WATER SCALE PRO

Technical White Paper

Thermodynamic Prediction of Mineral Scale Formation in Industrial and Oilfield Waters

Version 1.7

July 2026

waterscalepro.com

Contents

1. Executive Summary

Water Scale Pro is a cloud-delivered scale prediction platform that brings rigorous aqueous geochemistry to water treaters, production chemists, and facility engineers. It predicts the formation of thirteen common scale-forming minerals — including calcite, gypsum, barite, celestite, siderite, and halite — from a standard water analysis, at user-specified temperature and pressure.

Unlike simple index calculators, Water Scale Pro performs full aqueous speciation with a research-grade geochemical equilibrium engine, automatically selecting between an extended Debye–Hückel (B-dot) activity model for fresh and brackish waters and the Pitzer ion-interaction model for high-TDS brines. Predictions are reported as saturation index (SI), saturation level (SL = IAP/Ksp), and Momentary Excess — the mass of mineral that must precipitate to restore equilibrium, expressed in industry units including lbs per 1,000 bbl.

The platform also computes the traditional operational indices practitioners expect — Langelier (LSI), Ryznar (RSI), Puckorius (PSI), Larson–Skold, Stiff–Davis, and Oddo–Tomson — and clearly delineates where each is applicable. Results are delivered through a browser-based application with water blending (Multi-Mix), temperature and pressure sensitivity sweeps, branded PDF reporting, and an optional data-warehouse integration (ScaleConnect) that scores water analyses at scale directly from the customer's cloud data platform.

This white paper describes the computational methodology, the software architecture, and the validation approach behind the product, and states the assumptions and limitations that govern its applicable range.

2. The Mineral Scale Problem

Inorganic scale deposition is one of the most persistent and costly flow-assurance and asset-integrity problems in water-handling systems. In oil and gas production, mixing of incompatible waters (for example, sulfate-rich seawater with barium-rich formation brine), pressure drawdown, and temperature change drive precipitation of barite, celestite, calcite, and halite in tubing, chokes, and surface equipment. In industrial and municipal systems, calcium carbonate and calcium sulfate scales foul heat exchangers, membranes, and distribution piping, degrading heat transfer and throughput.

The economics are asymmetric: preventing scale with correctly selected chemistry and operating envelopes costs a small fraction of remediating it after deposition. Effective prevention, however, depends on accurate prediction — knowing which minerals will form, where in the temperature/pressure path they will form, and how much mass is available to deposit.

Historically, practitioners have relied on either (a) simple hand-calculated indices such as the Langelier Saturation Index, which are only valid in dilute waters and address only calcium carbonate, or (b) expensive desktop geochemistry packages that require specialist training and manual data entry. Water Scale Pro was built to close that gap: research-grade speciation thermodynamics, delivered through an

interface a field chemist can use in minutes, with outputs expressed in the units the industry actually works in.

3. System Overview

Water Scale Pro consists of four cooperating subsystems:

1. **Calculation engine.** A thermodynamics engine (ScaleEngine) that performs unit normalization, electroneutrality checking, rigorous aqueous speciation, temperature- and pressure-corrected solubility products, and saturation/mass-excess calculations for thirteen minerals.
2. **Web application.** A Streamlit-based front end providing guided data entry with quick-start presets (fresh water, seawater, oilfield brine), a Multi-Mix water blending workspace, interactive results with step-by-step derivations, charting, and PDF report export.
3. **Platform services.** A lightweight API service layer providing voice transcription for hands-free data entry, transactional and notification email, and durable persistence of saved analyses in a managed PostgreSQL store.
4. **ScaleConnect.** An optional enterprise integration that connects to a customer's cloud-based data platform, runs every pending water analysis through the same ScaleEngine, and writes saturation-index results back to the customer's environment on a configurable schedule.

A single calculation core serves every entry point — the interactive app, generated reports, and the ScaleConnect pipeline — so a given water analysis produces identical results regardless of how it enters the system.

