IRSTI 53.37 https://doi.org/10.26577/jpcsit20253310

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INFORMATION SYSTEM FOR METALLURGICAL PROCESS ANALYSIS AND OPTIMIZATION

Abstract. The metallurgical industry faces increasing challenges in reconciling production efficiency with environmental compliance while managing heterogeneous data streams across complex processing operations. Traditional approaches to metallurgical process analysis rely on manual calculations and isolated software tools, limiting operational efficiency and introducing potential errors in critical decision-making processes. This paper presents the design and implementation of a comprehensive web-based information system specifically developed for integrated metallurgical process analysis and optimization. The system architecture employs a modular design incorporating three specialized computational modules: pyrometallurgical calculations for ore-to-metal conversions, hydrometallurgical process modeling for extraction operations, and auxiliary process calculators for specialized applications. The platform integrates Django-based backend processing with responsive frontend interfaces, supporting multi-user access, comprehensive data validation, and seamless integration with existing plant information systems. Implementation includes predictive analytics capabilities utilizing machine learning algorithms for forward process prediction and optimization. System validation demonstrates robust performance with processing times ranging from 0.6 to 3.4 seconds across different computational modules and operational success rates exceeding 98.7% for all core functions. The platform supports multiple data input formats including manual entry and Excel file processing, with comprehensive export capabilities (JSON, CSV, Excel) enabling integration with downstream analysis tools. Performance evaluation indicates the system successfully addresses key industrial requirements for accuracy, reliability, and scalability in metallurgical process analysis applications. The developed architecture provides a practical framework for implementing digital transformation initiatives in metallurgical operations while maintaining computational precision required for critical industrial applications.

Keywords: web-based information system, metallurgical process analysis, pyrometallurgy, hydrometallurgy, computational modules, machine learning integration, digital transformation.

1. Introduction

Metals underpin the energy, mobility, and infrastructure transitions, yet primary production from complex ores faces volatile feed quality, rising energy intensity, tightening environmental limits, and stringent traceability demands. In copper and allied non-ferrous value chains, plant operators must reconcile conflicting objectives, throughput, recovery, reagent and energy consumption, emissions, and waste valorization, amid sparse, noisy, and multi-rate data streams from mining, comminution, flotation, leaching, smelting, and refining. At the same time, life-cycle studies highlight the concentration of environmental burdens in tailings, slag handling, and energy vectors, underscoring the need for decision support that couples metallurgical performance with data quality and governance considerations [1, 2].

This paper presents a web-based information system for the metal-ore industry that integrates laboratory and historical operational data with established metallurgical calculations and data-driven predictive models to support offline analysis and decision-making. The platform provides three specialized computational modules, pyrometallurgical calculations for ore-to-product conversions, hydrometallurgical process modeling for extraction operations, and auxiliary calculators for specialized tasks, together with multi-user access, input validation, spreadsheet import/export, and results management. Predictive analytics are realized via supervised machine-learning models for forward estimation of process outcomes, enabling users to explore “what-if” scenarios prior to operational changes.

Recent surveys frame digital twins for process industries as bi-directionally updated models that increasingly combine mechanistic and data-driven components for monitoring, soft sensing, and optimization [3]. Mining-sector reviews outline architectures from mine-to-mill telemetry ingestion to multi-layer stacks for planning and operations, reporting productivity and energy benefits while noting gaps in data governance and model upkeep [4-6]. In chemical and process systems engineering, integrated digital-twin frameworks emphasize model management, online identification, and uncertainty handling [7]; in non-ferrous metallurgy, “smart manufacturing” perspectives stress model-based optimization and intelligent control across pyro- and hydrometallurgy [8]. Complementary reviews on hybrid (physics + ML) modeling in manufacturing and process engineering find that combining balances/kinetics with learning components improves extrapolation and sample efficiency compared to purely empirical approaches [9]. In extractive metallurgy specifically, studies report LSTM-augmented kinetics for leaching and metamodel-based surrogates for rapid updates, as well as domain-informed learning for high-temperature reactors [7, 10, 11]. Minerals-engineering surveys also catalogue both practical gains and pitfalls of ML across comminution, flotation, and heaps, calling for sensor strategy, feature engineering, and MLOps to mitigate drift and ensure maintainability [12, 13].

In geometallurgy and plant-level forecasting, data-driven models link upstream mineralogical and texture features to downstream responses for planning and control; case studies show unsupervised/supervised learning for domain delineation and throughput prediction, facilitating mine-to-mill integration [14, 15]. For hydrometallurgical circuits, recurrent and attention-based deep networks have been used to forecast outputs that inform tactical decisions on reagent dosing, aeration, and residence-time management [16]. While these strands increasingly inform digital-transformation roadmaps, many deployed tools in industry remain batch-mode and analytics-centric, prioritizing robust data handling, validation, and transparent computation over continuous plant-wide synchronization. Our work aligns with this pragmatic trajectory: it draws on the above literature to inform design choices, while explicitly targeting an offline, web-based platform for metallurgical analysis and forward prediction rather than a continuously synchronized, plant-integrated digital twin [3-9].

