



Smart Pharma

AI in Formulation, Manufacturing & Quality Control

How can AI help us make medicines more consistent, reliable and safe?

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Learning objectives

- 1 Explain formulation optimisation and its trade-offs.
- 2 Describe Process Analytical Technology (PAT).
- 3 Explain smart manufacturing and digital twins.
- 4 Describe computer vision for quality inspection.
- 5 Explain predictive maintenance and batch-quality prediction.
- 6 Identify supply-chain applications and key limitations.



Why can two batches differ?

Two batches may use the same formula but experience different materials or process conditions.

Batch A

Meets expected specifications
Consistent appearance and performance

Batch B

Uneven coating or variable dissolution
Potential quality concern

The challenge

What changed—and how could we detect it earlier?

AI can help identify patterns in ingredients, equipment settings and process data. It does not replace testing or investigation.



1. Formulation optimisation

Define the target

Set the desired dose, release profile and dosage form.

Choose ingredients

Select API properties and suitable excipients.

Set process conditions

Mixing, granulation, compression and coating.

Measure outcomes

Dissolution, uniformity, hardness and stability.

Model relationships

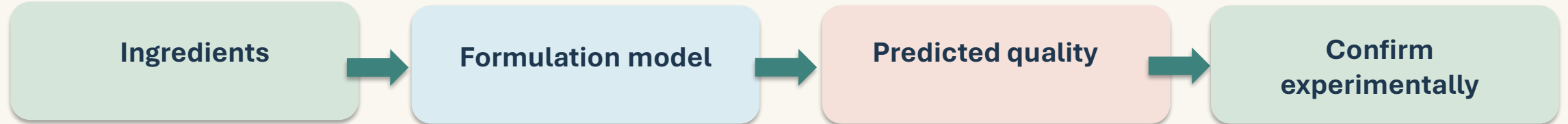
Use experimental data to learn variable–outcome patterns.

Confirm experimentally

Test promising formulations and verify performance.



What influences formulation performance?



Examples

Dissolution • uniformity •
hardness • stability

The key idea

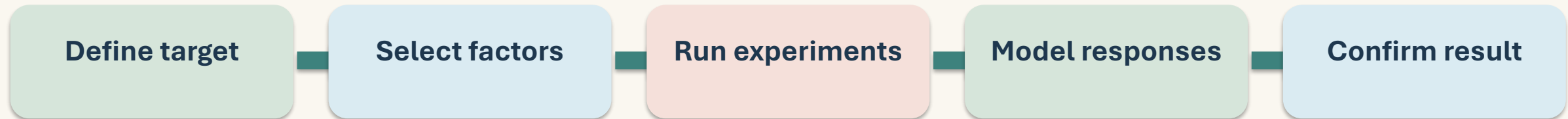
Formulation variables
interact; optimise for several
outcomes.

Human role

Review the evidence and
confirm with experiments.



Formulation optimisation: from goal to evidence

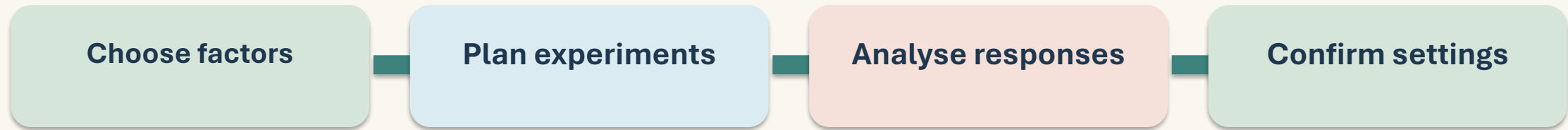


- Define measurable quality targets before optimizing.
- Use DoE and models to understand factor interactions; test the selected formulation experimentally.

“AI narrows the search; experiments establish the evidence.”



Design of Experiments (DoE)



What DoE contributes

Tests selected combinations systematically to estimate factor effects and interactions.

