MERIDIAN CHEMICAL TECHNOLOGIES PROCESS SAFETY SPECIFICATION

Project Aether: Reactor Safety & Flowsheet Design

Exothermic Oxidation Reactor (R-101) Safety Integrity & Relief Sizing

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Executive Summary

This design specification outlines the process flowsheet, safety instrumented interlocks, and pressure relief parameters for the new exothermic liquid-phase oxidation reactor R-101. A detailed Hazard and Operability (HAZOP) study identifies cooling water loss as the controlling hazard, posing a critical risk of thermal runaway and autocatalytic product decomposition. To mitigate this risk, an active Safety Instrumented System (SIS) is configured with redundant 2oo3 temperature sensors to trigger feed isolation. As a final barrier, a rupture disk in series with a balanced bellows pressure safety valve is sized using the DIERS Homogeneous Equilibrium Model (HEM). The system is designed for a peak two-phase flow rate of $42,500$ kg/h at a set pressure of 10.0 barg, venting safely to the low-pressure flare header.

Contents

1 Introduction & Project Scope

This document details the process flowsheet design and safety specifications for Project Aether at the **Meridian Chemical Technologies** facility in Bayport, Texas. The project entails the installation of a new, highly exothermic liquid-phase oxidation reactor system (R-101) designed to convert hydrocarbon reactant A to intermediate compound B. Due to the high reaction enthalpy ($\Delta H_r = -125$ kJ/mol) and the volatile nature of the solvent system, this process poses significant risk of thermal runaway and subsequent overpressurization.

To mitigate these risks and ensure compliance with global safety standards, including OSHA Process Safety Management (PSM) regulations and Center for Chemical Process Safety (CCPS) guidelines [1, 2], a comprehensive process safety and flowsheet design specification has been established.

1.1 Objectives

The primary objectives of this design specification are to:

- Define the process flowsheet and establish material balance parameters under normal operating conditions.
- Detail the instrumentation and automated safety control loops (Basic Process Control System, BPCS, and Safety Instrumented System, SIS) surrounding the reactor.
- Document a preliminary Hazard and Operability (HAZOP) study for the reactor node to identify potential deviations, consequences, and required safeguards.
- Specify the sizing methodology and design parameters for the primary reactor relief system, consisting of a rupture disk in series with a pressure safety valve (PSV), in compliance with API Standards 520 and 521 [3, 4].

1.2 Safety Design Philosophy

Our engineering approach aligns with the principles of inherently safer design (ISD) proposed by Trevor Kletz [5], emphasizing minimization and moderation. Where inherent safety cannot fully eliminate hazards, we deploy robust active and passive protection layers. As illustrated in this specification, these layers include:

1. **Prevention (BPCS):** Standard temperature, pressure, and flow controllers to maintain steady-state operation.
2. **Mitigation (SIS):** Automated reactor emergency shutdown (ESD) loops to cut off feed and initiate emergency nitrogen purge in the event of coolant failure.
3. **Protection (Relief System):** A dual-barrier relief system designed to vent vapor and liquid fractions safely to the flare header in a worst-case runaway scenario.

2 Process Description & Material Balance

The process involves the catalytic liquid-phase oxidation of Reactant A using compressed air as the source of oxygen. The reaction is carried out in a continuous stirred tank reactor (R-101), equipped with a high-efficiency cooling jacket and an emergency deluge coil.

2.1 Chemical Reaction and Kinetics

The primary oxidation reaction is highly exothermic and proceeds via a free-radical mechanism catalyzed by a soluble cobalt-manganese metal complex. The reaction stoichiometry is simplified as:

$$\text{A (liq)} + \text{O}_2\text{ (g)} \xrightarrow{\text{Cat.}} \text{B (liq)} \quad \Delta H_r = -125 \text{ kJ/mol} \tag{1}$$

A secondary decomposition reaction of the product B can occur if the reactor temperature exceeds the thermal threshold of 115°C. This decomposition is autocatalytic, extremely exothermic

($\Delta H_d = -340$ kJ/mol), and generates rapid non-condensable gas release:

$$\text{B (liq)} \xrightarrow{\text{Thermal Runaway}} \text{C (g)} + \text{D (g)} \quad \Delta H_d = -340 \text{ kJ/mol} \tag{2}$$

Thus, strict temperature control is critical to prevent the reaction from transitioning from the controlled oxidation state to the runaway decomposition regime.

