Development of Software for Predicting the Thermophysical Properties of Foods Based on Their Composition Using the Choi–Okos Model.

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ABSTRACT:
The thermophysical properties of food vary with temperature and composition; therefore, estimating them is essential for modeling heating, cooling, refrigeration, and freezing processes. These elements enable this study, which aims to develop software to estimate the specific heat (C_p), density (rho), thermal conductivity (k), and thermal diffusivity (alpha) of food based on its proximate composition and temperature. This is achieved through the computational implementation of correlations based on the Choi-Okos model. The application was developed in Python using Flask and SQL Alchemy, with moisture, carbohydrates, proteins, fats, fiber, ash, and temperature as input variables. It accepts temperatures between -40 °C and 150 °C, restricting each component to the range of 0 to 100% and verifying that the total composition sums to 100% before running the calculations. The computational core calculates the individual properties of the main constituents as a function of temperature and automatically generates the food's thermophysical values. It also stores, displays, and exports the results. Functional testing confirmed the integrated operation of the recording, processing, query, and export modules. However, a mathematical review of the algorithm revealed the need to refine certain mixing rules and the handling of frozen water before establishing the model's final predictive accuracy. The developed software constitutes a functional computational platform for composition-based thermophysical estimation.

Keywords: thermophysical properties, Choi and Okos, food, computational modeling, scientific software.

1. Introduction

In the agri-food industry, it is essential to employ mathematical models that allow for the design and optimization of equipment used in freezers, evaporators, heat exchangers, sterilization systems, and heating or cooling units. This involves analyzing thermophysical properties representative of the actual process conditions, such as specific heat (Cp), density (ϱ), thermal conductivity (k), and thermal diffusivity (α), which directly influence energy balances and heat transfer models used to estimate heating rates, processing times, and temperature distribution in

food products (Datta et al., 2022; Erdogdu, 2023; Szpicer et al., 2023).

Therefore, having computer systems that allow for these calculations using variables such as temperature is currently indispensable, given that recent studies have confirmed significant variations in thermophysical properties between products with different compositions and during the transformations induced by processing. Högg and Rauh (2023), for example, characterized the thermophysical properties of high-moisture meat analogues and demonstrated the need to consider their composition and structure during thermal modeling. Al-Shemmeri et al. (2024) reported on changes in properties and porosity during the roasting of coffee beans, while Sheen et al. (2025) experimentally determined the differences in thermophysical properties between cured and uncured meat products. These results limit the indiscriminate use of constant values obtained from general tables.

The Chois and Okos model was designed for a wide temperature range, approximately -40 to 150 °C, allowing its application under different processing conditions. This means that the thermal property is not assigned solely based on the name or category of the food, but rather derived from quantifiable compositional variables. However, applying the compositional approach requires acknowledging its underlying assumptions: the proximate composition alone does not necessarily describe the spatial distribution of phases, porosity, air content, or structural modifications that occur during processing. These characteristics can alter energy transport. Studies by Högg and Rauh (2023) and Al-Shemmeri et al. (2024) demonstrate that the product's physical structure must be considered when interpreting calculated or measured thermophysical properties. This is especially relevant for products subjected to intense thermal transformations, where the structure can change simultaneously with the temperature.

The freezing regime introduces an additional challenge because when the temperature drops below the initial freezing point, some of the liquid water transforms into ice, and the matrix begins to behave as a multiphase system. The ice fraction directly modifies the product's heat capacity, thermal conductivity, density, and diffusivity. For this reason, the thermal description of frozen foods requires differentiating unfrozen water from the solid phase and establishing mixing rules compatible with the preservation of mass and volume. This mathematical treatment of these transitions is one of the aspects that must be carefully verified before extending a computational model to the entire proposed temperature range.

The availability of reliable properties also conditions the performance of numerical simulations. Datta et al. (2022) pointed out that computer-aided food engineering depends on models capable of adequately representing product properties and operating conditions. From an applied perspective, Szpicer et al. (2023) documented the use of computational fluid dynamics in various food processes, while Rivera et al. (2024a, 2024b) used computational tools to analyze the distribution of the thermal load and the non-uniformity of heating during sterilization processes. In these cases, the accuracy of the properties used directly influences the calculated temperature fields.

2. Methodology

This study has an applied methodology of quantitative approach to computational development which focused on the implementation and functional verification of the software to estimate temperature-dependent thermophysical properties (C_p, rho, k and alpha) from food compositions using the Choi-Okos framework with respect to the workflow it is carried out through four stages: implementation of the mathematical model, software development, functional verification and preliminary computational evaluation with respect to the database used. Information previously gathered in the territory in the subtropical zone of the Cotopaxi province and part of the cantons of the Los Rios province in Ecuador, including records of foods defined by mass fractions of water, carbohydrates, proteins, fats, fiber and ash in 11 food categories.