4. Computational Methodology

4.1 Calculation Workflow

Every prediction follows a six-stage pipeline:

1. **Input normalization.** Ion concentrations are accepted in field units (mg/L or ppm) and converted to molarity using an internal molecular-weight table covering 28 aqueous species. Molarity is then converted to molality using the solution density, which matters materially for concentrated brines where 1 L of solution contains substantially less than 1 kg of water.
2. **Electroneutrality check.** The charge balance of the reported analysis is computed. Imbalances within ±5% are automatically reconciled by adjusting sodium or chloride (the standard makeup ions), and the adjustment is disclosed to the user. When pH must be estimated by the engine, the tolerance is tightened to ±0.01% to prevent charge-balance artifacts from contaminating the computed pH.
3. **Aqueous speciation.** The full analysis is passed to the embedded geochemical equilibrium solver, which solves the coupled mass-action and mass-balance equations to yield free-ion molalities, ion-pair distributions, individual ion activities, ionic strength, and (when not supplied) pH.

4. **Carbonate system resolution.** Alkalinity and carbonate speciation are derived from the speciated bicarbonate and carbonate concentrations using exact analytic temperature expressions for the carbonate equilibrium constants.
5. **Solubility products at T and P.** For each mineral, log Ksp is evaluated at the system temperature from fitted polynomial expressions anchored to published thermodynamic data, then corrected for pressure via a molar-volume (ΔV) correction term.
6. **Saturation state and mass excess.** The ion activity product (IAP) is assembled from speciated activities and compared against Ksp to produce the saturation level, saturation index, qualitative risk classification, and Momentary Excess for each mineral.

4.2 Aqueous Speciation and Activity Models

The central accuracy problem in brine chemistry is non-ideality: in concentrated solutions, the effective (thermodynamic) concentration of an ion diverges sharply from its analytical concentration. Water Scale Pro addresses this by computing activities, not concentrations, through full speciation — and by selecting the activity model appropriate to the water's ionic strength:

- **B-dot (extended Debye–Hückel) model** for ionic strength below 0.5 molal — fresh, potable, brackish, and most surface waters. This regime uses a standard thermodynamic database validated for dilute-to-moderate ionic strengths.
- **Pitzer ion-interaction model** for ionic strength of 0.5 molal and above — produced brines, seawater and evaporated seawater, and other high-TDS systems. The Pitzer formalism, with its virial expansion in binary and ternary ion-interaction parameters, remains accurate to halite saturation and beyond, where Debye–Hückel-family models fail.

The switch is automatic and reported with every result, so users always know which formalism produced their numbers. Speciation itself accounts for ion pairing (e.g., $CaSO_4^o$, $MgHCO_3^+$), which can sequester a significant fraction of scale-forming ions in dilute-to-moderate waters and is a major source of error in index-only calculators.

When no measured pH is provided, the engine estimates pH by charge balance during speciation. When no carbonate data is provided, dissolved CO_2 is initialized at atmospheric equilibrium ($\log_{10} pCO_2 = -3.40$, ≈ 400 ppm), and the CO_2 fugacity is user-adjustable for gas-lifted or CO_2-rich systems.

4.3 Mineral Database and Solubility Products

Thirteen scale-forming minerals are evaluated on every run, spanning the carbonate, sulfate, halide, phosphate, and fluoride scale families encountered in industrial and oilfield waters:

Mineral	Formula	Family	Typical occurrence
Calcite	$CaCO_3$	Carbonate	Ubiquitous; heaters, tubing, membranes

Mineral	Formula	Family	Typical occurrence
Aragonite	CaCO3	Carbonate	Higher-temperature CaCO3 polymorph
Magnesite	MgCO3	Carbonate	High-Mg waters
Strontianite	SrCO3	Carbonate	Sr-rich formation waters
Witherite	BaCO3	Carbonate	Ba-rich, high-alkalinity waters
Siderite	FeCO3	Carbonate	Iron-bearing, anoxic systems
Gypsum	CaSO4·2H2O	Sulfate	Low-temperature CaSO4 scale
Anhydrite	CaSO4	Sulfate	High-temperature CaSO4 scale
Barite	BaSO4	Sulfate	Seawater/formation-water mixing
Celestite	SrSO4	Sulfate	Sr brines mixed with sulfate waters
Halite	NaCl	Halide	Ultra-high-TDS produced water
Fluorite	CaF2	Fluoride	F-bearing waters
Hydroxyapatite	Ca5(PO4)3OH	Phosphate	Phosphate-treated systems

