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Quantitative Horizons in Pharmacy: A Review of Applied Mathematical Advances (2010–2025)

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ABSTRACT:

Background: The convergence of applied mathematics and pharmacy has revolutionized approaches to drug development, therapy optimization, and patient-centered care. Mathematical and computational models are increasingly vital in interpreting complex biomedical data and supporting pharmaceutical innovation.

Aims: This review aims to summarize and critically appraise recent developments in the application of applied mathematics to pharmaceutical sciences and pharmacy practice. It explores how mathematical techniques influence drug formulation, pharmacokinetics / pharmacodynamics, clinical trials, and personalized medicine.

Methods: A comprehensive literature search was conducted in databases such as PubMed, Scopus, and Web of Science using keywords including, Applied Mathematics, pharmacy, pharmacokinetics, pharmacodynamics, drug modeling, and personalized medicine. Articles published from 2010 to 2025 were screened for relevance. Key themes and representative studies were identified and synthesized.

Results: Applied Mathematics underpins diverse aspects of pharmacy, including Pharmacokinetic and pharmacodynamics modeling, drug formulation and release kinetics, clinical trial design and statistical analysis, and systems pharmacology and personalized medicine. Emerging trends show a growing reliance on mathematical and data-driven approaches to tackle pharmaceutical challenges.

Conclusions: Applied mathematics provides essential tools for innovation in pharmaceutical sciences and clinical pharmacy practice. Its integration advances drug development, enhances therapeutic outcomes, and enables personalized medicine.

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Strengthening mathematical-pharmaceutical collaborations will be crucial for the future of precision health care.

Abbreviations

PK: Pharmacokinetic

PD: Pharmacodynamic

PBPK: Physiologically based Pharmacokinetic

MD: Molecular Dynamics

QSAR: Quantitative Structure-Activity Relationship

ML: Machine Learning

LR: Linear Regression

NLME: Nonlinear Mixed-Effects Models

DD: Drug Delivery

INTRODUCTION

Over the past decade and a half, the landscape of pharmaceutical sciences and pharmacy practice [1] has undergone a profound transformation, shaped increasingly by the integration of applied mathematics. Traditionally, pharmacy focused on the discovery, formulation, and dispensing of medications based on empirical observations and established protocols. However, the exponential growth of biomedical data [2], advances in computational technologies, and the complexity of modern therapeutics have necessitated the adoption of more rigorous, quantitative approaches [3]. Applied mathematics has emerged as a linchpin in addressing these evolving challenges, offering sophisticated tools for modeling, simulation, data analysis, and decision-making across the pharmaceutical field [4]. From 2010 to 2025, applied mathematics has profoundly influenced various aspects of pharmacy. Mathematical modeling and simulation have become indispensable for understanding the kinetics and dynamics of drugs within the body, leading to more accurate predictions of efficacy, safety, and individual variability. The use of differential equations, compartmental analysis, and stochastic models has transformed pharmacokinetic (PK) and pharmacodynamic (PD) evaluations [5], supporting more precise dose individualization and improving drug development timelines. The last fifteen years have witnessed a paradigm shift in pharmaceutical sciences, with applied mathematics becoming central to drug discovery, development, formulation, and delivery. As pharmacy has evolved from a predominantly empirical tradition to one driven by quantitative and predictive methodologies, the integration of mathematical models and computational techniques has fundamentally changed research and practice [6-7]. Modern pharmaceuticals involve increasingly complex compounds, diverse delivery systems, and a deeper understanding of human variability in response to therapy. Applied mathematics offers a toolkit to address these challenges, encompassing differential equations, stochastic modeling, statistical learning, and optimization algorithms. Mathematical modeling in pharmacokinetics and pharmacodynamics (PK/PD) has enabled precise simulation of drug behavior, improved dose individualization, and more efficient clinical trial designs [8]. Population-based models, non-linear mixed-effects modeling, and physiologically-based pharmacokinetic (PBPK) approaches are now routinely applied in both preclinical and regulatory contexts [9-10]. Parallel advances in statistics and machine learning techniques have transformed the design, monitoring, and interpretation of clinical trials [11-12]. Adaptive and Bayesian trial methodologies allow dynamic incorporation of cumulative data, improving trial efficiency and patient safety [13-14]. In formulation science, mathematical techniques guide the optimization of drug release profiles, dissolution, and delivery mechanisms under varying physiological environments [15-16]. Big data analytics and computational systems biology have further expanded the role of applied mathematics in pharmacy. The rise of systems pharmacology and network modeling allows for a holistic understanding of drug interactions at molecular, cellular, and organ levels [17-18]. Machine learning-based approaches utilize large-scale patient and omics data to unlock advances in personalized medicine, creating pathways toward truly individualized therapeutics [19-20]. Challenges remain, particularly around model validation, reproducibility, and bridging the gap between computational predictions and real-world outcomes [21-22]. Addressing these requires interdisciplinary communication, collaborative research, and continued methodological innovation. This review critically surveys the interface

between applied mathematics and pharmacy from 2010 to 2025. It covers innovations in PK/PD modeling, clinical trial analytics, drug formulation science, big data, and emerging fields such as systems pharmacology and Pharmacometrics. It also discusses persistent challenges and future directions for this dynamic, interdisciplinary domain. This review aims to summarize and critically appraise recent developments in the application of applied mathematics to pharmaceutical sciences and pharmacy practice. It explores how mathematical techniques influence drug formulation, Pharmacokinetics / pharmacodynamics (PK/PD), clinical trials, and personalized medicine.

