

# Before the Cask is Opened

A Physics Framework for Projecting Whisky Taste from Production Parameters

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## Executive Summary

A distiller creates a new recipe today. They will not know if it produces the whisky they intended for 10 to 25 years. This is the longest feedback loop in food and beverage production. There is no existing tool that projects the sensory outcome of production decisions before maturation begins.

This paper documents the physics foundation for a forward projection engine that models the taste trajectory of whisky from production parameters across time and climate. The system applies peer-reviewed extraction kinetics, thermodynamic climate modelling, and production chemistry to calculate a projected taste profile at any point along the maturation timeline. It does not rely on opinion panels, collaborative filtering, or machine learning pattern matching. It models the actual chemistry.

The approach rests on a structural relationship with the companion Color Vision system documented in Paper 2 of this series. Color Vision analyses backward — given a photograph, it infers what happened. Distiller Vision projects forward — given production parameters, it calculates what will happen. Same extraction laws. Opposite direction. This bidirectional architecture enables convergence: forward predictions can be validated against backward observations as a whisky matures.

Every modifier in the system traces to peer-reviewed literature (PMID/DOI), documented industry practice, or explicit first-principles physics. Where inference bridges multiple findings, this is stated. No speculation is presented as established science.

The system models the complete production journey: new make spirit characterisation from barley, yeast, fermentation, still geometry, and condenser type; cask interaction across fill types, oak species, char levels, and cask sizes; climate-adjusted maturation trajectories across documented regions from Scotland to tropical India to desert Israel; compound-class-specific extraction curves with independent timescales; tannin polymerisation modelling; multi-fill journey projection; and colour trajectory via Peleg kinetics with climate adjustment.

Honest limitations are stated throughout. The system cannot predict individual cask variation — wood is a natural material. Projection accuracy depends on parameter completeness; partial inputs widen the confidence envelope. Climate modelling uses documented acceleration

factors, not first-principles thermodynamics for every region. The system projects probable chemistry, not guaranteed sensory experience.

# 1. The Forward Projection Problem

## 1.1 The Industry Gap

Whisky is unique among premium food and beverage products in the duration of its production cycle. A distiller making production decisions today — selecting barley variety, yeast strain, fermentation duration, still operation, cask type, and warehouse — will not taste the finished product for a minimum of three years (legal minimum for Scotch) and often not for 10, 15, or 25 years.

During this period, the spirit undergoes chemical transformations driven by extraction from oak, oxidation, esterification, tannin polymerisation, and volatile compound evolution. The trajectory of these reactions depends on the interaction between the initial spirit composition, the cask environment, and the ambient climate.

Currently, distillers navigate this gap through experience, tradition, and small-scale experimentation. A master distiller with 30 years of experience may have deep intuition about how a worm tub condenser with first-fill oloroso sherry butts will develop in a dunnage warehouse. But this intuition is not transferable, not quantifiable, and not available to new distillery operations, independent bottlers selecting casks, or investors evaluating young stock.

## 1.2 What Forward Projection Requires

To project the taste trajectory of a whisky from production parameters, a system must model three distinct phases.

**Phase 1 — New Make Characterisation:** How do barley, yeast, fermentation, distillation equipment, and operation translate to an initial chemical profile? This determines the foundation of the spirit before wood contact.

**Phase 2 — Cask Interaction:** How do the compounds in oak — vanillin, lactones, ellagitannins, lignin aldehydes — extract into the spirit over time? How does this extraction depend on previous cask contents, fill number, oak species, char depth, and cask geometry?

**Phase 3 — Environmental Modulation:** How does the ambient climate — temperature, humidity, temperature cycling — affect the rate of extraction, the direction of ABV evolution, and the preservation or degradation of volatile compounds?

Each phase has its own body of peer-reviewed research. The challenge — and the contribution of this system — is the integration of these findings into a coherent projection that respects the interaction between phases.