For each mineral, the solubility product is evaluated as a fitted polynomial in temperature, anchored to accepted 25 °C values from the geochemical literature (SUPCRT92-derived datasets, Plummer & Busenberg for the carbonates, Blount and Dickson for the sulfates, and the Pitzer/Harvie compilations for the evaporite minerals):

$$\log Ksp(T) = a + b \cdot Tc + c \cdot Tc^2 + d \cdot Tc^3$$

Pressure dependence is applied through a molar-volume correction of Helgeson–Kirkham–Flowers form, using tabulated reaction volumes ΔV for each dissolution reaction:

$$\Delta \log Ksp(P) = (P - 1) \cdot \Delta V / (2.303 \cdot R' \cdot T)$$

This captures the two dominant field drivers of scale: retrograde solubility with temperature (e.g., calcite and anhydrite become less soluble as water heats) and pressure-release scaling (e.g., calcite and halite dropout across chokes and at drawdown).

4.4 Saturation State: SI, SL, and Risk Classification

For each mineral, the ion activity product is assembled from the speciated activities according to the dissolution stoichiometry, and compared with the solubility product:

$$SL = IAP / Ksp \qquad SI = \log 10(SL)$$

SI > 0 (SL > 1) indicates supersaturation — the water can precipitate the mineral; SI < 0 indicates undersaturation — existing deposits of that mineral can dissolve. Computed indices are clamped to the

physically meaningful range [−20, +10] to suppress numerical noise at trace concentrations. Each mineral is assigned a qualitative risk grade for at-a-glance triage:

Saturation index	Risk grade	Interpretation
SI > 1.0	Severe	More than 10× supersaturated; rapid deposition likely
0.5 < SI ≤ 1.0	High	Strong thermodynamic drive to precipitate
0 < SI ≤ 0.5	Medium	Supersaturated; kinetics and seeding determine outcome
−1.0 < SI ≤ 0	Low	Near equilibrium; marginal risk
SI ≤ −1.0	None	Undersaturated; scale will not form

Alongside the numeric results, the application shows the full step-by-step derivation — free-ion activities, IAP assembly, Ksp at conditions — so results are auditable rather than a black box, and a free-vs-total ion table makes the effect of speciation visible.

4.5 Momentary Excess: From Index to Mass

A saturation index says whether scale can form; it does not say how much. Water Scale Pro therefore computes Momentary Excess (ME) for every supersaturated mineral: the quantity of mineral that would have to precipitate instantaneously to bring the water back to equilibrium. ME is obtained by solving the equilibrium condition against the conditional solubility product Kspc = Ksp / (γ^mcation · γ^nanion): a closed-form quadratic for 1:1 minerals, and Newton–Raphson iteration for asymmetric stoichiometries (CaF2, hydroxyapatite).

ME is reported in three unit systems — molality, ppm, and lbs per 1,000 bbl — the last being the standard oilfield deposition unit, enabling direct comparison with squeeze-treatment design bases and historical field data. This converts an abstract thermodynamic statement into an operational one: “this water can deposit 42 lbs of barite per 1,000 bbl produced.”

4.6 Traditional Operational Indices

Because decades of field correlations, specifications, and treatment programs are written in terms of the classical indices, Water Scale Pro computes all of them alongside the rigorous results:

Index	Formulation (as implemented)	Intended use
Langelier (LSI)	pH − pHs, with pHs = (pK2 − pKs) + pCa + pAlk	CaCO3 tendency in potable/cooling water
Ryznar (RSI)	2·pHs − pH	Empirical CaCO3 scaling/corrosion severity

Index	Formulation (as implemented)	Intended use
Puckorius (PSI)	2·pHeq − pHs; pHeq = 1.465·log10(M-alk) + 4.54	Buffering-corrected CaCO3 tendency
Larson–Skold	(epm Cl + epm SO4) / (epm HCO3 + epm CO3)	Corrosivity of aggressive anions to mild steel
Stiff–Davis	LSI with empirical ionic-strength correction	CaCO3 tendency in saline waters
Oddo–Tomson	LSI with ionic-strength, pressure, and CO2-fugacity corrections	Oilfield CaCO3 tendency under pressure

Consistent with their original derivations, these indices are computed from total analytical concentrations rather than speciated free-ion activities, and the interface interprets each with its applicability limits. For high-TDS brines, the speciation-based SI/SL results are authoritative; the classical indices are provided for continuity with existing practice, and the Stiff–Davis and Oddo–Tomson implementations are documented as simplified single-phase forms of the original correlations.

