

Models for the Development of Sorption Isotherms: A Review

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Received June 04, 2025; Revised July 06, 2025; Accepted July 13, 2025

Abstract Moisture sorption isotherms are fundamental for understanding the relationship between water activity and moisture content in food materials, directly impacting the design and optimization of drying, storage, and preservation processes. This review comprehensively evaluates sorption models, categorizing them into empirical, semi-empirical, theoretical, statistical physics-based, hybrid, and machine learning-based approaches. Empirical models, such as BET and GAB, remain widely used due to their simplicity and broad applicability across various food classes. However, these models often lack mechanistic insights, limiting their accuracy for complex or heterogeneous foods. Theoretical and statistical physics-based models provide deeper understanding of molecular sorption mechanisms but involve increased complexity and parameterization challenges. Recent advancements in hybrid and machine learning models demonstrate the potential to integrate physical laws with data-driven approaches, improving predictive performance and adaptability, particularly for novel and composite food matrices. Key challenges in model application include accurate model selection, robust parameter estimation, accounting for temperature dependency, and multi-component sorption phenomena. Moreover, data quality and limited experimental datasets often constrain model reliability. Emerging trends suggest that integrating physics-informed machine learning, real-time sensor data, multi-scale modeling, and digital twin technologies will enhance model robustness and facilitate real-time process control. Recommendations highlight the importance of selecting sorption models aligned with specific food types and processing requirements, employing rigorous fitting techniques, and combining mechanistic and data-driven approaches for optimal balance between accuracy and interpretability. Continued advancements in sorption isotherm modeling are expected to support sustainable, energy-efficient food processing and improve product stability and quality, addressing growing industry demands.

Keywords: Sorption Isotherm, Water activity, Moisture Content, Equilibrium Moisture content, Sorption Model

Cite This Article: Sunday Ibe Iji, Uwem Ekwere Inyang, and Benjamin Reuben Etuk, "Models for the Development of Sorption Isotherms: A Review." *American Journal of Food Science and Technology*, vol. 13, no. 2 (2025): 27-37. doi: 10.12691/ajfst-13-2-2.

1. Introduction

Adsorption is a mass-transfer surface process in which molecules, ions, or gases accumulate at the interface of a solid adsorbent, driven by attractive forces until dynamic equilibrium is reached when there is no further net transfer [1,2]. This phenomenon involves the formation of an adsorbate layer on the adsorbent surface, primarily through weak van der Waals interactions (physisorption), although forces such as electrostatic, dipole-dipole, hydrogen bonding, and even chemisorption may also play roles [3,4]. Adsorbents used in this process are typically porous solids with high surface areas, enhancing their capacity to attract and retain molecules [5].

According to [6], adsorption of a solute onto an adsorbent progresses through several sequential stages: external diffusion (movement of molecules from the bulk fluid to the interface), internal diffusion (migration within the pore structure), surface diffusion (movement along the

adsorbent surface), and the final adsorption-desorption events at active sites. The adsorption phenomenon may be physical (physisorption) or chemical (chemisorption). Physisorption involves weak, short-range electrostatic forces, typically Van der Waals interactions, whereas chemisorption involves the formation of chemical bonds between adsorbate and adsorbent [7].

It is essential to distinguish adsorption from absorption. While adsorption involves the surface-level adherence of molecules, absorption refers to the uptake of molecules into the entire volume of a material or across a membrane. Adsorption technologies have found broad applications, particularly in water and wastewater treatment, due to their low cost, simplicity, and high efficiency. Beyond environmental applications, adsorption is vital in separating chemical mixtures, removing contaminants, and preserving the quality and shelf life of food and fruit products [8,9].

Moisture content and its interaction with water activity are fundamental to the physical, chemical, and microbiological stability of food products. The sorption

isotherm, which defines the equilibrium relationship between moisture content and water activity at a constant temperature, is a key tool in food engineering. It informs decisions on packaging, drying techniques, and long-term storage conditions. Due to the complex and heterogeneous nature of food matrices, selecting an appropriate sorption model is critical for accurate prediction and analysis [10].

Since the 1980s, isotherm modeling has evolved significantly. Early models such as Brunauer–Emmett–Teller (BET) and Guggenheim–Anderson–de Boer (GAB) provided foundational insights into multilayer adsorption and water-binding mechanisms. Over time, more adaptable empirical models have emerged, allowing better fits for complex food systems. More recently, data-driven models incorporating machine learning and artificial intelligence have [11].

