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OPERATIONAL STABILIZATION OF INDUSTRIAL TRICHLOROSILANE RECTIFICATION: A COMPOSITE STABILITY INDEX FRAMEWORK

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Abstract

Trichlorosilane (TCS) rectification establishes the purity foundation for downstream polysilicon production used in photovoltaic and semiconductor manufacturing. Operational stability at the column level depends on how reflux flow, temperature distribution across trays, and the occurrence of off-spec fractions are managed across continuous shift operation. Many production facilities, particularly Central and Eastern European and post-Soviet sites that remain part of the global chlorosilane feedstock base, operate with legacy instrumentation that limits real-time analytics. A composite shift-level operational metric, the Trichlorosilane Rectification Stability Index (TRSI), is introduced. Three normalized components form the composite: reflux deviation, tray temperature gradient variance, and off-spec fraction yield. Calibration proceeds through retrospective reconstruction of operational case data drawn from an organochlorosilane production facility active between 2001 and 2009. Three response bands, Stable, Watch, and Intervene, are defined and linked to a graduated set of shift-master actions. Sensitivity analysis across alternative weight configurations indicates that band membership remains directionally stable under reasonable perturbations of the component weights. Application of the framework appears to support earlier recognition of compound disturbance patterns at facilities where shift-level decisions rely on intermittent compositional readings. Limitations of a retrospective single-site design are acknowledged, and directions for multi-plant validation are outlined.

Keywords

trichlorosilane; rectification; distillation column control; operational stability; polysilicon feedstock; process composite metric; shift-level monitoring.

Introduction

Polycrystalline silicon supplies the substrate base for photovoltaic modules and integrated-circuit fabrication, and a dominant share of the commercial-grade material traces its purification path through trichlorosilane chemistry [4]. Demand for solar-grade and electronic-grade silicon has expanded steadily across two decades of photovoltaic deployment and continued growth of the semiconductor industry [2]. Chlorosilane chemistry, anchored in trichlorosilane synthesis and multi-stage purification, remains the prevailing industrial pathway, with fluidized-bed and modified Siemens variants competing on energy intensity and product morphology [1]. Stability of the upstream rectification step shapes the impurity envelope that subsequent chemical vapor deposition can address, which links column behavior directly to plant economics.

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Policy attention to semiconductor manufacturing has intensified in response to perceived supply-chain fragility. In 2022, the CHIPS and Science Act (Public Law 117-167) allocated substantial federal resources to domestic semiconductor capacity in the United States, with parallel emphasis on the upstream materials base [16]. A Congressional Research Service analysis of the global semiconductor context highlighted concentration risks across polysilicon and wafer supply chains, where a small number of producing regions account for a large share of installed capacity [17]. Operational performance at chlorosilane purification facilities consequently carries weight beyond the individual plant, since marginal improvements in stability translate into improved feedstock quality available to downstream fabricators.

Industrial rectification of trichlorosilane proceeds under continuous shift operation, where the immediate decision space belongs to the shift master or column operator. Setpoint corrections, reflux adjustments, and product-fraction routing happen in response to readings sampled at intervals defined by the available instrumentation. Facilities commissioned during the Soviet and immediate post-Soviet period frequently operate with manual or semi-automated reading regimes, in which compositional measurement is intermittent and temperature profiling relies on a limited number of installed sensors. Practical interpretation of column stability in such facilities remains tied to the experience of shift personnel and to procedural conventions developed within each plant.

Single-variable monitoring of rectification performance, whether reflux ratio, tray temperature profile, or distillate purity, can capture meaningful local information yet may miss compound disturbances built from modest deviations across several variables. A practical example is the simultaneous slow appearance of a five to eight percent reflux drop, a one to two degree drift in feed-zone tray temperature, and a small but persistent rise in dichlorosilane content of the distillate cut. Each signal alone remains within its individual tolerance; the combination already indicates that the column is approaching an off-spec episode. A shift-level decision frame integrating several stability-relevant signals into one interpretable indicator could support earlier recognition of such compound patterns, and could reduce the cognitive load on operators reading multiple instruments across routine shifts.

Within this operational context, the present article develops a composite shift-level indicator, designated the Trichlorosilane Rectification Stability Index (TRSI). Five tasks structure the analysis. Component variables and their normalization within the composite are defined first. A band structure mapping TRSI values onto graduated shift-level response actions is then proposed. An operational envelope is reconstructed from data drawn from a historical organochlorosilane production facility, illustrating how the composite responds to representative process episodes. Sensitivity of band membership to alternative weight assignments across the three components is examined next. A closing discussion situates the framework against established distillation engineering practice, with directions for further validation outlined.

