



MODULE MANUAL

Dynamic simulation, ODE/PDE and operating modes

Calculate batch, fed-batch, perfusion and continuous processes reproducibly

DOCUMENT BASIS

Product workflows, visible results, review criteria, evidence boundaries and controlled handover.

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Document control

One controlled basis for public product guidance.

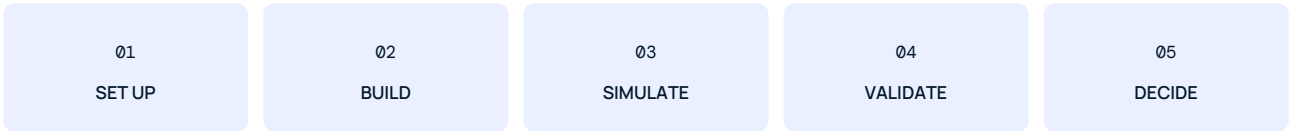
FIELD	VALUE
Document ID	M03-EN-4.2
Release	4.2
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Audience	Process Development, Modelling, Scale-up, MSAT
Purpose	How do process states evolve over time and within which operating envelope is the scenario plausible?
Owner	Acatian Product and Engineering

APPLICABILITY LIMIT

This manual explains the product workflow and the evidence needed to interpret its outputs. It does not replace qualified engineering judgement, customer quality systems, safety review, equipment-vendor data or validation for a regulated intended use.

Scope and use

Use the navigation path, input register, visible-result description, review criteria and handover record together. A screen or exported number without its model version, basis, unit, evidence status and limitations is not a controlled engineering result.



LANGUAGE

This document is written consistently in English. Product navigation names remain as displayed in the interface.

Dynamic simulation, ODE/PDE and operating modes

Calculate batch, fed-batch, perfusion and continuous processes reproducibly



ENGINEERING DECISION	PATH IN ACATIAN
How do process states evolve over time and within which operating envelope is the scenario plausible?	Simulate > Dynamic simulation / Advanced modelling
PRIMARY USERS	PERMITTED MATURITY
Process Development, Modelling, Scale-up, MSAT	Screening without calibration; Calibrated after estimation; Validated only with an independent dataset

START WITH THE DECISION

Acatian couples component balances with time-dependent states. ODEs represent ideal mixed states; PDEs represent spatial gradients as discretised fields. The operating mode and events must match real operation.

Expected artifacts

ARTIFACT	RECIPIENT
Module result package	Engineering reviewer
Readiness register	Model owner
Controlled version	Project team

Prepare the model

INPUT	WHY IT MATTERS	READY WHEN
Initial states	Start biomass, substrates, product, metabolites, volume and temperature.	Every state has value, unit and source.
Kinetics	Defines growth, uptake, formation and death.	Equation, parameter range and applicability are documented.
Operating profile	Distinguishes charge, feed, bleed, harvest and continuous flow.	Events, rates and control logic are defined.
Numerics	Controls stability, accuracy and runtime.	Solver, step size, tolerance and stop conditions are set.
Measured data	Supports calibration and independent validation.	Training and validation datasets are separated.

Preflight check

CHECK	Confirm the correct project, branch and controlled version
CHECK	Verify units, provenance and permissions
CHECK	Save a restore point before a decision-relevant change
CHECK	Keep blocking gaps visible

Workflow

01

Select operating mode

Choose batch, fed-batch, perfusion or continuous and verify working volume.

VISIBLE RESULT: Volume and transfer equations visibly change with mode.

02

Configure states and kinetics

Open ODE/PDE variables, parameters, bounds and sources.

VISIBLE RESULT: The state register is complete and dimensionally consistent.

03

Define events

Schedule feed, inoculation, harvest, bleed, samples and transfers.

VISIBLE RESULT: The event line is causal and chronological.

04

Run preflight

Check structure, units, initial values, bounds and numerics.

VISIBLE RESULT: No blocking finding remains.

05

Start simulation

Start the run and observe convergence, step size and residuals.

VISIBLE RESULT: Run ID, solver state and complete trajectory are produced.

06

Compare scenarios

Change only intended parameters and compare to branch baseline.

VISIBLE RESULT: Before/after exposes states, outputs and boundary violations.

Review the result

CRITERION	PASS CONDITION	IF IT FAILS
Scope and structure	The documented criterion is satisfied and supported by traceable evidence.	Correct the model or keep the output Not decision-ready.
Units and balances	The documented criterion is satisfied and supported by traceable evidence.	Correct the model or keep the output Not decision-ready.
Evidence and uncertainty	The documented criterion is satisfied and supported by traceable evidence.	Correct the model or keep the output Not decision-ready.
Reproducibility	The documented criterion is satisfied and supported by traceable evidence.	Correct the model or keep the output Not decision-ready.
Review state	The documented criterion is satisfied and supported by traceable evidence.	Correct the model or keep the output Not decision-ready.

APPLICABILITY LIMIT

A stable numerical solution is not biological validity. Project calibration and independent validation remain required.

Troubleshooting

OBSERVATION	LIKELY CAUSE	CORRECTION
The result looks plausible but cannot be explained	Inputs, units, model version or evidence are missing.	Open the relevant register, restore traceability and rerun.
A change affects unexpected outputs	Dependencies or imported mappings were not reviewed.	Inspect the change plan and before/after diff; undo if required.
The module appears complete but readiness is low	Required industrial evidence is still missing.	Assign the visible gaps and keep maturity at Screening or Not decision-ready.

Controlled handover

ARTIFACT	RECIPIENT	MUST CONTAIN
Module result package	Engineering reviewer	Inputs, calculations, results, units, intervals, maturity
Readiness register	Model owner	Gap, required work, owner, due date, intended use
Controlled version	Project team	Branch, version, change note, reviewer and restore point

Completion check

CHECK	The active project, branch, version and intended use are visible.
CHECK	Inputs carry units, provenance, review state and uncertainty where relevant.
CHECK	Blocking model, physical, numerical and evidence gaps are closed or assigned.
CHECK	The result maturity matches the available evidence.
CHECK	The output package opens correctly and includes its limitations.

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