Whiskey Maturation in Changing Climates: Four Years of Data and Advanced Modeling

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DISTINCT DISTILLAGE

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Introduction

- Institutional knowledge is invaluable in whiskey aging and distillation, shaping tradition and expertise
- Whiskey aging dynamics are complex, driven by temperature, humidity, barrel properties, and warehouse conditions
- Modeling offers a window into the barrel, revealing processes that cannot be directly observed
- **Goal: Develop a model that accurately replicates real-world warehouse conditions**
- Combining tradition with advanced analytics leads to better-informed decisions and deeper insights

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Outline

- 3-D Barrel Model Predictive Capabilities
- Data Analysis & Proof Gallon Predictions
- Spirit Penetration & Devil's Cut
- Congener Behavior & Reactions
- Exploring Model Predictions Across Floors
- Discussion & Model Refinements
- Conclusions

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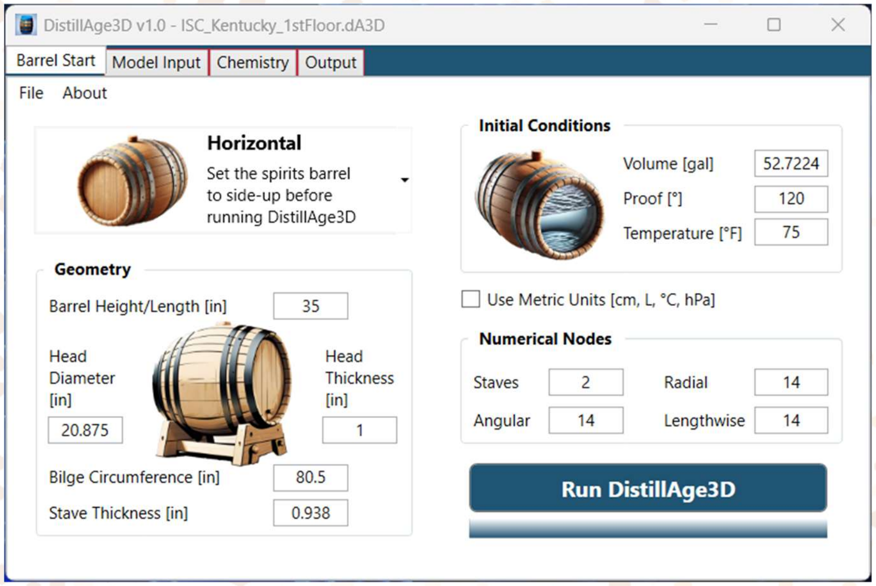
Model Predictive Capabilities

- Uses Ambient Pressure, Temperature, Relative Humidity, and Alcohol Vapor (when available) to Predict:
  - Average spirit temperature
  - Ethanol / water evaporation: Angel's share
  - Total volume and proof gallons
  - Alcohol-by-Volume and Alcohol-by-Mass
  - Influence of side-up vs. top-up barrels
  - Impact of entry proof
  - Chemistry (congeners)
  - Staves spirit penetration & Devil's cut
  - Economics: Barrel value & evaporation cost
  - pH & Color
  - Ullage pressure and hydrostatic forces



DistillAge3D: A cutting-edge 3-D barrel model, powered by physics and thermodynamics, runs independently on your desktop – no additional software required

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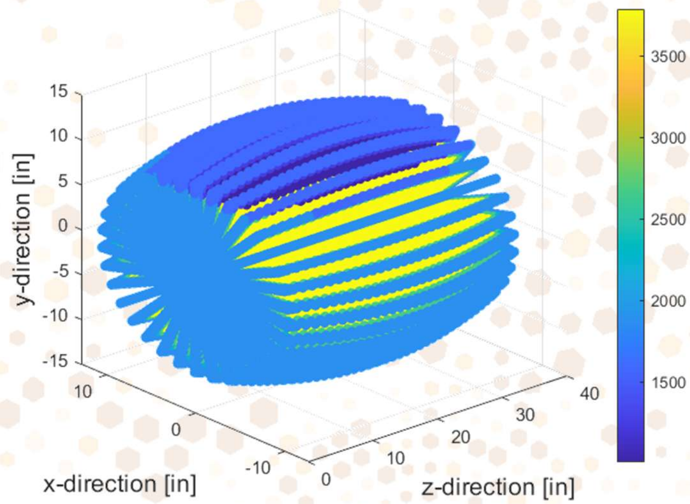
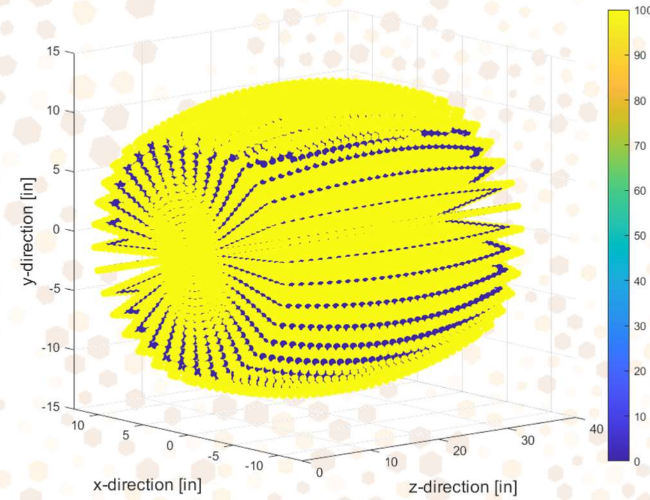
Setting Up the Model

Parameter	Value
Barrel Height	35 in
Head Diameter	20.875 in
Head Thickness	1 in
Bilge Circumference	80.5 in
Stave Thickness	0.938 in
Fill Weight (avg.)	509.229 lbf
Barrel Weight (avg.)	110.607 lbf
Fill Proof	120
Fill Temperature	75 °F
Whiskey Volume (calc.)	52.7224 gal
Barrel Orientation	Side Up
Stave & Head Moisture Content	12%



Surface plot of the constant pressure specific heats of barrel at the start: whiskey = yellow, air gap – dark blue



Indication of the wetted staves and the surface of whiskey in the barrel; scale is just for illustrative purposes

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Understanding the Data

- Proof was measured after 4 years; ambient data only 3+ years
- Re-used Year 3 for Year 4 data
- Floor 5*: Data missing between 3/2/2021 & 10/4/2021

	Floor 1	Floor 2	Floor 3	Floor 4	Floor 5
Temperature Range [°F]	24.6 – 101.9	26.2 – 102.3	28.1 – 102.2	28.9 – 101.5	28.1 – 108.0*
Relative Humidity (RH) Range [%]	23.6 – 92.1	21.3 – 91.2	22.2 – 91.2	21.5 – 91.8	23.7 – 89.2*
Proof After 4 Years [°]	122.40	**127.00**	125.70	127.30	130.72

* Used Floor 4 data for missing Floor 5 data

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Floor 2 Proof Higher Than Expected

- Data suggests Floor 3 > Floor 2 proof, observed Floor 2 proof is higher
  - Floor 3 is, on average, +1.70 °F warmer → increased ethanol and water evaporation
  - Floor 3 relative humidity is, on average, –2.83 % lower → higher water evaporation
- Potential explanations:
  - Barrel location – Differences in heat transfer
  - Airborne ethanol – Potential resistance to ethanol loss
  - Barrel variation – Different wood porosities affecting evaporation
- Modeling approach: Evaluate data, identify trends, and refine predictions to match observations