METHODOLOGY

Research Question, how have applied mathematical advances been utilized in pharmacy from 2010 to 2025, and what are the key trends, techniques, and outcomes? From 2010 to 2025, applied mathematics has played a pivotal role in advancing pharmacy, particularly in drug discovery, pharmacokinetics / pharmacodynamics (PK/PD), personalized medicine, and optimization of drug delivery systems.

Drug Discovery and Design

Molecular Dynamics (MD) Simulations: Applied mathematics has been used to model molecular interactions, predict drug-target binding, and optimize drug candidates, MD simulations help in understanding the behavior of biomolecules at atomic resolution [23] figure (1).

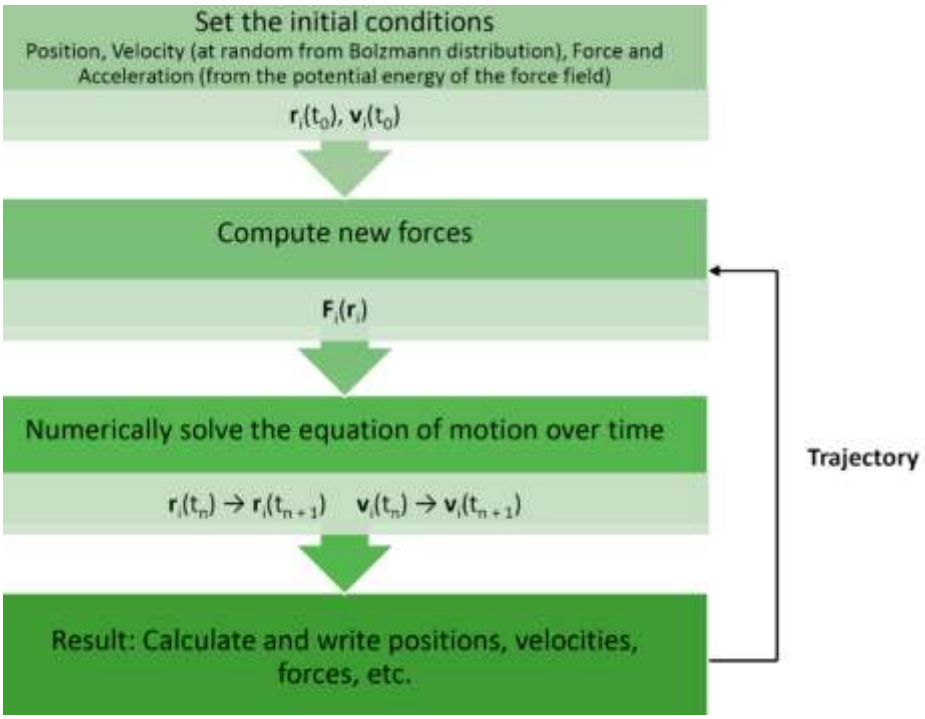

Figure 1: Basic molecular dynamics simulation algorithm [23]

Each particle moves according to Newton's second law or the equation of motion, F = ma (where 'F' is the force exerted on the particle, 'm' is its mass, and 'a' is its acceleration under a potential field), such that the particles in the system are captured in the trajectory, r: position, v: velocity, t: time.

Quantitative Structure-Activity Relationship: Mathematical models are used to predict the biological activity of compounds based on their chemical structure, aiding in the design of new drugs, figure (2) [24].

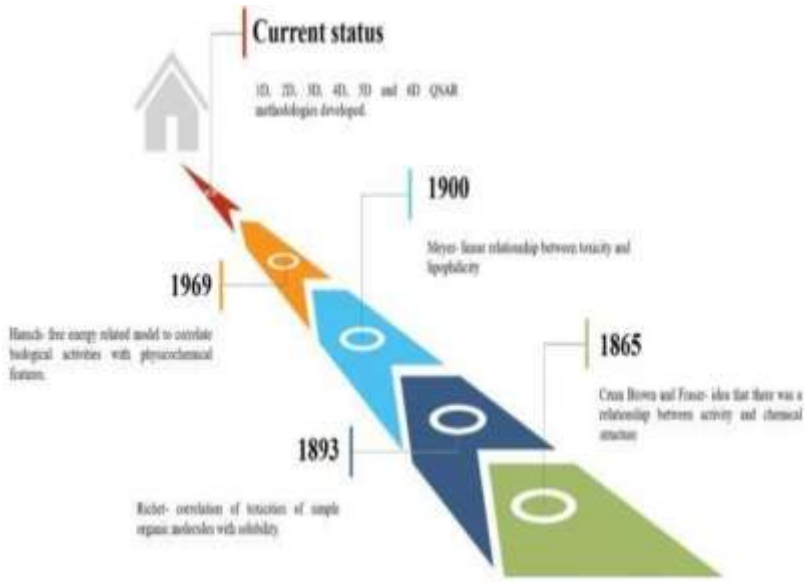

Figure 2: History of quantitative structure–activity relationship [24]