2.2 Process Flow and Stream Data

Reactant A (Stream 1) and the solvent containing dissolved catalyst (Stream 2) are fed continuously to R-101. Compressed air is sparged into the bottom of the reactor. The reaction temperature is maintained at 85°C by circulating cooling water through the reactor jacket (Streams 3 and 4). Under steady-state conditions, the liquid product mixture is continuously withdrawn from the reactor (Stream 5) to maintain a constant liquid holdup of 70%.

Table 1 summarizes the stream properties and material balance under normal operating conditions.

Table 1: Material Balance and Stream Properties under Normal Operating Conditions.

Stream	Description	Phase	Temp. (°C)	Press. (barg)	Flow (kg/h)	Key Components
1	Reactant A Feed	Liquid	25.0	5.0	2,500	Hydrocarbon A
2	Solvent & Catalyst	Liquid	20.0	5.0	1,200	Toluene, Co/Mn Cat.
3	Cooling Water In	Liquid	15.0	4.5	35,000	H_2O
4	Cooling Water Out	Liquid	28.5	3.8	35,000	H_2O
5	Product Stream	Liquid	85.0	3.0	3,700	Product B, Solvent
6	Reactor Vent Line	Vapor	85.0	3.0	150	N_2, unreacted O_2

2.3 Reactor Design Specifications

The reactor R-101 is designed to withstand both high pressures and severe thermal gradients. The mechanical and process design specifications are detailed in Table 2.

Table 2: Reactor Mechanical and Process Design Parameters.

Parameter	Value	Unit
Vessel Volume	10.0	m^3
Normal Operating Liquid Level	7.0	m^3 (70%)
Operating Temperature	85.0	°C
Operating Pressure	3.0	barg
Design Pressure	10.0	barg
Design Temperature	150.0	°C
Heat Transfer Area (Jacket)	24.0	m^2
Overall Heat Transfer Coeff. (U)	450.0	$W/m^2{\cdot}K$
Vessel Material of Construction	316L SS	–

3 Flowsheet Design & Safety Configuration

The piping and instrumentation design for the oxidation reactor (R-101) incorporates multiple layers of protection, spanning basic process control, safety instrumented shutdowns, and passive relief barriers. Figure 1 illustrates the flowsheet and safety instrumentation schematic.

3.1 Basic Process Control System (BPCS)

The BPCS manages the normal steady-state operation of the reactor. The key loops include:

- **Reactor Temperature Control (TC-101):** Consists of temperature transmitter TT-101, which transmits a signal to the DCS. The DCS executes a PID algorithm to modulate the cooling water inlet valve TCV-101.

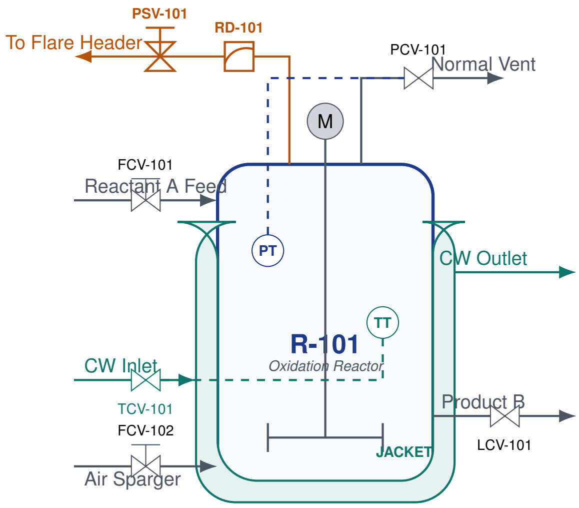

Figure 1: Process Flow and Piping & Instrumentation Diagram (P&ID Schematic) of the Reactor Safety Systems.

- **Reactor Pressure Control (PC-101):** Pressure transmitter PT-101 monitors head-space pressure and modulates vent valve PCV-101 to maintain pressure at 3.0 barg.
- **Liquid Level Control (LC-101):** Level transmitter LT-101 (not shown) modulates LCV-101 on the product outlet line to prevent gas blow-through and maintain liquid volume at 7.0 m^3.