4.7 Temperature and Pressure Sensitivity

Scale rarely forms at sampling conditions; it forms somewhere along the system's temperature/pressure path. Reports therefore include parametric sweeps that re-run the full speciation engine across a range of temperatures and pressures, charting SI, SL, and Momentary Excess for the leading minerals. This exposes, for example, the calcite dropout window as CO2 breaks out with declining pressure, or the gypsum-to-anhydrite crossover with rising temperature. ScaleConnect batch runs use configurable envelopes (by default 65–250 °F and 14.7–1,450 psia) to score warehouse data across operating conditions.

4.8 Water Blending (Multi-Mix)

Incompatible-water mixing is the dominant mechanism behind sulfate-scale failures. The Multi-Mix workspace lets users combine multiple water sources at specified ratios into a blended composition, which is then run through the identical speciation pipeline. Because barite and celestite supersaturation is often extreme at intermediate mixing fractions and modest at the endpoints, evaluating the blend itself — rather than the source waters separately — is essential, and Multi-Mix results carry the same SI/SL/ME outputs and reporting as single-water analyses.

5. Software Architecture

5.1 Application Layer

The user-facing application is built on Streamlit and delivered entirely in the browser — no desktop installation, licensing dongles, or database files to manage. Data entry is organized around a guided input form covering physical conditions (temperature, pressure, pH, density, TDS), major ions, and expandable panels for minor and trace species. One-click presets (fresh water, seawater, oilfield brine)

seed realistic full analyses for training and quick what-if work. A guided six-step onboarding tour introduces new users to the workflow from first analysis through report download, and voice dictation (Web Speech API with a server-side Whisper fallback) supports hands-free entry of lab results.

The input model accepts twelve cations (Ca, Mg, Na, K, Ba, Sr, Fe, Li, Al, Mn, Zn, Pb), the major anions (HCO3, CO3, SO4, Cl), and additional species including silica, fluoride, phosphate, boron, H2S, and dissolved CO2.

5.2 Service Layer

Platform services run as a dedicated API application, cleanly separated from the calculation front end. It provides speech-to-text transcription for hands-free data entry, transactional and notification email, and a rate-limited, spam-protected contact channel. Cross-origin access is restricted to the product's own domains.

5.3 Data Management

Application data is persisted in a managed PostgreSQL database protected by row-level security policies. Saved analyses preserve the full input composition together with derived quantities (estimated pH, computed density, CO2 fugacity) so that historical results remain reproducible as the engine evolves. Product usage analytics are captured as insert-only events, readable exclusively by privileged service processes, and summarized in an automated weekly operations dashboard.

5.4 Reporting

Every analysis exports to a branded PDF report generated server-side with ReportLab: predicted scaling tendencies ranked by the user's chosen metric (saturation level, saturation index, or Momentary Excess), temperature/pressure trend charts rendered with matplotlib, the treatment recommendations summary, and a footnoted legend of methods. Tabular results export to CSV for downstream analysis.

5.5 ScaleConnect: Warehouse-Scale Prediction

For operators whose water analyses already live in a cloud data platform, ScaleConnect runs the engine as a pipeline. A scheduled worker polls a customer-designated table in the customer's cloud environment on a configurable interval (default 15 minutes), maps the customer's columns onto the engine's input schema through a configurable field mapping, computes saturation indices for every pending row through the same ScaleEngine used interactively, and writes results back to a designated results table, marking source rows processed. Because the connector is decoupled from the calculation core by that mapping layer, ScaleConnect is designed to integrate with cloud-based data storage systems generally — data warehouses, data lakes, and managed databases — rather than any single vendor's platform. Access credentials are stored with symmetric encryption at rest, and sync activity is reported by email. This allows fleet-wide scale screening — thousands of analyses — without any manual data entry.