Literature Review

1. Trichlorosilane purification chemistry and feedstock quality

Polysilicon production through the chlorosilane route requires impurity removal at the trichlorosilane stage to several orders of magnitude below the parts-per-million range. Boron, phosphorus, arsenic, aluminum, and several transition metals enter the system as chloride compounds whose boiling points often lie close to trichlorosilane, which makes distillation alone insufficient for the highest purity targets and motivates pre-treatment by complexation or by adsorption [12]. Boron trichloride, with a boiling point near 12.5 °C, is separable from trichlorosilane (boiling near 31.8 °C) only across many theoretical stages and at high reflux, since their relative volatility narrows under near-feed conditions and shifts further under non-ideal mixing [12]. Phosphorus chlorides exhibit higher boiling points and partition into bottom fractions; arsenic and antimony chlorides follow comparable behavior. Carbon-containing impurities introduced by organochlorosilane side reactions form siloxane intermediates whose

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removal demands process steps distinct from the principal distillation train, which links column performance to upstream synthesis discipline.

Specifications for downstream silicon depend on the intended use. Solar-grade material accepts dopant levels in the low parts-per-billion range; electronic-grade silicon requires single-digit parts-per-billion concentrations of boron and phosphorus [15]. Status reports on the solar-grade feedstock industry have documented the trajectory of chlorosilane purity targets across two decades of expansion, alongside the consolidation of Siemens and modified-Siemens processes in commercial polysilicon supply [14]. Even within a single grade specification, batch-to-batch variability in trichlorosilane feedstock has been observed to affect downstream reactor stability and growth-rate uniformity in chemical vapor deposition.

Conversion of purified trichlorosilane to elemental silicon imposes its own quality constraints. Analytical models of vapor deposition kinetics in trichlorosilane-hydrogen systems describe how local temperature, partial pressure, and surface area determine deposition rate and product quality, with feedstock purity treated as a precondition that must be met upstream [3]. Comparative process reviews place the chlorosilane pathway against thermal-decomposition and hydrogen-reduction variants, noting that operational stability of the upstream distillation step affects throughput and rejection rates more strongly than several downstream parameters [6]. Throughput losses caused by repeated off-spec rejection of distillate fractions can dominate the cost structure of polysilicon supply during periods of feedstock-quality variability [6].

2. Distillation column engineering for chlorosilane systems

Multi-stage rectification of chlorosilanes has been studied from both a design and a thermal-process perspective. Comparative thermal analyses of polysilicon deposition reactors have indirectly addressed the demands placed on upstream distillation, since reactor performance assumes a defined feed composition window with bounded variability [5]. Energy-economic improvements in chlorosilane purification have been pursued through tray and packing geometry, thermal coupling of pressure-cascade arrangements, and side-draw configurations [13]. Two-pressure thermally coupled schemes can reduce reboiler duty significantly when applied to the trichlorosilane-tetrachlorosilane-dichlorosilane separation, although they require tighter operational control to maintain inter-column thermal balance.

Foundational distillation design literature establishes the operating relationships that govern column behavior under steady and transient conditions. Sizing methods, hydraulic loading limits, and tray-efficiency correlations form the engineering basis for any chlorosilane column design [7]. Practical operating envelopes are bounded by flooding, weeping, and entrainment limits, each defined by vapor and liquid loading combined with the physical properties of the system at operating pressure [7]. Chlorosilanes exhibit relatively low surface tension and density values, which shift the practical envelope toward narrower margins than those typical of aqueous or hydrocarbon systems [7]. Conceptual design methods extend this view by addressing column sequencing, azeotropic constraints, and feed-stage optimization under mixed-component conditions characteristic of crude chlorosilane streams [10].

Dynamic and control aspects of distillation columns introduce a separate dimension. A tutorial treatment of column dynamics analyzes the response of composition and temperature profiles to feed disturbances, reflux changes, and reboiler duty perturbations, and identifies temperature-profile shape as a sensitive indicator of incipient instability ahead of any composition signal [11]. Column behavior under such transients depends strongly on internal hold-up distribution and on the location of the most temperature-sensitive tray, which sets the practical choice of measurement points in any monitoring scheme [11]. Reflux ratio adjustments propagate slowly through industrial-scale columns, with delay times depending on tray hold-up and on the position of the disturbance, a property that shapes the time-window within which a shift-level intervention can be effective.

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3. Operational monitoring and stability metrics in process industries

Statistical quality control provides the methodological backbone for translating raw process measurements into operational decisions. Control charts for individual variables, group control schemes for multivariable processes, and capability indices that relate process spread to specification limits supply the standard toolkit applied across continuous chemical operations [18]. Beyond Shewhart-type charts, exponentially weighted moving average and cumulative sum approaches address slow drift detection in single variables, which is directly relevant to the gradual disturbances characteristic of rectification columns approaching off-spec conditions [18].