Each model differs in complexity, parameter sensitivity, and suitability for different classes of food. For example, cereal grains are typically well-described by the Henderson or GAB models, while fruits and vegetables are more accurately represented by the Peleg or Smith-type models. In contrast, tuber crops such as potatoes, yam, and cassava are often best described by the Guggenheim–Anderson–de Boer (GAB) model and sometimes the Modified Chung–Pfoest model, due to their high starch content and unique water-binding characteristics [12, 13].

Adsorption isotherms are critical for describing the interaction between adsorbate and adsorbent. They help determine the optimal adsorption capacity and efficiency of a given adsorbent, as well as assess the suitability of its application in specific systems [14]. These isotherms quantify the amount of adsorbate bound to the surface based on its concentration in the surrounding medium and are essential for designing efficient adsorption systems [15,16].

In the context of foods and fruits, sorption isotherms are crucial in modeling drying behavior, designing and optimizing drying equipment, predicting shelf-life stability, estimating moisture shifts during storage, and selecting suitable packaging materials. Sorption data also help evaluate the enzymatic, microbiological, and chemical stability of food items. Based on their curvature, sorption isotherms are generally classified into five types. For most fruits and food products, the isotherms are nonlinear and typically sigmoid in shape, reflecting the multilayer nature of water binding [17].

Numerous mathematical models have been developed to describe sorption isotherms and interpret adsorption behaviour. These models include both empirical and theoretically derived equations, ranging from simple linear regressions to complex multiparameter nonlinear models that explain the characteristic three-region profile of typical isotherms. The performance of each model depends on the food matrix and moisture activity range. A model effective for one food type may not perform adequately for another, and many models only yield accurate predictions within specific water activity intervals [18].

In some conditions, sorption isotherms can be approximated using linear models, especially within narrow water activity ranges, simplifying analysis and prediction [19]. Thus, understanding the strengths and limitations of each model is essential for their appropriate experimental and industrial use. This

review focuses on the existing sorption models, application, advantages and comparative analysis of various sorption isotherm models, particularly as they relate to food and fruits, providing insight into their relevance and practical utility.

1.1. Water Activity

Water plays a vital role in food systems, with product stability during storage largely influenced by its interaction with other food components. The binding state of water is key to preserving both raw and processed materials, and water activity is a critical parameter for describing this state. Notably, changes in sensory and quality attributes such as colour, flavour, texture, and stability often occur within narrow water activity ranges [20].

Water activity (a_w) is a key parameter for predicting the availability of unbound water in foods and understanding the physical state of solid food systems [21]. It is widely regarded as one of the most critical factors in food preservation and processing. Various food preservation methods—such as drying, freezing, and the addition of solutes—are designed to reduce water activity in order to suppress microbial growth and slow down enzymatic and non-enzymatic chemical reactions [22]. Together, water activity and sorption behaviour form the foundation for understanding and managing the shelf life and stability of food products during storage.

Unlike total moisture content, water activity is a physical measure of the energy state or availability of water for microbial, enzymatic, and chemical activity. It is the state of water—rather than its quantity—that determines the potential for microbial proliferation. Studies have shown that water activity is closely related to the vapor pressure of water in food. A higher proportion of free (unbound) water corresponds to a higher vapor pressure, while increased bound water leads to a reduction in vapor pressure [23].

Thermodynamically, the definition of water activity is based on the chemical potential of water in a food system, which, at equilibrium, must be equal to the chemical potential of water in the surrounding environment. Accordingly, water activity is defined as the ratio of the vapour pressure of water in food to the vapor pressure of pure water under the same temperature and pressure conditions [24]. This ratio provides valuable insight into how water interacts with food components and serves as a predictive tool for food stability, safety, and quality during storage. At equilibrium, the water activity is related to the relative humidity of the surrounding atmosphere which as shown in Equation 2.1.

$$a_w = \frac{P}{P_o} = \frac{ERH}{100} \quad (1)$$

where P is Vapor pressure of water in food material at any given temperature; P_o is vapor pressure of pure water at that temperature and ERH is Equilibrium relative humidity.

Due to its direct impact on product stability and quality, water activity is considered one of the most significant intrinsic variables used to forecast the growth of microorganisms in food [25].

1.2. Equilibrium Moisture Content (EMC)

Every food material exerts a characteristic vapour pressure at a given temperature and moisture content. When porous food substances come into contact with moist air, they tend to either adsorb or desorb water molecules until an equilibrium moisture content (EMC) is achieved. This EMC is a critical parameter that reflects the balance between the moisture content of the food and the surrounding environment. It depends primarily on the partial pressure of water vapour in the air and, to a lesser extent, on the ambient air temperature typically encountered during food drying and storage operations [23,26].