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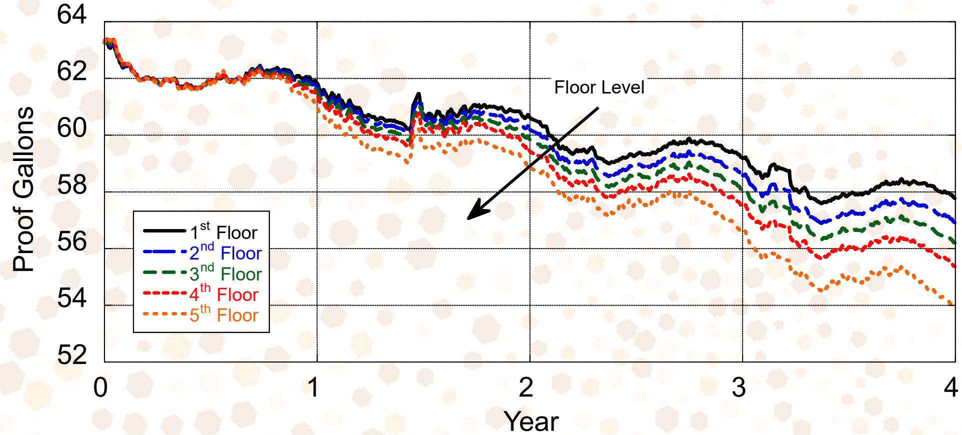
Proof Gallons

- Baldwin & Andreasen (1974): ~3% annual proof gallon loss, providing a benchmark for modeling
- 2nd-floor barrels: Adjusted permeability to align with observed evaporation trends
- Evaporation patterns: Driven primarily by floor-level temperature and relative humidity differences
- Spirit height & proof measurements: Can be used to calibrate model & better quantify losses

Proof gallons at each floor over time



Proof results at end of four years

Floor	Exp. [°]	Model [°]	Difference [°]	Loss [° gal]
1st	122.40	122.82	+0.42	5.49
2nd	127.00	126.94	–0.06	6.35
3rd	125.70	124.72	–0.98	7.07
4th	127.30	126.83	–0.47	7.90
5th	130.72	131.49	+0.77	9.37

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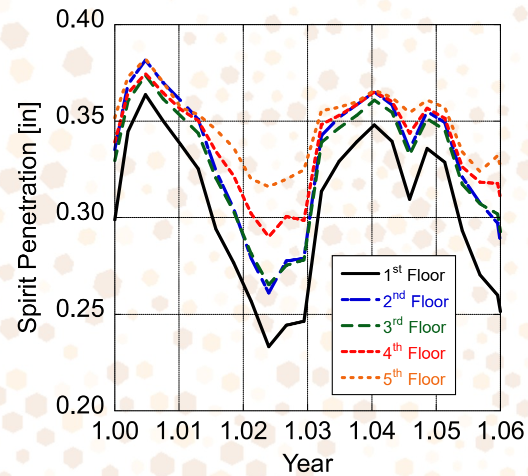
Spirit Stave Penetration & Devil's Cut

- Roussey et al. (2021): In-situ monitoring of wine barrel mass & ullage pressure
- Penetration model factors
  - ABV↑ Density↓ Gravitational Force↓ ✚
  - Temp↑ Permeability↓ Pore size↓ ▬
  - RH↓ Permeability↓ Pore size↓ ▬
  - Temp↑ Surface Tension↓ Cohesion↓ ▬
  - Temp↑ Viscosity↓ Flow Resistance↓ ✚
  - Wood porosity (constant)
  - Spirit contact angle (constant)
  - Variation in hoop placement (not considered)

✚ Greater penetration
▬ Lower penetration



Floor	Penetration [in]	Devil's Cut [kg]
1st	0.370 ± 0.156	1.221 ± 0.495
2nd	0.392 ± 0.158	1.228 ± 0.494
3rd	0.398 ± 0.164	1.305 ± 0.515
4th	0.408 ± 0.167	1.334 ± 0.521
5th	0.419 ± 0.170	1.363 ± 0.525

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Congeners & Reactions

- Reaction expressions include precursor effects and oxidation
- Ethanol concentration included to account for proof fluctuations
- Flexible framework allows for easy modifications and additions

#	Species	Formula	Pre-cursor
1	m-cresol	C_7H_8O	amino acids
2	o-cresol	C_7H_8O	amino acids
3	p-cresol	C_7H_8O	amino acids
4	vanillin	$C_8H_8O_3$	coniferaldehyde
5	cis-isoeugenol	$C_{10}H_{12}O_2$	coniferyl alcohol
6	coniferaldehyde	$C_{10}H_{10}O_3$	coniferyl alcohol
7	coniferyl aldehyde	$C_{10}H_{10}O_3$	coniferyl alcohol
8	eugenol	$C_{10}H_{12}O_2$	coniferyl alcohol
9	guaiacol	$C_7H_8O_2$	coniferyl alcohol
10	trans-isoeugenol	$C_{10}H_{12}O_2$	coniferyl alcohol
11	methoxyeugenol	$C_{11}H_{14}O_3$	eugenol
12	cis-lactone	$C_9H_{16}O_2$	fatty acids
13	trans-lactone	$C_9H_{16}O_2$	fatty acids
14	4-vinyl-guaiacol	$C_9H_{10}O_2$	ferulic acid

#	Species	Formula	Pre-cursor
15	acetyl furan	$C_6H_6O_2$	furfural
16	furfuryl alcohol	$C_5H_6O_2$	furfural
17	4-ethyl-guaiacol	$C_9H_{12}O_2$	guaiacol
18	4-methyl-guaiacol	$C_8H_{10}O_2$	guaiacol
19	coniferyl alcohol	$C_{10}H_{12}O_3$	lignin
20	ferulic acid	$C_{10}H_{10}O_4$	lignin
21	methanol	CH_4O	lignin
22	methoxy group	$-OCH_3$	lignin
23	p-coumaryl alcohol	$C_9H_{10}O_2$	lignin
24	sinapyl alcohol	$C_{11}H_{14}O_4$	lignin
25	5-HMF	$C_6H_6O_3$	Maillard
26	5-methyl-furfural	$C_6H_6O_2$	Maillard
27	furaneol	$C_6H_8O_3$	Maillard
28	furfural	$C_5H_4O_2$	Maillard
29	maltol	$C_6H_6O_3$	Maillard

#	Species	Formula	Pre-cursor
30	phenol	C_6H_6O	p-coumaryl alcohol
31	4-ethyl-phenol	$C_8H_{10}O$	phenol
32	syringaldehyde	$C_9H_{10}O_4$	sinapaldehyde
33	sinapaldehyde	$C_{11}H_{12}O_4$	sinapyl alcohol
34	syringol	$C_8H_{10}O_3$	sinapyl alcohol
35	ethyl vanillate	$C_{10}H_{12}O_4$	vanillic acid
36	methyl vanillate	$C_9H_{10}O_4$	vanillic acid
37	vanillic acid	$C_8H_8O_4$	vanillin
38	syringic acid	$C_9H_{10}O_5$	syringaldehyde
39	acetaldehyde	C_2H_4O	ethanol
40	acetic acid	$C_2H_4O_2$	acetaldehyde
41	ethyl acetate	$C_4H_8O_2$	acetic acid
42	isobutyl alcohol	$C_4H_{10}O$	amino acid
43	isobutyraldehyde	C_4H_8O	isobutyl alcohol
44	isobutyl acetate	$C_6H_{12}O_2$	isobutyl alcohol
45	apocynin	$C_9H_{10}O_3$	coniferyl alcohol

