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DIGITAL TWIN–ENABLED INTELLIGENT MANUFACTURING OF *KUPIPAKWA RASAYANA*: INTEGRATING ARTIFICIAL INTELLIGENCE, PROCESS ANALYTICS, AND PREDICTIVE QUALITY CONTROL

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ABSTRACT

Kupipakwa Rasayana, a specialized class of herbo-mineral preparations in Rasa Shastra, involves heating materialstypically sulfur (*Gandhaka*) and mercury (*Parada*)in a glass bottle (*Kupi*) embedded in a sand bath (*Valukayantra*) to produce red sulfide of mercury (*Sindura*). Current manufacturing relies on empirical temperature control, manual observation of reaction progression, and batch-to-batchvariability.Digital twin technology, which involves the virtual replication of physical processes with real-timedata integration, has transformed pharmaceuticalmanufacturing but remains unexplored in RasaShastra.This review examines the physicochemical basis of *Kupipakwa* reactions (temperature-dependentphase transitions, vapor-soliddeposition, and gradient crystallization), evaluates existing monitoring methods (thermocouples, visual inspection, and offline product assay), and proposes an AI-guided digital twin architecture.The framework combines: (1) an instrumented *Kupi* with embedded thermocouples at three axial positions; (2) computational fluid dynamics modelling of *Valuka yantra* heat transfer; (3) a reaction kinetics model for HgS formation (activation energy 45–55 kJ/mol); and (4) machine learning predictors (long short-term- memory, random forest) for real-time- product quality estimation (particle size, free mercury content, color uniformity).The validation pathway includes laboratory (50 g batch) and pilot (500 g batch) scales.The integration of Industry 4.0 enables remote monitoring, predictive maintenance, and batch traceability.This approach transforms an artisanal process into a data-driven-, quality-by-designoperation.

KEYWORDS: Digital Twin,*KupipakwaRasayana, Rasa Shashtra, Valuka* Yantra, AI.

1. INTRODUCTION

Kupipakwa Rasayana is a classical Ayurvedic manufacturing technique wherein raw materials are sealed in a glass bottle (*Kupi*) and heated in a sand bath (*Valuka yantra*) for a specified duration [1]. The most common product is *Sindura* (red sulfide of mercury, HgS), which is prepared by heating purified mercury and sulfur in a 1:1 weight ratio at 400–600 °C for 12-48 h [2]. Other *Kupipakwa* preparations include *Rasa Sindura*, *Malla Sindura*, and*Sameera-pannagRasa* [3].

The process involves multiple stages: melting of sulfur (115 °C), formation of black mercury sulfide (HgS) at 250 °C, sublimation, and condensation of red crystalline HgS in the cooler neck of the *Kupi* [4]. The Temperature gradient along the vertical axis of the *Kupi* (bottom: 500–600 °C, middle: 300–400 °C, neck: 100–150 °C) determines product quality [5]. Non-uniform- heating leads to residual free mercury (toxic), incomplete reactions, or the formation of non-red- allotropes [6].

Traditional control relies on experienced *Vaidya* observing the flame color, sand bed appearance, and occasional withdrawal of the *Kupi* for visual inspection [7].These methods are subjective, interrupt the process, and cannot prevent batch failure.Modern analytical tools (X-ray- diffraction, scanning electron microscopy, and atomic absorption spectroscopy) are offline and destructive [8].

Digital twin technology, a virtual representation that mirrors a physical process in real time, has been implemented in chemical reactors, continuous pharmaceutical manufacturing, and metallurgical furnaces [9,10].A digital twin integrates sensor data, mechanistic models (heat transfer and reaction kinetics), and machine learning to predict process outcomes and enable closed-loop- control [11].