At equilibrium, the moisture content of a food product remains constant over time for a specific combination of temperature and water vapor pressure. In this state, the food is said to have reached its equilibrium moisture content. This condition signifies that there is no net exchange of moisture between the food and its environment. The attainment of EMC is the natural conclusion of any adsorption or desorption process, although it can be a slow process. Depending on the nature of the food material, equilibrium may take several days or even weeks to be fully realized [27].

Understanding EMC is crucial in the modeling of sorption isotherms and in designing drying and storage systems for food products. The slow approach to equilibrium underscores the importance of controlling environmental factors such as relative humidity and temperature to accelerate drying or avoid undesired moisture uptake during storage. In industrial applications, achieving EMC efficiently ensures the preservation of product quality, safety, and shelf life [28,29].

1.3. Moisture Sorption Isotherms

At equilibrium, the relationship between water content and equilibrium relative humidity of a material can be displayed graphically by a curve as shown in Figure 2.1 which is called the moisture sorption isotherm [30].

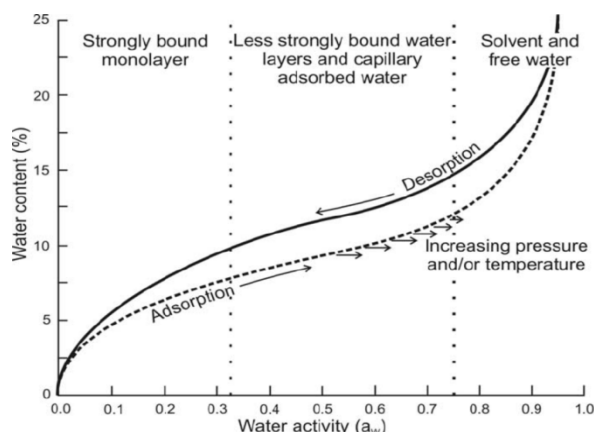


Figure 1. A schematic representation of a sorption isotherm with a hysteresis between the adsorption and desorption isotherms. [31]

The moisture sorption isotherms show the equilibrium amount of water sorbed onto a solid as a function of steady state vapour pressure at a constant temperature [32]. There are many empirical equations that attempt to describe this behaviour, but the water sorption properties at various relative humidities should be experimentally

determined for each material. The general shape of the isotherm, specific surface area of the sample, reversibility of moisture uptake, presence and shape of a hysteresis loop provide information on the manner of interaction of the solid with water [33]. Knowledge of water sorption properties is important in predicting the physical state of materials at various conditions, because most structural transformations and phase transitions are significantly affected by water [21].

A lot of models for moisture sorption isotherms can be found in the literature [34,35]. Langmuir originally developed an equation based on the theory that gas molecules are adsorbed on the active sites of a solid to form a monolayer [36]. The Brunauer–Emmett–Teller (BET) sorption model is widely used for modeling water sorption in food and pharmaceutical materials, particularly to determine the monolayer moisture content [37]. The monolayer value represents the amount of water sufficient to form a single molecular layer on the adsorbing surface and is considered optimal for stability in low-moisture foods [38]. The BET model is based on the assumption that sorption occurs in two thermodynamic states: a tightly bound monolayer and multilayers resembling bulk water [39].

Generally, food materials stored at varying relative humidity will either adsorb or desorb moisture depending on their water activity [40]. The resulting isotherm can follow either an adsorption or desorption curve. These processes are not fully reversible, making it essential to distinguish between isotherms based on whether the product is gaining or losing moisture [37,41]. originally classified five types of isotherms (as shown in Figure 2): Type I (Langmuir-type), typical for monomolecular adsorption on porous solids; Type II, a sigmoid curve common in most food products; Type III, associated with crystalline substances; Type IV, for swelling hydrophilic solids; and Type V, for multilayer adsorption such as water on charcoal [40]. Most food products typically exhibit Type II sigmoid isotherms [42].

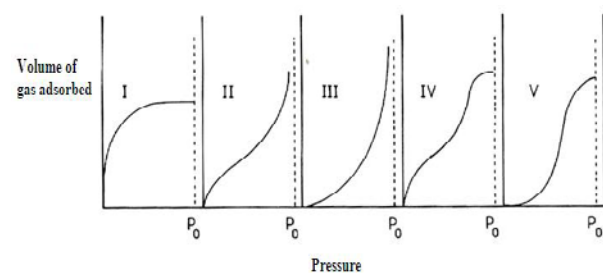


Figure 2. Types of adsorption isotherm according to Brunauer classification [41]

2. Importance of Sorption Isotherm

Water sorption isotherms illustrate the equilibrium amount of water held by food solids as a function of water activity at a constant temperature [37]. Moisture sorption isotherms are an essential tool for food scientists, as they enable prediction of chemical and physical stability, assist in ingredient selection to adjust aw for enhanced shelf life, and allow estimation of moisture gain or loss in packaging systems with known water vapor permeability [35,42]. Sorption isotherms are also critical in storage, drying, and

preservation by dehydration, particularly in predicting the shelf life of dried foods or estimating drying time during processing [43].

