, and policy-relevant modelling.

Research Methodology

1. Research design

This paper uses a narrative, literature-based review design. It organises the supplied source material around model foundations, scientific and technological applications, sustainability, validation, uncertainty, and governance. It does not report a new field survey, experiment, or analysis of an externally collected dataset.

2. Analytical procedure

The material was synthesised thematically. First, modelling concepts and workflows were identified. Second, applications were grouped into scientific, technological, environmental, and planning domains. Third, a statistical assessment framework was formulated to show how model predictions can be compared with observed values. The numerical example in Section 5 is simulated for demonstration only and must not be interpreted as measured evidence.

3. Modelling workflow

Table 1. General mathematical-modelling workflow

Stage	Purpose	Typical output
1. Problem framing	Define the question, system boundary, users, and success criteria.	Research question and scope
2. Assumptions and inputs	Specify simplifying assumptions, variables, and data requirements.	Assumption list and dataset
3. Model formulation	Translate relationships into equations, algorithms, or agent rules.	Candidate model
4. Calibration	Estimate parameters using calibration data.	Fitted parameter values
5. Validation	Test predictions using data not used for calibration.	Independent performance estimates
6. Sensitivity and uncertainty	Examine effects of uncertain inputs and structural choices.	Sensitivity rankings or uncertainty ranges
7. Interpretation	Connect model outputs to the original question and decision context.	Findings and limitations
8. Communication	Report methods, assumptions, code, data, and conclusions clearly.	Reproducible report

Source: *Prepared by the author based on the mathematical-modelling workflow discussed in this paper.*

Applications of Mathematical Modelling

1. Scientific and biological systems

In biological research, models can represent population growth, species interactions, disease transmission, and processes occurring at molecular or ecosystem scales. Population models may describe births, deaths, migration, and environmental constraints. Pharmacokinetic models describe how a substance is absorbed, distributed, metabolised, and eliminated over time. Such applications require careful parameter estimation and validation against appropriate observations; model outputs should not be treated as substitutes for clinical judgement or empirical evidence.

2. Physical systems and engineering

Engineering models express physical processes through algebraic equations, ordinary differential equations, or partial differential equations. They can estimate internal system behaviour that is difficult to measure directly, compare alternative designs, and reduce the time and cost of repeated physical trials. Model reduction can simplify computationally demanding systems while preserving the variables most relevant to the question. The reduced model must still be checked against the full model or suitable benchmark data.

3. Computational modelling and artificial intelligence

Numerical simulation supports the solution of complex equations in meteorology, civil engineering, mechanical systems, and biomedical research. Data-driven models and machine-learning methods can identify patterns in large datasets, while surrogate models approximate expensive simulations. Combining data-driven methods with mechanistic knowledge may improve interpretability, but predictive performance should be evaluated using independent data and transparent procedures to avoid overfitting.

4. Environmental systems and climate change

Environmental models describe processes such as pollutant transport, soil erosion, hydrological flows, ecosystem change, and greenhouse-gas emissions. Scenario analysis can compare mitigation and adaptation strategies under alternative assumptions. Since environmental systems contain structural and parameter uncertainty, results are best communicated with sensitivity tests, plausible ranges, and explicit descriptions of data limitations rather than as single certain forecasts.

5. Energy systems and sustainable development

Energy-system models help compare supply technologies, demand profiles, resource limits, costs, and emissions targets. Multi-objective optimisation is useful when environmental protection, affordability, reliability, and social equity may conflict. Model results can inform planning, but the selected objective functions and constraints embody choices that should be disclosed and discussed with affected stakeholders.

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6. Urban planning and transport

Urban models represent relationships among land use, transport demand, infrastructure, and service provision. Network and agent-based approaches can explore how changes in land-use patterns or transport policy affect movement and access. Such models can support scenario comparison, provided that local data, distributional effects, and the needs of different population groups are considered.

Statistical Framework for Model Evaluation

Statistical analysis helps summarise data, estimate model parameters, compare predicted and observed values, and quantify uncertainty. The selected measures should match the study objective, data scale, and consequences of prediction errors. No single statistic is sufficient for every modelling problem.

1. Descriptive statistics

For observations $x_1, x_2, \ldots, x_n$, the arithmetic mean is $\bar{x} = (\Sigma x_i)/n$. The sample variance is $s^2 = \Sigma(x_i - \bar{x})^2/(n - 1)$, and the sample standard deviation is $s = \sqrt{s^2}$. The mean describes the central tendency, while the standard deviation summarises dispersion around the mean. Median and interquartile range may be preferable when distributions are strongly skewed or contain outliers.

2. Predictive-performance measures

Let y_i be an observed value, $\hat{y}_i$ the corresponding model prediction, and n the number of paired observations. The residual is $e_i = y_i - \hat{y}_i$.

Mean Absolute Error (MAE): $MAE = (1/n)\ \Sigma\ |y_i - \hat{y}_i|$. It represents the average absolute prediction error in the original measurement units.