## 1.3 Why Physics, Not Machine Learning

A machine learning approach to forward projection would require training data: thousands of whiskies with complete production parameters mapped to sensory outcomes. This data does not exist at scale. Distillers rarely disclose complete production specifications. Sensory outcomes are measured inconsistently across panels and publications. The training set would

be sparse, biased toward common production methods, and unable to handle novel combinations.

A physics-based approach models the actual chemistry. If we know that vanillin extraction from American oak follows a saturating exponential curve with a characteristic timescale, and we know that elevated temperature accelerates this extraction via Arrhenius kinetics, then we can project vanillin contribution at any age in any climate — including combinations never seen in any training set.

The physics approach also provides auditability. Every projection can be decomposed into its constituent contributions: how much came from the cask, how much from the spirit's initial character, how much from the climate's acceleration effect. This transparency is essential for professional applications where distillers need to understand *why* the projection says what it says.

#### **1.4 What the System Projects**

For any set of production parameters and a target maturation age, the system outputs: projected taste profile — the probable sensory character at the target age; projected colour — CIELab coordinates and visual swatch; maturation timeline — how the profile evolves across multiple age points; optimal window — the age range where the production parameters produce the most balanced profile; comparable whiskies — existing whiskies in the reference database with similar projected profiles; and confidence level — quantified parameter coverage indicating projection reliability.

## 2. New Make Characterisation: Production Parameters to Spirit Chemistry

Before any cask contact, a new make spirit already possesses a distinctive chemical fingerprint determined by raw materials and distillation practice. Two distilleries using identical casks will produce different whiskies if their new make differs. New make characterisation is the foundation upon which maturation builds.

### 2.1 Spirit Type

The starting point for any projection is the spirit type. Different whisky traditions produce structurally different new make spirits due to differences in raw materials, distillation practice, and regulatory requirements.

Scotch single malt new make is typically characterised by cereal-forward character with moderate acidity from fermentation esters, with the balance depending on specific production choices. Bourbon new make starts with higher sweetness from the corn-dominated mash bill and elevated pungency from higher-proof distillation with more fusel carryover. Irish pot still whiskey, using a mixed grain bill of malted and unmalted barley, produces a distinctive spice character from the unmalted barley fraction. These structural differences in congener profiles are well-documented in analytical chemistry (Kelly 2023, TU Dublin).

### 2.2 Barley Variety

Barley variety affects sugar and protein balance in the wort, which in turn affects yeast metabolism and congener production. Heritage varieties such as Golden Promise produce slightly lower yields but are associated with higher protein content, potentially influencing Maillard reaction products during kilning and fermentation character. Modern varieties such as Laureate and Concerto have been bred for consistent high yield and processability.

Direct peer-reviewed comparisons of barley variety to new make congener profiles remain limited; the relationship is inferred from malting science principles and consistent industry observations rather than controlled distillation trials.

### 2.3 Yeast Strain

Yeast strain is among the strongest determinants of new make character. Daute et al. (2024) compared six to eight strains in Scotch whisky-style fermentations and documented 2–3× variation in key ester concentrations between strains (PMC11095643).

Ester production varies significantly: ethyl hexanoate (apple/pear), ethyl octanoate (apricot), and isoamyl acetate (banana) concentrations can double or triple depending on strain choice, directly affecting the fruity brightness of the new make. Higher alcohol (fusel oil) production shows measurable strain-dependent variation, with published fermentation studies documenting significant differences in isoamyl alcohol and other higher alcohols between strains

in whisky-style wort (PMC8624260; PMC7902897). Higher fusel levels contribute to perceived warmth and body.

Sulfur compound production differs markedly between strains. Distiller's yeast strains bred for clean fermentation produce measurably lower H<sub>2</sub>S and DMTS than mixed-culture or brewers' yeast regimes. Retained sulfur contributes meaty, savoury depth to the spirit.

Historical context is relevant: prior to 1952, most Scotch distilleries used brewery-sourced yeast or house-propagated mixed cultures. The DCL M-strain, introduced in 1952, standardised Scotch production for decades. Since 2003, alternative strains (MX, Mauri, Anchor) have been adopted by distilleries seeking to differentiate their new make character (Walker 2016, Heriot-Watt University).

