

Local chemical industry: reagents, processes and safety



Conceptual visualization — local chemical industry connects feedstock quality, reaction, separation, storage, utilities, safety, maintenance and analytical control.

Produce, purify, store and distribute essential reagents on Mars without turning each process into a new single point of failure.

Before starting — reconnect stoichiometry, ISRU and manufacturing quality before treating a chemical process as a source of qualified local supply. Important quantities and assumptions are stated at first use.

Mastery objectives

- construct material balances from feedstock through reagents, intermediates, useful product, recycle and purge
- separate production quantity from purity, compatibility and qualification for the intended downstream use
- prioritise local chemical processes by mission consequence, substitution difficulty and autonomy leverage
- connect process hazards, storage, instrumentation, corrosion and quality control to operating decisions

1. A settlement cannot live on machines alone

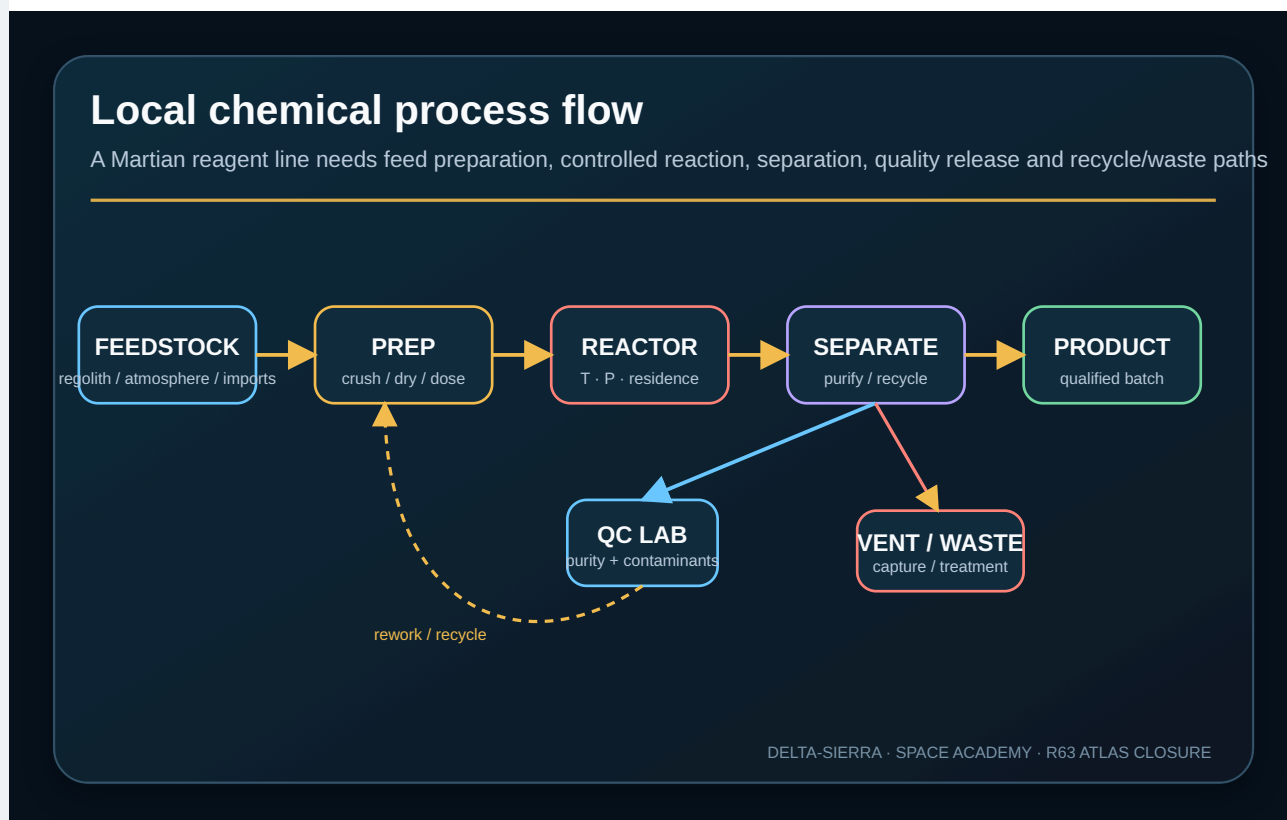
A Mars habitat constantly consumes and produces substances: treated water, oxygen, buffer gases, nutrients, cleaning materials, analytical reagents and maintenance chemicals. Early missions import nearly everything. As the settlement grows, the goal is not to recreate the entire terrestrial chemical industry but to identify a few process chains whose loss would disable several other systems. Local chemistry becomes continuity infrastructure, much like power or communications.