The monolayer moisture content of a food product is a useful indicator of the amount of strongly bound water to specific polar sites in a dehydrated food matrix. At this moisture level, the product generally exhibits stability against microbial spoilage and quality degradation [37,38]. This information is vital in mixing operations, product formulation, and determination of sorption enthalpy at different temperatures, establishing limits for textural properties like crispness and hardness, and optimizing moisture content to maintain product quality without over-drying. It also facilitates rapid moisture content estimation from water activity through isotherm curves [35].

2.1. Measurement of Sorption Isotherms

Water sorption isotherms can be determined using gravimetric, manometric, or hygrometric methods [37,42]. The gravimetric method tracks weight changes in food samples and may use continuous systems like electro-balances or discontinuous setups with saturated salt solutions [35,37]. The manometric approach measures water vapor pressure changes in the vapor space using a manometer, often with oil for improved accuracy [36]. The hygrometric method assesses equilibrium relative humidity using dew-point or electric hygrometers [42]. Among these, the standardized static gravimetric method from the European COST90 project is widely adopted for its precision and reliability in detecting weight changes under controlled conditions [43]. The advantages of the COST90 static gravimetric method include:

- Determining the exact dry weight of the sample;
- Minimizing temperature fluctuations between samples and their environment;
- Accurately registering weight change at equilibrium and
- Achieving both hygroscopic and thermal equilibrium between the sample and water vapour source.

2.2. Classification of Sorption Models for the Development of Sorption Isotherms

Over the past four decades, sorption isotherm models have evolved significantly and can be broadly classified into six categories: empirical, semi-empirical, theoretical, statistical physics-based, hybrid, and machine learning-based models [37,44].

3. Empirical Models

These primarily serve as mathematical fits to experimental data, without explicitly incorporating the underlying physicochemical mechanisms of sorption. Classic examples include the Henderson, Oswin, and Smith models, widely used due to their simplicity and ease of parameter estimation [37,45]. These models perform well within limited moisture ranges and specific food types such as grains and cereals but often lack predictive robustness when extrapolated beyond tested

conditions [46]. Their strengths, weaknesses, applications and equations are as shown in Table 1 and 2.

Table 1. Empirical models and their characteristics

Strength	Weakness	Applications
Simple functional forms. Require few parameters, easily obtained from experimental data. Useful for quick assessments and comparative studies.	Lack mechanistic basis; purely descriptive. Limited applicability outside tested moisture or temperature ranges. Poor accuracy for heterogeneous or complex food matrices.	They are widely used for staple grains (e.g., wheat, maize), legumes, and dried fruits where data sets are limited or for routine industrial moisture estimation [45].

Table 2. Empirical models and their equations

Models	Equations	References
Henderson	$M = \left[\frac{\ln(1 - a_w)}{-A} \right]^{1/B}$	[47]
Oswin	$M = A \left[\frac{a_w}{1 - a_w} \right]^B$	[48]
Smith	$M = A + B \log(1 - a_w)$	[49]
Freundlich	$M_w = K(a_w)^{1/n}$	[50]
Kuhn	$M = B + \frac{A}{\ln(a_w)}$	[51]
Iglesias-Chinife	$\ln \left[M_w + (M_w^2 + M_{w,0.5})^2 \right] = C_1 a_w + C_2$	[52]
Double Log Polynomial (DLP)	$M = A \ln(a_w) + B \ln(a_w)^2 + C$	[51]
Modified Halsey	$M_w = \left(-\frac{C}{\ln a_w} \right)^{1/n}$	[47]
Peleg	$M_w = C_1 a_w^{C_2} + C_2 a_w^{C_3}$	[53]
White and Eirring	$M = \frac{1}{A - B a_w}$	[54]

Where M is moisture content; a_w is the water activity; T is Temperature; A, B and C are empirical constants.

3.1. Semi-empirical Models

These models integrate empirical fitting with theoretical assumptions about multilayer adsorption, offering improved accuracy and physical interpretability. The Guggenheim–Anderson–de Boer (GAB) model is a prime example, extensively validated for foods ranging from dehydrated vegetables to powdered dairy [37]. Other notable semi-empirical models include BET, Chung–Pfof, and Modified Oswin, which incorporate monolayer moisture content concepts or modified empirical parameters [55]. The strengths, weaknesses, applications and equations of semi-empirical models are as shown in Table 3 and 4.