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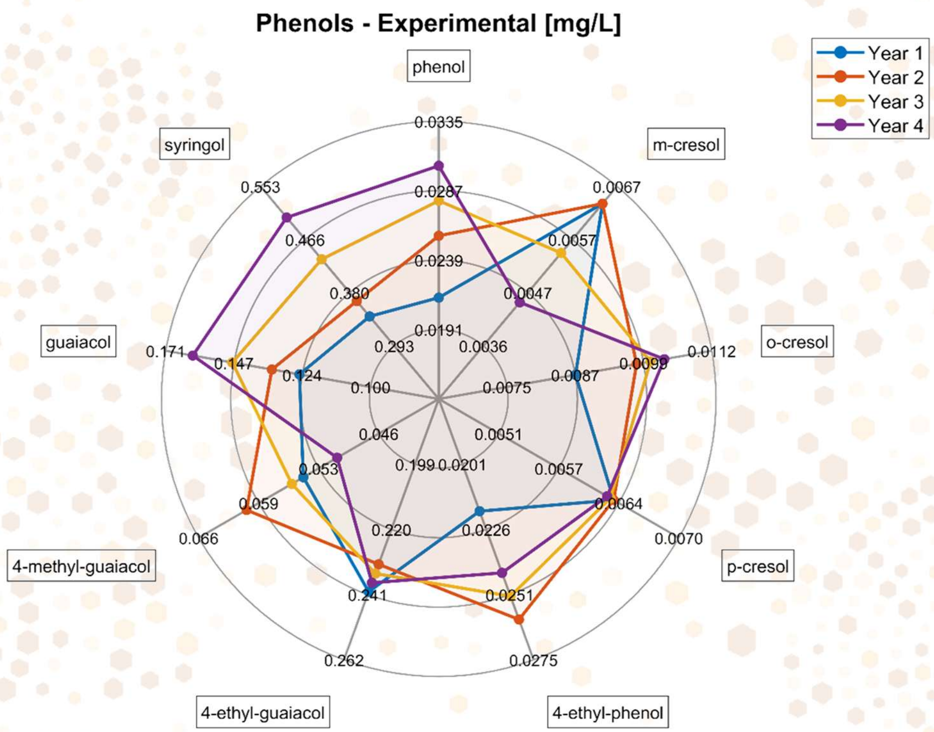
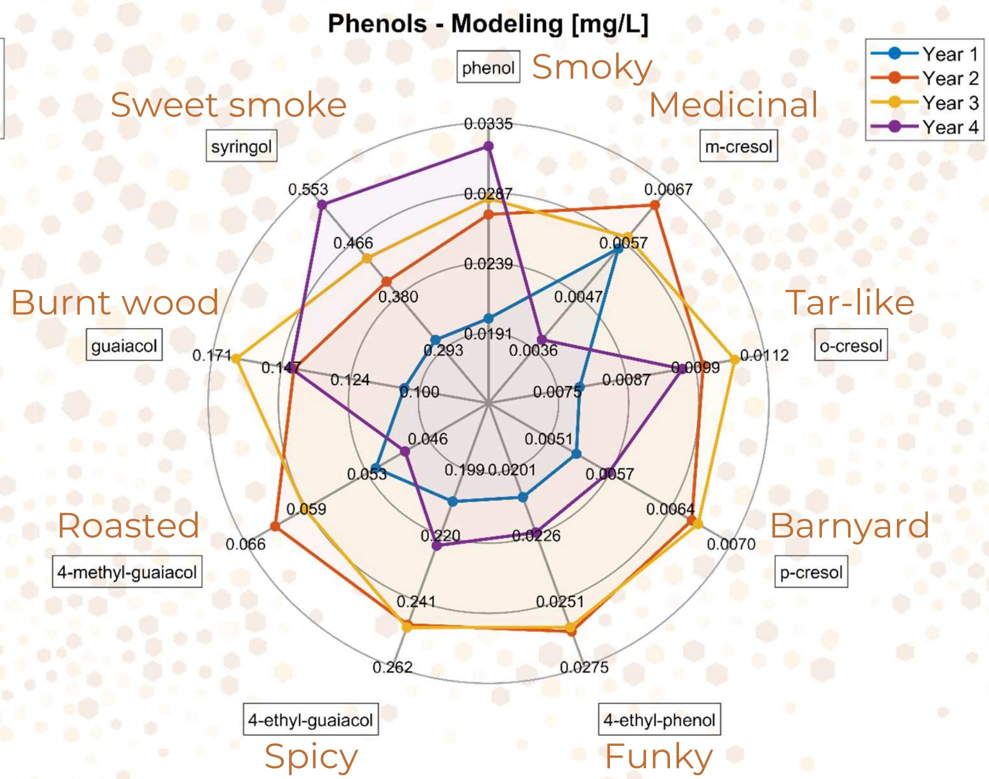
Phenols: Smoky, Spicy, & Woody





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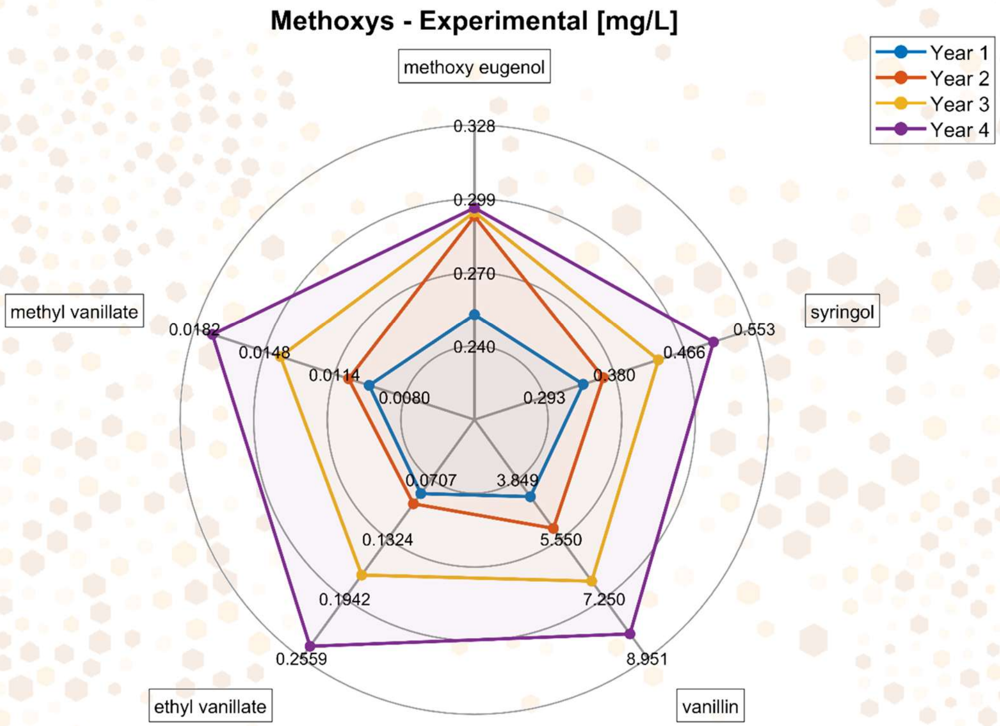
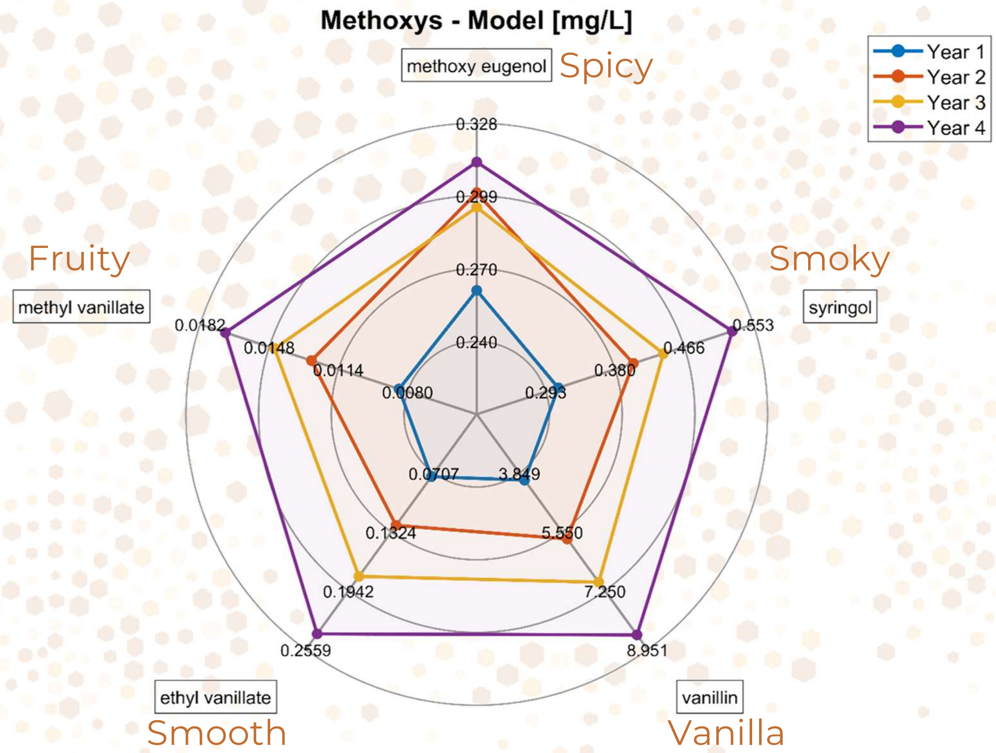
Phenols Underpredicted at Year 1: Model shows a 6.8% average difference from experimental data