Machine Learning: The algorithms, such as deep learning, have been employed to analyze large datasets of chemical compounds and predict drug efficacy, toxicity, and bioavailability, below some common mathematical formulas used in machine learning [25].

Linear Regression, it is principle technique for the predication of the continuous variable, mathematical formula for simplest linear regression defined as:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots.. + \beta_n x_n + \varepsilon \quad (1)$$

In which:

y : Target variable

$x_1, x_2, .. x_n$: Input features

$\beta_0, \beta_1, \beta_2, \ldots\ldots, \beta_n$: Coefficients to be learned

ε : Error term.

Logistic regression or sigmoid function, plays a pivotal role in the algorithm, defined as:

$$o(z) = \frac{1}{e^{-z}} \quad (2)$$

In where:

z : A linear combination of input and their corresponding coefficients, logistic function maps the linear output to a value between 0 and 1, allowing us to interpret it as a probability.

Cost functions quantify error or discrepancy between predicted values and actual values, Mean Squared Error (MSE) is a commonly used cost function for regression problems, defined as:

$$\text{MSE} = \left(\frac{1}{n}\right)\sum\left(y_i - \bar{y}\right)^2 \quad (3)$$

In which

n : Number of samples

y_i : Actual value

$\bar{y}$: Predicted value

For classification problems, Cross-Entropy Loss is often employed, given by:

$$\mathrm{CE} = \sum y_i \log(p_i) + (1 - y_i)\log(1 - p_i) \quad (4)$$

In which, y_i actual label (0 or 1) and p_i is the predicted probability.

Gradient descent is an optimization algorithm used to minimize the cost function and find the optimal values of the coefficients. The update rule for gradient descent can be expressed as:

$$\theta = \theta - \alpha \times \nabla J(\theta) \quad (5)$$

θ Represents the coefficients, α learning rate, $J(\theta)$ defined as cost function, while $\nabla J(\theta)$ cost gradient.

Pharmacokinetics and Pharmacodynamics (PK/PD)

Compartmental Models: Mathematical models, such as the one-compartment and two-compartment models, are used to describe the absorption, distribution, metabolism, and excretion (ADME) of drugs. Suppose x(t) is the drug concentration at time *t* seconds.

$$\frac{dx}{dt} = \text{Input rate of drug - Output rate of drug} \quad (6)$$

If the drug is administered orally, it diffuses into the blood via the GI tract, forming the first and second compartments. Assume that x_0 represents initial drug concentration, and $x_i(t), i = 1,2$ then [26],

$$\frac{dx_1(t)}{dt} = -k_1 x_1(t) \quad (7)$$

$$\frac{dx_2(t)}{dt} = -k_1 x_1(t) - k_e x_2(t) \quad (8)$$

k_1, k_e : Travel of drug movement from one compartment to another

Solution of equations (7-8):

$$x_1(t) = x_0 \exp(-k_1 t) \quad (9)$$

$$x_2(t) = \frac{x_0 k_1}{k_1 - k_e}\left[\exp(-k_e t) - \exp(-k_1 t)\right] \quad (10)$$

When dealing with clinical cases, the situation is different because oral administration of the drug is not possible. Rather, the clinical patient must be given the drug directly into the bloodstream. In this case, the blood is treated as the primary compartment into which the drug is administered, while the tissues are viewed as the second compartment that has the therapeutic effect. It is worth noting that the drug reaches the tissues at a constant rate k_b from the blood, and is excreted at a different constant rate k_t . Mathematical model for the drug is described using the following set of equations:

$$\frac{dx_b(t)}{dt} = -(k_b + k_e)x_b(t) + k_t x_t(t) \quad (11)$$

$$\frac{dx_t(t)}{dt} = k_b x_b(t) - k_t x_t(t) \quad (12)$$

The third model is called the three-compartment model, as after giving the patient the drug intravenously in the three compartments, which are the central compartment (plasma), the peripheral compartment which represents the organs and tissues, and finally the peripheral compartment with little perfusion (organs and tissues) [27]: If $x_i(t), i = 1,2,3$ represent concentrations in central & peripheral compartments, then equations define characteristics of drug concentration in the three compartments are as follows [27]:

$$\frac{dx_t(t)}{dt} = -(k_{10} + k_{12} + k_{13})x_1(t) + k_{21}x_2(t) + k_{31}x_3(t) \quad (13)$$

$$\frac{dx_2(t)}{dt} = k_{12}x_1(t) + k_{21}x_2(t) \quad (14)$$

$$\frac{dx_3(t)}{dt} = k_{13}x_1(t) + k_{31}x_3(t) \quad (15)$$

Physiologically based pharmacokinetic models

These models use mathematical equations to simulate drug behavior in different tissues and organs, enabling personalized dosing strategies, figure (3) [28].