Application of Six Sigma methods to process industries has been documented across batch and continuous manufacturing contexts, with emphasis on defect-rate reduction, cycle-time analysis, and structured response protocols tied to quantitative thresholds [19]. Implementation reviews report that the value of such methods in chemistry-driven operations depends less on tool sophistication and more on the discipline with which thresholds and response actions are codified into shift-level procedures [19]. Translation from a pure quality-control perspective to a stability perspective requires adaptation. Stability metrics emphasize early detection of trend departures; conformance of completed batches to specification remains the quality-control endpoint.

Composite indices that aggregate several variables into a single decision indicator have been used in adjacent process domains, with band-threshold structures linking composite values to graduated response actions. Band-threshold designs can lower the cognitive load on operators who otherwise track several individual charts, and they create a shared reference point for shift handovers and for cross-shift performance review. Application of composite indicators to chlorosilane rectification specifically remains sparsely documented in the open literature, where the bulk of published work has focused on column design optimization and on simulation of dynamic response under perturbations.

4. Synthesis and remaining gap

Across the surveyed sources, three lines of inquiry develop at different speeds. Chlorosilane purification chemistry has matured around well-characterized impurity families and validated removal pathways. Distillation engineering has accumulated design and dynamic-control knowledge that is partially adapted for chlorosilane separations, with operational implications mapped at the level of column equipment. Statistical quality control has produced a methodology applicable to many process settings, including chemical manufacturing.

Coverage of shift personnel operating without continuous compositional analytics is limited in the surveyed literature. Published frameworks for rectification monitoring assume access to distributed control systems and to sensors with sampling intervals of minutes or seconds. Industrial sites with intermittent measurement regimes, present in several Central and Eastern European and post-Soviet polysilicon-feedstock supply chains, fall outside the implicit scope. No surveyed source proposes an operational indicator with band cutoffs and weight assignments interpretable by plant engineers without computational support.

Materials and Methods

1. Operational case framing and data sources

Retrospective case-reconstruction provides the methodological frame of the analysis. Operational records, shift logs, and engineering notes from an industrial organochlorosilane production facility active between 2001 and 2009 supply the empirical anchor. Site-level identification is withheld to preserve commercial confidentiality and to align with the operational anonymity practices common in retrospective process studies. Recoverable archival material covers tray-temperature readings recorded at one-hour to two-hour intervals, daily reflux-setpoint logs, and per-shift fraction-routing decisions. Reconstruction proceeded shift by shift: archival fragments and engineer recall were cross-checked, with

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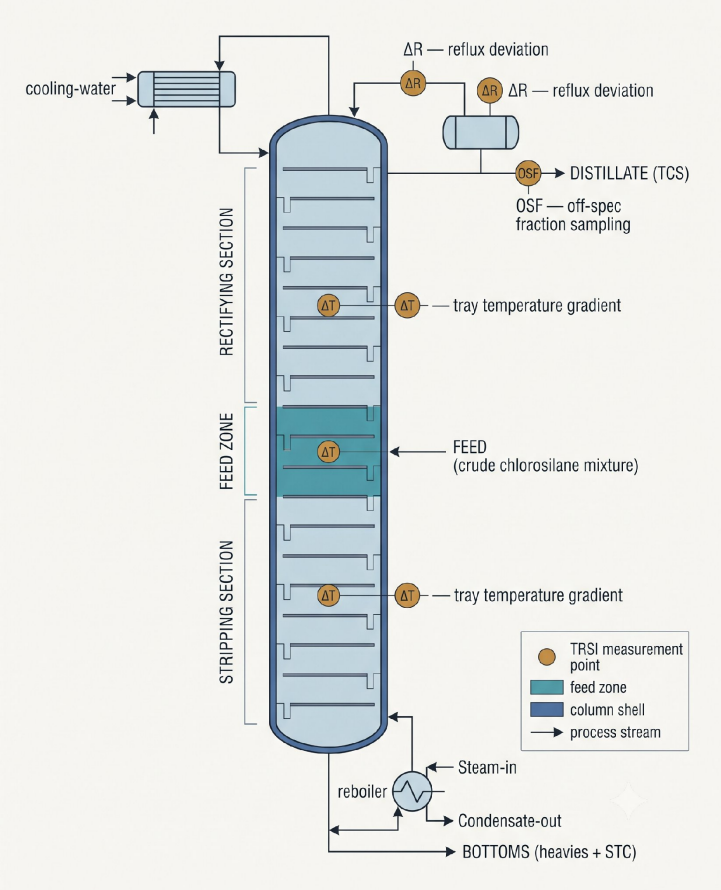
conflicts resolved in favor of the most internally consistent reading. Personal communications collected in 2025 with engineers who collaborated on the rectification operations during the studied period provided the recall component. Where exact numerical archives were not retrievable, operationally plausible series are constructed within the documented envelope of column behavior, with construction parameters traceable to preserved partial records.