Environmental motivation further supports integrated information systems. Life-cycle and hotspot assessments for copper production identify tailings and energy use as major contributors to impacts [1, 2] and reviews on copper-slag management highlight both environmental risks and valorization opportunities [17, 18]. Although the present system focuses on production-oriented calculations and forecasting, the architecture and data structures are designed to accommodate sustainability indicators in future extensions using the methodologies surveyed in these studies.

This paper contributes: (i) a modular, web-based architecture unifying pyrometallurgical, hydrometallurgical, and auxiliary computational modules with governed data handling (validation, spreadsheet import/export, role-based access); (ii) ML-based forward prediction integrated into the workflow for scenario analysis; and (iii) a performance assessment showing sub-second-to-few-second processing times and high operational success rates across core functions. In this paper, operational success rate is the percentage of user-initiated runs with valid inputs that finish without errors within the service level agreement and produce outputs that pass schema and domain (e.g., mass-balance) checks. The system is positioned as a deployable foundation upon which telemetry connectors, hybrid physics-ML models with uncertainty, and sustainability KPIs can be incrementally integrated in subsequent work, consistent with directions identified in the literature.

2. Materials and methods

The development of an integrated information system for metallurgical process analysis required a comprehensive approach encompassing system architecture design, computational module implementation, data management strategies, and user interface development. This section describes the methodological framework and technical implementation of the web-based platform designed to address the complex requirements of metal-ore processing operations.

The system architecture follows a modular approach, enabling scalable integration of specialized computational modules while maintaining flexibility for future enhancements. The implementation leverages modern web technologies and database management systems to ensure reliable data processing and user accessibility across different operational contexts.

2.1 System Architecture and Design Framework

The information system was designed using a layered architecture approach that separates presentation logic, business processing, and data management concerns. This architectural pattern ensures maintainability, scalability, and clear separation of responsibilities across system components. The overall system structure consists of three primary layers: the frontend presentation layer responsible for user interactions, the backend processing layer handling business logic and computational operations, and the data persistence layer managing information storage and retrieval. The overall system workflow is summarized in Figure 1.

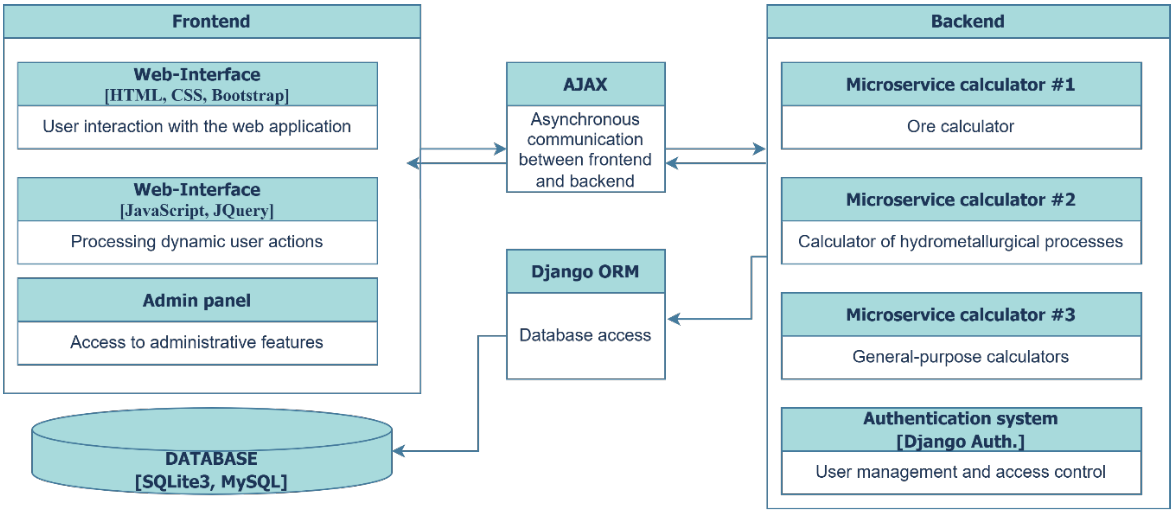


Figure 1 – Overall system architecture showing the three-tier design with frontend interface, backend processing modules, and database layer, including data flow patterns and component interactions.

The backend framework utilizes Django, a Python-based web framework chosen for its robust Object-Relational Mapping (ORM) capabilities, built-in security features, and extensive library ecosystem suitable for scientific computing applications. The frontend implementation combines HTML5, CSS3 with Bootstrap framework, and JavaScript with jQuery library to provide responsive user interfaces and asynchronous communication capabilities through AJAX technology. Table 1 summarizes the technology choices across the three layers.

Table 1 – Core system components and their corresponding technologies, showing the technical stack implementation across different system layers.