Methoxys: Sweet, Spicy, & Aromatic





Methoxys Trends Matched: Model shows a 7.5% average difference from experimental data

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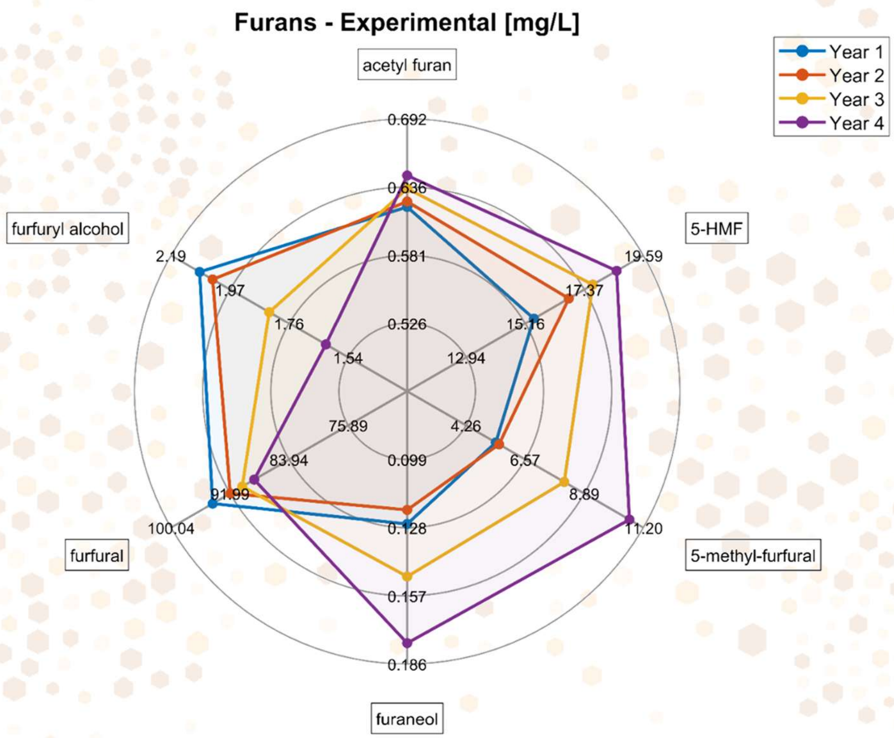
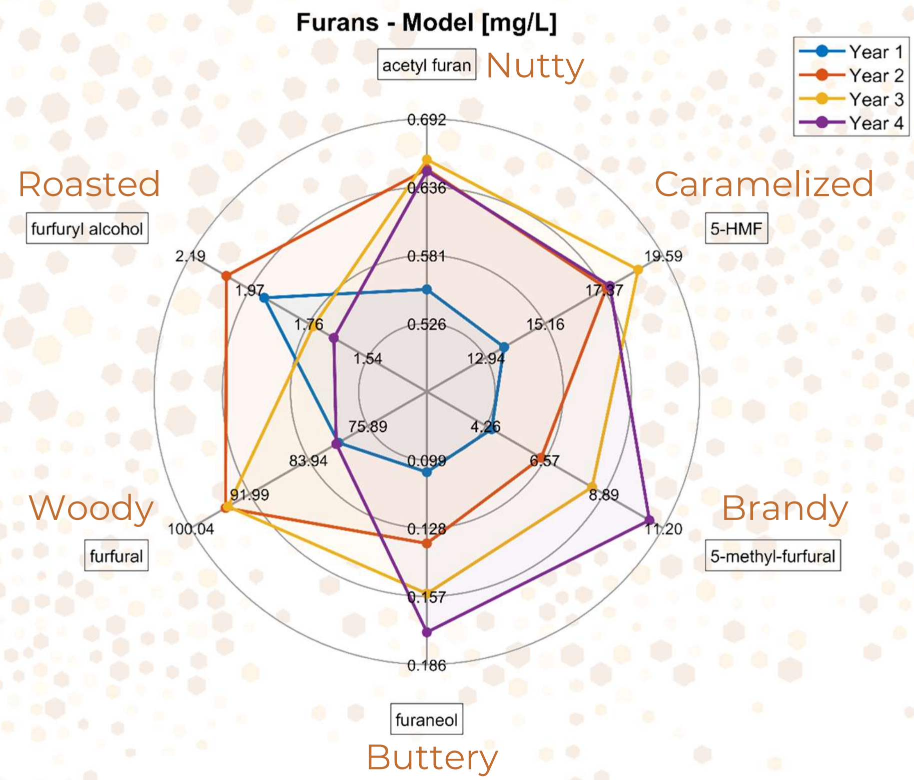
Furans: Caramel, Toast, & Sugar





Furans Predicted Reasonably: Model shows a 7.1% average difference from experimental data