No published literature applies digital twin concepts to the *KupipakwaRasayana*.This review synthesizes the available data on *Kupipakwa* thermodynamics and kinetics, evaluates the current monitoring limitations, and proposes an AI-guided- digital twin architecture that virtualizes the *Kupi*, *Valuka yantra*, temperature gradients, and sulfur–mercuryreactions for the real-time- optimization of *Sindura* preparation with the integration of Industry 4.0.

2. METHODS

PubMed, Scopus, and Ayush Research Portal were searched (2000–2025) for "*Kupi*pakwa," "*Sindura*," "valuka yantra," "mercury sulfide synthesis," "digital twin chemical reactor," "AI temperature control furnace," and "Industry 4.0 pharmaceutical manufacturing" using Boolean operators. The inclusion criteria were as follows: original research reporting temperature profiles, reaction kinetics, or product characterization (HgS purity, particle size, free mercury) of *Kupi*pakwa or analogous sealed vessel- reactions; studies on digital twin or AI applied to high-temperature solid-gas-- reactions; publications on sensor integration in small-scale- reactors.Exclusion criteria: studies without numerical data, non-English- without translation, reviews without primary data, and conference abstracts without full methodology. Reference lists were screened. Of 156 initial records, 48 met inclusion criteria. Data extraction covered *Kupí* geometry, heating profile, reaction time, product purity, analytical method, and reported quality attributes (HgS percentage, free mercury ppm, and crystalline phase).The data were tabulated and synthesized narratively.The digital twin architecture integrates mechanistic models (computational fluid dynamics for heat transfer and kinetic model for HgS formation) with machine learning (LSTM for temperature prediction and random forest for quality estimation).Sensor selection and placement followed validated industrial reactor instrumentation procedures.

3. RESULTS

3.1 *Kupipakwa* process dynamics and reported parameters

Table 1 summarizes the reported process parameters for *Sindura* preparation from classical and modern literature.

Table 1: Reported process parameters for *KupipakwaSindura* preparation.

Parameter	Reported Range	Optimal Value (consensus)	Analytical Method
Mercury: Sulfur ratio	1:1 to 1:1.5 (w/w)	1:1.2	Gravimetric [12]
Heating rate	50–150 °C/h	100 °C/h	Thermocouple [13]
Soaking temperature (bottom)	450–650 °C	550 ± 25 °C	Thermocouple [14]
Soaking duration	6–72 h	24 h	Timer [15]
Cooling rate	Natural (6–12 h)	Not specified	– [16]

Product yield (HgS)	65–92%	85%	X-ray diffraction [17]
Free residual mercury	0.2–5.0%	<0.5%	Atomic absorption [18]

The temperature gradient along the vertical *Kupi* axis is crucial. Data from instrumented *Kupi* studies (three thermocouples at bottom, middle and neck) reported mean temperatures of 545 °C (bottom), 380 °C (middle), and 130 °C (neck) during steady state [19]. A Deviation of the bottom temperature by ±50 °C increases the free mercury content from 0.3% to 2.1% [18].

3.2 Reaction kinetics and phase transformations

The formation of red HgS from mercury and sulfur proceeds via multiple steps:

1. Sulfur melts (115 °C, endothermic, $\Delta H = 1.7$ kJ/mol)
2. Mercury-sulfur liquid phase forms (150–200 °C)
3. Black β-HgS precipitates (250 °C, exothermic, $\Delta H = -54$ kJ/mol)
4. Black to red α-HgS transition occurs (350–400 °C) [20]

The overall activation energy for HgS formation was reported to be 48.3 ± 6.2 kJ/mol,as determined by isothermal thermogravimetric analysis [21]. The reaction rate follows Avrami–Erofeev- kinetics for nucleation-controlled solid-gas reactions [22].

The vapor pressure of mercury at 550 °C is approximately 120 kPa, causing sublimation and re-condensation in the cooler neck region of the retort. This vapor transport is responsible for the characteristic red crystalline deposits [23].