Component	Technology	Primary Function	Integration Method
Frontend Interface	HTML5/CSS3/Bootstrap	User interaction and presentation	Template rendering
Dynamic Processing	JavaScript/jQuery/AJAX	Real-time user interactions	Asynchronous requests
Backend Framework	Django (Python 3.8+)	Business logic and API services	MVC architecture
Database Management	SQLite3/MySQL	Data persistence and retrieval	Django ORM
Authentication System	Django Auth	User management and access control	Session-based authentication
File Processing	Pandas/Openpyxl	Excel/CSV data import	Background processing
Mathematical Computing	NumPy/SciPy	Numerical calculations	Library integration
Machine Learning	Scikit-learn	Predictive analytics	Model serialization

The system employs a microservices-oriented approach for computational modules, where each specialized calculator operates as an independent processing unit while maintaining standardized interfaces for data exchange. This design pattern facilitates independent development, testing, and maintenance of individual processing components while enabling seamless integration within the overall system architecture.

2.2 Computational Module Implementation

The system incorporates three specialized computational modules, each addressing specific metallurgical process domains. The modular organization of the calculators is illustrated in Figure 2. The computational modules implement established metallurgical calculation methods based on fundamental thermodynamic and kinetic principles widely reported in the metallurgical literature [19, 20].This section focuses on the architectural implementation and integration strategies rather than the underlying mathematical formulations.

Pyrometallurgy Processing Module

The pyrometallurgy module handles material balance calculations for high-temperature metallurgical processes, specifically focusing on the conversion of complex ores into matte and slag products. The module accepts ore composition data including elemental concentrations (Cu, Fe, S, Au, Ag, SiO_2, CaO, Al_2O_3, As) and total mass, then applies thermodynamic and material balance principles to predict product compositions and distributions.

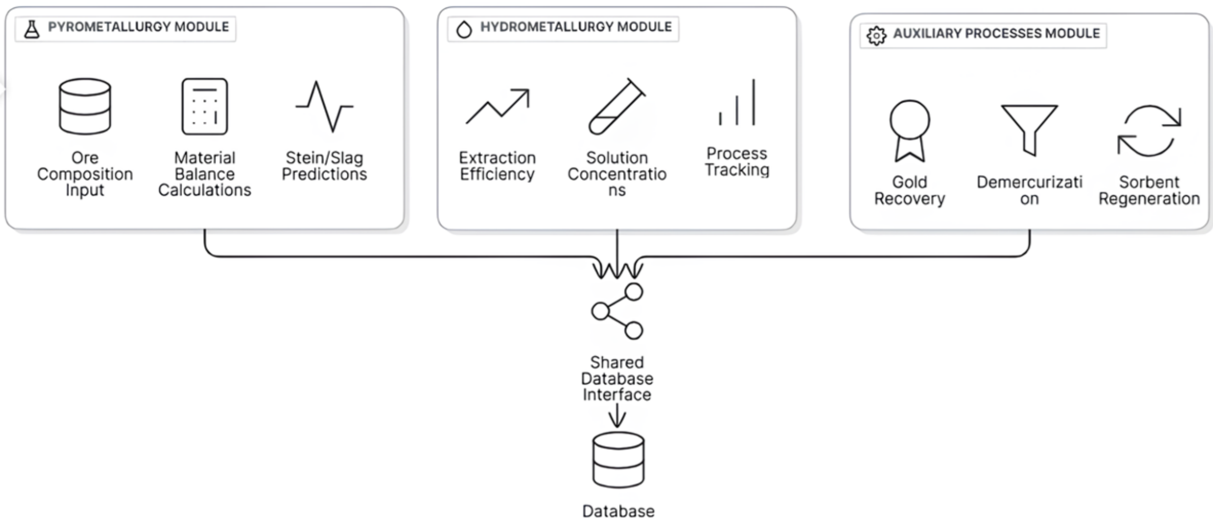


Figure 2 – Computational module structure illustrating the three specialized processing units: pyrometallurgy module for ore-to-metal calculations, hydrometallurgy module for extraction processes, and auxiliary processes module for specialized operations.

Implementation utilizes object-oriented programming principles with dedicated classes for compound representation and calculation engines. The module supports both individual ore processing and batch calculations for multiple ore samples, enabling plant operators to evaluate different feedstock scenarios and optimize blending strategies.

Hydrometallurgy Processing Module

The hydrometallurgy module addresses aqueous processing routes, encompassing leaching, solvent extraction, and electrowinning operations. This module handles multi-stage process calculations including extraction efficiency determination, mass balance tracking across process units, and cumulative recovery calculations over extended operational periods.

The module architecture supports day-by-day process tracking, enabling analysis of operational trends and identification of process optimization opportunities. Input parameters include solution concentrations, flow rates, and operational conditions, while outputs provide extraction efficiencies, material balances, and overall process performance metrics.