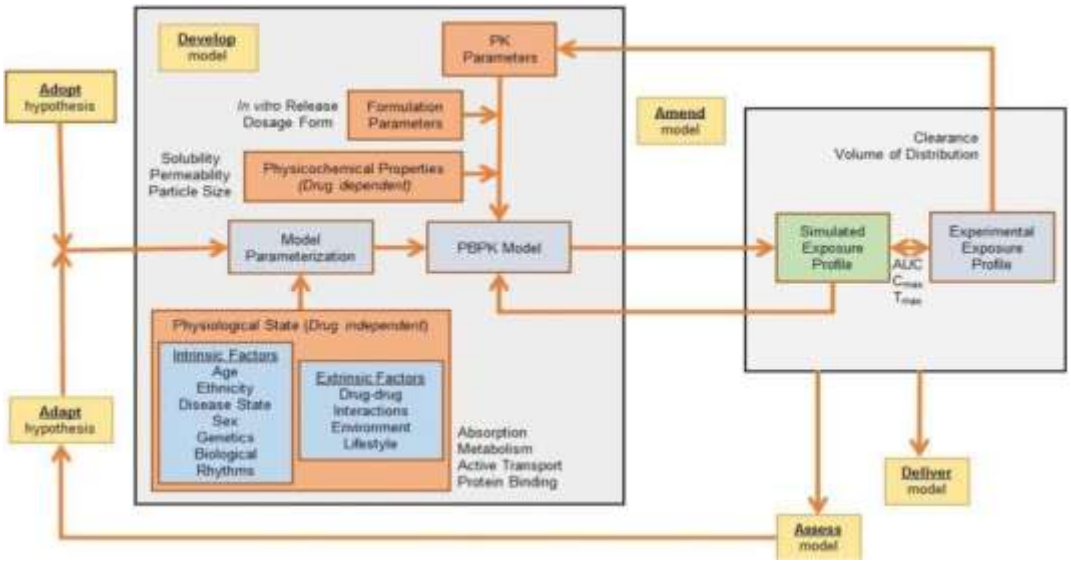

Figure 3: Subpopulation modeling in the framework of the $(AAD)^2$ methodology [28]

Nonlinear Mixed-Effects Models (NLME)

These models are used to analyze population PK/PD data, accounting for variability between individuals [30], non-linear mixed-effects models written as:

$$y_{ij} = F(\phi_i, t_{ij}) + G(\phi_i, t_{ij}, \beta)\varepsilon_{ij}$$
$$j \in (1,2,\ldots,n_i) \quad (16)$$
$$\phi_i = \mu \exp(\varsigma_i), i = 1,2,\ldots,N$$

y_{ij} : Observed value

$F(\phi_i, t_{ij})$: Individual prediction for individual i

ε_{ij} : Independent random variable

$G(\phi_i, t_{ij}, \beta)$: Function determines scale of random error for an individual i

Drug Delivery Systems

Mathematical Modeling of Drug Release

Mathematical models of the drug release have been used in the drug delivery (DD) field for more than 50 years by the scientists in the drug development process. These models not only help scientists to learn the dynamics of the drugs release, but also help them to save money and time by helping to design more effective experiments. Models such as the Higuchi equation and Korsmeyer-Peppas model are used to predict drug release from controlled-release formulations [31].

Optimization Algorithms

Techniques like linear programming and genetic algorithms are used to optimize drug formulations and delivery systems for targeted therapy. Application of optimization in computational systems biology is biomarker identification, which is frequently related to the problem of classifying samples measured using the omics technologies (genomics, proteomics, lipidomics, and metabolomics), optimization problems can be formulated as follows [32]:

$$\min c(\theta)$$
$$g(\theta) \le 0$$
$$Ib \le \theta \le ub$$
$$\theta_j \in \Re \text{ or } Z,\ j = 1,2,\ldots,p \quad (17)$$

θ : Vector of dimension $p \ge 1$ contains the parameter estimates that are sought

c : Cost function

$Ib \ \& \ ub$: Constraints

This review examines the current state-of-the-art computational methods employed in various stages of pharmaceutical research, from initial compound screening to final drug evaluation, figure (4) [33].