Regarding the software and the validation process, data integrity restrictions were established, processing only inputs with complete profiles of six components that add up to exactly 100% and operating temperatures between -40 °C and 150 °C. For the development of the system, the Python programming language was used using Flask and SQLAlchemy. The data incorporate constituent polynomial correlations, including distinct ice phase coefficients for sub-zero conditions, to calculate Cp, rho, k and alpha. The complementary libraries (Pandas and OpenPyXL) handle the structuring of tabular data and the export of multiple sheets to Excel, while the integrated modules provide real-time input validation, visualization of approximate composition, database querying, and auditing of intermediate calculations to ensure numerical traceability with respect to experimental literature before empirical validation.

2.1 Procedure

Stage 1. Definition of input and output variables.

The input structure was defined using temperature and six food composition variables such as water, carbohydrates, protein, fat, fiber, and ash. These percentage values were internally converted into mass fractions using the following equation, $Xi = \frac{\text{Pi}}{100}$, where Pi represents the percentage of component i, and Xi its corresponding mass fraction.

Stage 2. Implementation of compositional constraints.

Before performing any calculations, the software verified that each composition variable was within the 0–100% range. This data and its total composition were calculated and accepted only when, $\sum_{i=1}^{n} Pi = 100\%$, with a computational tolerance of 0.01 percentage points. Temperature values were restricted to: $-40 \leq T \leq 150$ °C. These checks were implemented both during the creation of new food records and during their editing.

Stage 3. Calculation of component thermophysical properties.

For each food constituent, temperature-dependent polynomial expressions were implemented for specific heat capacity, density, thermal conductivity, and thermal diffusivity. The generic equations were expressed as:

- $Cp,I = ai + bi + ciT^2 + diT^3$
- $Pi = ai + biT + ciT^2$
- $ki = ai + biT + ciT^2$
- $\alpha i = ai + biT + ciT^2$

where the coefficients a_i, b_i, c_i, and d_i depend on the food component.

For temperatures of 0 °C or higher, the current software implementation calculates the contribution of each component and stores intermediate values for subsequent review.

Stage 4. Processing at Sub-Zero Temperatures

For temperatures below 0 °C, the software activates a separate calculation branch that estimates the parameters related to the water-ice transition and subsequently calculates the thermophysical contribution of liquid water, ice, and the other food components.

Stage 5. Storing and Visualizing Results

The calculated values of Cp, ϱ, k, and α were stored in the food log, allowing the system to generate detailed tables with the contribution of each component and produce a graphical representation of the proximate composition.

Stage 6. Data Export

The software generated Excel workbooks containing the input variables, the calculated thermophysical properties, the intermediate calculation tables, and the summary results. This data is presented separately for specific heat, thermal conductivity, thermal diffusivity, and the final summary of properties.

Stage 7. Functional Verification

The application was tested with food samples of varying compositions and temperatures to verify input control, numerical execution, database storage, results display, and data export**.**

2.5. Data Analysis

Data analysis was conducted using descriptive and computational verification procedures. These procedures began with checking the consistency of input data, confirming the 100% mass balance condition, verifying temperature constraints, examining the calculations for intermediate components, and comparing the output behavior in food products with different compositions. These results were organized into structured tables to examine their variation with temperature and composition.. Therefore, the model's performance is expected to be quantified using the mean absolute error (MAE). $MAE = \frac{1}{n}\sum_{i=1}^{n}(yi - \hat{y}i)$, the root mean square error (RMSE), $RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(yi - \hat{y}i)}$, the mean absolute percentage error (MAPE), $MAPE = \frac{100}{n}\sum_{i=1}^{n}\left(\frac{yi-\hat{y}i}{yi}\right)$ and the coefficient of determination (R^2). Predicted-versus-reference plots and residual analysis will also be used to identify systematic deviations associated with temperature, food composition, or product category.

3. Results

The developed software completed the full computational workflow for food registration, composition validation, thermophysical-property calculation, database storage, graphical visualization, and Excel export. The application accepted temperature values within the interval from (-40) to (150°C), restricted each compositional variable to 0–100%, and rejected records whose total proximate composition differed from 100% by more than 0.01 percentage points.

The computational model processed six food constituents: water, carbohydrates, proteins, fat, ash, and fiber. Temperature-dependent coefficients were implemented for specific heat capacity, density, thermal conductivity, and thermal diffusivity. A separate set of equations was included for ice under subzero-temperature conditions.