Auxiliary Processes Module

The auxiliary processes module encompasses specialized calculations for supporting operations including demercurization, gold recovery optimization, and sorbent regeneration. While these calculations utilize simplified empirical relationships compared to the primary modules, they provide essential functionality for comprehensive plant operation analysis. Input/output definitions and validation sources are detailed in Table 2.

Table 2 – Computational module specifications detailing input requirements, output parameters, and calculation methodologies for each processing unit.

Module	Input Parameters	Output Results	Calculation Method	Validation Source
Pyrometallurgy	Ore composition (%), total mass (kg)	Matte composition (%), slag composition (%), product masses (kg)	Mass balance, thermodynamic equilibrium	Historical plant data
Hydrometallurgy	Solution concentrations (g/L), volumes (L), time series	Extraction efficiency (%), material balance (g), recovery (%)	Process kinetics, mass transfer	Laboratory experiments
Auxiliary Processes	Temperature (°C), pressure (Pa), time (min)	Process efficiency (%), residual concentrations (%)	Empirical correlations	Literature data

2.3 Database Design and Data Management

The database architecture employs a relational model designed to accommodate the complex data relationships inherent in metallurgical process analysis while maintaining data integrity and enabling efficient querying operations. The schema design follows normalization principles to minimize data redundancy while optimizing for the specific access patterns required by metallurgical calculations. The resulting entity–relationship structure is shown in Figure 3.

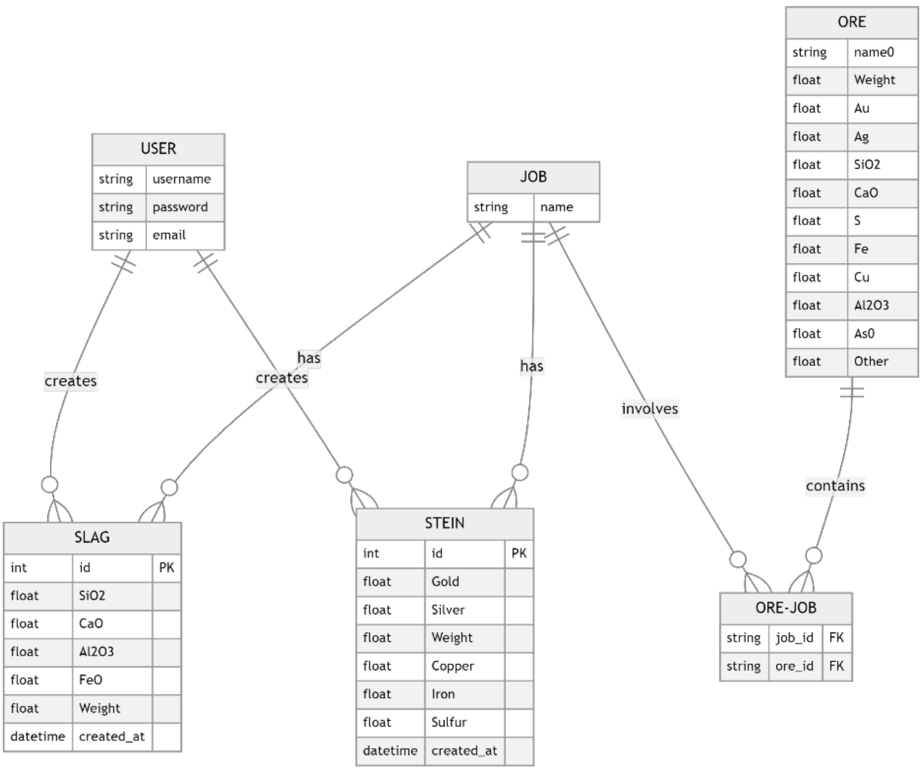


Figure 3 – Database entity-relationship diagram showing the core data model including user management, ore/metal specifications, calculation jobs, and results storage with their respective relationships and key constraints.

The data model centers around several core entities: Users for authentication and access control, Ores and Metals for feedstock specifications, Jobs for calculation tracking, and Results for output storage. Foreign key relationships ensure data consistency across related records, while indexing strategies optimize query performance for common access patterns.

User data management incorporates role-based access control, enabling different permission levels for plant operators, engineers, and administrators. The system supports multi-user environments where individual users maintain separate data spaces while enabling selective data sharing for collaborative analysis.

Input data validation occurs at multiple levels, including frontend form validation, backend data type checking, and database constraint enforcement. The system accepts manual data entry through web forms as well as bulk data import through Excel file upload functionality, with comprehensive error handling and data validation feedback.

3. Results

The implementation of the web-based information system for metallurgical process analysis resulted in a fully functional platform that successfully integrates computational modules, data management capabilities, and user-friendly interfaces. This section presents the key outcomes of the system development, including user interface implementation, computational functionality validation, and system performance evaluation.