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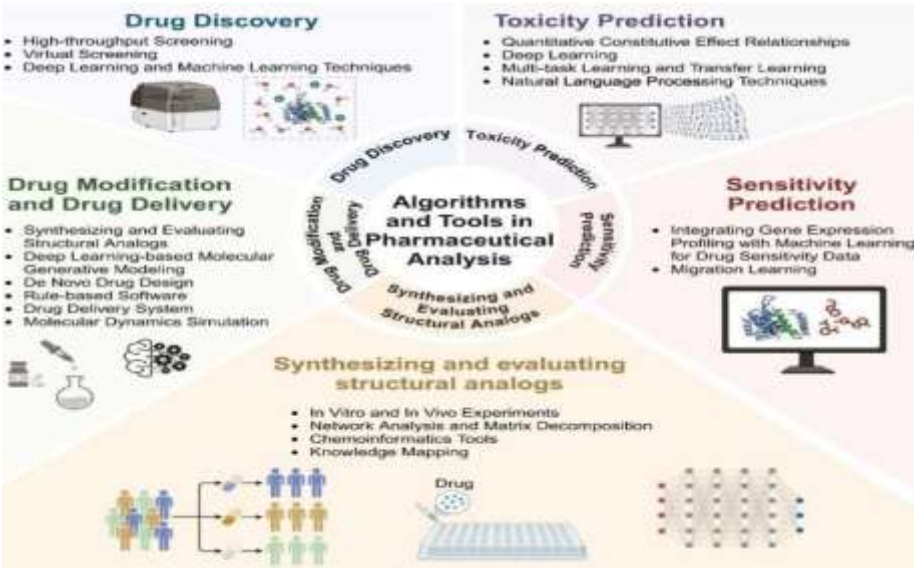

Figure 4: A schematic overview of computational algorithms and tools utilized in various stages of pharmaceutical analysis, encompassing drug discovery, structural modification, delivery, sensitivity prediction, and toxicity assessment [33]

Systems Pharmacology

Network Theory: Applied mathematics is used to model complex biological networks, such as protein-protein interactions and metabolic pathways, to understand drug effects at the systems level [34]. Consider a basic motif containing two nodes x and y, which represent two interacting species of the pathway or chemical reaction network. The interaction between these nodes are defined based on the ODE system that represents the reactions. Assuming a general ODE system in the form of:

$$\frac{dx}{dt} = f_x(x,y) = \frac{\partial f(x,y)}{\partial x}$$
$$\frac{dy}{dt} = f_y(x,y) = \frac{\partial f(x,y)}{\partial y} \quad (18)$$

The sign of the entries of the Jacobian matrix of (13) specify the type of interaction between x and y. If $f_y(x,y) > 0$, then y activates x, while if $f_x(x,y) < 0$ y inhibits x. If any of the partial derivatives is zero, there would be no connection in the corresponding direction. Figure (5) presents all the variations possible between x and y, as well as the graph representation for each interaction [34].

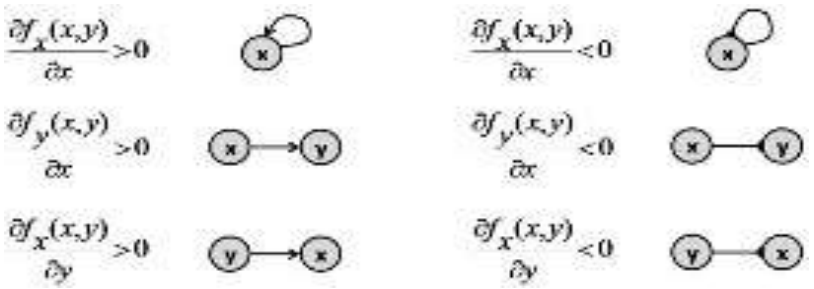

Figure 5: Representations for the basic interactions between the nodes in a two-element motif

Stochastic Modeling: Used to model random fluctuations in biological systems, such as gene expression or drug metabolism, to predict variability in drug response [35-37].

Clinical Trial Design

Mathematical models are used to design adaptive clinical trials that can modify dosing or patient recruitment based on interim results, improving efficiency and reducing costs, figure (6) [38].

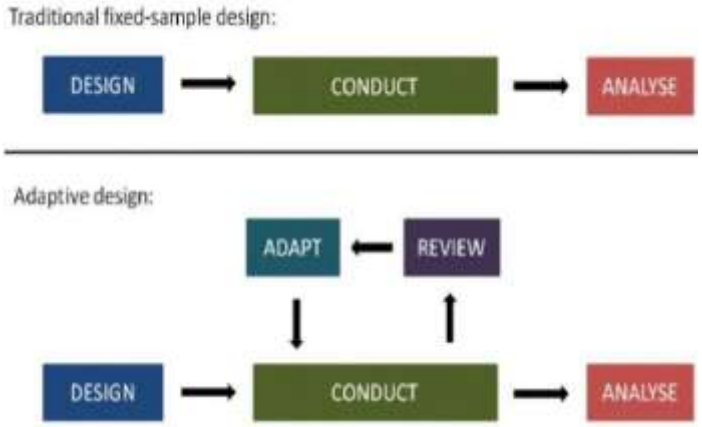

Figure 6: Schematic of a traditional clinical trial design with fixed sample size, and an adaptive design with pre-specified review(s) and adaptation(s) [38]

PK Models

Compartmental Models

These models divide the body into compartments (e.g., central and peripheral) to describe drug distribution and elimination [39-40].