2. Map flows before selecting reactors

A process diagram starts with inputs, outputs, recycle loops and purge streams. Atmospheric carbon dioxide can feed some chains; water can provide hydrogen and oxygen through electrolysis; regolith contains oxides and salts but requires extraction and purification. Every flow should carry a rate, composition, pressure, temperature and purity requirement. Without that accounting, a stream described as recyclable may simply accumulate contaminants until the loop becomes unusable.

3. Purity should match the function

Pressurization gas, synthesis reagent, electrolysis water and analytical solution do not need the same purity. Over-purification costs energy, consumables and maintenance; under-purification can poison a catalyst, accelerate corrosion or invalidate a measurement. Each impurity limit should therefore be tied to a real failure mode or performance requirement.



Chemical autonomy depends on complete process flows, including recycle, purge, waste and product-quality verification. Pedagogical synthesis by Delta-Sierra from the primary sources cited in this course; schematic, not to scale.

4. Reaction, separation and recirculation

The chemical reaction is only one part of a process unit. Fluids must be heated or cooled, compressed, separated, filtered, dried, measured and often recycled. Separation can dominate energy consumption. A credible Mars process therefore represents the whole chain rather than stopping at the reaction equation that produces the desired molecule.

5. Catalysts and hidden consumables

A process using local resources may still depend on imported catalysts, membranes, resins, standards or seals. These items belong in the Earth-dependence matrix. Their annual mass may be small while their criticality is enormous. Planning combines stock, measured lifetime, regeneration, alternatives and the ability to continue at reduced performance.

6. Storage and chemical compatibility

A tank is not an abstract volume. Metals, seals, lubricants, sensors, temperature and pressure must be compatible with the chemical. Incompatible reagents are physically separated, vents and drains go to safe destinations, and connectors may be keyed where a cross-connection would be dangerous. Buffer stocks also decouple process units so maintenance on one does not immediately stop the next.

7. Instrumentation that supports decisions

A distant process must detect drift before it contaminates a common resource. Flow, pressure, temperature, conductivity and composition measurements matter only when linked to actions. Critical sensors also need a way to be checked through cross-comparison, standards, functional tests or redundant measurement. Otherwise automation can act confidently on a perfectly displayed but wrong value.

8. Safety and containment

Hazards combine pressure, temperature, toxicity, flammability, reactivity and oxygen deficiency. The first barrier is often to reduce hazardous inventory by producing in smaller batches and isolating volumes. Ventilation, detection, containment, procedures and personal protection follow. The analysis must also consider loss of electrical power, exhaust or telemetry while the process is already abnormal.

Deepening: turn purge streams into resources

No practical loop is perfectly closed. Impurities accumulate and force purge streams. Instead of treating every purge as waste, engineers characterize its composition and possible recovery: water, salts, neutralized products or material held for a future processing line. The objective is not unlimited recycling but a precise understanding of what leaves the loop and why.

Deepening: local qualification campaign

A new chemical unit should not jump directly from assembly to life-critical production. It begins with controlled batches, conservative operating limits and enhanced instrumentation. Yield, contamination and drift are compared with assumptions, then capacity increases progressively. Qualification prevents one design mistake from contaminating a large common reserve.

9. Worked example: yield and buffer stock

A unit must deliver 18 kg/day of useful product. Measured overall material yield is 72%. The equivalent useful feed requirement is $18 \div 0.72 = 25$ kg/day. Four days of finished-product buffer require at least $18 \times 4 = 72$ kg before adding the chosen uncertainty and maintenance margin. Feed rate and finished-product inventory are different quantities and should never be mixed.

Calculated case study: simplified mass balance for the Sabatier reaction

TEACHING ASSUMPTION — Consider the ideal reaction $\text{CO}_2 + 4 \text{H}_2 \rightarrow \text{CH}_4 + 2 \text{H}_2\text{O}$. The batch contains 100 kg of CO_2 and the process achieves 85% of theoretical methane mass yield.

Let $M_{\text{CO}_2} = 44$ g/mol, $M_{\text{H}_2} = 2$ g/mol and $M_{\text{CH}_4} = 16$ g/mol be molar masses; m_{CO_2} the CO_2 mass; η process yield, dimensionless; and m_{CH_4} methane mass.