3.2 Safety Instrumented System (SIS) Interlocks

To protect against common-cause failures (e.g., cooling water loss, controller freeze), a separate safety instrumented system (SIS) operates independently of the BPCS. The SIS triggers safety-critical actions if safe operating envelopes are violated:

- **Interlock I-101 (High Temperature / Emergency Shutdown):** If the reactor temperature exceeds 98°C, the SIS closes FCV-101 and FCV-102 to cut off reactant and air feeds, and opens an emergency nitrogen sweep to purge oxygen from the headspace.
- **Interlock I-102 (High Pressure / Emergency Depressurization):** If the pressure exceeds 5.5 barg, the SIS initiates emergency depressurization through an automated blowdown valve (not shown) routed directly to the low-pressure flare.

3.3 Passive Relief Barrier

As a final layer of defense against mechanical failure, reactor R-101 is equipped with a rupture disk (RD-101) in series with a spring-loaded pressure safety valve (PSV-101) set at the vessel design pressure of 10.0 barg. Placing a rupture disk upstream of the PSV protects the valve from corrosive reactant vapors and prevents any leakage of toxic components during normal operation. A pressure gauge and bleed valve are installed in the interspace between the disk and the valve to monitor for disk pinhole leaks.

4 Hazard & Operability (HAZOP) Study

A Hazard and Operability (HAZOP) study was conducted for the reactor node (Node 1) to systematically evaluate potential deviations from the design intent, analyze their consequences, and verify the adequacy of existing safeguards in accordance with CCPS guidelines [1].

4.1 Node Definition

- **Node 1:** Reactor R-101 vessel shell, cooling jacket, feed lines (Reactant A, Solvent, Catalyst, Air), and product outlet line up to the first isolation valve.
- **Design Intent:** Continuous liquid-phase oxidation of Reactant A at 85°C and 3.0 barg with continuous cooling jacket heat removal.

4.2 HAZOP Analysis Matrix

Table 3 summarizes the key findings of the HAZOP study. Special attention is given to deviations that could trigger a thermal runaway reaction.

Table 3: HAZOP Analysis Matrix for Node 1: Reactor R-101.

Deviation	Potential Cause	Consequence	Safeguards	Recommendations
High Temp.	TCV-101 fails closed, or jacket fouling.	Reaction acceleration. Temp > 115°C triggers autocatalytic decomposition of Product B. Solvent vaporization causes rapid overpressure.	• TT-101 high alarm in DCS. • SIS Interlock I-101 feed cutoff. • Rupture disk RD-101 and PSV-101.	Install redundant TT-102 to form a 2oo3 voting logic in the SIS shutdown loop.
High Flow (Reactant A)	FCV-101 fails wide open.	Excess reactant concentration increases heat generation beyond cooling capacity (1.2 MW), leading to thermal runaway.	• High flow alarm on FT-101. • Reactor temp alarm TT-101. • SIS Interlock I-101 feed cutoff.	Ensure FCV-101 has Class VI rating; configure hardware-based limit on control signal.
No Flow (Cooling Water)	Pump trip or cooling water header failure.	Loss of cooling. Temp rises at 4.2°C/min, reaching decomposition within 7 minutes.	• Cooling water flow FT-103 alarm. • SIS emergency feed shutdown.	Provide emergency backup firewater connection, automated via TCV-102.
High Pressure	PCV-101 fails closed, or nitrogen regulator fails high.	Reactor pressure rises. Vessel rupture if pressure exceeds design pressure (10 barg).	• PT-101 high alarm in DCS. • Rupture disk RD-101 bursts at 10.0 barg. • PSV-101 opens at 10.0 barg.	Install continuous pressure transmitter (PT-103) in the RD/PSV interspace.

4.3 Discussion of Key Findings

The HAZOP study indicates that the loss of reactor cooling is the most critical hazard path, representing a high-consequence scenario with a short time-to-runaway. Reliance on the basic process control system (BPCS) is insufficient to achieve tolerable risk. Therefore, the implementation of the Safety Instrumented System (SIS) is mandatory. The sizing of the relief system (discussed in Section 5) must assume the failure of both the BPCS and SIS to act, acting as the ultimate passive protection layer.

5 Pressure Relief & Flare System Sizing

The emergency relief system for reactor R-101 is sized using the DIERS methodology for runaway chemical reactions, in compliance with API Standards 520 and 521 [3, 4]. Due to liquid swell, two-phase (gas-liquid) flow is expected during venting.

5.1 Design Basis and Sizing Methodology

The controlling scenario is a **loss of cooling water leading to runaway reaction**. This scenario produces the highest required mass venting rate due to solvent vaporization and autocatalytic product decomposition.