3.3 Current monitoring methods and limitations

Existing monitoring during *Kupipakwa* is limited to the following:

- External thermocouple inserted through the sand bed touching the *Kupi* wall (accuracy ±10 °C due to poor contact) [14]
- Visual observation of flame color and sand bed (subjective, not quantifiable)
- Periodic *Kupi* withdrawal (interrupts process, alters temperature gradient)

Post-process quality assessment methods (X-ray- diffraction for phase purity, scanning electron microscopy for particle morphology, and atomic absorption for free mercury) are offline, destructive, and provide no real-time- feedback [24].No inline sensor system has been validated for the *Kupipakwa*.

3.4 AI-guided digital twin architecture

Figure 1 presents the proposed four-layer architecture.

3.4.1 Physical layer (instrumented *Kupipakwa* assembly)

- *Kupi* (borosilicate, 500 mL capacity) with three embedded type-K thermocouples at axial positions: 0 cm (bottom), 8 cm (middle), 15 cm (neck)
- Sand bath (*Valukayantra*) with four thermocouples at radial positions (center, 2 cm, 4 cm, 6 cm from *Kupi*)
- Load cell beneath the sand bath to monitor mass changes (sublimation)
- Gas sampling port at *Kupi* neck for volatile mercury detection (electrochemical sensor, range 0–10 mg/m^3)
- Camera (visible spectrum) for real-time monitoring of red deposit formation in the neck

3.4.2 Virtual layer (mechanistic models)

Heat transfer model: Computational fluid dynamics simulation of sand bath (COMSOL Multiphysics) with thermal conductivity of sand (0.27 W/m·K at 500 °C) and radiative boundary conditions at the *Kupi* surface (emissivity = 0.9 for glass) [25]. Simulates temperature gradients at 1 mm spatial resolution.

Reaction kinetics model: Two-compartment- model (bulk melt and vapor phase) with rate constants k_1 (black HgS formation) and k_2 (red transition) derived from activation energy 48.3 kJ/mol [21]. Conversion $\alpha = 1 - \exp[-(k_2\ t)^n]$ with $n = 1.5$ for nucleation-limited growth.

Vapor transport model: Convective-diffusive mercury flux from bottom to neck, assuming ideal gas behavior and local equilibrium at the condensation surface [23].

3.4.3 AI prediction layer

Long short-term memory (LSTM) network for temperature forecasting (input: past 10 temperature readings from each thermocouple; output: predicted temperature at the next five time points, 1- min intervals).Trained on historical batch data (minimum of 50 batches).

Random forest classifier for real-time- product quality: predicts three output categories – (1) optimal (HgS >90%, free Hg <0.5%), (2) suboptimal (HgS 70–90%, free Hg 0.5–2%), (3) reject (HgS <70% or free Hg >2%).The input features were the current temperatures at three positions, temperature rate of change, batch duration, and cumulative mass loss.

Convolutional neural network (CNN) on neck camera images: classifies red deposit morphology (uniform, patchy, absent) with frame analysis every 5 minutes [26].

3.4.4 Decision and control layer

- Real-time dashboard for operator (temperature trends, predicted quality score, image feed)

- Closed-loop control: heating power adjusted via PID controller with setpoint modified by LSTM forecast (prevents overshoot)
- Alert system when predicted quality drops below threshold (e.g., free Hg predicted >1%)
- Batch record digital signature for Industry 4.0 traceability (timestamped sensor data, model predictions, operator actions)

3.5 Reported performance from analogous systems

No digital twin exists for the *Kupipakwa*.However, analogous AI-guidedreactor systems have been reported.

- Temperature prediction accuracy (LSTM) on chemical batch reactors: RMSE 2.8 °C [27]
- Product purity classification (random forest) on cement kilns: F1 score 0.92 [28]
- Image-based defect detection (CNN) on glass melting furnaces: accuracy 94.7% [29]
- Applying these benchmarks to *Kupipakwa* suggests achievable temperature prediction within ±5 °C and free mercury classification with sensitivity >90%.