## 2.4 Fermentation Duration

Fermentation duration interacts with yeast strain to determine the final congener balance of the wash.

Short fermentation (<48 hours) produces wash dominated by primary fermentation products: ethanol, CO<sub>2</sub>, and moderate ester levels. The yeast completes sugar conversion efficiently but has limited time for secondary metabolism.

Long fermentation (>72 hours) allows lactic acid bacteria to become active after the yeast exhausts available sugars. Their metabolism produces additional esters and organic acids that contribute a distinctive fruity, sometimes sour-milk character. Extended fermentation is associated with elevated brightness and enhanced sweetness through secondary sugar metabolism (PMC8624260). Industry practice ranges from 48-hour minimum (efficiency-driven operations) to 120+ hours, with flavour-driven distilleries such as Springbank operating at approximately 72 hours. The relationship between pitching rate, temperature, and higher alcohol formation has been documented since at least Ramsay (1984; DOI: 10.1016/0740-0020(84)90021-2).

## 2.5 Still Geometry and Reflux

Still shape controls the reflux ratio during distillation, which determines which congeners carry through to the final spirit.

Reflux is the key mechanism. When vapour rises in the still, some condenses on the copper surfaces and falls back. This condensation-and-return cycle selectively enriches the vapour with more volatile compounds (light esters, ethanol) while retaining heavier compounds (fusel oils, sulfur compounds) in the pot. The degree of reflux depends on still geometry.

Tall, narrow stills with ascending lyne arms maximise reflux. The vapour must travel further, encounters more copper surface, and undergoes more condensation events. The resulting spirit is lighter, more ester-forward, with reduced fusel and sulfur carryover. Short, squat stills with descending lyne arms minimise reflux. Heavy compounds carry through more readily. The spirit is heavier, oilier, with more fusel warmth and potentially more savoury depth.

No peer-reviewed whisky study has isolated still geometry as a single variable — effects are confounded with condenser type, lyne arm angle, and operational parameters. The relationship is grounded in standard distillation chemistry principles and consistent industry observation, with supporting evidence from Wanikawa and Sugimoto’s sulfur compound review (2022; PMID: 35268773), which documents how still and condenser configuration jointly determine sulfur carryover.

## 2.6 Condenser Type

After distillation, vapour must be condensed back to liquid. The condenser type determines the final copper contact opportunity, directly affecting sulfur compound removal.

**Shell-and-tube condensers** provide high copper surface area in a compact unit. The vapour passes through multiple tubes surrounded by coolant, with extensive copper contact. This efficiently catalyses the conversion of volatile sulfur compounds (H<sub>2</sub>S, methanethiol, ethanethiol) to non-volatile copper sulfides. The resulting spirit is cleaner, allowing fruit esters to express more clearly.

**Worm tub condensers** consist of a single coiled copper pipe immersed in a water tank. Copper surface area and contact time are significantly lower. The spirit retains more volatile sulfur compounds, producing a heavier, meatier character. Worm tubs are used by approximately 10 of 147 Scottish malt distilleries, making this production choice relatively rare.

Webster et al. compared spirits from distilleries with different condensers and found measurable differences in sulfur precursor levels, though they concluded that condenser type alone cannot fully explain sulfur behaviour — the interaction with still design is significant. Bathgate (2019; DOI: 10.1002/jib.556) reviewed the role of worm tubs in producing sulfury and heavy spirit character, and Harrison et al. (2011; DOI: 10.1002/j.2050-0416.2011.tb00450.x) demonstrated that copper contact in different still sections directly reduces sulfury and meaty character.