Table 3. Semi-Empirical Models and their characteristics

Strength	Weakness	Applications
Balanced complexity and accuracy. Can describe multilayer adsorption and provide meaningful parameters (e.g., monolayer moisture). Widely accepted by food scientists and engineers.	Parameters may vary with temperature, food composition, and measurement technique. Moderate complexity can hinder practical use in some cases. May not capture adsorption on highly heterogeneous surfaces accurately.	GAB and related models are preferred for fruits, vegetables, dairy powders, and bakery products due to their ability to represent realistic moisture sorption behavior over a broad moisture activity range [55, 56]

Table 4. Semi-empirical models and their equations

Model	Equation	References
GAB	$M = \frac{M_o G K a_w}{(1 - K a_w) (1 - K a_w + G K a_w)}$	[57]
BET	$\frac{M}{M_o} = \frac{C a_w}{(1 - a_w) (1 - a_w + C a_w)}$	[41]
Modified BET	$\frac{M}{M_o + T} = \frac{(1 - a_w) (1 - a_w + C a_w)}{C a_w}$	[58]
Chung-Pfost	$a_w = \exp \left(-\frac{A}{T + C} \exp(-B \cdot M) \right)$	[59]
Modified Oswin	$M = (a_3 + b_3 T) \left(\frac{a_w}{1 - a_w} \right)^{c_3}$	[48]
Halsey	$a_w = \exp \left(-\frac{A}{RT \theta^r} \right)$	[59]
Caurie	$\frac{1}{M} = \frac{1}{M_o} + K \ln \frac{1}{a_w}$	[60]
Adam and Shove	$\ln(a_w) = A - \frac{B}{T + CM}$	[61]
Chen-Clayton	$a_w = \exp[-k_1 T^{m_1} \exp(-k_2 T^{m_2} M)]$	[62]
Ferro-Fontan	$\ln(a_w) = \alpha M - R \ln T - \gamma$	[45]

Where M_o is the monolayer moisture content; T is Temperature in Kelvin; K, α , γ , m_1 and m_2 are empirical constants; R is universal gas constant; Where $\theta = \frac{M}{M_o}$.

Table 5. Theoretical models and their characteristics

Strengths	Weaknesses	Applications
Strong mechanistic foundation. Provide physical insight into sorption processes (e.g., binding energy, surface heterogeneity). Useful for designing tailored adsorbents and functional foods.	Require detailed parameter estimation, often needing extensive experimental or computational input. Complex mathematical formulations limit routine industrial application. May oversimplify real food surfaces due to assumptions of homogeneity.	Used in research involving novel food matrices, bioactive compound encapsulation, and adsorbent design, especially for heterogeneous foods such as spices, herbs, and functional powders [64].

Table 6. Equations of theoretical models

Model	Equations	References
Langmuir	$a_w \left(\frac{1}{M_w} - \frac{1}{M_o} \right) = \frac{1}{C M_o}$	[63]
Frenkel–Halsey–Hill (FHH) Model	$\ln(a_w) = -\frac{A}{M^n}$	[65]
Henderson–Thompson Model	$\ln(1 - a_w) = -a M^n$	[37]
Polanyi Theory (Potential Theory)	$M = f(A), \text{ where } A \text{ is adsorption potential}$	[66]
Statistical Thermodynamics (ST) Model	Complex forms are with M and energy distribution	[67]
Dubinin–Radushkevich (D–R) Model	$M = M_m \exp \left[-B \left(\ln(1 + \frac{1}{a_w}) \right)^2 \right]$	[68]
Multilayer Sorption Theory (MLST)	Model-dependent; formulated in M , a_w and T	[69]
Empirical–Thermodynamic Models	Generally, of the form $M = f(\mu, a_w, T)$	[70]
Kiselev Model	$\frac{1}{C_e(1 - \theta)} = \frac{K_i}{\theta} + \frac{K_i K_n}{\theta}$	[5]
Hill–de Boer Model	$\frac{K_1 C_e}{\theta(1 - \theta)} = \exp \left(-\frac{K_2 \theta}{RT} \right)$	[71]

Where θ is fractional surface coverage; C_e is equilibrium concentration (mg/L); K_i and K_2 , are equilibrium constant (L/mg); K_i and K_n constants are determined from experimental data.

Table 7. Statistical physics-based models and their characteristics

Strengths	Weaknesses	Applications
Capable of representing surface heterogeneity and energy distribution. Offer detailed mechanistic interpretation of sorption phenomena. Can model cooperative and competitive adsorption effects.	Computationally intensive and mathematically complex. Require advanced statistical or numerical methods for parameter estimation. Less accessible to routine food engineering practice.	Applied in advanced research on adsorption in heterogeneous food matrices such as nuts, dried fruits, and protein-rich foods where sorption behavior deviates from classical models [74].