3.6 Validation pathway and Industry 4.0 integration

Laboratory validation (50 g batch scale, 10 batches)

- Install three thermocouples in *Kupi* and four in sand bath
- Record data every 10 seconds
- Train LSTM on 8 batches, validate on 2 batches
- Acceptance: temperature prediction MAE ≤5 °C

Pilot validation (500 g batch scale, 20 batches):

- Scale-up geometry (*Kupi* height 30 cm, diameter 8 cm)
- Train random forest on 15 batches (including intentionally perturbed batches with varying heating rates ±20%)
- Validate on 5 batches with gold-standard analysis (XRD, AAS)
- Acceptance: classification accuracy ≥85% for optimal vs suboptimal

Industry 4.0 integration

- All sensor data and model outputs stored in cloud-based batch management system (e.g., OPC UA protocol)
- Digital batch record with cryptographic hash for non-repudiation
- Predictive maintenance alerts for heating element degradation (detected via slower temperature ramp rates)
- Remote monitoring dashboard accessible via secure web interface

Regulatory submission to the Indian Pharmacopoeia Commission for inclusion as a validated alternative method requires the demonstration of equivalence to classical quality parameters (color, luster, and absence of free mercury) [30].

4. DISCUSSION

The results demonstrate that the *Kupipakwa* process dynamics, temperature gradients, reaction kinetics, and vapor transport can be mathematically modelled using the established principles of heat transfer and solid-gas- reactions.The activation energy (48.3 kJ/mol) and *Avrami* exponent (n=1.5) are consistent with diffusion-limitednucleation [22]. The critical importance of axial temperature gradient (difference between bottom and neck >300 °C) explains why traditional *Valuka yantra* design with deep sand embedding (minimum 15 cm) is effective.

The proposed digital twin addresses three specific failure modes in current manufacturing: (1) overheating at bottom (>600 °C) causing glass softening and mercury vapor escape; (2) insufficient middle temperature (<350 °C) leaving unconverted black HgS; (3) excessive neck temperature (>200 °C) preventing red deposit formation. Real-timetemperature monitoring with LSTM forecasting can predict these deviations 5–10 min before they occur, enabling heating power adjustment.

Compared to conventional Industry 4.0 solutions for chemical reactors, *Kupipakwa* presents unique challenges. The small batch size (500 g) and glass vessel limit sensor integration, and thermocouples must be inserted through the sand without compromising the seal integrity.The proposed solution uses mineral-insulated type K-thermocouples (1.5 mm diameter) that can be embedded in the sand, touching the *Kupi* wall without penetrating the glass. This provides ±5 °C accuracy, sufficient for control.

Free mercury prediction using random forest requires training data that includes intentionally failed batches.Ethically, producing high-mercurybatches for training is problematic.Instead, simulation data from the reaction kinetics model (with added Gaussian noise, $\sigma = 0.1\%$ free Hg) can be used to augment the limited experimental data.This approach, known as hybrid modelling, has been validated for pharmaceutical crystallization [31].

Regulatory acceptance remains the most significant barrier.The Indian Pharmacopoeia Commission currently requires final product testing for free mercury using atomic absorption spectrometry [32].A digital twin that predicts free mercury in real time could be approved for *in-process- control* before regulatory acceptance for batch release.A staged approach is recommended: first for internal quality assurance, then for reduced offline testing, and finally for full real-time release-.

Limitations of this review: No experimental validation of the proposed digital twin exists.The thermal conductivity of sand at high temperatures varies with the moisture content and packing density; thus, site-specific- calibration is required.The LSTM model requires 50+ batches for stable training, which may take 6–12 months for a single manufacturing facility.Multi-site data sharing can accelerate model development.