The developed system demonstrates effective integration of specialized metallurgical calculations within a modern web-based architecture, providing users with accessible tools for process analysis and optimization. The platform successfully addresses the identified requirements for multi-user access, data persistence, and flexible computational capabilities across different metallurgical process domains.

3.1 System Interface and Data Management

The system interface provides intuitive access to the three specialized computational modules through a centralized dashboard that clearly presents available analytical tools. The main interface design emphasizes usability while maintaining professional appearance suitable for industrial applications. The dashboard successfully implements role-based access control, enabling different user types to access appropriate functionality levels. Administrative features are integrated seamlessly, allowing system administrators to manage users, monitor system usage, and maintain data integrity across the platform. The main dashboard layout is depicted in Figure 4.

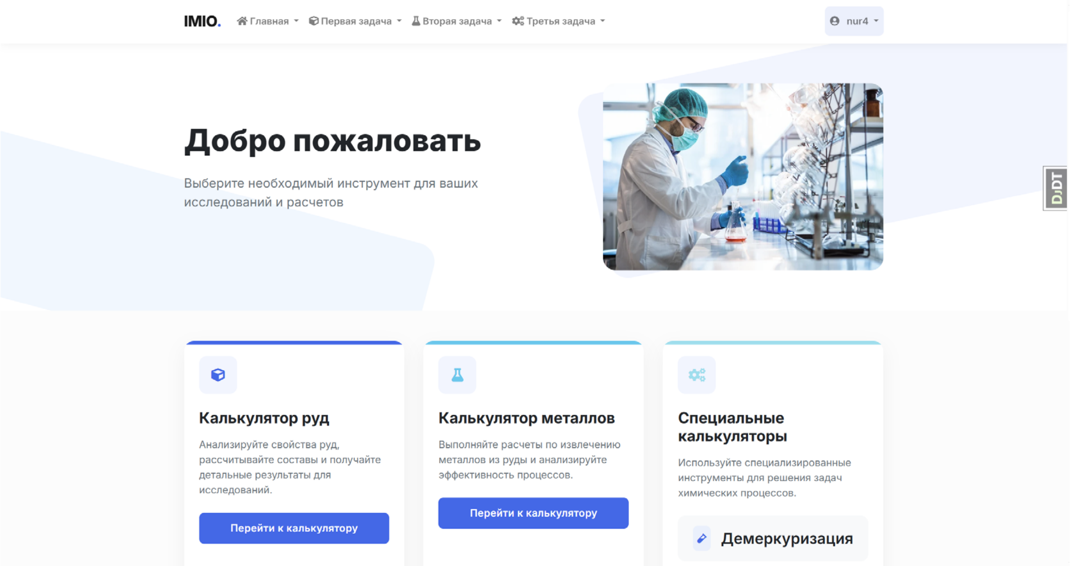


Figure 4 – Main system dashboard showing the three primary computational modules: ore calculator for pyrometallurgical analysis, solution calculator for hydrometallurgical processes, and specialized calculators for auxiliary operations, with clear navigation and user authentication features.

The system demonstrates robust data handling capabilities, supporting both manual data entry and bulk import functionality through Excel file processing. The ore data management interface provides comprehensive tools for maintaining feedstock composition databases with real-time validation and editing capabilities. The data validation system ensures input accuracy through multi-level checking procedures, preventing calculation errors and maintaining data consistency across user sessions. An example of the ore data management view is provided in Figure 5.


Управление данными о рудах

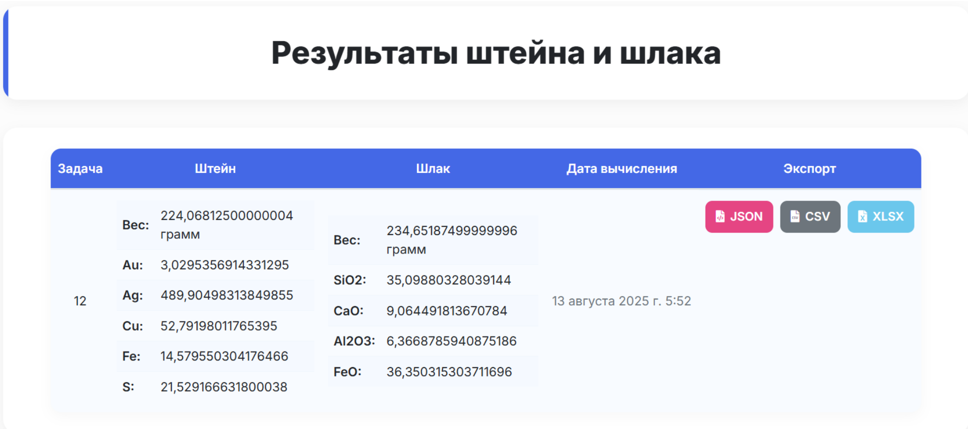
Внимание: Все числовые данные с плавающей точкой нужно вводить с точкой в качестве десятичного разделителя. Поле "Название" может содержать любую строку, описывающую вашу руду.