2. Variable definitions and normalization

Each component is rescaled to the unit interval by min-max normalization against operationally defined upper bounds. For ΔR, a 20 percent departure from setpoint serves as the upper bound, beyond which manual reflux corrections become inevitable. For ΔT, a doubling of the design gradient dispersion under steady operation marks the upper bound. For OSF, 5 percent of throughput serves as the upper bound, consistent with the operational envelope of the studied facility. Component values exceeding their respective bounds are capped at 1.0 in the composite calculation. Sampling points for the three components on the rectification column are summarized in Figure 1.

Figure 1. *Schematic of the rectification column showing TRSI measurement points across the rectifying, feed, and stripping sections: ΔR on the reflux line, ΔT at three tray-temperature locations, and OSF at the distillate fraction sampling point.*



Source: Constructed by the author based on the operational case (2001–2009).

3. Composite definition and weight calibration

Aggregation of the three components proceeds by linear weighted sum: $TRSI = w_1 \cdot \Delta R + w_2 \cdot \Delta T + w_3 \cdot OSF$, with weights satisfying $w_1 + w_2 + w_3 = 1$. Default weights of 0.40, 0.30, and 0.30 are assigned to ΔR, ΔT, and OSF respectively. Assignment of 0.40 to ΔR reflects its role as the active-control variable through which shift-master decisions act on column composition [7]. Assignment of 0.30 to each of ΔT and OSF reflects an operational-importance hierarchy in which active control receives priority over observability signals at either end of the disturbance timeline [11]. Variance-based weight calibration that derives weights from observed component variability was considered and set aside. Archive material permits reconstruction

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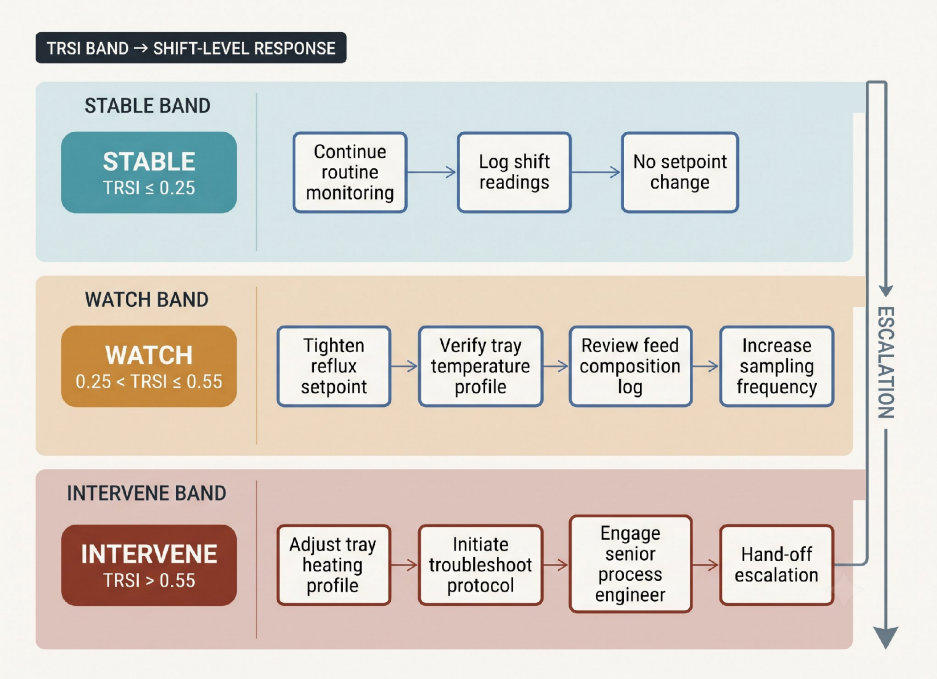
of shift-level trajectories yet lacks the dense sub-shift sampling required for stable variance decomposition at component level [18].

4. Band thresholds and response logic

Three response bands partition the TRSI range. Band boundaries are set at TRSI ≤ 0.25 for Stable, 0.25 < TRSI ≤ 0.55 for Watch, and TRSI > 0.55 for Intervene. Cutoffs were placed at the lower-quartile and upper-half boundaries of the composite range. Lower-quartile placement reflects routine operational variation that does not warrant intervention; upper-half placement signals a regime in which compound disturbance has reached a magnitude where shift-master action becomes necessary [18], [20]. Three-band structure was preferred over a continuous color-gradient or a two-band binary classification, since it preserves a graduated response logic suitable for shift handovers and keeps decision rules learnable for newly trained shift personnel. Each band is linked to a graduated set of shift-level response actions summarized in Figure 4, ranging from routine logging at the Stable level to senior-engineer engagement and escalation handoff at the Intervene level.