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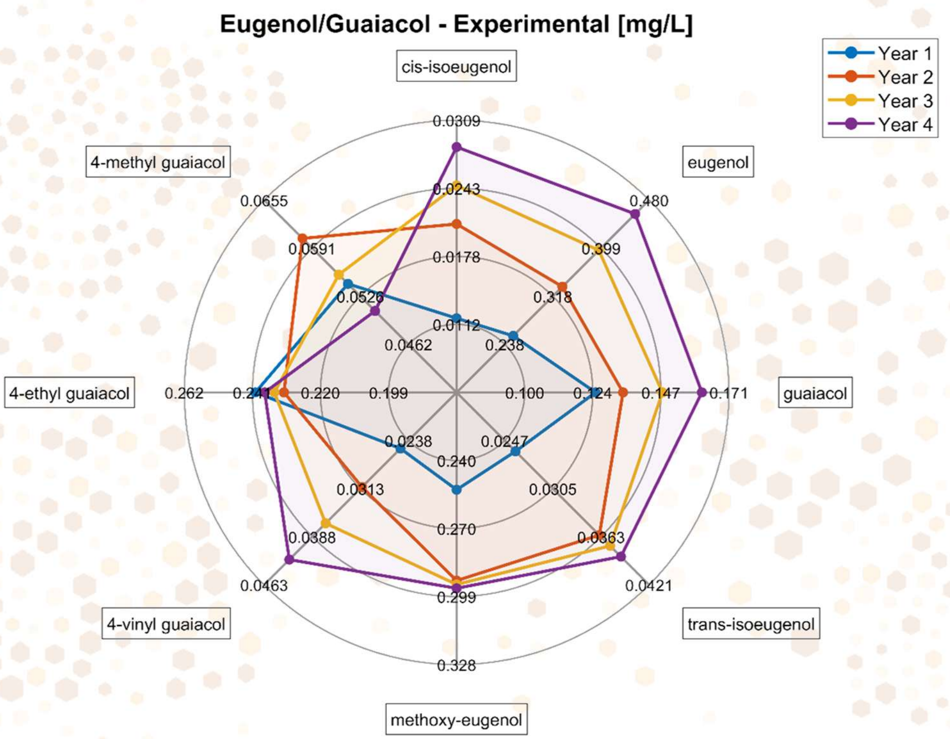
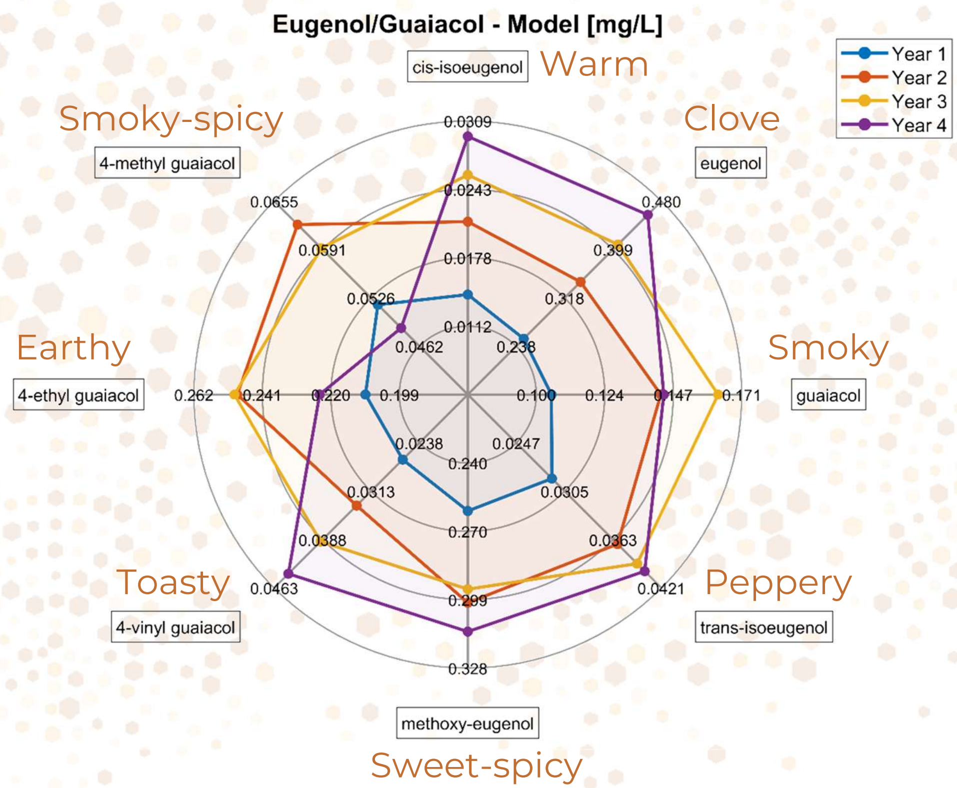
Eugenols: Spicy, Smoky, & Clove





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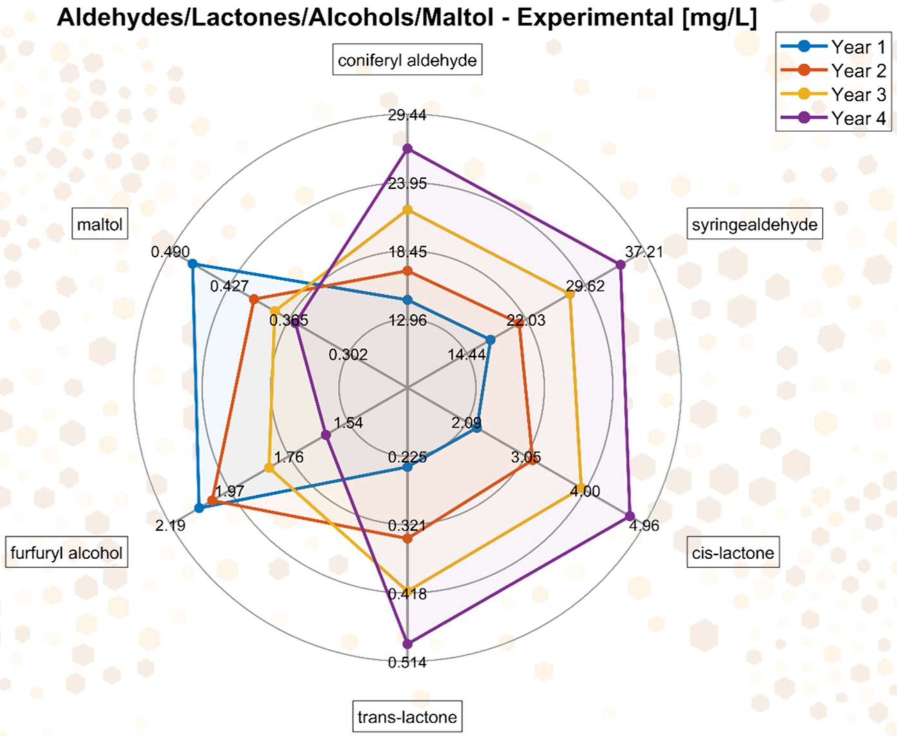
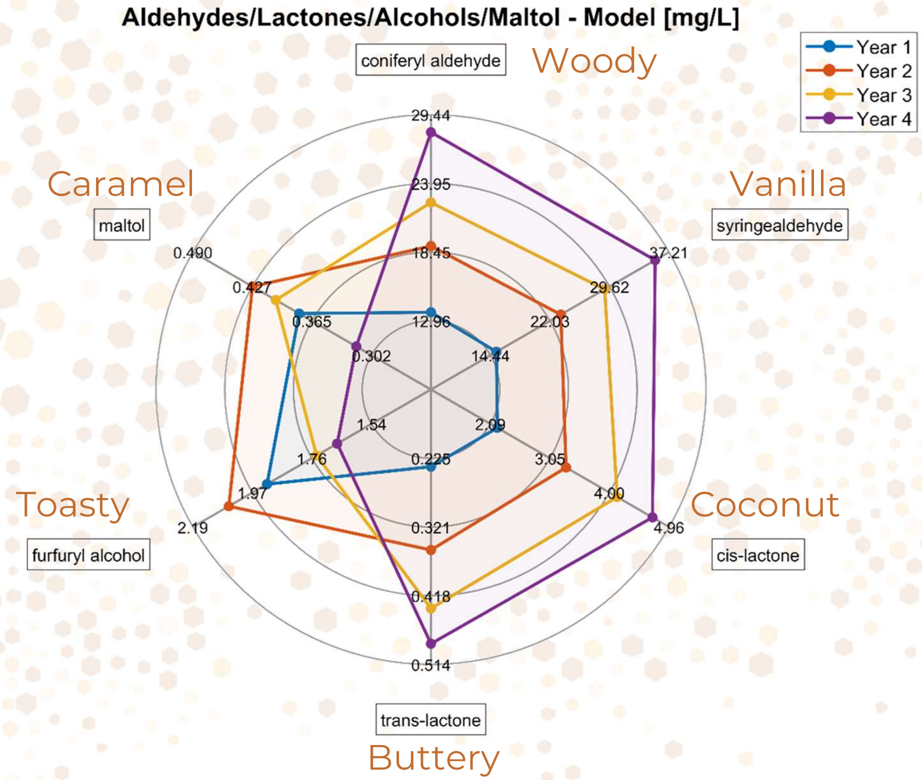
Eugenols Predicted Consistently: Model shows a 6.0% average difference from experimental data