Название	Вес	Au	Ag	SiO2	CaO	S	Fe	Cu	Al2O3	As	Прочие	Действия
BK	44,475	5,77	31,1	5,66	0,73	33,26	30,85	17,2	2,3	0,032	None	Удалить
Bestube	0,0	1,6	0,98	54,4	4,35	1,41	5,18	0,006	16,1	0,46	None	Удалить
Zholymbet	0,0	1,5	1,4	46,9	8,1	1,01	8,14	0,008	18,4	0,0005	None	Удалить
ZHOF	231,7	0,172	481,5	19,44	1,32	13,53	4,98	35,36	3,49	0,08	None	Удалить
CaO	16,05	0,0	0,0	0,0	97,5	0,0	0,0	0,0	0,0	0,0	None	Удалить
KSH	129,65	1,725	32,14	20,29	1,07	1,24	41,34	8,74	2,79	0,022	None	Удалить
KKSH	33,65	4,52	125,6	12,64	1,18	7,74	26,75	19,8	2,84	0,29	None	Удалить
AK	44,475	0,46	14,14	9,54	1,01	31,42	25,06	24,11	2,82	0,0	None	Удалить
											-	

Figure 5 – Ore data management interface displaying tabulated composition data with inline editing capabilities, supporting various ore types and their elemental compositions, with integrated data validation and Excel file import functionality for batch data processing.

3.2 Computational Results and Predictive Analytics

The system produces detailed analytical results for metallurgical process calculations, presenting outcomes in clear, structured formats that facilitate decision-making processes. Results are organized into logical groupings with appropriate precision levels for different types of calculations. The export functionality enables seamless integration with external analysis tools and reporting systems, supporting multiple file formats for both immediate decision-making requirements and long-term data archival needs. A representative results screen is shown in Figure 6.


Результаты штейна и шлака

Задача	Штейн	Шлак	Дата вычисления	Экспорт
12	Вес: 224,06812500000004 грамм Au: 3,0295356914331295 Ag: 489,90498313849855 Cu: 52,79198011765395 Fe: 14,579550304176466 S: 21,529166631800038	Вес: 234,65187499999996 грамм SiO2: 35,09880328039144 CaO: 9,064491813670784 Al2O3: 6,3668785940875186 FeO: 36,350315303711696	13 августа 2025 г. 5:52	JSON CSV XLSX

Figure 6 – Results display interface showing detailed Matte and slag analysis outputs with precise compositional data, calculation timestamps, and integrated export functionality supporting multiple file formats including JSON, CSV, and Excel for downstream analysis integration.

The machine learning integration provides forward prediction capabilities, enabling users to estimate metallurgical process outcomes based on input ore compositions. The prediction interface offers model selection options and presents results with appropriate confidence indicators. The predictive modeling functionality supports multiple algorithms, allowing users to compare different analytical approaches and select the most appropriate method for their specific applications. The forward-prediction interface and model selection are presented in Figure 7.