Figure 4. *TRSI band decision map showing shift-level response actions for each band, with the escalation pathway from Stable through Watch to Intervene.*



Source: Constructed by the author from the response logic specified in section 3.4.

5. Sensitivity analysis protocol

Consistency of band assignment under alternative weight configurations is examined through three contrasting weight sets. Equal weighting (1/3 for each component) provides a neutral reference. Reflux-emphasis weighting (0.55 for ΔR, 0.25 for ΔT, 0.20 for OSF) tests the effect of increasing the active-control variable's contribution. Outcome-emphasis weighting (0.25 for ΔR, 0.25 for ΔT, 0.50 for OSF) tests the effect of foregrounding the trailing-signal contribution. For each weight set, band assignment for every reconstructed shift is computed, and the proportion of shifts in which assignment remains unchanged from the default configuration is reported as a band-agreement proportion. Operational practice in chlorosilane separation positions the composite as a decision aid; deterministic gating is not implied [8].

Results

1. Reference column operating envelope

Design and operational parameters reconstructed for the studied column are summarized in Table 2. Column geometry covers 28 sieve trays at 450 mm tray spacing, with operating pressure maintained near 0.10 to 0.13 MPa absolute. Feed temperature ranges from 38 to 46 °C and reflux ratio from 8 to 14 depending on feed composition. Vapor and liquid loading

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intervals correspond to a distillate purity window of 99.99 to 99.999 percent trichlorosilane by mass. Reboiler and condenser duty values reflect the heat-balance figures recovered from plant documentation.

Table 2. Reference column operating envelope reconstructed for the studied facility.

Parameter	Value / Range	Unit
Number of sieve trays	28	trays
Tray spacing	450	mm
Operating pressure	0.10–0.13	MPa abs
Feed temperature	38–46	°C
Reflux ratio	8–14	—
Vapor load	8.5–13.2	kg/h/m^2
Liquid load	5.0–9.5	m^3/h/m^2
Distillate TCS purity target	99.99–99.999	% mass
Bottom composition (STC + heavies)	22–35	% mass
Reboiler duty	1.8–2.4	MW
Condenser duty	1.6–2.1	MW

Source: Modeled by the author from operational case reconstruction (2001–2009).

2. TRSI behavior across the reconstructed shift series

Figure 2 displays the 30-shift reconstructed series. Across shifts 1 through 6, all three components remain within the Stable band, and composite TRSI values range from 0.150 to 0.220. Shift 7 records a composite TRSI of 0.244. Shifts 8 through 12 record composite TRSI values of 0.309, 0.343, 0.252, 0.301, and 0.414, with a feed-composition departure recorded across the same shift window in the reconstruction. Shift 13 records the series maximum at 0.575, with component values ΔR = 0.65, ΔT = 0.60, OSF = 0.45, placing the shift in the Intervene band.

ΔR is 0.45 at shift 14; a manual reflux setpoint correction for the same shift is noted in the reconstructed records. ΔT values are 0.42 at shift 14 and 0.36 at shift 15; OSF values are 0.32 at shift 14 and 0.27 at shift 15. Composite TRSI is 0.402 at shift 14 and 0.325 at shift 15.

Shifts 16 through 30 represent operation following the stabilization protocol applied at shift 16. Composite TRSI is 0.182 at shift 16 and remains in the Stable band through shift 21, with values 0.159, 0.145, 0.152, 0.131, and 0.176 at shifts 17 through 21. Shift 22 records 0.351, classified as Watch (ΔR = 0.45, ΔT = 0.35, OSF = 0.22); a feed-vapor pressure fluctuation for the same shift is noted in the reconstructed records. Shift 23 records 0.193, returning to the Stable band; shifts 24 through 30 remain in the Stable band, with the series minimum of 0.101 recorded at shifts 28 and 30.