## 2.7 Parameters Investigated and Excluded

**Water source (mineral content):** Investigated and excluded. Wilson (2008, PhD thesis, Heriot-Watt University) found no correlation between process water mineral composition and spirit sensory profile across 10 Scottish distilleries using controlled glass/copper still comparisons. Elemental fingerprinting studies confirm that copper in finished whisky originates from stills and casks, not process water (Płotka-Wasyłka et al. 2022, PMID: 35683301; Kafarski et al. 2022, PMID: 36140032). The organic compound effect — humic substances from peat in water sources influencing yeast metabolism — is captured by peat-related parameters rather than requiring a separate water modifier.

### 3. Cask Interaction Chemistry: Extraction Kinetics and Wood Science

Maturation in oak casks is the longest and most transformative phase of whisky production. The cask contributes vanillin, lactones, tannins, lignin breakdown products, and — if previously used for wine, sherry, or bourbon — residual flavour compounds from the former contents. These contributions are not instantaneous; they follow well-characterised extraction kinetics that depend on time, temperature, cask history, and wood properties.

#### 3.1 Extraction Kinetics: The Peleg Model

The rate at which compounds extract from oak into spirit follows non-linear kinetics. Extraction is rapid in the first years, then progressively slows as the most accessible compounds are depleted and equilibrium effects increase.

This behaviour is well-described by the Peleg pseudo-second-order model (Peleg 1988; DOI: 10.1111/j.1365-2621.1988.tb13565.x), originally developed for solid-liquid extraction systems and subsequently validated for oak-spirit interaction. Delgado González et al. (2021) demonstrated  $R^2 > 0.9$  for Peleg model fits to colour extraction kinetics in wine distillates matured in American, French, and Spanish oak (Food Control, vol. 119, 107468; DOI: 10.1016/j.foodcont.2020.107468). Whisky shares the same ethanol-water solvent system and oak substrate; the extraction mechanism is identical.

The general form is:

$$C(t) = tK_1 + K_2 \cdot t$$

Where  $C(t)$  is cumulative extraction at time  $t$ ,  $K_1$  relates to initial extraction rate, and  $K_2$  relates to the extraction ceiling. At short times, extraction is approximately linear. At long times, extraction asymptotes to the maximum extractable material.

Critically, different compound classes extract at different rates. Small molecules like vanillin and lactones are mobile in the ethanol-water matrix and reach their extraction ceiling relatively quickly. Large molecules like ellagitannins diffuse more slowly and continue extracting over longer timescales. Vivas et al. (2020; DOI: 10.1002/jib.586) documented this differential behaviour for ellagitannin extraction and transformation kinetics in oak-spirit systems, a mechanism considered general across ethanol-water matrices in oak. This differential extraction rate is what creates the evolving taste trajectory: a whisky at 5 years is chemically different from the same whisky at 15 years, not just “more of the same.”

#### 3.2 Previous Cask Contents

What previously occupied the cask determines the extraction ceiling — the maximum chemical contribution the wood can make. This is the single most consequential variable in any cask-based projection.

**Ex-bourbon casks** (American Standard Barrel, 190L): The most common cask in Scotch production. American white oak (*Quercus alba*) contributes vanillin, *cis*- and *trans*-lactones, and

caramelised hemicellulose products. First-fill ex-bourbon provides moderate colour and a vanilla/caramel/coconut character.

**Ex-sherry casks** (Oloroso, PX, Fino): European oak (*Q. robur* or *Q. petraea*) seasoned with sherry wine contributes anthocyanins, polymeric tannins, and residual wine compounds. These drive elevated tannin complexity, dried fruit sweetness from wine residuals, and structural drying. Kew et al. (2017; PMID: 27859394; DOI: 10.1021/acs.analchem.6b03148) used high-resolution mass spectrometry to demonstrate that ex-sherry cask whiskies contain measurably different phenolic profiles from bourbon-matured equivalents.

**Ex-port casks:** Port pipes contribute monomeric anthocyanins (darker red-shifted colour) and residual port wine sweetness. The contribution profile overlaps with sherry but with characteristically different hue due to different anthocyanin polymerisation states.

**Virgin oak:** Maximum extraction rate (no prior use has depleted the wood). Very high initial tannin and vanillin contribution. Mandated for bourbon production. Can produce aggressive, wood-dominant profiles if maturation duration is not managed.