By stoichiometry, 44 g of CO_2 corresponds to 16 g of CH_4 and requires 8 g of H_2 . Theoretical methane: $100 \times 16 \div 44 = 36.36$ kg. At 85%: $36.36 \times 0.85 = 30.91$ kg CH_4 . Theoretical hydrogen feed: $100 \times 8 \div 44 = 18.18$ kg H_2 .

This balance is deliberately simplified: it omits purity, recycle streams, energy and kinetics. It shows how stoichiometry first fixes the order of magnitude of material flows.

10. Exercise

A loop consumes 12 kg/day of reagent. Local production is available 80% of the time and produces 18 kg/day while running. Calculate average production, average surplus and a buffer able to cover five days of planned maintenance.

11. Reasoned solution

Average production is $18 \times 0.80 = 14.4$ kg/day, leaving 2.4 kg/day above demand. Five days offline require at least $12 \times 5 = 60$ kg in buffer, excluding margin. Rebuilding 60 kg at 2.4 kg/day takes 25 days if no other losses occur. Availability and recovery rate matter as much as nameplate capacity.

12. Mini-project

Choose one settlement chemical chain and produce a flow diagram, imported consumables list, two failure modes, required sensors, containment strategy and justified buffer stock. Explain what happens if the unit remains unavailable through one complete resupply window.

Local chemical industry is a controlled network of material transformations

A Mars settlement cannot become more autonomous by owning reactors alone. Chemical industry requires feedstock characterization, compatible storage, separation, purification, catalysts, sensors, heat and power, maintenance and safe handling of products and waste

streams. The useful question is which local processes remove the most critical Earth dependencies at an acceptable complexity and risk.

Early chemical systems should therefore be chosen from a settlement-wide flow map. Carbon dioxide, water, oxygen, hydrogen-containing streams, salts, cleaning agents, polymers and process gases all connect to life support, agriculture, propulsion, maintenance and construction. A by-product that is waste in one unit can become feedstock for another, but only if purity, timing and storage are compatible.

This module stays at systems-engineering level. It explains balances, conversion, recirculation, purity and safety without presenting hazardous operating recipes. Detailed process conditions belong in validated engineering procedures and safety documentation for the specific equipment.

Ten principles for a first Martian chemical plant

1. Map flows before selecting equipment

Draw every major input, product, recycle stream, purge and waste stream. Add the source and destination of each material. This exposes where a process depends on an imported consumable or where two systems could share a resource.

Mass flow should be expressed over a consistent time basis. A process that produces enough material per batch may still fail the settlement if batch frequency, downtime or storage capacity cannot meet continuous demand.

2. Purity should match the use

Absolute purity is expensive and often unnecessary. A construction process, crop nutrient stream and medical application can require very different quality. Over-purifying every stream wastes energy and equipment capacity, while under-purifying a critical stream can damage hardware or create safety problems.

Specifications should therefore be use-specific and measurable. The plant needs sampling and analytical capability appropriate to the decision being made.

3. Conversion and yield are not the same metric

Conversion describes how much of a reactant is consumed. Yield describes how much desired product is obtained relative to a theoretical or defined basis. Side reactions, separation losses or off-spec material can make high conversion coexist with disappointing useful yield.

Operations should track the metric that corresponds to settlement value. A high reactor conversion is not success if downstream purification rejects a large fraction of product.

4. Recirculation improves efficiency but increases coupling

Unreacted material can often be separated and returned to the process. Recycling reduces fresh feed demand but introduces additional compressors, pumps, valves, controls and contamination paths. The recycle loop can also accumulate species that are not removed elsewhere.

This is why processes need purge streams. A small purge can prevent unwanted accumulation, but purged material should be examined for safe reuse elsewhere before it is treated as waste.

5. Catalysts are high-leverage consumables

A catalyst may not be consumed in the ideal reaction equation, but real catalysts can foul, poison, sinter or lose activity. A plant that depends on one imported catalyst has an Earth dependency even if its bulk feedstocks are local.

Catalyst life, regeneration capability and spare inventory should appear in the autonomy model. The same logic applies to membranes, filters, sorbents and analytical reagents.

6. Storage compatibility is part of process design

Products and reactants need tanks, liners, seals, valves and ventilation compatible with their properties. The storage system should prevent mixing of incompatible materials and make leaks detectable. Inventory instrumentation must be trustworthy enough to support both operations and emergency decisions.

Buffer storage also decouples processes with different operating schedules. A batch reactor can feed a continuous consumer if enough safe intermediate storage exists.

7. Instrumentation must answer operational questions

Useful measurements include flow, pressure, temperature, composition and inventory, but sensors should be chosen because they support decisions. Measuring everything without defining alarm thresholds produces data rather than control.