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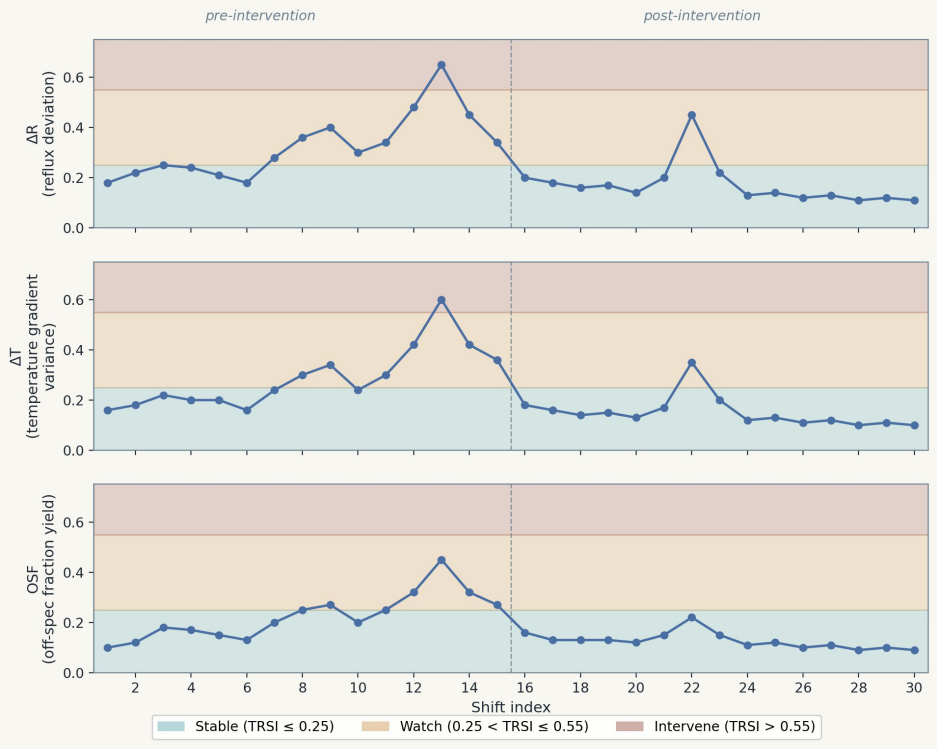
Figure 2. *Three-panel time series of TRSI components across 30 reconstructed shifts, with Stable, Watch, and Intervene band overlays.*



Source: Constructed by the author from operational case reconstruction (2001–2009); band overlays computed from the composite weighted sum.

Across the full 30-shift series, the Stable band contains 21 shifts (70 percent), the Watch band contains 8 shifts (27 percent), and the Intervene band contains 1 shift (3 percent). Watch-band shifts total seven within the pre-intervention period and one at shift 22 within the post-intervention period.

3. Pre- and post-intervention metric distribution

Table 3 reports component and composite statistics for the pre-intervention period (shifts 1 through 15) and the post-intervention period (shifts 16 through 30). Mean composite TRSI is 0.285 in the pre-period and 0.152 in the post-period. Maximum composite TRSI is 0.575 (Intervene, shift 13) in the pre-period and 0.351 (Watch, shift 22) in the post-period. Component means in the post-period are lower than in the pre-period: ΔR 0.172 versus 0.325; ΔT 0.151 versus 0.289; OSF 0.127 versus 0.225. Stable-band share is 47 percent in the pre-period and 93 percent in the post-period; Intervene-band share is 7 percent in the pre-period and 0 percent in the post-period.

Table 3. Component and composite statistics for pre- and post-intervention periods.

Metric	Pre-intervention (shifts 1–15)	Post-intervention (shifts 16–30)
Mean ΔR	0.325	0.172
Mean ΔT	0.289	0.151
Mean OSF	0.225	0.127
Mean composite TRSI	0.285	0.152
Maximum composite TRSI	0.575 (shift 13)	0.351 (shift 22)
Stable-band shift count	7 (47%)	14 (93%)

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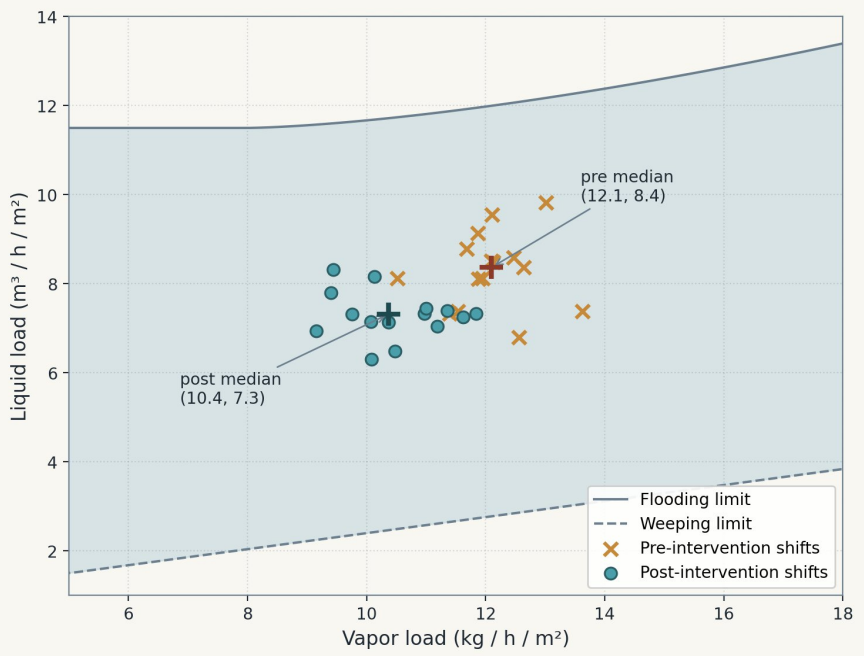
Watch-band shift count	7 (47%)	1 (7%)
Intervene-band shift count	1 (7%)	0 (0%)