6. Verification and Quality Assurance

Confidence in a prediction engine comes from testing it against known ground truth and guarding its inputs. Water Scale Pro's quality program includes:

- **Reference verification of speciation.** The pH estimation and speciation path is tested against published benchmark solutions with known speciation, and the engine's two activity-model paths are compared against each other across the ionic-strength boundary to verify continuity of results.
- **Input integrity guards.** Electroneutrality screening rejects or reconciles internally inconsistent lab analyses before they can produce misleading indices, and all unit conversions flow through a single audited conversion module (temperature, pressure, concentration, and density-aware molarity-to-molality).
- **Transparent derivations.** Step-by-step display of saturation-level and Momentary Excess calculations allows any result to be hand-checked against the underlying activities and constants.
- **Automated end-to-end testing.** The web application is exercised with Playwright browser automation (including the guided tour and core analysis flow), and the backend carries a pytest suite covering chemistry accuracy and service behavior.
- **Deterministic engine reuse.** A single thread-safe engine instance serves interactive, report, and batch workloads, eliminating configuration drift between entry points.

7. Assumptions and Limitations

Water Scale Pro is an equilibrium thermodynamics tool, and its results should be read with the following boundaries in mind:

- **Thermodynamics, not kinetics.** SI and SL state whether precipitation is thermodynamically favorable, not how fast it will occur. Induction time, seeding, hydrodynamics, and inhibitor kinetics determine whether a supersaturated water actually deposits scale in a given residence time. Momentary Excess is an upper bound on depositable mass, not a deposition-rate prediction.
- **Classical indices are dilute-water tools.** LSI, RSI, and PSI are computed from total concentrations, as originally defined, and lose validity in high-TDS brines; the Stiff–Davis and Oddo–Tomson implementations are simplified single-phase forms. For brines, rely on the Pitzer-based SI/SL results.
- **Fitted thermodynamic data.** Solubility products are polynomial fits anchored to published datasets, with a molar-volume pressure correction; they are engineering-accurate over typical oilfield envelopes rather than full equation-of-state treatments at extreme conditions.
- **Silica scaling.** Silica is accepted as an input species and participates in speciation, but amorphous silica/silicate scale is not currently scored as a saturation-index mineral.

- **Treatment guidance is qualitative.** Recommendations identify the appropriate mitigation family (pH adjustment, CO2 management, sulfate reduction, inhibition); quantitative inhibitor dose optimization remains the domain of product-specific performance testing.
- **Analysis quality governs output quality.** Charge-balance reconciliation catches gross inconsistencies, but no software can correct a mislabeled or degraded sample. Field-preserved, charge-balanced analyses remain the foundation of reliable prediction.

8. Conclusion

Water Scale Pro packages the thermodynamic machinery of research geochemistry — full aqueous speciation, Pitzer-model brine activities, temperature- and pressure-corrected solubility products across thirteen minerals — behind an interface designed for the people who actually fight scale: water treaters, production chemists, and facilities engineers. It reports both the rigorous quantities (SI, SL, Momentary Excess in field units) and the classical indices the industry's institutional knowledge is written in, makes every derivation auditable, and scales from a single what-if analysis in a browser to automated scoring of an entire data warehouse.

The result is a decision tool: which minerals, where in the T/P path, how much mass, and what class of mitigation — available in minutes from a standard water analysis, with no software to install.

For product information, sample reports, and trial access, visit **waterscalepro.com**.

Appendix A. Accepted Input Parameters

Group	Parameters
Physical conditions	Temperature (°C/°F), pressure (psia/bar/atm), pH (measured or engine-estimated), density, TDS
Major cations	Ca^{2+}, Mg^{2+}, Na^{+}, K^{+}
Scale-critical cations	Ba^{2+}, Sr^{2+}, Fe^{2+}
Trace cations	Li^{+}, Al^{3+}, Mn^{2+}, Zn^{2+}, Pb^{2+}
Major anions	$HCO3^{-}$, $CO3^{2-}$, $SO4^{2-}$, Cl^{-}
Other species	SiO2, F^{-}, $PO4^{3-}$, B, H2S, dissolved CO2 (with adjustable CO2 fugacity)

Concentrations are accepted in mg/L or ppm and internally converted to molality with density correction. Outputs per mineral: saturation index, saturation level, risk grade, and Momentary Excess (molal, ppm, lbs/1,000 bbl), plus solution ionic strength and the activity model applied.