Table 8. Statistical physics-based model equations

Models	Equations	References
One-Site Langmuir Model (Statistical Physics Interpretation)	$M = \frac{M_m C a_w}{1 + C a_w}$	[67]
Two-Site Langmuir Model	$M = \frac{M_1 C_1 a_w}{1 + C_1 a_w} + \frac{M_2 C_2 a_w}{1 + C_2 a_w}$	[75]
Multi-Layer Statistical Model	Model-dependent (often recursive or summation-based)	[76]
n-Layer Molecular Model	$M = \sum_{i=1}^n \frac{M_i C_i a_w}{1 + C_i a_w}$	[75]
Hill-de Boer Model	$\theta = \frac{K a_w e^{\alpha \theta}}{1 + K a_w e^{\alpha \theta}}$	[67]
Statistical Thermodynamic Energy Distribution Model	$M = \int_a^\infty M(\epsilon) f(\epsilon, a_w T) d\epsilon$	[67]
Guggenheim Statistical Thermodynamic Model	Advanced partition function forms	[77]
Zimm–Bragg Model (Cooperative Binding)	$M = \frac{M_m S a_w}{1 + S a_w + \sigma (S a_w)^2}$	[78]
Statistical Conformational Model	Equation varies with assumed conformers	[67]
Fermi–Dirac Adsorption Model	$M = \frac{M_m}{1 + \exp\left(\frac{E - \mu}{kT}\right)}$	[79]

Where α is interaction parameter; Energy distribution function $f(\epsilon)$; μ is chemical potential; E is energy level; s is binding constant; σ is cooperativity.

3.2. Theoretical Models

Rooted in fundamental thermodynamics and adsorption theories, theoretical models such as Langmuir, Polanyi potential theory, and their derivatives explicitly describe sorption based on molecular interactions and surface properties [44,63]. Langmuir's model, focusing on monolayer adsorption on homogeneous surfaces, laid the foundation for later multilayer models [37]. The strengths, weaknesses, applications and equations of theoretical models are shown in Table 5 and 6.

3.3. Statistical Physics-Based Models

Statistical physics models integrate microscopic molecular behavior and energetic heterogeneity to link sorption thermodynamics with observable isotherms [72]. These models emerged in the 1990s and have since been refined to describe multilayer adsorption and cooperative effects in complex food systems [73]. The characteristics, application and equations of the are shown in Table 7 and 8.

3.4. Hybrid Models

Hybrid models combine features of empirical, theoretical, and statistical approaches to optimize prediction accuracy and applicability. Since the 2010s, several hybrid models have been proposed, integrating GAB with statistical physics concepts or machine learning techniques to handle complex sorption phenomena and temperature dependence [80,81]. The characteristics, application and equations of the are shown in Table 9 and 10.

3.5. Machine Learning-Based Models

Machine learning (ML) approaches represent a paradigm shift by modeling sorption isotherms through pattern recognition and nonlinear function approximation

without explicit physical assumptions. Algorithms such as artificial neural networks (ANN), support vector machines (SVM), and random forests (RF) have demonstrated promising results in recent years [37,52]. The characteristics, application and equations of the are shown in Table 11 and 12.

3.6. Summary of the Recent Advances in Sorption Isotherm Modeling

Recent developments in sorption isotherm modeling have enhanced the understanding and prediction of moisture interactions in complex food systems. Traditional semi-empirical models such as GAB and BET have been refined to include temperature effects and surface heterogeneity, improving their applicability to diverse food products [55,56]. Theoretical models have advanced by incorporating multilayer adsorption and energy heterogeneity, providing better mechanistic insights [73].

Statistical physics-based models have gained traction for capturing molecular-level interactions and cooperative adsorption, particularly effective for heterogeneous foods like nuts and dried fruits. Hybrid models that combine empirical fits with mechanistic principles have improved prediction accuracy for processed and composite foods [45,81].

The integration of machine learning techniques, including neural networks and support vector machines, marks a transformative step by accurately modeling complex nonlinear sorption behaviors and incorporating multiple variables such as temperature and composition [44,52]. Physics-informed ML models further enhance robustness by embedding physical laws within data-driven frameworks [63].

These modeling advances, coupled with process simulation integration, enable optimized moisture control during food processing and storage, significantly

improving quality and shelf-life management [88]. modeling as a crucial tool in modern food engineering. Collectively, these innovations position sorption isotherm

Table 9. Hybrid models and their characteristics

Strengths	Weaknesses	Applications
Enhanced accuracy and robustness across varied conditions.	Increased model complexity may require extensive data and computational resources.	Successfully applied in modeling sorption isotherms of composite foods, processed snacks, and freeze-dried products where conventional models fail to capture complexity [45].
Flexibility to adapt to different food types and storage environments.	Difficult to interpret physically due to mixed origins.	
Can incorporate mechanistic understanding with data-driven refinement.	Model development and validation remain challenging.	