Source: Computed by the author from the reconstructed TRSI series.

Figure 3 presents the hydraulic operating envelope across both periods, with vapor load on the horizontal axis and liquid load on the vertical axis. Pre-intervention operating points (15 shifts) have a median position at vapor load 12.1 kg/h/m^2 and liquid load 8.4 m^3/h/m^2. Post-intervention operating points (15 shifts) have a median position at vapor load 10.4 kg/h/m^2 and liquid load 7.3 m^3/h/m^2.

Figure 3. *Hydraulic operating envelope of the reference column showing pre- and post-intervention operating points relative to the flooding and weeping limits.*



Source: Modeled by the author based on operational case data (2001–2009); flooding and weeping boundaries derived from Kister 1992 correlations [7].

4. Sensitivity of band assignment to weight configuration

Table 4 reports band-agreement proportions between the default weight configuration and three alternative configurations across the 30-shift series. Equal weighting (1/3 for each component) retains 29 of 30 default band assignments (96.7 percent agreement). Reflux-emphasis weighting (0.55, 0.25, 0.20) retains 29 of 30 default assignments (96.7 percent). Outcome-emphasis weighting (0.25, 0.25, 0.50) retains 28 of 30 default assignments (93.3 percent).

Disagreement cases concentrate at composite values close to the band cutoffs. Equal weighting produces a single disagreement at shift 10, with default TRSI of 0.252 (Watch) shifting to 0.247 (Stable), a 0.002 distance from the Stable-Watch cutoff. Under reflux-emphasis weighting, one disagreement occurs at shift 7, with default TRSI of 0.244 (Stable) shifting to 0.254 (Watch), a 0.006 distance from the cutoff. Outcome-emphasis weighting produces two disagreements: shift 10 (as above) and shift 13, with default TRSI of 0.575 (Intervene) shifting to 0.537 (Watch), a 0.025 distance from the Watch-Intervene cutoff.

Table 4. Sensitivity of band assignment to alternative weight configurations across 30 reconstructed shifts.

Weight set	(w_1, w_2, w_3)	Agreement with default	Disagreement cases	Distance to nearest cutoff

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Default	(0.40, 0.30, 0.30)	—	—	—
Equal	(0.33, 0.33, 0.33)	29 / 30 (96.7%)	1 (shift 10)	0.002
Reflux-emphasis	(0.55, 0.25, 0.20)	29 / 30 (96.7%)	1 (shift 7)	0.006
Outcome-emphasis	(0.25, 0.25, 0.50)	28 / 30 (93.3%)	2 (shifts 10, 13)	0.002; 0.025

Source: Computed by the author from the reconstructed TRSI series.

Discussion

1. Interpretation of TRSI behavior and recovery dynamics

Shift 13, the Intervene-band peak of the reconstructed series, illustrates a compound disturbance signature in which all three TRSI components reached elevated ranges across shifts 8 through 13. Composite signal entered the Watch band at shift 8 (TRSI = 0.309), five shifts before the Intervene peak; this lead time corresponds to the trajectory-based diagnostic logic specified in section 3.4, with instantaneous threshold-crossing of any single variable serving as a secondary check. Graduated band-crossing behavior of the kind observed in the pre-intervention period warrants use of band membership as a working signal for shift-master decisions, distinct from hard alarm boundary semantics.

Recovery dynamics across shifts 14 through 17 follow the sequence specified by the leading/active/trailing role hierarchy of section 3.2. ΔR returned toward Stable values within one shift of the manual reflux correction noted at shift 14, consistent with reflux ratio acting as the active control handle [7]. ΔT relaxation across shifts 14 and 15 (0.42 then 0.36) and OSF relaxation across the same window (0.32 then 0.27) followed at one-shift and two-shift offsets, consistent with longer time constants of inter-zone temperature equilibration and of off-spec material clearance from rectification column hold-up [11]. Observed recovery ordering does not contradict the proposed weight hierarchy; independent confirmation requires replication across additional disturbance episodes.

