WHITEPAPER

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Using Large Language Models to improve and accelerate MES migrations

Using Large Language Models:
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Introduction

The digital transformation of pharmaceutical manufacturing continues to accelerate, with Manufacturing Execution Systems (MES) like PAS-X serving as the cornerstone for ensuring compliance, traceability, and operational excellence.

During the migration of MES PAS-X across different versions, the integrity and accuracy of the master batch records (MBRs) must be maintained.

One of the most critical steps in this process is identifying, documenting and preventing inaccuracies and differences between the MBRs in both versions.

This Whitepaper explores how Large Language Models (LLMs) can help to automate or partially automate and enhance deviation detection in both MES Systems, with a focus on enabling faster and more accurate migration processes.

What is an LLM (Large Language Model)?

A Large Language Model (LLM) is an advanced type of artificial intelligence designed to understand, interpret, and generate human-like text. These models are trained on massive amounts of data — including technical documents, code, and natural language — allowing them to perform complex reasoning, summarization, comparison, and automation tasks.

LLMs don't just repeat information; they understand structure, logic, and context. This makes them ideal for industries such as pharmaceutical manufacturing, where documentation, compliance, and data accuracy are critical.

Complexity in MBR Migration

Migrating a MBR isn't straightforward because it is much more than just a software upgrade.

Key challenges are usually as follows:

- **Different material flow mapping in the two systems.**

Challenge: Material handling changes between MES versions can affect how raw materials, intermediates, and packaging components are tracked. This impacts compliance, traceability, and workflow design.

Example: In v2, material dispensing might be logged as one combined step where the operator verifies the Batch status, enters the required quantity, and confirms dispensing.

In v3, the same process is broken into separate stages:

1. Batch Verification – Confirm the Batch is released and available.
2. Weighing – Capture the exact measured amount.
3. Dispensing Confirmation – Approve and record the transaction.

This shift from a single activity to a multi-step workflow means MBRs must be redesigned to ensure all material checks remain compliant and no controls are lost or duplicated during migration.

- **Element Mapping Variations**

Challenge: Functions may shift categories between system versions, complicating direct comparison.

Example: A *container status check* in v2 could be logged as a "user activity," where the operator manually verifies and records. In v3, the same check might be configured as a *basic function* tied to equipment logic based on state diagrams defined. Migration must ensure this transition is reflected correctly without losing compliance traceability.

- **Incorporation of New Functionalities**

Challenge: PAS-X v3 introduces enhanced functional building blocks such as signal senders and receivers. These allow the MES to react dynamically to process execution events (e.g., equipment signals, process conditions, or intermediate step triggers). When migrating MBRs, these new functionalities must be embedded properly, replacing older manual or sequential activities. This ensures that the upgraded MBRs leverage automation, reduce operator workload, and improve compliance.

Example:

- In v2, a mixing process might rely on manual step confirmation.
  - The operator completes "Add Material A and Mix for 10 Minutes."
  - Once finished, they manually confirm the step in MES before the next instruction (e.g., "Start Cooling") becomes available.
- In v3, this same workflow can be optimized using signal senders and receivers within the MBR:
  - When the "Mixing Completed" step finishes execution, it automatically sends a signal within the MBR.
  - The next step ("Start Cooling") is configured to receive this signal, allowing it to start immediately once the prior step is done — without waiting for manual confirmation.

This internal signaling improves process flow automation, reduces operator workload, and ensures that dependent steps execute in the correct logical order even when running in parallel or asynchronously.

- **Extended Functionalities in the new MES**

Challenge: The new system offers enhanced flexibility and features, so migration should not just replicate old records but optimize them.

Example: v3 may support advanced exception handling — e.g., automatic exception triggering if a material fails a Batch status check. In v2, this was a manual process requiring operator judgment. Migration offers the opportunity to embed these additional controls for efficiency and compliance.

These challenges highlight that MBR migration is not just about transferring data but about **reinterpreting manufacturing logic** across different system architectures while ensuring **compliance, traceability, and efficiency**.

How LLMs can be used to overcome challenges in MES migration projects

Large Language Models (LLMs), are advanced AI systems trained to understand language, context, and structure.

Current LLMs can detect meaningful changes at semantic level and not just text changes in different files.

LLMs can process PDF reports or can analyze the MBR exports from both PAS-X versions, identify differences, classify them as deviations, and generate structured, audit-ready reports. This capability introduces unprecedented efficiency, accuracy, and scalability.