Root Mean Square Error (RMSE): $RMSE = \sqrt{[(1/n)\ \Sigma\ (y_i - \hat{y}_i)^2]}$. Squaring errors before averaging gives larger errors greater influence.

Coefficient of determination (R^2): $R^2 = 1 - [\Sigma(y_i - \hat{y}_i)^2\ /\ \Sigma(y_i - \bar{y})^2]$, where $\bar{y}$ is the mean of observed values. Under this predictive definition, R^2 can be negative when predictions perform worse than using the observed mean as a benchmark.

Mean Absolute Percentage Error (MAPE): $MAPE = (100/n)\ \Sigma\ |(y_i - \hat{y}_i)/y_i|$. MAPE is unsuitable when observed values are zero and can behave poorly when they are close to zero.

3. Illustrative calculation using simulated values

The following five paired values are invented solely to demonstrate statistical calculations. They are not taken from a field study, experiment, or published dataset.

Table 2. Simulated observed and predicted values

Case	Observed (y)	Predicted ($\hat{y}$)	Residual ($y - \hat{y}$)	Absolute error	Squared error
1	10	11	-1	1	1
2	12	11	1	1	1
3	13	14	-1	1	1
4	15	14	1	1	1
5	20	18	2	2	4

Source: *Author's own illustration using simulated values; data are not empirical.*

Table 3. Summary of illustrative statistical measures

Statistic	Illustrative result	Interpretation
Mean observed value	14.00	Average of the five simulated observations.
MAE	1.20	Average absolute prediction error, in the same units as the outcome.
RMSE	1.26	Penalises larger errors more heavily than MAE.
R^2	0.862	Proportion of observed variation accounted for under the stated formula; interpretation is limited by the tiny simulated example.
MAPE	8.54%	Average absolute percentage error; included only because all example observations are non-zero.

Source: *Author's calculations based on the simulated values presented in Table 2; results are illustrative only.*

The example produces MAE = 1.20, RMSE = 1.41, R^2 = 0.918, and MAPE = 9.90%. These figures demonstrate the formulas only. They do not establish that any real mathematical model has achieved this performance. In an empirical study, all measures should be calculated from a clearly described dataset, and the validation observations should be independent of those used to fit the model.

4. Calibration, validation, and uncertainty

A robust evaluation separates data used for parameter estimation from data reserved for validation. For time-series data, chronological splitting may be more appropriate than random splitting; for spatial data, spatially separated validation can help reveal limited transferability. Residual plots should be examined for systematic patterns, heteroscedasticity, and outliers. Sensitivity analysis assesses how changes in inputs or parameters affect outputs, while uncertainty analysis communicates the range of plausible outcomes under uncertain assumptions.

Results and Discussion

The thematic review indicates that mathematical modelling has value across disciplines because it converts complex processes into explicit structures that can be analysed and compared. Its practical contribution depends on matching model complexity to the research question. Agent-based models are useful when individual behaviour and local interactions matter; differential-equation models are appropriate for many continuous processes; and statistical or machine-learning models can be effective when reliable data are available and prediction is the main goal. The statistical framework shows why model assessment should go beyond visual agreement or a single goodness-of-fit value. MAE is easy to interpret, RMSE highlights large deviations, and R^2 compares residual variation with the variation in observed outcomes. These measures are complementary rather than interchangeable. Their values can also be misleading when the sample is small,

observations are dependent, data are unrepresentative, or validation data have been used during model development.

For sustainability applications, modelling is most useful when scenarios expose trade-offs among economic, environmental, and social objectives. A technically accurate model can still support poor decisions if its assumptions exclude vulnerable groups, its data are biased, or its uncertainty is concealed. Reproducible code, documented data sources, transparent parameter choices, stakeholder engagement, and accessible presentation of results are therefore central to responsible practice.

Limitations

This paper is a narrative review based on the supplied chapter material and does not claim to be a systematic review. No new empirical dataset was supplied, so the numerical example is simulated and cannot be used as evidence about the real-world accuracy of a particular model. The referenced literature is retained from the source material, but bibliographic details should be checked against the original publications before journal submission. A future empirical study should specify a concrete application, obtain an appropriate dataset, document sampling and preprocessing, and report results from an independent validation procedure.

Conclusion

Mathematical modelling is a versatile foundation for scientific explanation, technological development, and sustainable planning. A disciplined workflow—from problem framing and assumptions to calibration, independent validation, sensitivity analysis, and communication—helps ensure that models address the question for which they were developed. Statistical measures such as MAE, RMSE, and R^2 provide useful but partial evidence of predictive performance and should be interpreted alongside residual diagnostics and uncertainty analysis. For policy-relevant use, models should be transparent, reproducible, appropriately validated, and attentive to equity and stakeholder needs. Further empirical research should apply the proposed framework to a defined scientific or sustainability problem using real, documented observations.

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Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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17. To describe statistical techniques used for model calibration, validation, and performance assessment.of mitigation and adaptation.