Why it matters

Can learn more efficiently than changing one variable at a time without a plan.



Predicting dissolution and drug release

Potential benefit

Estimate likely release behaviour and prioritise formulations for testing.

Potential problem

Predictions depend on training data and may miss formulation-specific behavior.

The question

Has the model been checked against the required dissolution method?

“Predictions do not replace required dissolution testing.”



Stability: predicting change over time

Stability studies assess how product quality changes under specified storage conditions.



Potential inputs

Temperature, humidity, packaging, formulation, impurity trends and historical study results.



2. Process Analytical Technology (PAT)

PAT uses timely measurements and process understanding to help monitor and control manufacturing.

Traditional testing

Often relies on samples tested at selected time points.

PAT-enabled monitoring

Can provide process information during manufacture, where suitable and validated.

“The goal is better process understanding—not simply more data.”



What can PAT measure?

NIR / Raman spectroscopy

Chemical composition, moisture or blend information

Temperature / pressure

Process conditions and equipment state

Particle-size measurement

Particle distribution and process consistency

Torque / power signals

Changes during mixing or granulation

Imaging

Shape, size, coating or visible defects

In-line sensors

Timely information about selected process variables



From measurements to process insight

A sensor produces data; process knowledge gives that data meaning.

Measure

Collect suitable signals at defined process stages.

Interpret

Relate signals to material attributes or process behaviour.

Act

Investigate, adjust or continue according to approved procedures.

PAT methods need calibration, qualification and ongoing performance checks.



3. Smart manufacturing

Connected equipment

Machines, sensors and control systems share relevant process data.

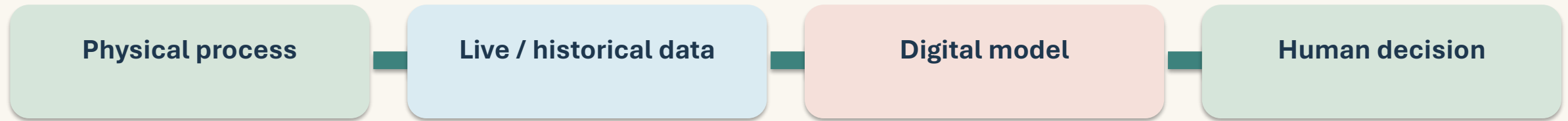
Integrated information

Batch records, laboratory results, maintenance and material data are linked.

“Smart manufacturing connects data, equipment and people.”



Digital twins and feedback loops



Inputs

Sensors, batch records and process history

Model role

Estimate behaviour or compare scenarios

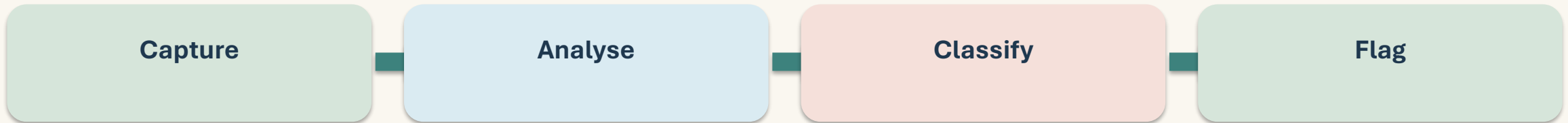
Human role

Review insights and choose an approved action.



4. Computer vision in pharmaceutical quality

Computer vision analyses images for a defined inspection task.



Applications

Chips, cracks, color variation, missing tablets and packaging defects.

Important limit

Visual inspection complements other tests; it cannot assess every quality attribute.



What can an inspection model detect?

Surface defects

Appearance

Packaging

Quality review

- Models can flag cracks, chips, coating variation, shape differences or missing tablets.
- Lighting, camera setup and representative training examples affect performance.



“A visual model is only as reliable as its validated task.”