Critical sensors need calibration and, when consequence justifies it, independent verification. A drifting analyzer can silently turn good material into off-spec product or mask a developing fault.

8. Containment and isolation limit the consequence of faults

Industrial zones should be physically separated from living areas. Ventilation, drainage or capture systems should prevent a small process release from contaminating the habitat. Isolation valves and segmented storage reduce the amount of material involved in one fault.

Emergency procedures should prioritize people, atmosphere integrity and fire prevention over preserving production. Restart occurs only after the fault is understood and affected equipment is verified.

9. Heat integration can reduce total energy demand

Some processes produce useful heat while others require heating. Exchanging heat between compatible streams can reduce electrical demand and radiator load. This integration must preserve isolation so contamination or pressure faults do not propagate across systems.

The plant should therefore be evaluated as both a material-flow and heat-flow network. Energy efficiency can improve without changing the core chemistry.

10. Qualification turns local production into trusted supply

A locally produced material should not immediately be used in a critical application. The settlement defines acceptance criteria, produces test batches, measures relevant properties and expands use as evidence grows. Qualification effort should be strongest where failure consequence is high.

This creates a path from experimental production to routine industrial supply without pretending that local manufacture automatically matches Earth-qualified material.

Calculation laboratory: conversion, yield, recycle and buffer inventory

Conversion

$$\text{Conversion} = \text{reactant_consumed} / \text{reactant_fed}$$

If 100 mol of a reactant enters a process and 82 mol is consumed, conversion is 0.82 or 82%. The remaining 18 mol may be separated, recycled, purged or lost depending on the process architecture.

Product yield

$$\text{Yield} = \text{useful_product} / \text{theoretical_product_from_feed}$$

If the theoretical product from a batch is 50 kg but only 44 kg meets specification, useful yield is 88%. This distinguishes reactor performance from what the settlement can actually use.

Recycle fraction

$$\text{Recycle_fraction} = \text{recycle_flow} / \text{total_returnable_flow}$$

A high recycle fraction can reduce fresh feed but increases dependence on the recycle hardware. The process model should include what happens when the recycle loop is unavailable and whether production can continue at lower efficiency.

Buffer storage

$$\text{Buffer_required} = \text{demand_rate} \times \text{autonomy_time} \times (1 + \text{margin})$$

If a consumer needs 8 kg/day, the upstream process can be offline for 5 days, and planners require 20% margin, buffer target is $8 \times 5 \times 1.20 = 48$ kg. Storage mass should then be checked against safe container and inventory constraints.

Worked material-balance example: Sabatier at systems level

The Sabatier reaction is often represented as carbon dioxide plus hydrogen producing methane and water. For settlement planning, the important lesson is stoichiometric bookkeeping: atoms entering the controlled reaction model must appear in products or other accounted streams. The process also needs separation, thermal control and management of unreacted feed.

Suppose an operations dashboard records 100 arbitrary molar units of limiting feed entering a reactor train and 85 units consumed. Conversion is 85%. If separation returns 12 of the 15 unconsumed units for another pass and purges 3 units to prevent accumulation of impurities, the recycle system changes fresh-feed demand even though single-pass conversion stays 85%.

This example deliberately avoids operating conditions. Real process design requires equipment-specific engineering, compatible materials, validated controls and safety analysis. The calculation exercise is about conservation and system interfaces.

Progressive exercises with solutions

- ▶ Exercise 1 - Conversion
- ▶ Exercise 2 - Useful yield
- ▶ Exercise 3 - Buffer
- ▶ Exercise 4 - Why purge exists

Interactive beginner glossary

- reactant - material consumed or transformed in a reaction.
- conversion - reactant consumed divided by reactant fed.
- yield - useful product performance measure.
- recycle stream - process flow sent back for reuse.
- purge - deliberate removal from a recycle loop.
- catalyst - reaction-enabling material with finite practical life.
- buffer inventory - stock between processes.
- qualification - proving suitability before critical use.

Chemical-industry calculation laboratory: yield, inventory and purity are separate controls

Industrial autonomy depends on knowing not only whether a reaction occurs, but how much qualified product is produced, how much feedstock is consumed and how long buffers last.

Process yield

$$\eta_{\text{yield}} = m_{\text{actual}} / m_{\text{theoretical}}$$

If stoichiometry and feed measurements imply a theoretical 90 kg product but only 72 kg of qualified product is collected, $\text{yield} = 72/90 = 0.80$, or 80%. The missing 18 kg equivalent may represent unreacted feed, by-products, separation losses or off-spec material; yield alone does not reveal where it went.