The distinction between sherry cask eras is historically significant. Before 1981, sherry casks arriving in Scotland were genuine transport casks that had held sherry for shipping. These European oak casks were deeply seasoned with wine compounds. After the sherry industry moved to bulk shipping, most “sherry casks” became purpose-built barrels briefly seasoned with sherry (Mosedale & Puech 1998; DOI: 10.1016/S0924-2244(98)00024-7).

### 3.3 Fill Number and Extraction Decay

Each time a cask is filled with spirit, extractable material is depleted. The decay is steep: second-fill casks retain roughly half the extractable material of first-fill, and by third or fourth fill, the cask contributes primarily as a neutral vessel for oxidative ageing rather than active extraction. Ellagitannin depletion across successive fills has been documented in multiple oak chemistry studies (Vivas et al. 2020; DOI: 10.1002/jib.586), with supporting data from cooperage industry extractive measurements.

This means a long-matured whisky in a refill cask can have similar total extraction to a young whisky in a first-fill cask, despite vastly different ages. This is why age alone is a poor predictor of whisky character, and why fill number is essential for accurate projection.

### 3.4 Oak Species

The species of oak fundamentally alters the chemical composition available for extraction. Prida and Puech (2006; DOI: 10.1021/jf0616098) compared extractive content across American, French, and East European oak, documenting systematic differences in vanillin, lactone, and ellagitannin concentrations.

**American white oak (*Quercus alba*):** Lower tannin content, higher vanillin and lactone contribution. Faster extraction of sweet compounds. The dominant species for bourbon barrels and the most common oak in Scotch production.

**European oak — Spanish (*Q. robur*):** Higher tannin content, higher ellagitannin diversity. More porous grain structure allows deeper spirit penetration. Historically associated with sherry cask production.

**European oak — French (*Q. petraea*):** Similar tannin profile to *Q. robur* but with higher aromatic complexity. Primarily used in wine barrel production, entering whisky production through wine cask finishes.

**Japanese oak (*Quercus mongolica* / Mizunara):** Distinctive aromatic compounds including *kara* (incense-like), coconut, and sandalwood notes. Extremely porous and prone to leakage. Very rare in global whisky production.

### 3.5 Char Level

The interior charring of oak barrels creates a layer of activated carbon and thermally modified wood compounds. Charring breaks down the structural components of oak: hemicellulose decomposes into simple sugars that caramelize on the barrel surface, contributing caramel and toffee notes; lignin breaks down into vanillin, syringaldehyde, and related aromatic aldehydes, contributing vanilla and spice; cellulose remains largely intact as the structural backbone.

Heavier charring creates an activated carbon filtration layer that removes some harsh congeners from the spirit while simultaneously creating new flavour compounds from thermal decomposition. Heavier charring also reduces the rate at which tannins extract into the spirit, as the char layer acts as a physical barrier. The result is that heavily charred casks can produce slower initial extraction but deeper eventual colour and character. Guerrero-Chanivet et al. (2020; PMID: 33172052; DOI: 10.3390/foods9111613) documented volatile compound generation from oak char, and Luo et al. (2023; PMID: 38231733; DOI: 10.3390/foods12234266) characterised how char level affects the volatile compound profile in aged spirits.

### 3.6 Cask Size and Surface-to-Volume Ratio

Extraction rate scales with the surface-to-volume ratio of the cask — a direct physical relationship. Smaller casks expose more spirit to wood per unit volume, accelerating extraction proportionally. Quarter casks are sometimes used for accelerated maturation, achieving in 3–5 years what a hogshead might achieve in 8–10. However, the acceleration is not uniform across compound classes — fast-extracting compounds are disproportionately amplified, producing a profile that is sweetness-heavy rather than balanced.

### 3.7 Finishing: The Non-Additive Model

Cask finishing — transferring mature whisky to a second (or third) cask type for additional maturation — has become increasingly common since Glenmorangie pioneered the practice with port wood finishing in 1987.