5. Predictive maintenance

Signals

Vibration, temperature, motor current, pressure and operating history

Pattern detection

Compare current behavior with expected operating patterns

Maintenance action

Inspect equipment, plan service or investigate an alert

The goal is fewer unplanned stoppages without ignoring safety or maintenance procedures.



From equipment signals to maintenance planning

Early warning

A bearing shows rising vibration over several shifts.

Investigation

Check sensor quality, operating load and maintenance history.

Planned action

Inspect and service the equipment if evidence supports it.

“A prediction is a reason to investigate—not proof of failure.”



6. Batch-quality prediction

Models can estimate selected quality attributes or flag batches with unusual profiles.

Process inputs

Material lots, mixing time, temperature, pressure and sensor trends

Model output

Estimated attribute, risk category or anomaly flag

Quality review

Check evidence, investigate deviations and follow the quality system.

A model score alone cannot authorise batch release.



What might a batch-quality model predict?

Continuous value

Estimate a numeric attribute, such as hardness or moisture.

Category

Flag likely in-spec or potential out-of-spec risk.

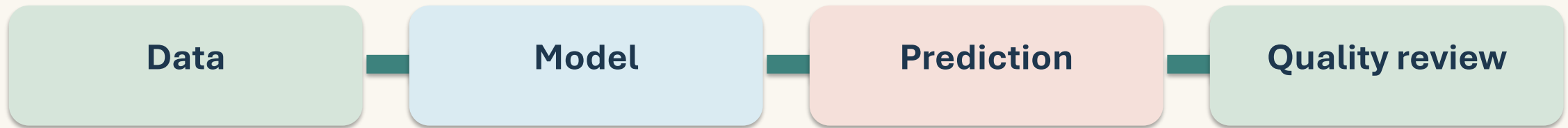
Anomaly

Identify a batch or process profile that differs from normal.

“Test on unseen batches and relevant operating conditions.”



Validation before quality decisions



Accuracy

Overall performance can hide important errors.

False negatives

A real defect may be missed.

Generalisation

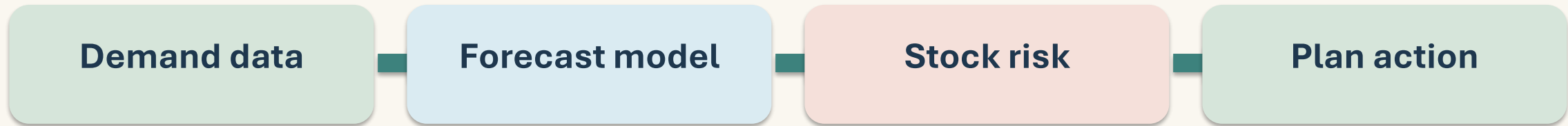
Performance can change across products or sites.

Context

Quality risk and evidence matter.



7. Supply-chain applications



Demand forecasting

Use historical demand, seasonality and relevant external factors.

Inventory planning

Estimate stock needs and potential shortage risk; flag supplier or distribution risks.