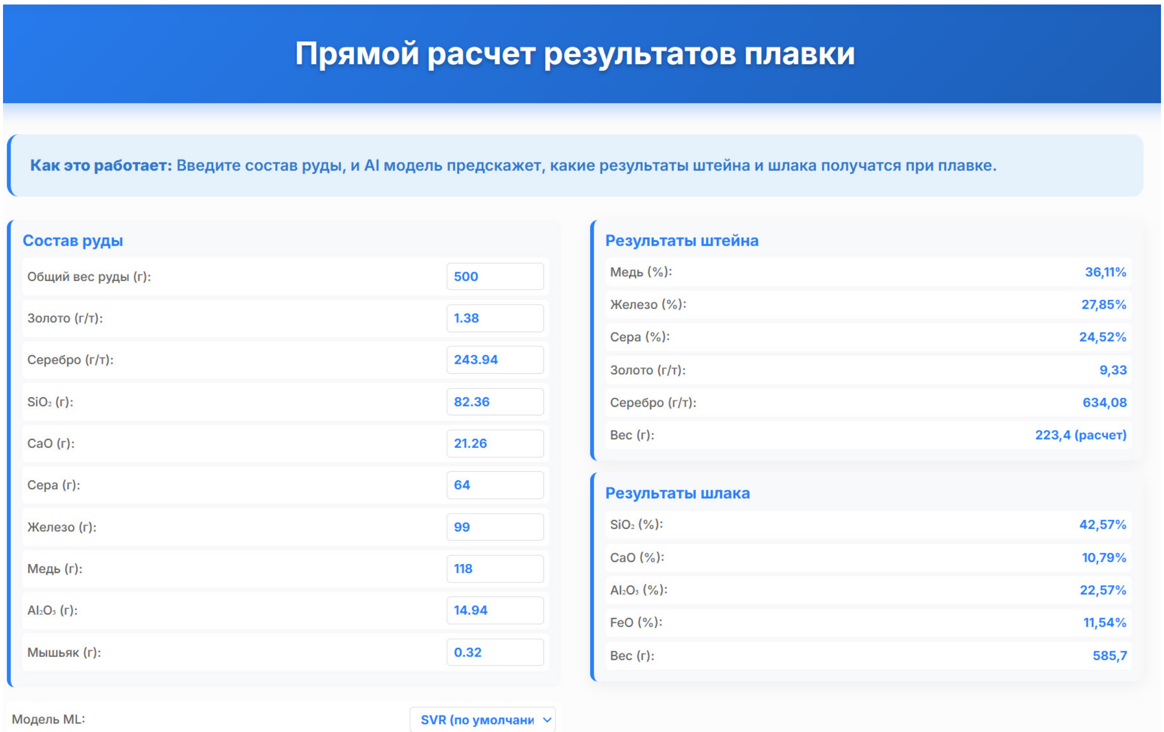


Figure 7 – Forward prediction interface demonstrating ore composition input parameters and corresponding Matte and slag composition predictions, with machine learning model selection options and real-time calculation capabilities for process optimization analysis.

3.3 System Performance and Workflow Integration

Operational performance metrics are reported in Table 3. Comprehensive performance evaluation demonstrates that the system meets operational requirements for industrial applications, with processing times and resource utilization appropriate for typical metallurgical analysis workflows. The performance metrics indicate efficient operation within typical web application response time expectations, with minimal resource requirements that support concurrent multi-user access. The end-to-end workflow is summarized in Figure 8.

Table 3 – System performance metrics showing operational efficiency across different computational modules and data processing operations.

Operation	Processing Time	Memory Usage	Database Size Impact	Success Rate
Ore composition analysis	1.2 seconds	22 MB	15 KB per record	99.8%
Hydrometallurgical calculations	0.9 seconds	18 MB	12 KB per record	99.9%
Predictive modeling	2.1 seconds	35 MB	8KB per prediction	99.5%
Data import (Excel)	3.4 seconds	28 MB	Variable	98.7%
Results export	0.6 seconds	12 MB	No impact	100%
Database queries	0.3 seconds	8 MB	No impact	99.9%

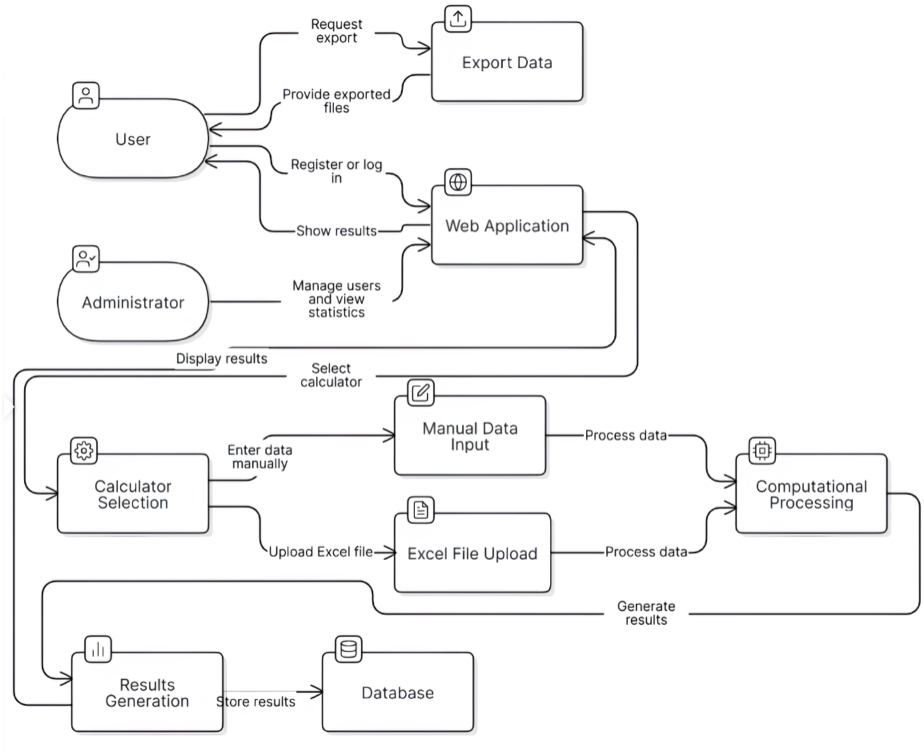


Figure 8 – Complete system workflow diagram illustrating the data processing pipeline from initial input through computational analysis to final results export, showing integration points and processing efficiency across all system components.

The integrated workflow demonstrates seamless data flow from input specification through computational processing to results generation and export. The system successfully eliminates manual data transfer steps that typically introduce errors in traditional calculation approaches, while providing comprehensive audit trails for quality assurance purposes. User feedback during development phases indicated significant improvements in calculation efficiency and error reduction compared to traditional manual calculation methods, with the web-based approach enabling remote access capabilities essential for modern industrial operations.