Final Notes: Woody, Creamy, & Sweet





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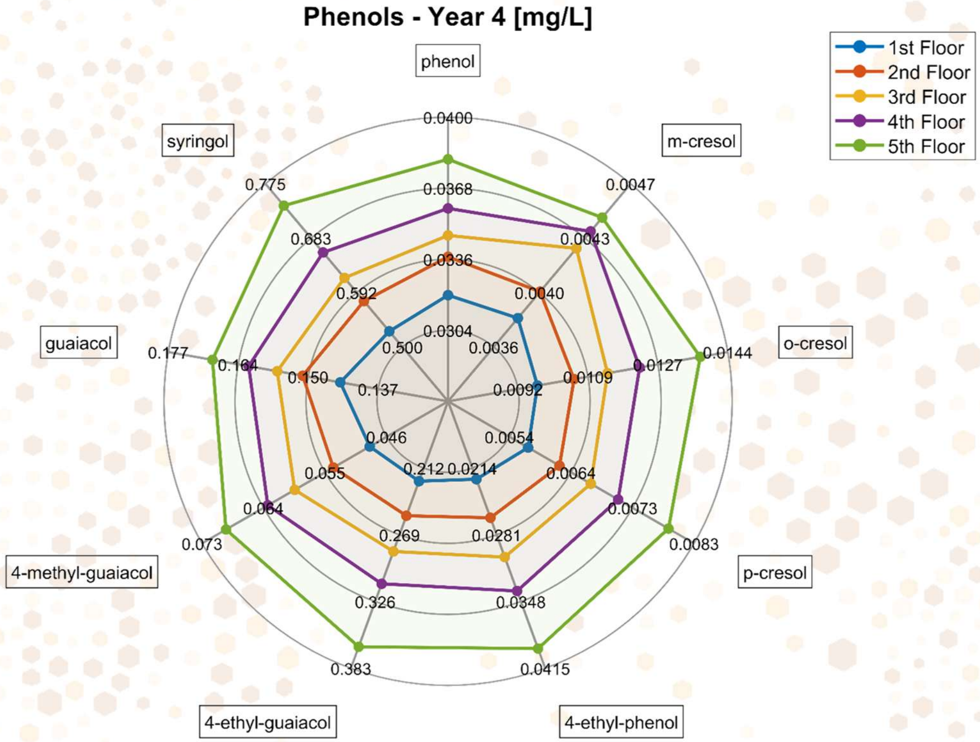
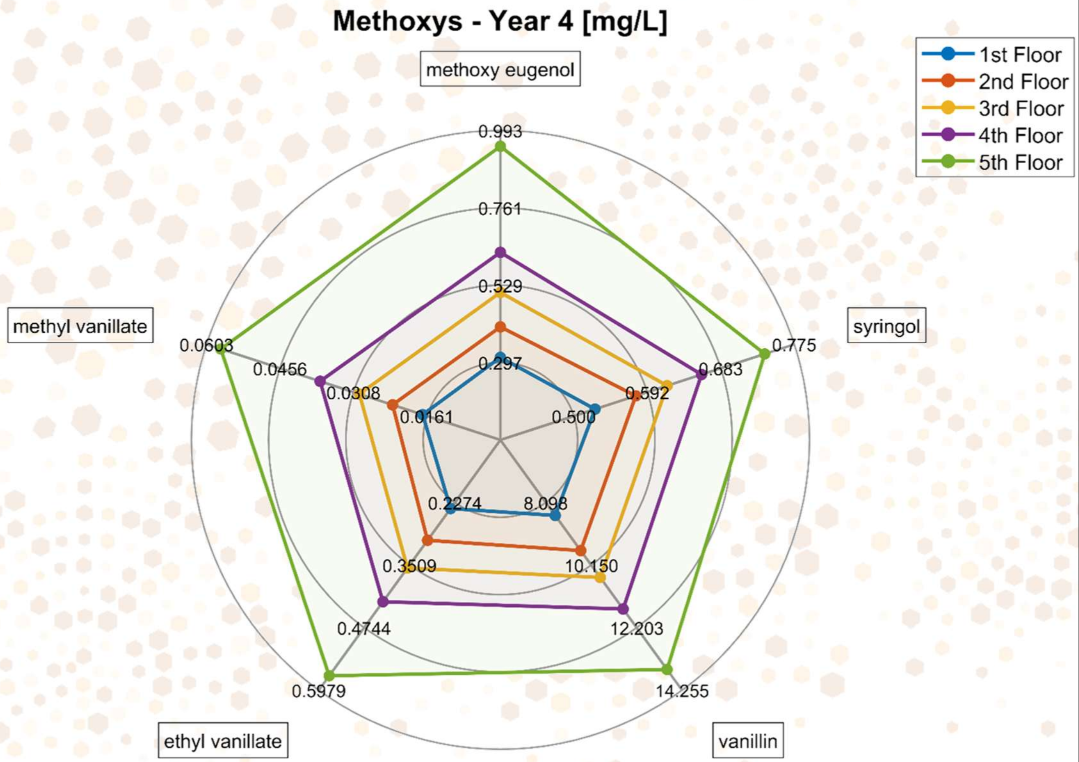
Other Chemical Species: Model predictions align with experimental data, showing a 5.9% average difference

Phenols & Methoxys: Different Floors





Floor-Level Predictions at Year 4: Model captures species behavior across floors, with trends showing variability rather than perfect linearity

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Discussion

- Captures non-linear chemistry, adapts to wetted surface areas & oxygen influx
- Strong predictive ability, with an average congener difference of 6.7% (mg/L)
- Model improvements:
  - Enhanced data collection on initial distillate composition
  - Frequent sampling in the first 6 months, then reduced frequency
- Expectation vs. Reality: Model provides insight and precise trend predictions, but expecting exact matches is unreasonable
- Physics & Thermodynamics-Based:
  - Requires minimal input data for accurate predictions
  - Unlike Machine Learning models, does not require massive datasets

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Conclusions

- **Physics-Based Model** – Accurately predicts aging trends, providing reliable insights into the maturation process
- **Value Proposition** – Can help guide decisions about future production strategies
- **Process Optimization** – Allows for adjustments to improve efficiency, yield, & quality
- **Operational Benefits** – Supports efforts to optimize proof gallons, congeners, and consistency
- **Predictive Decision-Making** – Helps explore proactive warehouse adjustments
- **Consistency & Efficiency** – Potential to improve batch uniformity and minimize the need for corrective blending
- **Versatility** – Adaptable to other barrel-aged spirits beyond whiskey

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Chris Depcik – LinkedIn

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Thank you!

Any Questions?