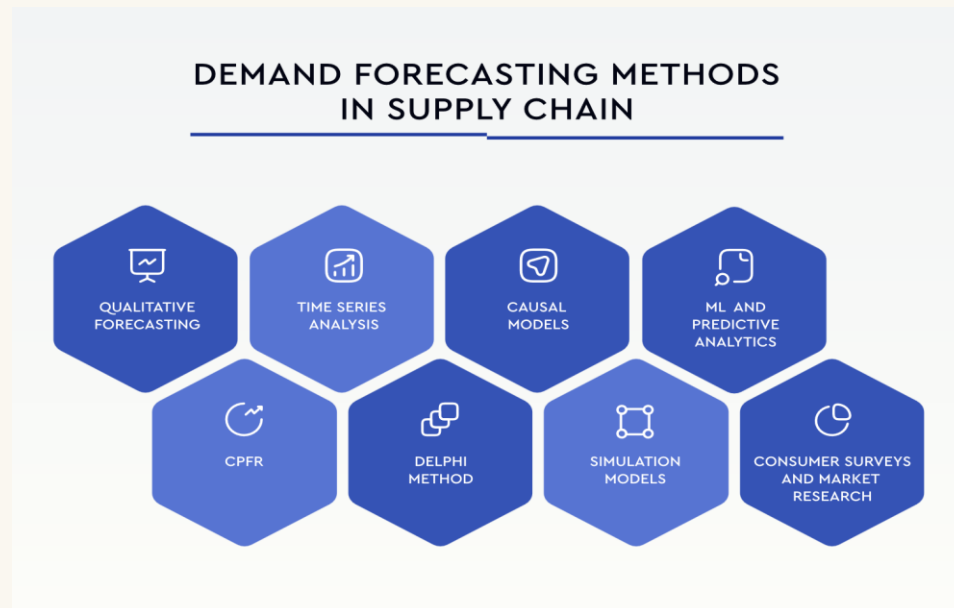
Contingency planning

Use alerts to verify stock and prepare alternatives for critical medicines.



When supply-chain predictions go wrong

A forecast is only as useful as the data and assumptions behind it.



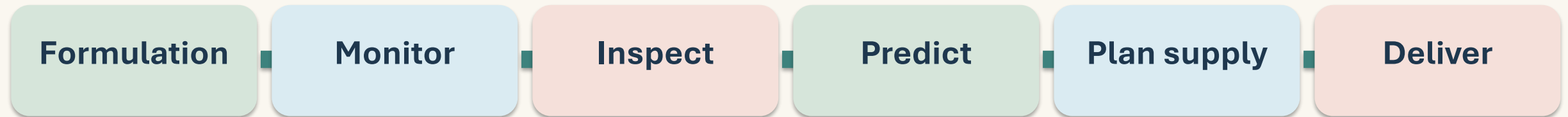
Discussion

What should a pharmacy team do when the forecast predicts adequate stock but the shelf is empty?

AI should support contingency planning, not replace local verification and professional judgement.



From formulation to patient supply



AI contributes

Pattern detection, prediction and prioritization.

Quality systems contribute

Validated methods, procedures and documented decisions.

People contribute

Context, investigation, accountability and judgement.

“The aim is reliable medicines—not automation for its own sake.”



Formulation optimisation in practice

Example: balance product performance, stability and manufacturability.



Define the goal

Set measurable quality targets before searching for a formulation.

Learn from experiments

Use DoE and suitable models to understand factor interactions.

Confirm the candidate

Test the selected formulation and check it meets requirements.

AI narrows the search; experiments establish the evidence.



PAT and smart manufacturing

Connected measurements can help teams understand a process while it runs.



Sense

Collect suitable signals such as temperature, pressure or spectroscopy.

Interpret

Relate signals to material attributes and process behaviour.

Respond

Review alerts and act through approved operating procedures.

Real-time data are useful only when they are reliable and interpreted.



Computer vision for tablet inspection

A camera model can screen for defined visual defects at production speed.



Capture consistently

Lighting, camera position and image quality affect performance.

Detect and flag

Identify cracks, chips, coating variation or missing tablets.

Verify the system

Measure false alarms and missed defects on representative samples.

Visual inspection does not replace tests for every quality attribute.



AI in pharmaceutical supply chains

Forecasting and risk signals can support more resilient medicine availability.



Forecast demand

Combine historical demand with relevant seasonal and local factors.

Monitor supply risk

Track supplier delays, inventory and critical dependencies.

Plan contingencies

Use alerts to prompt verification and backup planning.

A forecast supports planning; it cannot guarantee future availability.



Key takeaways

- Formulation optimisation balances multiple product attributes.
- PAT and smart manufacturing help teams understand process behaviour.
- Computer vision flags defined visual defects.
- Predictive maintenance and batch-quality models prioritise investigation.
- Supply-chain AI supports forecasting and risk monitoring.
- Validation, GMP and quality oversight remain essential.

“Use AI to improve decisions—not to bypass quality.”