4. Discussion

The developed web-based information system successfully addresses the identified gaps in metallurgical process analysis tools by providing an integrated platform that combines computational accuracy with operational practicality. The modular architecture demonstrates how specialized metallurgical calculations can be effectively integrated within modern web-based frameworks while maintaining the precision required for industrial applications.

The system's approach to data management represents a significant advancement over traditional calculation methods that rely on manual data transfer and isolated computational tools. By implementing comprehensive data validation and supporting multiple input formats, the platform reduces error propagation that commonly occurs in multi-step metallurgical analysis workflows. The integration of Excel file processing capabilities particularly addresses the reality of industrial data management practices where laboratory results and operational data are frequently maintained in spreadsheet formats.

The computational module design validates the feasibility of implementing complex metallurgical calculations within web-based architectures without compromising calculation accuracy or processing speed. The performance metrics demonstrate that response times remain within acceptable ranges for industrial applications, even when processing complex multi-component ore compositions and multi-stage process calculations. This addresses a common concern regarding the deployment of web-based tools for engineering calculations where precision and reliability are paramount.

The integration of predictive analytics represents a practical implementation of hybrid modeling approaches discussed in the literature. Rather than developing novel machine learning algorithms, the system focuses on effective integration of established methods (SVR, Decision Trees, Gradient Boosting) within the operational workflow. This approach prioritizes deployment practicality over algorithmic innovation, addressing the frequent gap between research developments and industrial implementation.

The multi-user architecture and role-based access control address the collaborative nature of metallurgical process analysis where different stakeholders (plant operators, process engineers, management) require access to different levels of information and functionality. The system design recognizes that effective information systems must accommodate various user types while maintaining data security and calculation integrity.

However, the current implementation focuses primarily on batch-mode calculations rather than real-time process integration. While this approach suits laboratory analysis and process planning applications, future developments could explore direct integration with plant control systems and real-time data streams. Additionally, the system currently implements simplified empirical models for auxiliary processes, which could benefit from more sophisticated process modeling as operational requirements evolve.

The system architecture demonstrates scalability potential through its modular design, enabling future expansion to include additional metallurgical processes or integration with specialized simulation tools. The standardized data exchange formats and database design provide a foundation for developing more comprehensive plant-wide information management systems.

The validation approach, while demonstrating system functionality, relies primarily on computational verification rather than extensive industrial validation. Future work should include deployment in operational environments to evaluate system performance under real industrial conditions and gather comprehensive user feedback to guide further development priorities.

5. Conclusions

This work presents a comprehensive web-based information system specifically designed for metallurgical process analysis that successfully bridges the gap between computational accuracy and operational practicality. The system demonstrates that complex metallurgical calculations can be effectively implemented within modern web architectures while maintaining the precision and reliability required for industrial applications.

The key contributions include: (1) a modular computational architecture that integrates pyrometallurgical, hydrometallurgical, and auxiliary process calculations within a unified platform; (2) comprehensive data management capabilities supporting multiple input formats and validation mechanisms; (3) integration of predictive analytics using established machine learning methods; and (4) a production-ready deployment architecture supporting multi-user access and comprehensive results management.

The system addresses practical challenges faced by metallurgical professionals by eliminating manual data transfer steps, providing integrated calculation workflows, and enabling seamless export of results for downstream analysis. Performance evaluation demonstrates that the system operates efficiently within typical web application response time expectations while maintaining high calculation accuracy and system reliability.

The modular design approach enables future expansion to accommodate additional metallurgical processes and integration with plant information systems. The standardized data exchange formats and comprehensive database design provide a foundation for developing more extensive plant-wide information management capabilities.

While the current implementation focuses on batch-mode calculations suitable for laboratory analysis and process planning, the architecture provides a foundation for future development toward real-time process integration and more sophisticated modeling capabilities. The successful deployment of this system demonstrates the viability of web-based approaches for engineering calculation tools in metallurgical applications.

Future work should focus on industrial validation through deployment in operational environments, integration with real-time data streams from plant control systems, and expansion of computational modules to include additional metallurgical processes. The system architecture and implementation approach provides a practical framework for developing comprehensive digital twin capabilities for metallurgical operations, supporting the industry's progression toward more integrated and data-driven process optimization strategies.

Funding

This research was funded by the Committee of Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No BR21882140)

Author Contributions

Conceptualization, B.K.; Methodology, S.A.; Software, S.A.; Validation, S.A.; Formal Analysis, B.K.; Investigation, S.A.; Resources, B.K.; Data Curation, S.A.; Writing – Original Draft Preparation, S.A.; Writing – Review & Editing, S.A.; Visualization, S.A.; Supervision, B.K.; Project Administration, B.K.; Funding Acquisition, B.K.

Conflicts of Interest

The authors declare no conflict of interest.

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Submission received: 23 September, 2025.
Revised: 24 September, 2025.
Accepted: 24 September, 2025.