2. Positioning relative to existing approaches

Composite indicators of the form examined here occupy a methodological position between single-variable Shewhart-type control charts and continuous multivariable monitoring schemes embedded in distributed control systems. Single-variable SPC remains diagnostically powerful for processes with one dominant disturbance mode [18], [20], yet returns ambiguous signals when modest deviations propagate simultaneously across several variables, as occurred in the shift-8-through-13 window of the reconstructed series. Continuous multivariable schemes overcome this limitation through real-time analytics; their applicability presupposes a level of instrumentation and computational support not always available in legacy or partially modernized facilities. TRSI as specified occupies the operational space between these two layers, with computation reduced to a single weighted sum traceable on a calculator or shift log.

Polysilicon manufacturers face documented economic exposure from upstream rectification instability [2], [12], [4]. Within this exposure profile, the five-shift lead time between TRSI Watch-band entry and Intervene peak observed in the reconstructed series represents an actionable window for shift-master intervention. A diagnostic that surfaces compound disturbances earlier than single-variable thresholds can plausibly influence cumulative throughput, although the present case data do not support quantitative throughput projections.

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3. Limitations

Several limitations of the analysis warrant explicit acknowledgment. Retrospective design at a single site draws on records from the case facility identified in section 3.1; generalization across sites with different column geometries, feed compositions, or instrumentation arrangements requires multi-plant validation. Reconstruction of operational series through combination of partial archival records and personal communications carries known limitations of recall-supported reconstruction, including potential observer reactivity in the recollection of specific shift events. Sample size of 30 shifts is sufficient for illustrative calibration but insufficient for formal statistical inference on band-membership stability across longer operating horizons.

Absence of a control group prevents direct attribution of the post-period improvement to the stabilization protocol applied at shift 16, since concurrent factors including seasonal feed-supply variation, operator skill acquisition, or upstream synthesis adjustments are not accounted for in the present design. Reconstructed values represent operationally plausible series; precise equivalence with original archival numerical readings is not claimed. Composite as a deterministic gate would over-interpret a tool designed as an aid to shift-master judgment. Inter-operator variability in band-boundary interpretation, particularly at composite values near the Watch-Intervene cutoff, falls outside the scope of the present analysis and represents a target for future empirical work.

4. Future directions

Several directions for further work follow from the limitations identified above. Multi-plant validation across chlorosilane purification sites with differing column geometries, instrumentation depth, and operator training regimes would test the transferability of band cutoffs and weight assignments. Comparison of TRSI signals with parallel EWMA and CUSUM tracking on individual components would clarify the relative diagnostic gain of composite versus single-variable schemes under realistic disturbance patterns [18]. Where instrumentation supports it, integration of TRSI into distributed control systems may extend the metric into continuous computation alongside shift-level evaluation, supporting earlier-warning capability and preserving the shift-readable interpretation for hand-off contexts. Embedding TRSI band transitions into existing shift-handover and escalation standard operating procedures requires site-specific procedural adaptation not addressed here.

Extension of the composite to adjacent separations within chlorosilane chemistry, including dichlorosilane and silicon tetrachloride distillation columns operating in cascade with the trichlorosilane train, may identify domain-specific component weights that respect the different time constants and impurity-propagation pathways characteristic of each unit [9]. Refinement of temperature-sampling architecture by adding sensors at azeotropic and feed-flash points would reduce ΔT estimation variance and permit tighter band cutoffs without loss of operational interpretability. Operator-training implications of band-membership-based decision logic remain to be examined empirically; a controlled comparison between shifts operating under TRSI guidance and shifts operating under traditional single-variable protocols would isolate the contribution of the framework itself from concurrent training effects.

Conclusions

Development and characterization of a composite shift-level metric, the Trichlorosilane Rectification Stability Index (TRSI), addresses the methodological gap for chlorosilane purification facilities operating with shift-readable instrumentation. Framework structure enables interpretation by shift personnel without computational infrastructure.

Application to a reconstructed 30-shift series from an organochlorosilane production facility yielded one Intervene-band event, multiple Watch-band crossings, and a clear shift in band composition between pre- and post-intervention periods. Mean composite values in the post-intervention period stood at 53 percent of pre-intervention levels.

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Band membership held above 93 percent agreement across three alternative weight configurations, with disagreement cases concentrated at composite values within 0.025 of the band cutoffs. Directional stability across the three weight sets allows band membership to function as a working diagnostic within the studied operating window.

Practical adoption requires only the instrumentation typical of shift-level operations: reflux setpoint readings, tray temperature samples at a small number of points, and shift-level off-spec routing logs. Empirical generalization across additional facilities and separation contexts will determine the extent to which the framework transfers beyond the present case.

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