The required relief area (A) is calculated using the Homogeneous Equilibrium Model (HEM) for choked flow:

$$A = \frac{W_v}{K_d \cdot G_c} \tag{3}$$

where W_v is the peak venting rate (42,500 kg/h), K_d is the discharge coefficient (0.85), and G_c is the critical two-phase mass flux (3,250 $\mathrm{kg/m^2 \cdot s}$) calculated by integrating the momentum equation:

$$G_c = \rho_t \sqrt{2(h_0 - h_t)} \tag{4}$$

Here, ρ_t and h_t represent fluid properties at the throat, and h_0 is the stagnation enthalpy.

5.2 Relief Device Sizing Parameters

Table 4 presents the design parameters for the RD-101 and PSV-101 relief system.

5.3 Piping Pressure Drop Constraints

Per API 520 Part II, the inlet piping pressure drop must not exceed 3% of the set pressure to prevent valve chatter. The 3-inch inlet line layout limits the friction loss to 0.21 bar (2.1%). The backpressure on the outlet line is limited by using a balanced bellows PSV, which tolerates backpressures up to 50%.

Table 4: Design and Sizing Parameters for Rupture Disk RD-101 and PSV-101.

Parameter	Value	Unit
Controlling Scenario	Thermal Runaway	–
Relief Phase	Two-phase (HEM)	–
Required Flow (W_v)	42,500	kg/h
Set Pressure of PSV-101	10.0	barg
Burst Pressure of RD-101	9.5	barg at 115°C
Accumulation	10% (11.0 barg)	–
Calculated Throat Flux (G_c)	3,250	kg/m^2·s
Minimum Required Area	1,776	mm^2
Selected Orifice (API 526)	L (1,841 mm^2)	–
PSV Inlet / Outlet Line Size	3 / 4	inches

The 4-inch discharge line to the flare header has a calculated backpressure of 3.5 barg (35%), which satisfies all design constraints.

6 Conclusion & Recommendations

The process safety and flowsheet design for the R-101 reactor system on Project Aether has been executed in accordance with industry best practices and corporate risk criteria. By combining active process controls, safety instrumented shutdowns, and a robust passive relief system, the project achieves a highly reliable, layered defense against thermal runaway and overpressure.

6.1 Summary of Action Items and Recommendations

Based on the HAZOP study (Section 4) and relief sizing calculations (Section 5), the following engineering actions must be completed prior to the Pre-Startup Safety Review (PSSR):

1. **SIS Instrumentation Upgrade:** Implement 2oo3 voting logic for reactor temperature (TT-101A/B/C) and pressure (PT-101A/B/C) transmitters to reduce failure probability and spurious trips.
2. **Backup Cooling Integration:** Finalize design for the emergency jacket deluge line, activated via fail-open valve (TCV-102) on loss of utility water pressure.
3. **Valves and Solenoids Specification:** Specify feed cutoff valves (FCV-101/102) as Class VI tight-shutoff and equip them with dedicated safety-rated solenoid valves.
4. **Relief Interspace Monitoring:** Install pressure transmitter (PT-103) in the RD-101/PSV-101 interspace with a DCS high-pressure alarm to detect disk leakage.
5. **Inspection Schedule:** Establish a PM routine: replace the rupture disk every 2 years and bench-test/recalibrate the PSV annually.

6.2 Regulatory Compliance Statement

The design detailed herein conforms to the safety guidelines of OSHA 29 CFR 1910.119 (Process Safety Management) and matches the quantitative risk reduction targets specified by the ISA-84/IEC-61511 standards for Safety Instrumented Systems in the process industry.

References

[1] Center for Chemical Process Safety (CCPS). *Guidelines for Hazard Evaluation Procedures*. 3rd. New Jersey: John Wiley & Sons, 2010.

[2] Daniel A. Crowl and Joseph F. Louvar. *Chemical Process Safety: Fundamentals with Applications*. 4th. Boston, MA: Pearson Education, 2019.

[3] American Petroleum Institute (API). *Sizing, Selection, and Installation of Pressure-Relieving Devices in Refineries – Part I: Sizing and Selection*. Standard API STD 520. Washington, D.C.: API, 2020.

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[5] Trevor Kletz. *Process Plants: A Handbook for Inherently Safer Design*. Boca Raton, FL: CRC Press, 2009.