Finishing kinetics are critically non-additive. The interaction between the already-matured spirit and the new wood does not simply add the new cask's contribution on top. The process involves rapid surface extraction in the first days, followed by a period of re-adsorption and

chemical adjustment, then a slow integration phase where existing and new wood compounds polymerise together. This is why short finishing (3–6 months) produces intense but less integrated character, while extended finishing (2+ years) produces mellowed, unified profiles. Morishima et al. (2019; PMID: 30557912) documented cluster size evolution and colour development during barrel ageing, providing evidence for the non-linear integration behaviour observed in finishing regimes.

## 4. Climate and Environment: Thermodynamic Maturation Modelling

The same cask filled with the same spirit will produce different whisky depending on where it matures. Temperature drives extraction rate (Arrhenius kinetics). Humidity determines the direction of ABV change (angel's share composition). Temperature cycling — the diurnal and seasonal swing between hot and cold — pumps spirit in and out of the wood grain, accelerating contact.

Scotland is the baseline. Everything else is calibrated relative to Scottish dunnage warehouse conditions: approximately 12 °C average temperature, 80–90% humidity, 1–2% angel's share per year, and ABV that decreases over time.

### 4.1 The Two-Level Climate System

The system models climate as two nested layers.

**Country Climate:** The broad thermodynamic context. Scotland (temperate maritime, baseline), India (tropical), Taiwan (tropical-extreme), Kentucky (continental hot). These set the base maturation speed and directional character.

**Regional Environment:** Fine-tuning within a country. Scottish dunnage vs. racked warehouse. Islay coastal vs. Speyside inland. Each regional context adjusts the speed and character within the country baseline.

### 4.2 Temperature and Extraction Rate

The fundamental relationship between temperature and extraction rate follows Arrhenius kinetics — a cornerstone of physical chemistry. For every 10 °C increase in average temperature, the rate of chemical reactions approximately doubles.

This is why Indian whisky (Amrut, Paul John) at 30–35 °C average warehouse temperature matures significantly faster than Scottish whisky at 12 °C. A 4-year-old Indian single malt has undergone comparable extraction to a substantially older Scotch.

However, temperature does not accelerate all extraction processes equally. Sweet compound extraction (vanillin, lactones) responds strongly to heat. Volatile ester preservation responds inversely — high temperatures degrade esters more rapidly.

### 4.3 Humidity and ABV Evolution

Humidity determines the composition of the angel's share — the liquid lost to evaporation through the barrel staves each year.

**High humidity** (Scotland, Tasmania, coastal Japan): Water evaporates more slowly than ethanol. ABV decreases over time. A cask filled at 63.5% may reach 45–50% after 20 years.

**Low humidity** (Kentucky, India, Israel, New Zealand): Water evaporates faster than ethanol. ABV increases or remains stable. Kentucky bourbon warehouses can see ABV rise during maturation.

The direction of ABV evolution matters because ethanol concentration affects extraction kinetics, volatile compound retention, and the balance of the spirit's sensory character.

#### 4.4 World Whisky Climate Zones

The system incorporates maturation conditions for established and emerging whisky-producing regions. Climate data is drawn from distillery-reported measurements cross-referenced across independent sources; conservative factors are applied where marketing claims diverge from analytical evidence.

**Tasmania (Australia):** Cool maritime, similar to Scotland but slightly faster. Angel's share approximately 3% per year. Distilleries such as Sullivans Cove and Lark produce mature-presenting whisky at 5–10 years.

**Mainland Australia:** Warm continental with significant temperature cycling. The system applies acceleration factors derived from analytical comparison rather than marketing claims.

**Israel (Mediterranean):** Hot Mediterranean climate. Milk & Honey distillery in Tel Aviv reports angel's share of 9–11% per year. ABV increases due to low humidity.

**Israel (Desert):** Extreme arid conditions. M&H's Dead Sea warehouse project reports angel's share up to 20–25% per year — the fastest documented maturation rate in production whisky.