Feedstock coverage time

$$D = m_{\text{stock}} / \dot{m}_{\text{use}}$$

A 500 kg feedstock inventory consumed at an average 25 kg/day provides $500/25 = 20$ days of ideal coverage. If the process is mission-critical and resupply is impossible in that interval, a 20-day figure is a trigger for production, rationing or alternative chemistry, not a reason for complacency.

Unit check. $\text{kg} \div (\text{kg}/\text{day}) = \text{day}$.

Process-engineering studio: close a chemical plant balance before trusting its output

A local chemical industry is valuable only when operators can account for feedstock, reaction, separation, recycle, purge, product qualification and storage. A reactor conversion percentage alone does not tell the settlement how much usable product reaches inventory.

1. Begin with a component balance

$$m_{in} = m_{product} + m_{recycle} + m_{purge} + m_{loss} + \Delta m_{inventory}$$

Every term is mass over the same accounting period. The equation forces unaccounted material to become visible. If 100 kg enters a teaching process and 58 kg leaves as qualified product, 24 kg is recycled, 8 kg purged, 5 kg measured process loss and inventory rises 5 kg, the balance closes: $58+24+8+5+5=100$ kg.

2. Distinguish conversion from yield

$$X = m_{reactant_consumed} / m_{reactant_fed}$$

X is conversion, a dimensionless fraction. If 80 kg of reactant is fed and 68 kg is consumed, $X = 68/80 = 0.85$ or 85%. High conversion does not guarantee high qualified-product yield because side products and separation losses may remain.

$$\eta_{yield} = m_{product,qualified} / m_{product,theoretical}$$

If the theoretical product for the measured feed is 60 kg but only 48 kg passes qualification, $\eta_{yield} = 48/60 = 0.80$ or 80%. The symbol η , “eta”, is used here for yield.

3. Track selectivity when several products compete

$$S_{desired} = n_{desired} / n_{reactant_converted}$$

For chemical reactions, amounts are often compared in moles because stoichiometry counts molecules rather than kilograms. n denotes amount of substance in moles. This simplified selectivity definition asks what fraction of converted reactant appears in the desired product pathway, using a stoichiometrically consistent basis. Operators must define the exact basis before using a selectivity value.

4. Recycle reduces fresh feed demand but couples the plant

$$\dot{m}_{\text{fresh}} = \dot{m}_{\text{total_feed}} - \dot{m}_{\text{recycle}}$$

If the reactor needs 50 kg/h total feed and 18 kg/h is qualified recycled stream, fresh-feed demand is 32 kg/h. Unit check: kg/h – kg/h = kg/h. But recycle also returns impurities and connects downstream equipment to the reactor; a recycle loop therefore needs purge and composition monitoring.

5. Purge fraction controls accumulation

$$f_{\text{purge}} = \dot{m}_{\text{purge}} / \dot{m}_{\text{returnable}}$$

If 2 kg/h is purged from 20 kg/h of returnable gas, $f_{\text{purge}} = 0.10 = 10\%$. A larger purge can reduce contaminant accumulation but wastes more valuable material. A smaller purge conserves feed but may allow inert or unwanted species to accumulate. The correct value comes from a full component balance, not from this single ratio.

6. Connect production rate to autonomy stock

$$D_{\text{stock}} = m_{\text{usable_stock}} / \dot{m}_{\text{demand}}$$

For 420 kg of qualified reagent and average demand of 28 kg/day, ideal coverage is 15 days. This does not include inaccessible heel, degraded material, demand spikes or protected reserve, so operational coverage should be more conservative.

► Integrated exercise — why a 90% conversion plant can still miss demand

Mission decision. The operator's dashboard should expose component balances, conversion, yield, recycle, purge, impurity trends, product qualification and stock coverage. A process is not autonomous merely because the reactor runs.

First-Man process plant: atoms, energy and impurities must all balance

Local chemical industry becomes valuable when it reliably converts Martian resources and settlement wastes into products that reduce difficult imports. The hard part is not writing a reaction equation. A real process must acquire feedstock, condition it, move it through equipment, control temperature and pressure, separate products, manage impurities, recycle useful material, purge accumulating contaminants, verify product quality, and place off-specification material somewhere safe.

Every process should therefore be drawn with three ledgers at once: a material ledger, an energy ledger and a hazard ledger. Closing only the material balance can still hide an impossible heat duty; closing material and energy can still hide an unsafe inventory of reactive gas. The process engineer's job is to make all three visible.