Pharmacodynamics (PD)

Pharmacodynamics is the study of the biochemical and physiological effects of drugs and their mechanisms of action. Mathematical models in PD are used to describe the relationship between drug concentration and effect [41].

PK and PD relationship [41]

Pharmacokinetics (PK) and pharmacodynamics (PD) are two fundamental areas of pharmacology that describe different aspects of drug actions within the body. This refers to the movement of drugs within the body and involves four main processes:

Absorption: How a drug enters the bloodstream from its site of administration.

Distribution: How the drug spreads throughout the body's tissues and fluids.

Metabolism: How the drug is chemically altered, primarily in the liver, into metabolites.

Excretion: How the drug and its metabolites are eliminated from the body, usually via the kidneys, PK helps in understanding the concentration of the drug over time in the body.

Pharmacodynamics (PD): describes the physiological effects of the drug on the body and how the drug exerts its therapeutic effect. Key aspects include:

Receptor binding: How the drug interacts with cellular receptors to produce an effect.

Dose-response relationships: The relationship between the dose of the drug and the magnitude of its effect.

Therapeutic window: The range of drug doses that elicits a therapeutic effect without causing significant adverse effects. PD helps in understanding the drug's mechanism of action and its efficacy.

The relationship between PK and PD is crucial for determining the appropriate dosage and schedule for administering drugs to achieve optimal therapeutic effects while minimizing adverse effects. This relationship can be complex and is often represented through models that link drug concentrations (PK) with the observed effects (PD), figure (7) [41].

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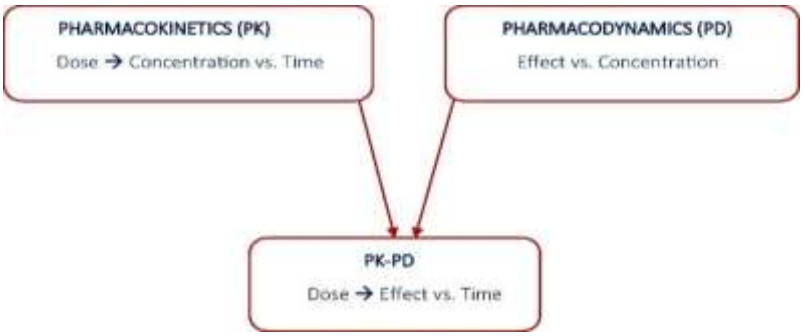

Figure 7: Pharmacokinetic and pharmacodynamics relationship [41]

Mechanistic Models

These models incorporate detailed knowledge of the drug's mechanism of action and the biological system it affects. Mechanistic models are a type of scientific model that aim to represent the underlying processes or mechanisms of a system. These models are based on the principles of cause and effect, where specific inputs and parameters are used to simulate the behavior of the system under study, they often involve mathematical representations of physical, chemical, or biological processes. The content of mechanistic models is shown in table (1) [41].

Table 1: Content of Mechanistic models

Machining operation	Tool type	Materials	Fiber content	Fiber orientation	Refs.
Orthogonal Cutting	PCD tools (COMPAX 1300)	MD-Graphite/Epoxy (IM-6/3501–6) $[45°/-45°/(0°/90°/45°/-45°)_2]_s$	68 %	0°-180°	[42]
	Solid carbide tool	UD-CFRP	47.4 %	90°	[43]
Milling	Straight milling tool Helical milling tool	UD-CFRP	55.7 %	–	[44]
	PCD (APKT1604)	UD-CF/PEEK (Carbon fiber reinforced polyetheretherketone)	55 %	90°	[45]
	OSG-Walter F2037 single square carbide insert	UD-CFRP	60 %	0°/45°/90°	[46]
	PCD milling tools (Schwegler)	UD-CFRP $[0°/45°]_{15}$	59 %	0°-180°	[47]

The purpose of mechanistic models are used to understand, simulate, and predict complex phenomena by focusing on the causal relationships and interactions within a system. These models typically consist of equations that describe the dynamics of the system. For example, they might use differential equations to represent changes over time. Mechanistic models are widely used in fields such as biology (e.g., enzyme kinetics, population dynamics), chemistry (e.g., reaction kinetics), environmental science (e.g., pollutant dispersion), and engineering (e.g., systems dynamics). They can provide deep insights into how systems operate and allow for the testing of hypotheses about system behavior under various conditions. Mechanistic models can be complex and require detailed knowledge of the system being modeled. They also rely heavily on the accuracy of input parameters and assumptions made during model development. In practice, developing a mechanistic model involves defining the system

boundaries, identifying all relevant processes and interactions, and validating the model against experimental or observational data to ensure its reliability.