3.1. Functional Results of the Software

Table 1. Functional modules implemented in the thermophysical-property prediction software

Módulo / Función	Descripción
Food registration	Stores code, name, category, temperature, and proximate composition.
Input validation	Checks temperature range, individual percentages, and total composition.
Thermophysical calculation	Calculates C_p, rho, k, and alpha.
Database management	Stores and retrieves food records and calculated properties.
Search and filtering	Filters products by name, code, category, and temperature condition.
Composition visualization	Generates a graphical representation of proximate composition.
Individual export	Exports detailed calculation tables to Excel.
Complete export	Generates consolidated thermophysical calculation files.

The database model stores the four calculated properties alongside the six composition variables and the temperature. For temperatures below 0°C, additional variables related to water and ice fractions are also stored.

3.2. Reproducible computational test

A calculation test was performed at 14°C using a composition of 76.0% water, 12.0% carbohydrates, 11.0% protein, 0.2% fat, 0.6% ash, and 0.2% fiber. The total composition was 100%.

Table 2. Proximate composition used in the computational test

Component	Composition (%)	Mass fraction
Water	76.0	0.760
Carbohydrates	12.0	0.120
Protein	11.0	0.110
Fat	0.2	0.002
Ash	0.6	0.006
Fiber	0.2	0.002
Total	**100.0**	**1.000**

Using the equations currently implemented in models.py, the software generated the thermophysical values presented in Table 3.

Table 3. Thermophysical properties generated by the current computational model at 14 °C.

Property	Calculated value	Unit
Specific heat capacity, (C_p)	3.599968	kJ/(kg·K)
Density, (\rho)	1113.163511	kg/m³
Thermal conductivity, (k)	0.502401	W/(m·K)
Thermal diffusivity, (\alpha)	(1.27167\times10^{-7})	m²/s

These values were obtained directly from the weighted calculations implemented in the current software version, where the contribution of each constituent is accumulated during the thermophysical calculation routine. The corresponding component-specific calculations are shown in Table 4.

Table 4. Component thermophysical properties calculated at (14°C)

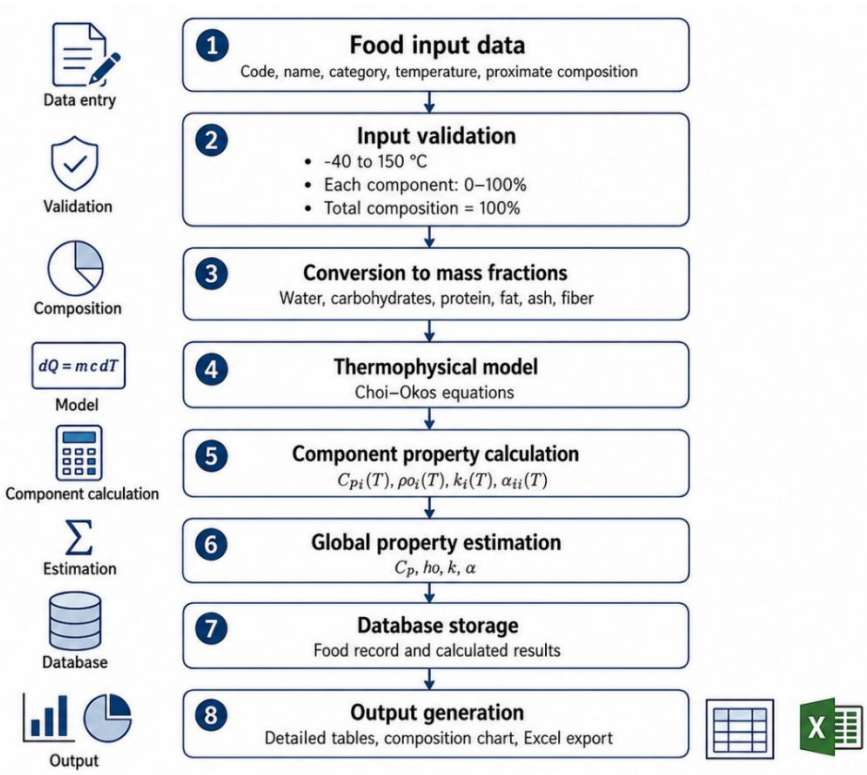
Component	(C_{p,i}) kJ/(kg·K)	(\rho_i) kg/m³	(k_i) W/(m·K)	(\alpha_i) m²/s
Water	4.176001	996.4876	0.594444	(1.39956\times10^{-7})
Carbohydrates	1.575111	1594.7536	0.219975	(9.50137\times10^{-8})
Protein	2.024867	1322.6460	0.195009	(7.50879\times10^{-8})
Fat	2.003885	919.7440	0.141707	(9.97863\times10^{-8})
Ash	1.118333	2419.8712	0.348644	(1.29595\times10^{-7})
Fiber	1.870617	1306.3775	0.200185	(8.08071\times10^{-8})

The software also generated intermediate calculation tables for specific heat, thermal conductivity, and thermal diffusivity, which can be exported individually for each food record.