Fresh feed depends on conversion and recycle

$$F_{\text{fresh}} = P_{\text{target}} / (Y \times x_{\text{useful}})$$

Starting question

How much fresh feed must enter a simplified process to sustain a target useful-product rate when only a fraction of feed becomes the desired product?

Read aloud

Read: "fresh feed equals target product rate divided by overall yield times useful feed fraction."

Symbols, pronunciation and meaning

P_{target} is desired product mass rate; Y is overall mass yield from usable reactant to collected product; x_{useful} is the fraction of incoming feed that is the useful reactant after conditioning.

Units

If product rate is kg/day and both Y and x are dimensionless fractions, fresh feed is kg/day.

Origin and status of values

Target rate comes from settlement demand and inventory policy. Yield and useful fraction must come from demonstrated operation or conservative test data for the selected process, not ideal stoichiometry alone.

Why this operation

Only the product of useful feed fraction and process yield contributes to collected product in this simplified boundary. Dividing by that combined fraction finds the incoming mass required to obtain the target output.

Substitution and calculation

Teaching case: target product 40 kg/day, $Y=0.82$, useful fraction 0.90. Combined factor = 0.738. Fresh feed = $40/0.738 \approx 54.2$ kg/day.

Calculator entry

Enter $40 \div (0.82 \times 0.90)$.

Mental estimate

A combined yield near 0.74 means roughly three quarters of feed becomes product; 40 divided by three quarters is a little above 53, so 54.2 is plausible.

Independent check

$54.2 \times 0.90 \times 0.82 \approx 40.0$ kg/day.

Physical or operational interpretation

The gap between 54.2 kg/day feed and 40 kg/day product becomes unreacted material, other products, purge or waste according to the real flowsheet.

Plain-English translation

A forty-kilogram daily product demand can require much more than forty kilograms of raw feed because the feed is not pure and the process is not perfectly efficient.

Variation / sensitivity

If yield falls from 0.82 to 0.70, fresh feed rises to about 63.5 kg/day. Yield degradation directly increases mining, transport and conditioning burden.

Limit / assumption

This compact equation collapses stoichiometry, recycle and separations into an overall yield. Detailed design needs component-by-component molar balances.

What this does not prove

Meeting mass production does not prove that purity, energy use, catalyst life, thermal control or safety requirements are satisfied.

Boundary case to test

If x_{useful} becomes very small, required fresh feed grows rapidly. At $x=0$, the equation is undefined because no useful reactant enters; the process cannot produce the target regardless of total feed mass.

Recycle is powerful because it moves the boundary

Unreacted feed can often be separated and returned upstream. This can reduce fresh-resource demand, but it increases internal circulation and creates dependence on compressors, pumps, separators and control valves. The recycle loop may handle several times the fresh-feed flow. A failure in that loop can therefore collapse throughput even when raw material remains abundant.

Condition feed

purity, particle size,
pressure, temperature

React

conversion, heat duty,
catalyst

Separate

product, recycle,
impurities

Qualify

composition, storage,
release to user

Purge is not wastefulness when it prevents accumulation

A closed recycle loop can concentrate species that do not react or separate completely. Without a purge, an inert or harmful impurity can rise cycle after cycle until it damages product quality or equipment. The purge fraction should therefore be chosen from an impurity balance and monitored with composition measurements. Sending less material to waste is not always safer if the “saved” material is carrying contaminants back into the plant.

Energy and storage link the plant to the settlement

Industrial operation should follow power availability and product inventory. A process with flexible timing can run when electrical generation is abundant and coast through low-power periods using stored product. That turns storage tanks into a form of operational flexibility. Conversely, a process producing oxygen, water-treatment chemicals or another vital reagent may need protected power because stock depletion has a finite time-to-consequence.

Failure review: off-specification product

Imagine a plant that meets its daily mass target but a composition sensor drifts. If product is automatically transferred into the settlement's main storage, one bad batch can contaminate a much larger good inventory. A robust design holds new production in a quarantine vessel until independent or redundant checks release it. Quality control is therefore an architectural barrier, not paperwork after production.

Exercise: decide what to protect

A reagent plant has two separators but only one composition analyser. The analyser is required before product can be released to the user tank. During a fault, production mass flow can continue but composition is unknown. The safe degraded mode is not “keep producing because the reactor works.” Hold product in a segregated tank, reduce or pause production before quarantine capacity is exhausted, and prioritise restoration or independent verification of analysis capability.

A locally produced reagent is useful only when its purity and compatibility meet the requirement of the downstream process. Pedagogical synthesis by Delta-Sierra from the primary sources cited in this course; schematic, not to scale.