Table 10. Hybrid models Equations

Models	Equations	References
Redlich–Peterson (R–P)	$M = \frac{K_R a_w}{1 + \alpha a_w^\beta}$	[82]
Sips Isotherm (Langmuir–Freundlich Model)	$M = \frac{M_m (K a_w)^{\frac{1}{n}}}{1 + (K a_w)^{\frac{1}{n}}}$	[83]
Henry–Sips Combination Model	$M = \beta_{HS} K_H a_w + (1 - \beta_{HS}) \frac{M_m (K_S a_w)^{\frac{1}{r}}}{1 + (K_S a_w)^{\frac{1}{r}}}$	[84]
Tóth Model	$M = \frac{M_m K a_w}{[1 + (K a_w)^t]^{\frac{1}{t}}}$	[85]
Temkin	$M = \frac{RT}{b} \ln(K_T a_w)$	[85]
Klotz Isotherm	$M = \frac{M_m (K a_w)^n}{1 + (K a_w)^n}$	[86]
Dubinin–Radushkevich (D–R) Isotherm	$M = M_m \exp\left(\frac{\epsilon}{B} - B \epsilon^2\right)$ Where $\epsilon = RT \ln\left(1 + \frac{1}{a_w}\right)$	[87]
Halsey	$\ln(M) = \frac{1}{n} \ln(a_w) - \ln(K_H)$	[86]
Harkins–Jura	$\frac{1}{M^2} = \frac{B}{\log(a_w)} - A$	[86]
Langmuir–Freundlich–Jovanovic (LFJ) Model	$M = M_m \exp\left(\frac{1}{n} - K a_w\right) a_w^{\frac{1}{n}}$	[86]

Where M_m is maximum adsorption capacity; K : affinity constant; n is heterogeneity factor; K_H is Henry's constant; K_S is Sips constant; r is heterogeneity parameter; β_{HS} is weighting factor, M_m is maximum adsorption capacity; K is affinity constant; t is heterogeneity parameter, R is universal gas constant; T is temperature; b is Temkin constant related to heat of adsorption; K_T is equilibrium binding constant, M_m is maximum adsorption capacity; B is activity coefficient related to mean adsorption energy, K_H is Halsey constant; n is heterogeneity parameter, A , B are Harkins–Jura constants; K is Jovanovic constant; n is heterogeneity parameter.

Table 11. Machine learning-based models and their characteristics

Strengths	Weaknesses	Applications
High accuracy and adaptability to nonlinear, complex sorption behavior.	Require large, high-quality datasets for training and validation.	Increasingly used for modeling sorption in novel foods, functional ingredients, and complex food matrices such as multi-ingredient snacks, freeze-dried fruits, and bioactive-enriched [44, 88].
Can incorporate multiple variables including temperature, composition, and processing conditions.	Lack transparency and mechanistic interpretability (“black box” nature).	Emerging physics-informed ML approaches aim to blend mechanistic insight with data-driven power to improve robustness [89].
Automated parameter tuning and fast prediction once trained.	Risk of overfitting and reduced generalizability if not carefully managed.	

Table 12. Machine learning-based model equations

Models	Equations	References
Artificial Neural Networks (ANNs)	$y = f(Wx + B)$	[90]
Graph Neural Networks (GNNs)	$h_v^k = \sigma \left(\sum_{u \in \mathcal{N}(v)} W^{(k)} h_u^{(k-1)} + b^{(k)} \right)$	[91]
Support Vector Machines (SVMs)	$f(x) = \sum_{i=0}^n (\alpha_i - \alpha_i^*) K(x_i, x) + b$	[51]

Random Forest (RF)	$y^{\wedge} = \frac{1}{T} \sum_{t=0}^T h_{(t)}(x)$	[51, 92]
Radial Basis Function Neural Networks (RBF-NNs)	$y(x) = \sum_{i=1}^N w_i \phi(\ x - C_i\)$	[93]
Long Short-Term Memory (LSTM) Networks	The core equations involve input, forget, and output gates, and the cell state update	[94, 95]
Adaptive Neuro-Fuzzy Inference System (ANFIS)	ANFIS combines neural networks and fuzzy logic principles. It uses a set of fuzzy if-then rules with appropriate membership functions to generate the stipulated input-output pairs.	[96]
Extreme Gradient Boosting (XGBoost)	$y_i = \sum_{\substack{t=0 \\ f_{(k)} \in F}}^K f_{(k)}(x_i)$	[92]
Bayesian Additive Regression Trees (BART)	$y_i = \sum_{t=0}^m g(x; T_j, M_j) + \epsilon$	[97]
k-Nearest Neighbors (k-NN)	$y^{\wedge}(x) = \frac{1}{k} \sum_{i=1}^k y_i$	[92]