Problem Statement: MBR Migration Example

Usually, a one-to-one migration of an MBR is not possible due to differences listed above in both systems. In addition to the architectural changes, intentional modifications, improvements, and standardizations also complicate the comparison and validation process.

Differences in both MBRs occur during a migration at various levels/elements such as:

System-level/architecture differences

- Data Model Changes: V3 often introduces new database schemas, field names, or structures that are not 1:1 with v2.
- Terminology Updates: Example: “Instruction” in v2 may become “Operation Step” in v3.
- UI and Workflow Enhancements: New approval points, role assignments, and signatures.
- New Elements: Such as Signal Sender and Receiver that did not exist in Version 2.

Intended and not intended content-level differences

- Formatting & Units
- Instructional Wording changes
- Material Codes & Naming Conventions

These challenges often result in migration and validation errors, which could be significantly reduced or entirely eliminated by using AI (LLMs). The AI assists by generating clear, human-readable outputs — such as deviation reports or migration summaries — that can be easily reviewed and validated by supervisors or QA personnel. However**, final approval and decision-making always remain with qualified human reviewers**, ensuring compliance and accountability.

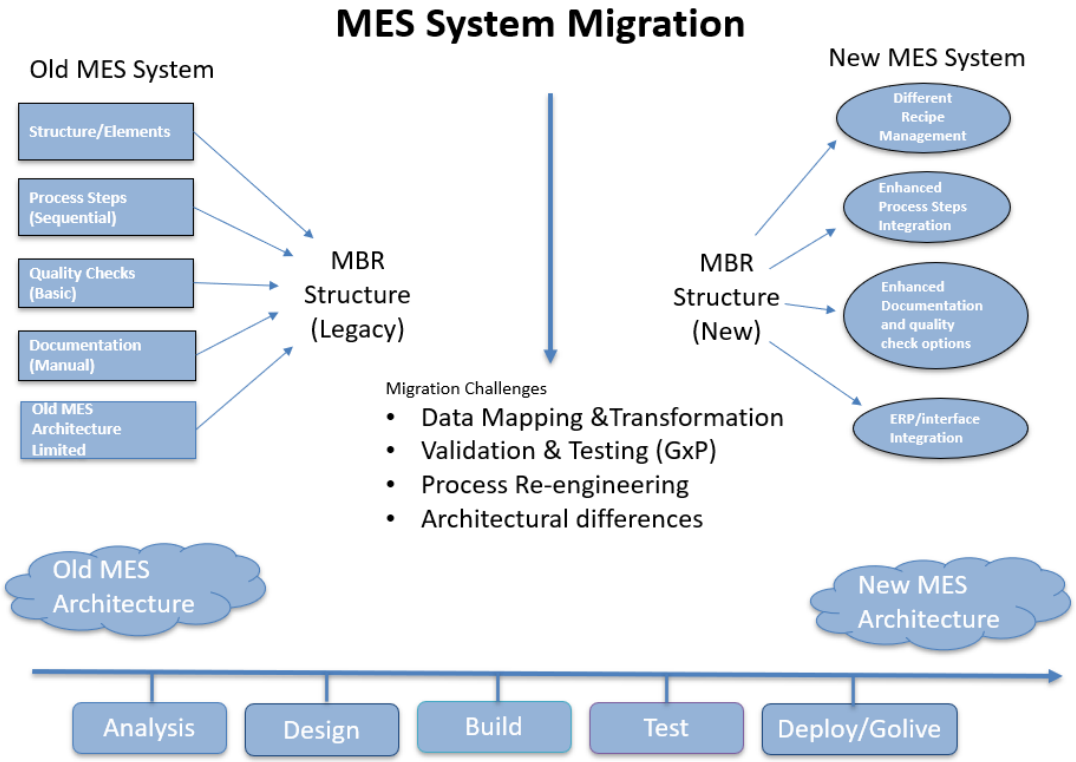

Figure 1 Challenges in MBR Migration

How LLMs could overcome these challenges

Automated Content Comparison

LLMs can compare MBRs from both PASX version V2 & V3 not only at text level but also at Semantic level. Just to give an idea LLMs recognizes “Check Batch Status” in v2 is equivalent to “Batch Verification” in v3 and this is just one of the wide range of examples. In overall LLMs are capable of things like:

Context-Aware Deviation Detection

- Detect meaningful changes rather than false positives from minor format differences.
- Ignores irrelevant whitespace or page number changes.
- Flags real risks like removal of a verification step.