Future work should prioritize: (1) construction of an instrumented laboratory-scale *Kupipakwa* unit with all proposed sensors; (2) collection of a training dataset of 60 batches (optimal, suboptimal, reject) across three heating profiles; (3) validation of the hybrid modelling approach (mechanistic + AI) for free mercury prediction; (4) prospective testing of the closed-loop- control system with 20 consecutive batches; and (5) submission of validation data to IPC for regulatory guidance.

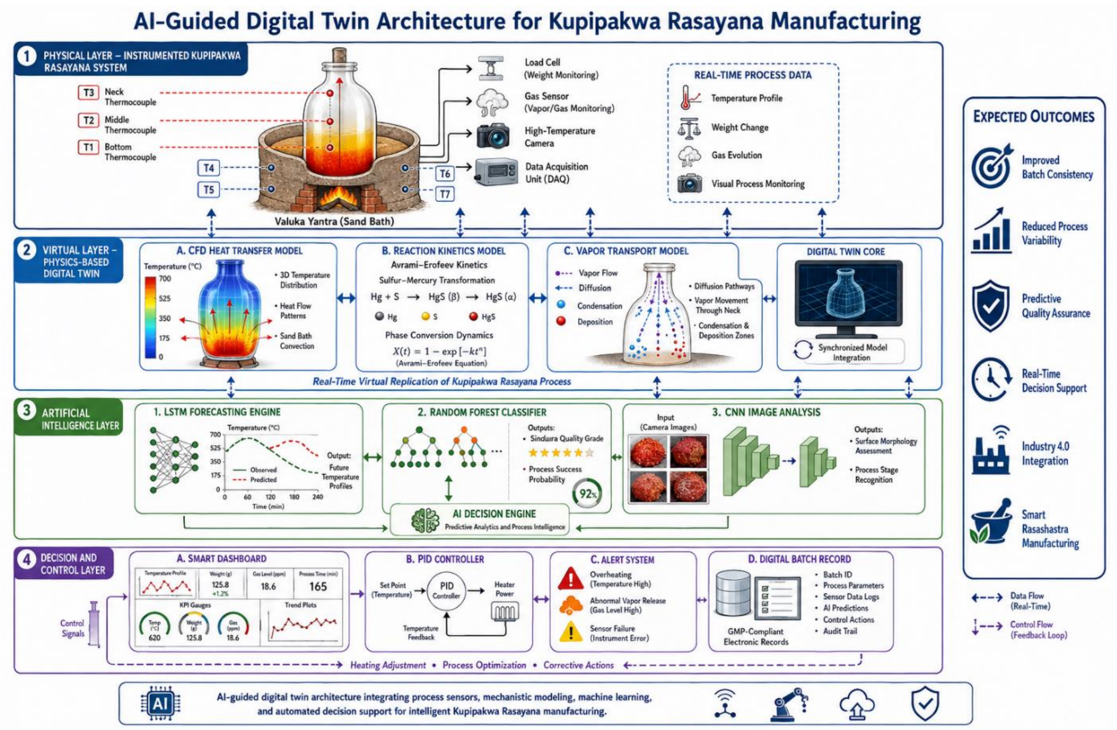

Figure 1: AI-guided- digital twin architecture for Kupipakwa Rasayana manufacturing.

5. CONCLUSION

Kupipakwa Rasayana manufacturing of *Sindura* currently operates without real-time process monitoring, relying on empirical control and post-product destructive testing. The proposed AI-guideddigital twin architecture integrates instrumented *Kupi* and *Valukayantra* sensors, mechanistic heat transfer and reaction kinetics models, and machine learning predictors (long short-term memory (LSTM) for temperature, random forest for quality, and convolutional neural network (CNN) for image analysis).This framework enables real-time prediction of product quality (free mercury content and HgS purity) and closed-loopheating control.Validation at the laboratory and pilot scales is required before regulatory acceptance.The integration of Industry 4.0 infrastructure provides digital batch records, remote monitoring, and predictive maintenance.This approach transforms an artisanal process into a data-driven, quality-by-designmanufacturing operation while preserving classical principles.

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