Operational qualification lab: run a chemical plant as a controlled chain, not a collection of reactions

Local chemical industry becomes useful only when feedstocks, purity, storage, energy, heat rejection, by-products, maintenance and quality assurance are all controlled. A reaction that works in a laboratory flask does not automatically become a settlement process. The operator must know what enters, what leaves, what impurities accumulate and what failure state the plant moves to when power, cooling or a reagent disappears.

Write the material balance before selecting equipment

Define the process boundary and every stream that crosses it. Include intended product, recycle streams, purge streams, water, carrier gases and waste. Recycle can reduce imported feedstock but may also concentrate contaminants. A purge that looks “wasteful” can be essential to stop impurity build-up. The material balance should therefore preserve chemical identity and quality, not only total kilograms.

Usable product yield across a batch

$$Y_{\text{usable}} = m_{\text{product,accepted}} / m_{\text{feed,limiting}}$$

1 – Concrete question

How much accepted product does the process deliver per unit mass of the limiting feed used?

2 – Intuition

Count only product that passes its specification, then compare it with the feed that actually limits production.

3 – Quantities

Measure accepted product mass and limiting-feed mass on the same batch boundary.

4 – Formula

Usable yield equals accepted product mass divided by limiting-feed mass.

5 – Read aloud

“Y usable equals accepted product mass divided by limiting feed mass.”

6 – Symbols

Y is a mass ratio; m denotes mass.

7 – Pronunciation

Subscripts describe quality status and process role.

8 – Units

kg/kg is dimensionless, though it may be expressed as kilograms of product per kilogram of feed.

9 – Convention

Do not mix theoretical stoichiometric yield with accepted operational yield; identify which one is being reported.

10 – Why division

The ratio shows how much useful output is obtained for each unit of constrained input.

11 – Assumptions

The teaching metric does not by itself account for co-products or recycle credit.

12 – Unit check

kg/kg = 1.

13 – Numerical case

Limiting feed entering the batch: $m_{\text{feed,limiting}} = 52$ kg.

Accepted product after purity/quality checks:

$m_{\text{product,accepted}} = 41.6$ kg.

$Y_{\text{usable}} = 41.6 / 52.$

$Y_{\text{usable}} = 0.80$ kg accepted product per kg limiting feed.

14 – Operations

Use 31 kg, not 35 kg, because off-spec material cannot yet serve the intended function.

15 – Algebra check

$40 \times 0.775 = 31$ kg.

16 – Mental estimate

31 is a little over three quarters of 40, so about 0.78 is plausible.

17 – Interpretation

Each kilogram of limiting feed produces 0.775 kg of accepted product under this batch condition.

18 – What it does not prove

It does not show energy efficiency, reaction selectivity, safety, catalyst life or whether off-spec product can be reworked.

19 – Sensitivity

If contamination lowers accepted mass to 26 kg while crude output is unchanged, usable yield falls to 0.65 kg/kg.

Quality loss can dominate apparent production.

20 – Practice

Guided exercise. Calculate usable yield for 52 kg limiting feed and 41.6 kg accepted product.

Detailed guided correction.

1. $Y_{\text{usable}} = 41.6 \div 52 = 0.80$ kg/kg.

2. The batch delivers 80% accepted product relative to the limiting feed basis.

3. Do not substitute crude output for accepted output; off-spec mass has not yet satisfied the defined product requirement.

Autonomous exercise. A 60 kg feed batch gives 48 kg accepted product and 8 kg off-spec product. A recycle step recovers half of the off-spec mass into accepted product during a second pass. Compute total accepted output and usable yield.

► Autonomous correction – open after attempting the exercise

21 – Mission decision

Use accepted yield, energy demand, recovery time and import displacement together when deciding whether a chemical should be produced locally or stocked from Earth.

Process safety and purity are coupled

Contamination can be a product-quality problem, a corrosion problem or a crew hazard.

Materials of construction, seals, lubricants and cleaning procedures matter. Before a process is scaled, identify incompatible chemicals, credible overpressure or thermal-runaway paths, ventilation needs and safe shutdown states. The most important emergency question is often not “how do we keep production running?” but “how do we stop the process without making the hazard worse?”

Qualification drill

Choose one locally useful chemical or reagent. Draw its feed, reaction, separation, recycle, purge, storage and waste streams. Assign a quality test to the final product and one impurity that can accumulate in recycle. Then inject a cooling loss halfway through a batch and describe the safe state, what material is quarantined and what evidence is required before the line restarts.