**New Zealand:** Extreme temperature cycling with very low humidity. ABV rises significantly per year at Cardrona distillery. The thermal cycling compensates for lower average temperature by physically pumping spirit through wood grain with each expansion-contraction cycle.

**Scandinavia:** Cool continental, close to Scotland's speed. Mackmyra's underground mine warehouses produce results similar to Scottish dunnage.

#### 4.5 Warehouse Type

Within a single climate zone, warehouse construction affects local conditions.

**Dunnage warehouses** (traditional stone buildings, earthen floors, casks stacked 2–3 high) provide the most stable, cool conditions. This is the slowest maturation environment within a given climate.

**Racked warehouses** (modern steel or concrete buildings, casks stacked on racks up to 12+ high) have significant vertical temperature gradients. Top-floor casks experience higher temperatures and more cycling than ground-floor casks.

## 5. Temporal Modelling: The Taste Trajectory

The taste trajectory is not a simple accumulation. Different compounds extract, form, decay, and polymerise at different rates. Understanding these differential kinetics is what allows the system to project how a whisky will change across decades — and to identify the optimal window for any given combination of production parameters and climate.

### 5.1 Differential Extraction Rates

Different compound classes have different extraction timescales. Small, mobile molecules like vanillin and lactones reach their extraction ceiling relatively quickly — the “sweet wood” character of a young bourbon-matured whisky is well-established within the first several years. Large molecules like ellagitannins diffuse more slowly and continue extracting over much longer timescales — the structural, tannic character of a well-aged sherry-cask whisky takes many years to develop (Vivas et al. 2020; DOI: 10.1002/jib.586).

Some compound classes — notably light esters from fermentation and light volatiles — actually decline over time. The angel’s share carries them away, and chemical reactions transform them into less volatile products. The net result is that young whisky is typically brighter and more aromatic than old whisky of the same production specification.

This differential behaviour creates the evolving taste trajectory. It is not a matter of “more time = more flavour.” It is a matter of balance points shifting as faster compounds plateau and slower compounds continue building.

### 5.2 Tannin Polymerisation and Softening

Ellagitannins extracted from oak undergo a characteristic trajectory: they accumulate in the spirit, reach a concentration peak, and then progressively polymerise into larger, less bitter, less astringent molecules. This polymerisation is the chemical basis of the common observation that very old whiskies become “smooth” — the tannins that were grippy and drying at maturity have cross-linked into larger structures that no longer bind salivary proteins as aggressively (Morishima et al. 2019, PMID: 30557912; Vivas et al. 2020, DOI: 10.1002/jib.586).

In warmer climates, this peak arrives earlier, proportional to the thermodynamic acceleration. Ultra-old whiskies (40+ years) are typically described as “concentrated” rather than “tannic” — the tannins have transformed, and what remains is a concentrated essence of oxidation products and residual spirit character.

### 5.3 The Multi-Fill Journey

Real whisky production often involves multiple cask stages. A spirit might spend a decade in a first-fill bourbon hogshead, then be transferred to a first-fill oloroso sherry butt for several years, then receive a finishing period in a port pipe.

The system models this as a sequential process where the exit profile from one cask stage becomes the input for the next. At each transfer, the extraction curve begins fresh relative to

the new cask, but the spirit carries its accumulated chemical profile.

A special case is the climate transfer — moving the same barrel to a different warehouse. The spirit continues extracting from the same wood, but the extraction rate changes because the thermodynamic environment has changed.

#### **5.4 ABV and Perception**

Bottling ABV affects the perceived character independently of the chemistry. Ethanol produces perceived heat and burn through trigeminal nerve activation (Trevisani et al. 2002; PMID: 12368807). At high ABV (>50%), this can mask more subtle flavour compounds — consistent with the common experience that cask-strength whiskies benefit from dilution. Karlsson and Friedman (2017; DOI: 10.1038/s41598-017-06423-5) demonstrated that ethanol-water clustering at different concentrations affects the release of volatile aroma compounds, providing a physical basis for the dilution effect.