Structured Deviation Reporting

Generates audit-ready deviation sheets for final approval and decision-making (Excel, CSV, PDF) that:

- List the exact field that changed.
- Categorize the deviation (naming, process logic, quantity, parameter).
- Provide a risk/impact analysis suggestion.

Scaling Across Hundreds of Records

Once trained/configured, the same LLM workflow can process hundreds of MBR pairs in parallel—impossible to do manually without huge QA teams.

Enabling Rapid QA Review

QA teams could get filtered, high-priority deviation lists instead of manually digging through pages.

LLMs can also auto-generate draft change control entries for QMS integration.

Generated sample Report

MBRs from both PAS-X v2 and v3 are exported in structured formats such as XML, CSV, or PDF. These are normalized and cleaned to standardize tags and formatting.

Deviation ID	Field	v2 Value	v3 Value	Type of Change	Impact Summary
DEV-MAT-001	Name	API_A_100mg	API-A-100mg	Naming convention	May impact material master matching or barcode scan
DEV-MAT-002	Check Batch Status	Yes	No	Verification rule	Disabling could skip GMP checks, review required

Process flow for LLM-Enabled Deviation Report Generation

The process begins with exporting Master Batch Records (MBRs) from PAS-X v2 and v3 in structured formats such as XML. These records will be preprocessed and normalized to align field names and standardize structures.

Next, a field-by-field alignment is carried out using unique IDs or fuzzy matching, with the LLM assisting in resolving uncertain mappings. Once aligned, the LLM comparison engine analyzes the content, detects deviations across materials, instructions, signatures, and control logic, and classifies them by severity. Based on these findings, a structured deviation report is generated in formats such as Excel, PDF, or JSON. This report includes deviation IDs, descriptions, impact assessments, and recommended actions.

Following report generation, QA and validation teams review and annotate the output, accepting or rejecting deviations and providing compliance context.

Finally, as an optional step, the LLM can auto-draft change control documents, producing GxP-ready documentation to support regulatory requirements.

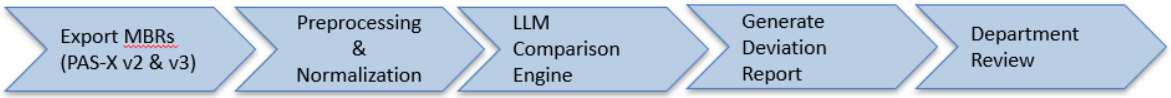

Figure 2 Process flow

Benefits of LLM-based deviation detection

Benefit	Description
Speed	Reduces MBR comparison time by 80–90%
Accuracy	Minimizes human oversight and missed changes
Scalability	Enables large-scale, multi-site MBR migration
Consistency	Standardized deviation reporting across teams
Audit-Readiness	Output suitable for QA review and regulatory inspections
Cost Efficiency	Reduces manual labor and rework

Conclusion

As the pharmaceutical industry moves toward intelligent, compliant digital manufacturing (Pharma 4.0), LLMs provide a transformative advantage. In the context of PAS-X MBR migration, they automate one of the most labor-intensive and critical steps—deviation detection and documentation. By enabling intelligent, structured, and scalable deviation sheet generation, LLMs support faster migration, higher quality, and better regulatory readiness.

Organizations adopting LLMs for MBR comparison will gain not only operational efficiency but also a strategic advantage in digital maturity and audit readiness.

Our Company

FrontWell Solutions is an expert in the digital transformation of the pharmaceutical manufacturing process. Our team of experts is engaged in providing digital solutions to 12 of the 20 leading pharmaceutical, biotechnology, chemical, and medical device companies and suppliers spanning Europe, the United States, and Asia.

Our expertise lies in delivering specialized consulting services, primarily centred around Manufacturing Execution Systems (MES), Laboratory Information Management Systems (LIMS), seamlessly integrating these Level 3 systems with Enterprise Resource Planning (ERP) platforms and driving Manufacturing Intelligence initiatives such as Overall Equipment Effectiveness (OEE) reporting.

Next Steps

Thinking about taking your next steps towards the CSV and AI journey? Our experts are ready to support you! Contact us under ReachUs@frontwell-solutions.com or via +49 (6101) 595 89 85.