Source context. NASA in-situ resource utilisation and life-support material provide relevant resource-processing context. The process numbers above are teaching values and do not describe a flight-certified plant. [NASA JSC — In-Situ Resource Utilization](#).

R61 chemical-industry readiness: qualified products, impurity control, process transitions and safe shutdown

A local chemical plant supports autonomy only when its products are released with known composition and the plant can be started, operated, stopped and maintained without creating unacceptable hazards. Reaction chemistry is therefore only one layer. The settlement also needs feed qualification, impurity tracking, process control, energy integration, product testing, storage compatibility and a recovery plan for off-specification material.

Rank reagents by mission consequence and substitution difficulty

Build a reagent hierarchy that asks what function the material serves, how much is consumed, whether another process can replace it, what feedstocks exist locally and how difficult purity is to achieve. A low-mass catalyst or analytical reagent may be more critical than a high-mass bulk chemical if no substitute exists. Autonomy planning should therefore prioritise consequence, not simply imported tonnes.

Primary-source bridge — JSC In-Situ Resource Utilization. NASA JSC ISRU material provides primary context for producing useful resources from local materials. R61 extends the lesson from resource extraction to qualification of the downstream chemical products used by a settlement. [Official source](#).

Impurities need their own material balance

A process can close the main reactant balance while an impurity slowly accumulates in a recycle loop. Track known contaminants, purge paths and the measurements that indicate accumulation. If an impurity affects catalyst life, corrosion, product purity or downstream life support, its concentration can become the true limiting variable even while main-product yield looks excellent.

Start-up and shutdown deserve separate procedures

Many process hazards occur during transitions rather than steady state: lines are not yet at temperature, inventories are moving, control loops are changing mode and compositions can pass through abnormal regions. Define inerting, purge, heat-up, feed introduction, product diversion and shutdown sequences with clear verification points. A plant that is stable only after it reaches steady operation is not operationally mature.

Primary-source bridge — Moon to Mars Architecture. NASA Moon-to-Mars architecture work provides primary context for integrated surface capabilities. R61 uses it to emphasise that local chemical production must fit power, storage, maintenance and crew operations rather than optimise a reactor in isolation. [Official source](#).

Product release must be tied to the intended use

Define acceptance tests by consequence. A cleaning reagent, crop nutrient, breathing-gas constituent and propellant feedstock do not necessarily require the same purity evidence. Off-specification product should be quarantined with a clear disposition: reprocess, downgrade to another qualified use, store for investigation or discard safely. Never blend off-spec material into good inventory merely to improve an average.

Energy integration can create hidden coupling

Using waste heat or shared compression can improve efficiency while coupling two processes that were previously independent. The architecture review should ask what happens when one plant shuts down, whether the other loses a required utility, and whether startup transients coincide. Efficiency gains are valuable only when the new dependency is visible and recoverable.

Qualification drill — product meets quantity target but fails purity

A plant produces the planned daily mass, but analysis shows a trace impurity above the release limit for its intended high-consequence use. Operators should divert the batch, preserve samples and process data, investigate feed/recycle/purge conditions, and decide whether the material can be reprocessed or downgraded. Production target achievement does not override product qualification.

Analytical capability limits what the plant can safely release

A process should not claim a purity that the settlement cannot measure. Match product specifications to available analytical methods, calibration standards and trained operators. If a critical impurity cannot be detected locally, either preserve imported testing capability, use a process with a stronger intrinsic quality argument, or restrict the product to a lower-consequence use.

Maintenance turnarounds need chemical inventory planning

Opening a reactor, replacing catalyst or cleaning a line can require purge gas, neutralising agent, PPE, waste storage and a temporary loss of production. Include these materials and downtime in the autonomy budget. A plant whose nominal output closes the mass balance may still be unsustainable if each maintenance event consumes scarce imported consumables.

Safe shutdown is a mission capability

Define how the plant reaches a stable condition after power loss, cooling loss, sensor disagreement or downstream storage unavailability. Identify which valves fail safe, which reactions continue producing heat, what inventory remains trapped and how the crew verifies that the hazard is controlled. Local industry is an asset only if it can stop safely as well as run efficiently.

Industrial sequencing should prioritize products whose absence creates high mission consequence and few substitutes. Pedagogical synthesis by Delta-Sierra from the primary sources cited in this course; schematic, not to scale.

Primary sources and bridges

- [NASA JSC — In-Situ Resource Utilization](#)
- [NASA — Moon to Mars Architecture](#)
- [NASA — Environmental Control and Life Support Systems](#)
- [Components](#)