3.3. Data Visualization and Export

For each registered food product, the application generated a bar chart representing the percentage contribution of water, carbohydrates, proteins, fats, ash, and fiber, allowing the total composition and calculation temperature to be displayed. These results can be exported in spreadsheet format, including food identification, temperature, composition, (C_p), (k), (rho), and (alpha) separated for specific heat, thermal conductivity, thermal diffusivity, and a final summary of the properties.

Figure 1. Computational workflow for thermophysical-property calculation and result export.



The current results correspond to the functional and numerical output of the implemented software. Experimental accuracy metrics were not calculated at this stage because an independent reference dataset has not yet been incorporated.

4. Discussion

The results obtained in this development stage confirm that the proposed computational architecture can integrate food composition, temperature control, thermophysical property calculations, structured storage, graphical visualization, and export to spreadsheets in a single workflow. This result addresses the main objective of the study: to develop a software tool capable of estimating Cp, ϱ, k, and α from proximate composition and temperature, using correlations based on the Choi-Okos method. This creates an opportunity in the field of education, particularly in areas such as the agro-industry, where these calculations can be performed more efficiently and quickly. Regarding system validations, we can see that they allow for the control of values specifically within the 100% range of a food's composition, reducing a common source of numerical inconsistency when thermophysical calculations are performed manually or using separate spreadsheets.

As a reference, we took random data from a food sample and evaluated it at a temperature of 14 °C in a reference matrix (76.0% water, 12.0% carbohydrates, 11.0% protein, 0.2% fat, 0.6% ash, and 0.2% fiber). This yielded C_p = 3.599968 kJ/(kg*K), rho = 1113.163511 kg/m^3, k = 0.502401 W(m.K), and alpha = 1.27167 × 10^{-7} m^2/s. These results confirm the correct algorithmic execution of the temperature-dependent component polynomials. By leveraging the Choi-Okos framework, the platform avoids the rigidity of static property tables at the category level, capturing subtle thermal variations induced by different moisture or lipid fractions within similar foods. Regarding food composition, we can determine that the moisture fraction predominates at 76%, exerting primary control over effective heat capacity and overall thermal conductivity. This demonstrates that small variations in water content drastically alter thermal energy requirements.

Methodologically, the system architecture retains intermediate component-level evaluations before data export, establishing an auditable computational record that simplifies error tracking in multi-step mixing rules. Operationally, the application standardizes workflow execution, enforces mass balance input constraints, and accelerates the generation of parameters for thermal process engineering, academic modeling, and heat transfer simulations.

5. Conclusion

- The developed software provides a functional computational environment for estimating the thermophysical properties of food based on its approximate composition, such as water, carbohydrates, proteins, fats, fiber, ash, and temperature. It also includes the automated calculation of specific heat capacity (C_p), density (ϱ), thermal conductivity (k), and thermal diffusivity (α), generating a functional alternative for calculations in areas related to agribusiness, education, and production. This saves calculation time, reduces errors, and improves decision-making.
- Regarding the computational architecture, the system supports database storage, inspection of intermediate calculations, graphical representation of approximate composition, and structured export of results. This allows for traceability between input data, component-level calculations, and final thermophysical results, which is relevant for repeated evaluations involving multiple food formulations or temperature conditions.
- The development process identified limitations in the mathematical treatment of density, thermal conductivity, thermal diffusivity, and the frozen food regime. The current code combines mass-weighted formulations with intermediate volumetric calculations, and the sub-zero temperature module requires further verification of the liquid water and ice fractions before its results can be considered highly validated. Therefore, a review of all mixing rules and temperature-dependent coefficients against the primary Choi-Okos references should be prioritized, followed by a reformulation of the phase change calculations to maintain consistency in mass and volume.
- Regarding food composition, we can determine that the moisture fraction predominates at 76%, exerting fundamental control over the effective heat capacity and overall thermal conductivity. This demonstrates that small variations in water content alter the thermal energy requirements.

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Author Declaration

- Originality Statement. The authors declare that this manuscript presents original work resulting from the development and functional assessment of the computational software described in this study. The manuscript has not been previously published and is not under simultaneous consideration by another journal. All external concepts, mathematical models, and scientific sources incorporated into the study have been appropriately cited.
- Conflict of Interest Statement. The authors declare that they have no financial, commercial, institutional, or personal conflicts of interest that could have influenced the design, development, analysis, interpretation, or reporting of the study.