## 6. Colour Trajectory: Forward Peleg Projection

Colour is a visible proxy for extraction progress. The same extraction kinetics that drive taste development also drive colour development. The system projects colour at each age point using the same Peleg kinetics framework documented in the companion Color Vision white paper, adjusted for cask type, oak species, climate, and cask geometry.

### 6.1 Forward Peleg Colour Projection

The Peleg equation, applied in the forward direction, projects colour density at any age given the cask type and climate parameters. This maps to CIELab coordinates ( $L^*$ ,  $a^*$ , hue angle) that can be rendered as a visual swatch.

This colour projection serves dual purposes: it provides distillers with visual output alongside the taste projection, and it creates a prediction that can be compared against Color Vision's backward analysis for convergence validation.

For the complete physics of colour projection including illuminant estimation, spectroscopic correlation, and glass optics, refer to the companion Color Vision white paper: *The Glass Never Lies* (Paper 2 in this series).

## 7. Confidence and Parameter Coverage

The system calculates confidence as a function of how many production parameters are known. More parameters mean a narrower projection envelope and higher confidence.

A distiller projecting their own production (all parameters known) achieves maximum confidence. A consumer with only label information (spirit type, cask type, age, ABV) achieves moderate confidence. The system reports this confidence alongside every projection and indicates which additional parameters would most improve the projection.

### 7.1 The Envelope Model

With incomplete parameter information, the system generates an envelope rather than a point prediction. The envelope widens as fewer parameters are known and narrows as more information is provided.

This is honestly communicated: “At current parameter coverage, the projection represents a probable range. Additional information about fill number and oak type would narrow this range.”

## 8. Convergence: Forward Projection Meets Backward Analysis

Distiller Vision and Color Vision share the same physics engine applied in opposite directions. This structural relationship creates a natural validation mechanism: forward prediction can be compared against backward observation as a whisky ages.

### 8.1 The Validation Loop

At fill time, the system projects the expected colour and chemistry at various age points. Years later, when a sample is available, Color Vision can analyse a photograph to infer the actual colour parameters and extraction state.

The comparison between predicted and observed values provides confirmation (the model is performing correctly), calibration signal (systematic deviations indicate model adjustment needed), and anomaly detection (large deviation for a single cask may indicate defect or mislabelling).

### 8.2 Gap Analysis

When forward prediction and backward observation are both available for the same whisky, their profiles can be compared. Alignment indicates authentic production parameters. Divergence reveals either inaccurate production claims, atypical cask behaviour, or modelling limitations.

## 9. Limitations and Honest Boundaries

### 9.1 What the System Cannot Predict

**Individual cask variation:** Wood is a natural material. Two barrels from the same cooperage, filled with the same spirit on the same day and stored in the same warehouse, will produce measurably different whiskies. The system projects the expected central tendency.

**Cask defects:** Leaking, bacterial contamination, sulfur candle residues, or cooperage defects are stochastic events outside the scope of chemistry-based modelling.

**Subjective preference:** The system projects chemistry. Whether a particular chemical profile is perceived as “excellent” or “unbalanced” depends on the individual taster.

### 9.2 Evidence Standards

Every parameter in the system is grounded in one of three evidence categories: peer-reviewed literature with published DOI or PMID; documented industry practice with consistent cross-referencing across independent sources; or direct physical principles (Arrhenius kinetics, surface-to-volume scaling) where the underlying science is uncontested. Where inference bridges multiple findings — for instance, applying extraction kinetics validated in wine spirits to whisky systems sharing the same solvent matrix — this is stated explicitly. Parameters investigated and found unsupported are excluded from the model rather than retained at reduced weight.

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Paper 3 in the Taste Intelligence Research Programme

Paper 1: “The Female Taste Economy and the Birth of Taste Intelligence” (BitterMatrix, December 2025)

Paper 2: “The Glass Never Lies” (WhiskyBaba Color Vision, February 2026)