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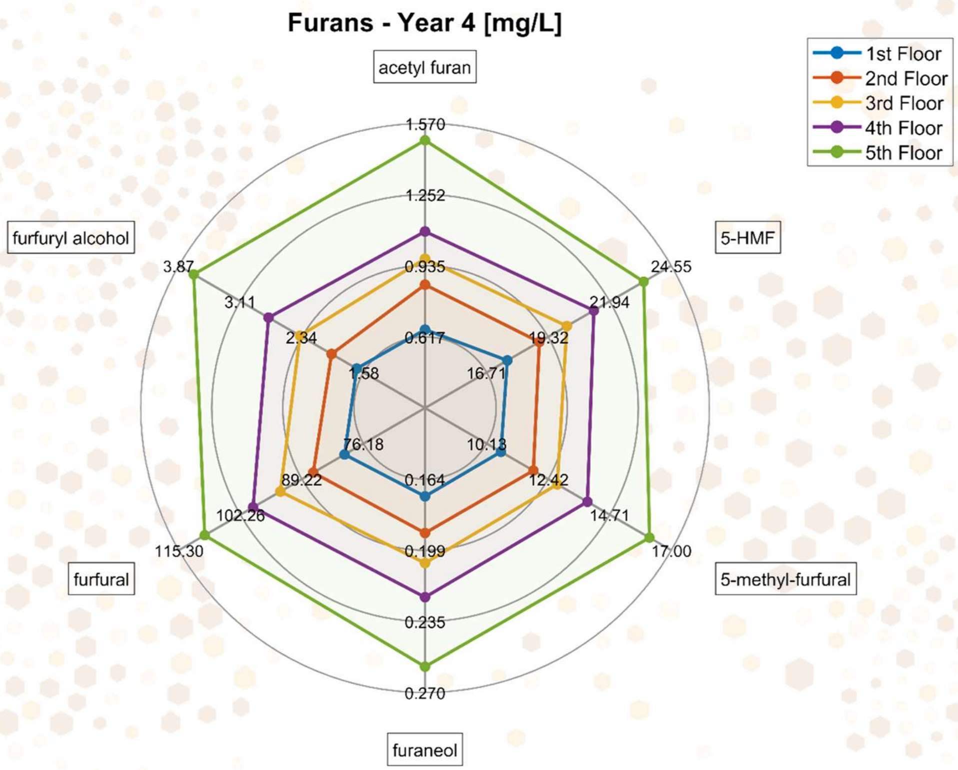
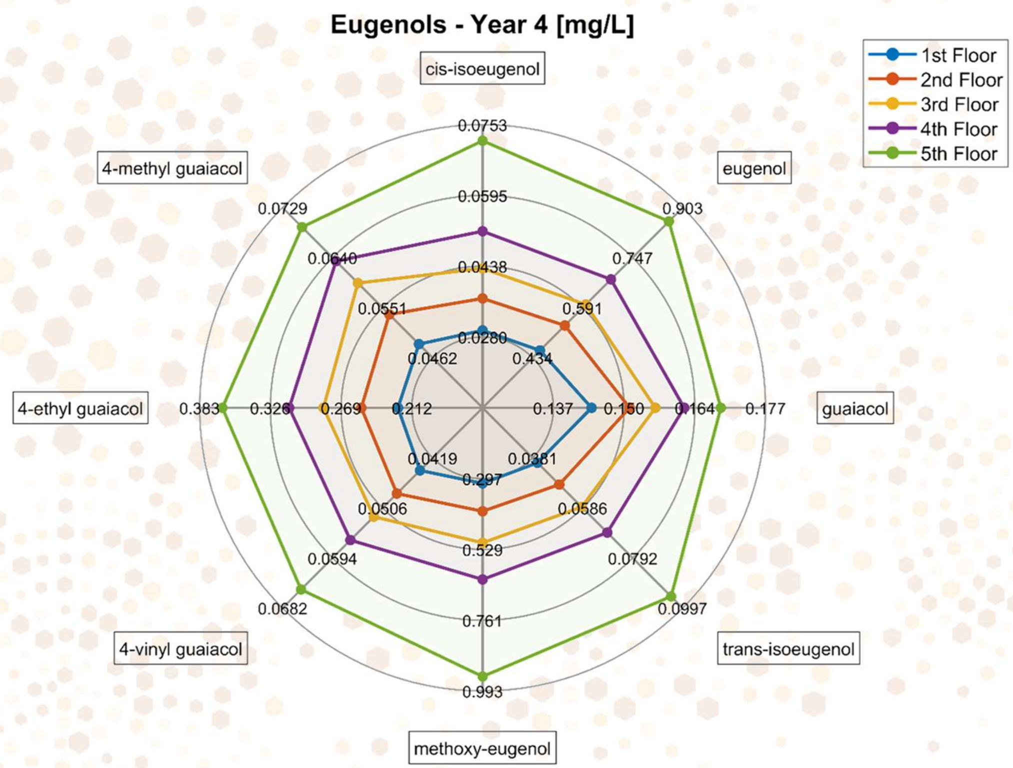
Furans & Eugenols – Different Floors





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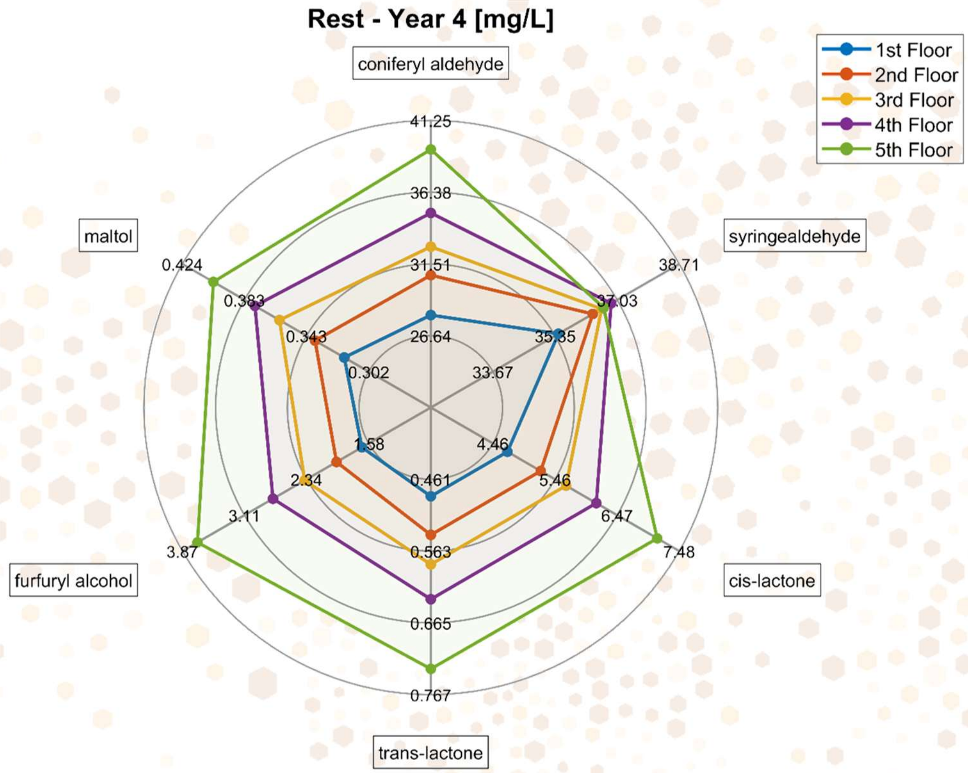
Floor-Level Predictions at Year 4: Model captures species behavior across floors, with trends showing variability rather than perfect linearity

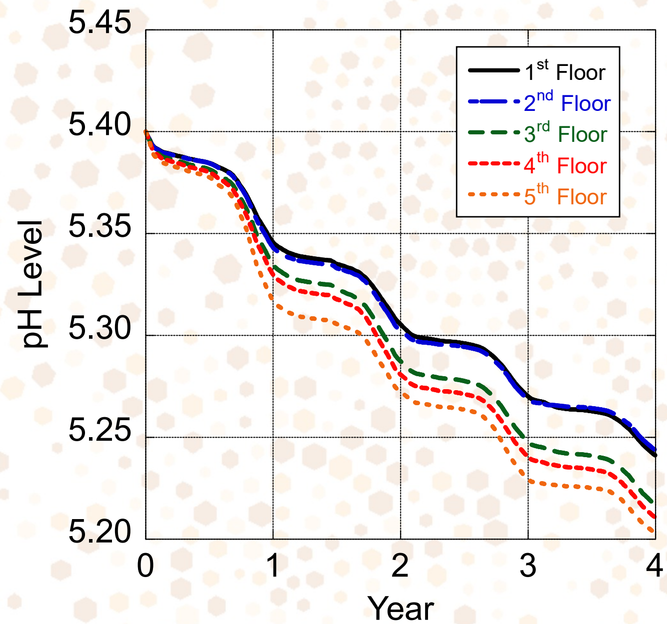
Rest – Different Floors



Floor-Level Predictions at Year 4: Model captures species behavior across floors, with trends showing variability rather than perfect linearity

pH Level Predictions

- Baldwin & Andreasen (1974): Changes in pH level over time
- General model based on ABV, acid extraction, and oxidation reaction expressions
- Can be extended to include tannin conversion to ellagic and gallic acids
- Floor impact:
  - ABV↑ pH↑
  - Volume loss↑ Wetted surface area↓ Lower acid extraction = pH↑
  - Temp↑ Extraction & Oxidation↑ pH↓