Integrated PK/PD Models

Integrated pharmacokinetic/pharmacodynamic (PK/PD) models are powerful tools used in the field of pharmacology to understand the relationship between drug concentrations in the body (pharmacokinetics, PK) and their subsequent effects (pharmacodynamics, PD). An integrated PK/PD model can provide valuable insights into the drug action mechanism, contribute to safer and more effective therapeutics, and support regulatory decision-making processes. Two approaches hybridize well, well-illustrated in figure (8) [48].

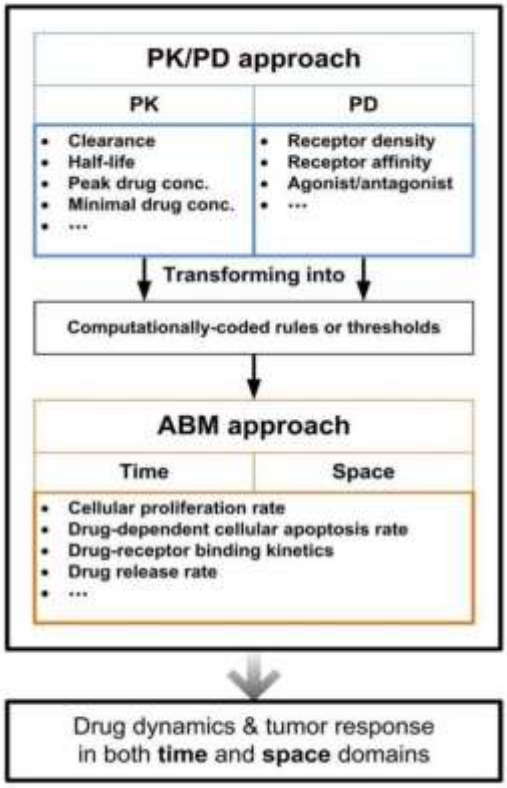

Figure 8: PK/PD approaches [48]

Applied Mathematics in Drug Formulation and Delivery

In the modern era, mathematical modeling of drug delivery and release prediction is an area of growing academic and industrial importance, with a tremendous future. This is due to the tremendous advances in information technology, and it is expected that computational optimization will be of paramount benefit to new drug delivery systems in terms of accuracy, ease of application, and remarkable applicability. As in other sciences (such as aviation and aerospace), computer simulation is likely to become an integral part of future research and development in pharmaceutical technology. It is only a matter of time before mathematical programs are routinely used to help optimize the design of new dosage forms. Given the desired type of administration, the dose of drug to be combined, and the targeted drug release pattern, mathematical predictions will enable accurate estimates of the composition, geometry, dimensions, and preparation procedures required for the respective dosage forms. Thus, one of the main driving forces for the use of mathematical modeling in drug delivery is time-saving and cost-reducing benefits: the number of experimental studies required to develop a new drug product and/or improve an existing one can be significantly reduced [50].

Vision for the future of mathematics-driven pharmacy

In the future, pharmacy will be deeply integrated with advanced mathematical modeling, simulation, and data analytics, leading to a highly personalized and proactive approach to healthcare [49]. In summary, we are currently observing a change in the

paradigm change, with engineering principles and product design becoming the guiding principle of pharmaceutical development. That is, we are adopting a way of thinking, according to which pharmaceutical ingredients, pharmaceutical products, the related manufacturing processes, and the biopharmaceutical properties are considered simultaneously and quantitatively, figure (9) demonstrates this engineering view of pharmaceutical development.

