Three-Dimensional Modeling of Whiskey Evaporation and Esterification

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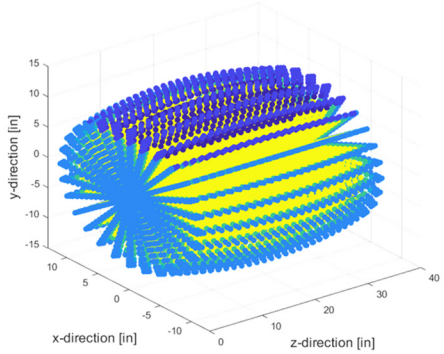
- Global sales projected to hit $128 billion by 2028
- Compound annual estimated growth rate > 6%
- Customer demand increasing for premium spirts and innovative whiskey varieties

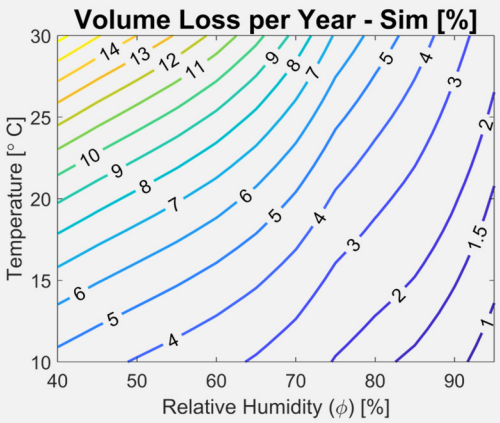
In combination with master distillers, predictive modeling of whiskey evaporation and esterification can help *tweak* whiskey characteristics

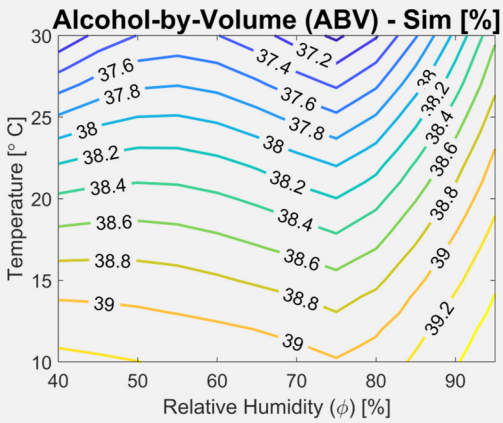
Unique and novel three-dimensional simulation tool:

- Variable properties and discretization in fully implicit solver: any characteristics or time-step is possible
- Horizontal and vertical barrel options
- Staves include influence of moisture content
- Alcohol-by-Volume and Alcohol-by-Weight predictions
- Evaporation of ethanol and water through barrel
- Heat transfer based on unconfined or confined barrels



Filled 50-gallon barrel with whiskey, air gap, unsaturated staves, and saturated staves shown



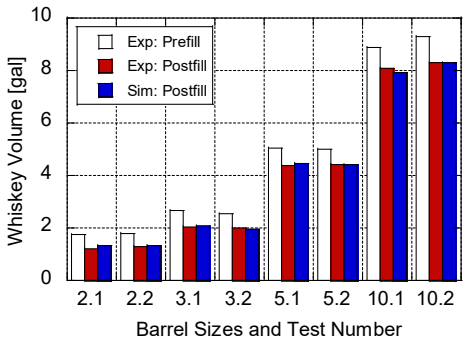


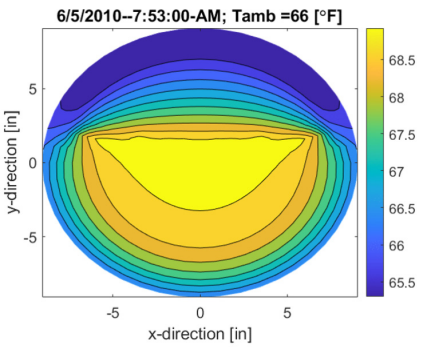
Validated with evaporation data:

- Year long experiments
- Impact of ambient temperature and relative humidity
- Volume loss in 205 L white oak barrels: simulations on average $0.14 \pm 0.11\%$ different
- Experimental ABV range: 37.3%-39.5% no discernable trend

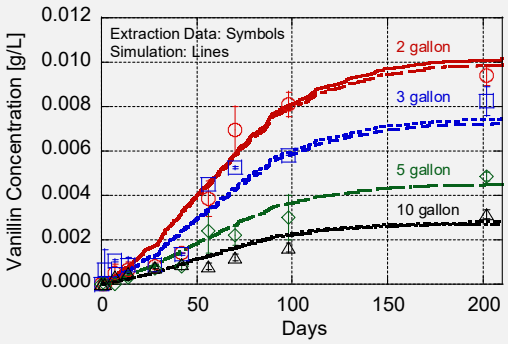
Variable environmental conditions:

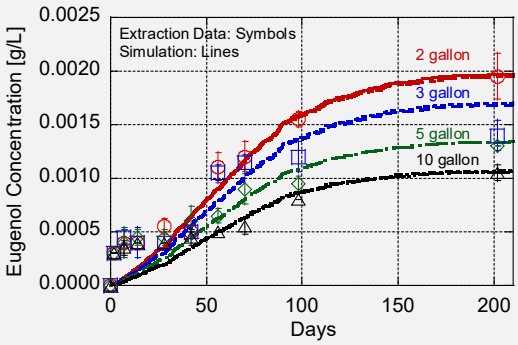
- 270-day ageing experiments
- 2-, 3-, 5-, and 10-gallon barrels
- Used wunderground for ambient temperature and humidity
- C numerical code, ***no special software or hardware needed***
- Simulated in 5 minutes on desktop computer; 75,000× faster than real-time (1,728 nodes)!





(Left) Simulation of different barrels and (Right) Illustration of temperature gradient within 10-gallon barrel that changes with ambient temperature





Extraction data verification:

- Based on surface area-to-volume ratio (simulation dynamically predicts)
- Chemistry developed and esterification well simulated; enhancements possible

Looking for collaborators, data for model improvements, commercialization potential

Watch a short presentation on the model!

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