Where y is Output (e.g., predicted sorption capacity); x is Input vector; W is Weights matrix; B is Bias vector; f is Activation function (e.g., sigmoid, ReLU); h_v^k is Feature vector of node v at layer k ; $\mathcal{N}(v)$ are neighbors of node v ; $W^{(k)}, b^{(k)}$ are learnable weights and biases; σ is activation function; α_i, α_i^* are Lagrange multipliers; $K(x_i, x)$ is Kernel function (e.g., radial basis function); b is Bias term; α_i, α_i^* : Lagrange multipliers $K(x_i, x)$: Kernel function (e.g., radial basis function); T is number of trees; $h_t(x)$ is prediction from the t -th tree; w_i is Weight for the i -th neuron; ϕ is Radial basis function (commonly Gaussian); C_i : is center of the i -th neuron; F is the ppace of regression trees; $f_{(k)}$ is the individual regression tree; $g(x; T_j, M_j)$: A regression tree with structure T_j and terminal node parameters M_j ; ϵ is Error term; $y^{\wedge}(x)$ is the predicted value of moisture content or sorption capacity for input; x ; y_i are Output value of the i -th nearest neighbor; k is the number of neighbors. Distance is typically computed using Euclidean distance or other metrics depending on feature type and scaling.

4. Challenges in Sorption Model Selection and Fitting

Selecting appropriate sorption isotherm models for food systems is challenging due to the complexity of food matrices and modeling limitations. Food heterogeneity, with diverse components like proteins and carbohydrates, makes it difficult for a single model to represent all systems, often requiring hybrid approaches [81]. While empirical models like GAB and BET are easy to use, they lack mechanistic insight, whereas theoretical models offer deeper understanding but involve complex, data-intensive parameter estimation [55].

Parameter estimation is further complicated by experimental limitations and data variability, often leading to convergence on suboptimal solutions [45,56]. Most models assume isothermal conditions, but temperature significantly affects sorption, necessitating more sophisticated, often overfitted, models when data are limited [55]. Model selection tools like R^2 , RMSE, and AIC may favor complexity over physical accuracy, especially in the absence of external validation [52]. Machine learning models enhance predictive power but require large datasets and often lack interpretability,

posing challenges for engineering applications [11,44].

5. Future Trends in the use of Sorption Models for the Development of Isotherms

Future developments in sorption isotherm modeling will leverage physics-informed machine learning to combine mechanistic understanding with data-driven accuracy, improving predictions even with limited data [89]. Models will increasingly incorporate multi-scale and multi-component interactions, better reflecting the complexity of real food systems [74]. Integration of real-time sensor data will enable adaptive moisture control during processing and storage [88].

Additionally, the creation of extensive model libraries and digital twins will support predictive simulations for industrial applications [44]. Advances will also focus on sustainable, energy-efficient drying processes and expanding modeling capabilities to novel, plant-based food products [55,81]. These trends collectively promise enhanced model robustness, applicability, and process optimization in food engineering.

6. Recommendations for Use of Sorption Models in the Development of Isotherms

Effective sorption modeling in food systems requires selecting models that match the specific food type and processing conditions. While empirical models like GAB and BET suit traditional foods, complex or processed foods benefit from more advanced semi-empirical or physics-based models. Incorporating temperature effects and multi-component interactions improves accuracy, especially when supported by strong experimental data.

Machine learning and hybrid models offer predictive advantages but should be guided by physical principles and large datasets to ensure interpretability. Reliable parameter estimation and validation with independent data are essential to avoid over fitting.

Integrating real-time sensor data with digital tools like digital twins enables dynamic control and optimization of processes. Ultimately, sorption models should support sustainable practices by enhancing energy efficiency in drying and storage.

7. Conclusion

This review comprehensively examines sorption models developed for moisture isotherm characterization in food engineering. Empirical models offer practical simplicity, whereas theoretical, hybrid, and machine learning-based models provide enhanced mechanistic understanding and predictive accuracy. Key challenges persist in model selection, parameter fitting, and capturing multi-component, temperature-dependent sorption behaviours. Emerging trends such as physics-informed machine learning and integration of real-time data are expected to advance model robustness and applicability. Tailoring sorption models to specific food matrices and processing conditions will be critical for optimizing moisture control, process efficiency, and sustainability in food manufacturing.

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