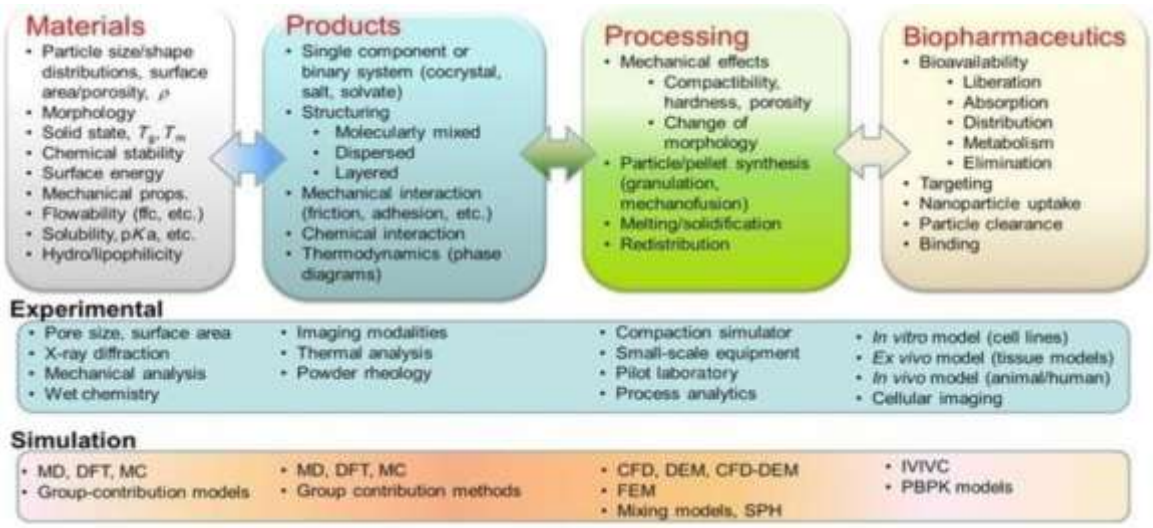

Figure 9: Engineering view of pharmaceutical development [49]

Risk Management

Quality risk management (QRM) can be defined as an integrated action aiming at, first, identifying, assessing and prioritizing risks and, second, at minimizing, monitoring, and controlling the related undesired event. Risk is defined as a combination of probability of occurrence and the severity of harm. The QRM workflow consists of (1) initiation, (2) assessment, (3) control, (4) review, and (5) communication of risks [50].

Personalized Medicine

Mathematical models will allow for the design of individualized drug therapies based on a patient's genetic makeup, lifestyle, and health conditions, algorithms can predict how different patients will respond to specific treatments, optimizing efficacy and minimizing adverse effects [51], figures (10-11).

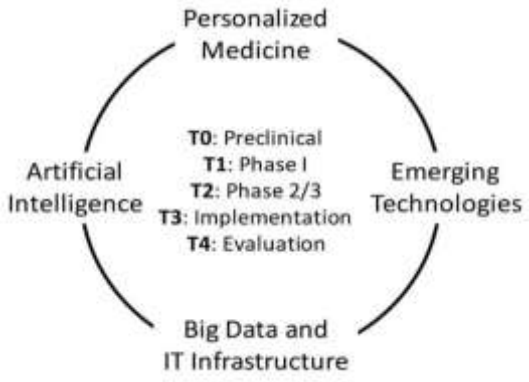

Figure 10: Four emerging complementary themes in biomedical science: personalized medicine, emerging data-intensive technologies, big data and information technologies (IT) infrastructure and artificial intelligence (AI) [51].

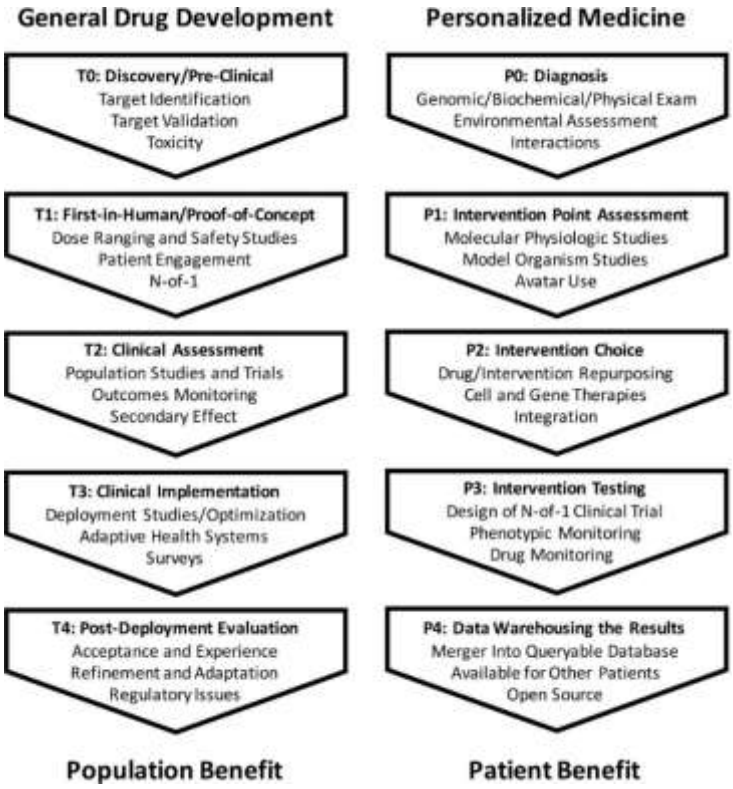

Figure 11: AI in all phases of the development (T0-T4) of personalized medicines [51]

Predictive Analytics: By leveraging big data and machine learning, pharmacists and healthcare providers can predict disease progression and treatment outcomes more accurately. This proactive approach helps in early intervention and better management of chronic diseases [52].

CONCLUSION

Applied mathematics has significantly impacted pharmacy from 2010 to 2024, enabling more efficient drug discovery, personalized medicine, and optimized drug delivery systems. The integration of mathematical modeling, machine learning, and systems pharmacology has led to improved therapeutic outcomes and reduced development costs. Future trends are likely to focus on the further integration of AI and big data analytics in pharmaceutical research and development.

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