Overall, the pH level decreases with increasing floor as the temperature effects cause the reaction rates to dominate

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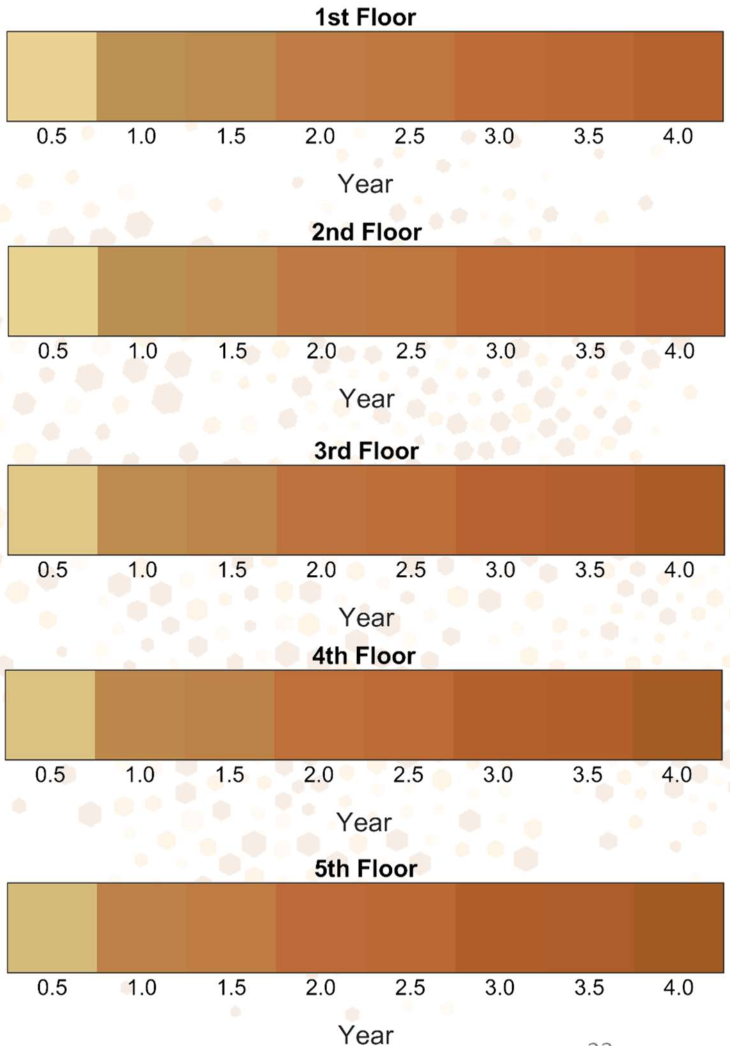
doi: 10.1093/jaoac/57.4/940

Color Predictions

- Baldwin & Andreasen (1974): 430 nm absorbance data over 12 years correlates with whiskey color development
- Color model: Integrated with pH predictions to track extraction trends
- Tannins: Primary contributor to color, strongly influenced by pH
- Floor-level effect: Higher floors show subtle darker color due to increased extraction (reflected in pH changes)



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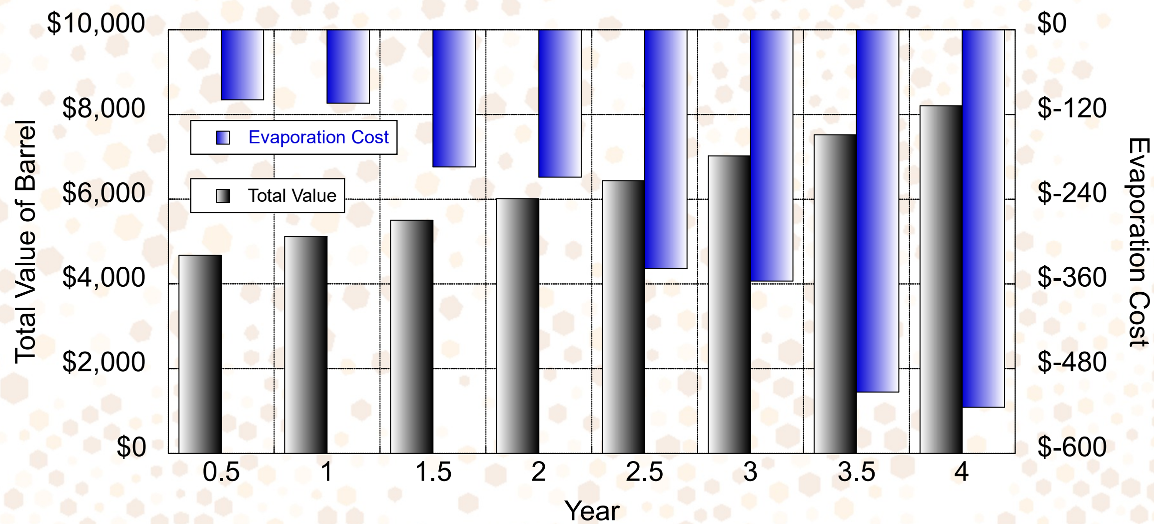
Economics

- Whiskey valuation modeling: Tracks value changes over time to inform financial decisions
- Technoeconomic analysis: Links exergy losses to economic impact, optimizing efficiency
- Strategic insights: Helps assess aging duration and floor selection for maximum returns



Estimate of the total value of the barrel on the 1st floor along with the cost due to evaporation

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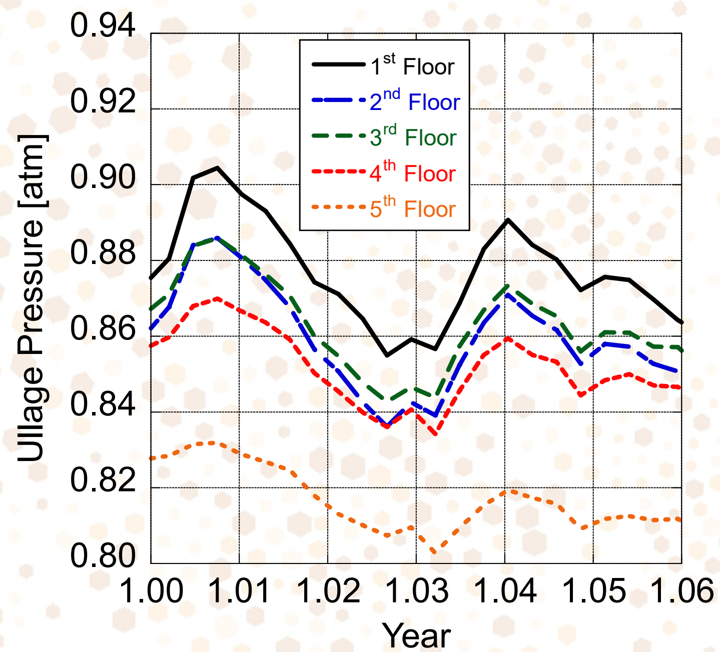
Ullage Pressure

- Roussey et al. (2021): Ullage pressure influenced by initial headspace volume and wood moisture variations
- Evaporation effect: Slows gas expansion in the barrel headspace over time
- Model integration: Accounts for both factors, showing increased evaporation impact at higher floors



Ullage pressure across floors: Snapshot at 1.00–1.06 Years, highlighting increased evaporation effects at higher levels

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