High yielding conversion of xylose to furfural via boronate esters

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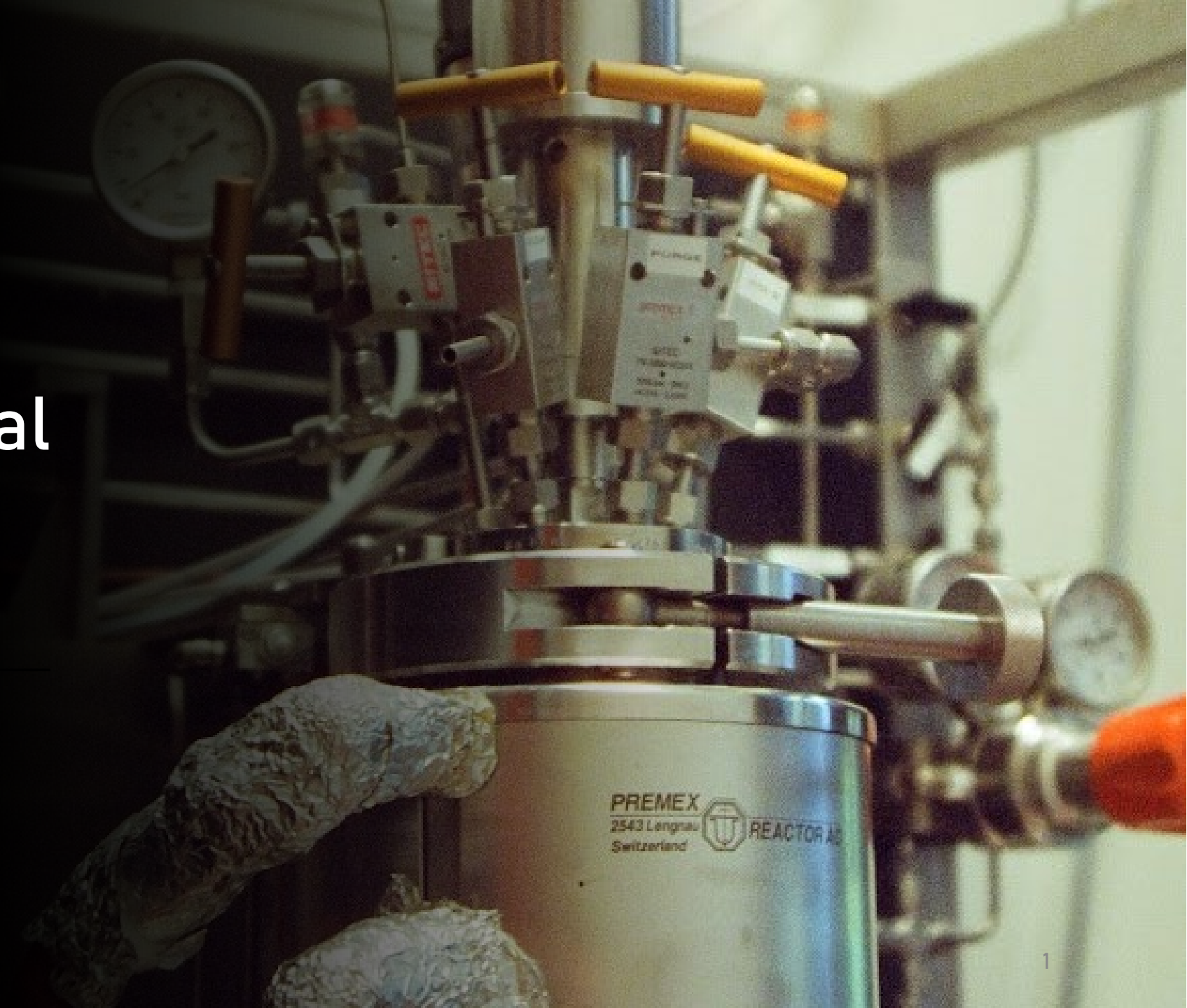


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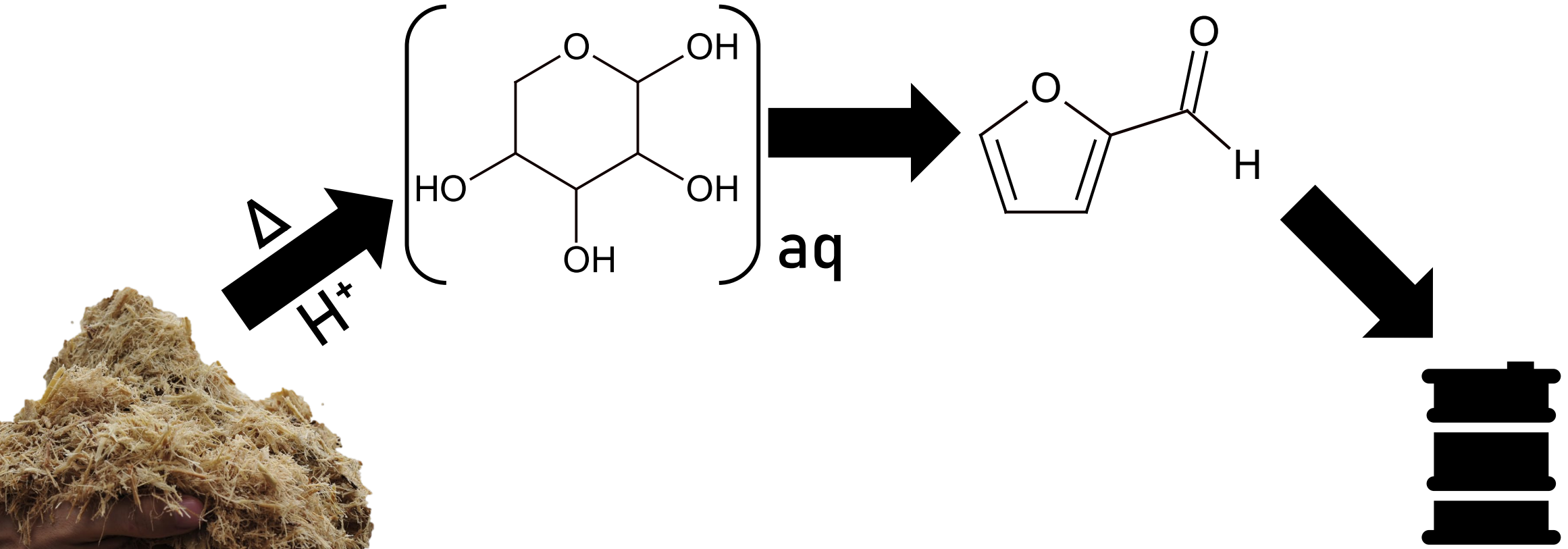
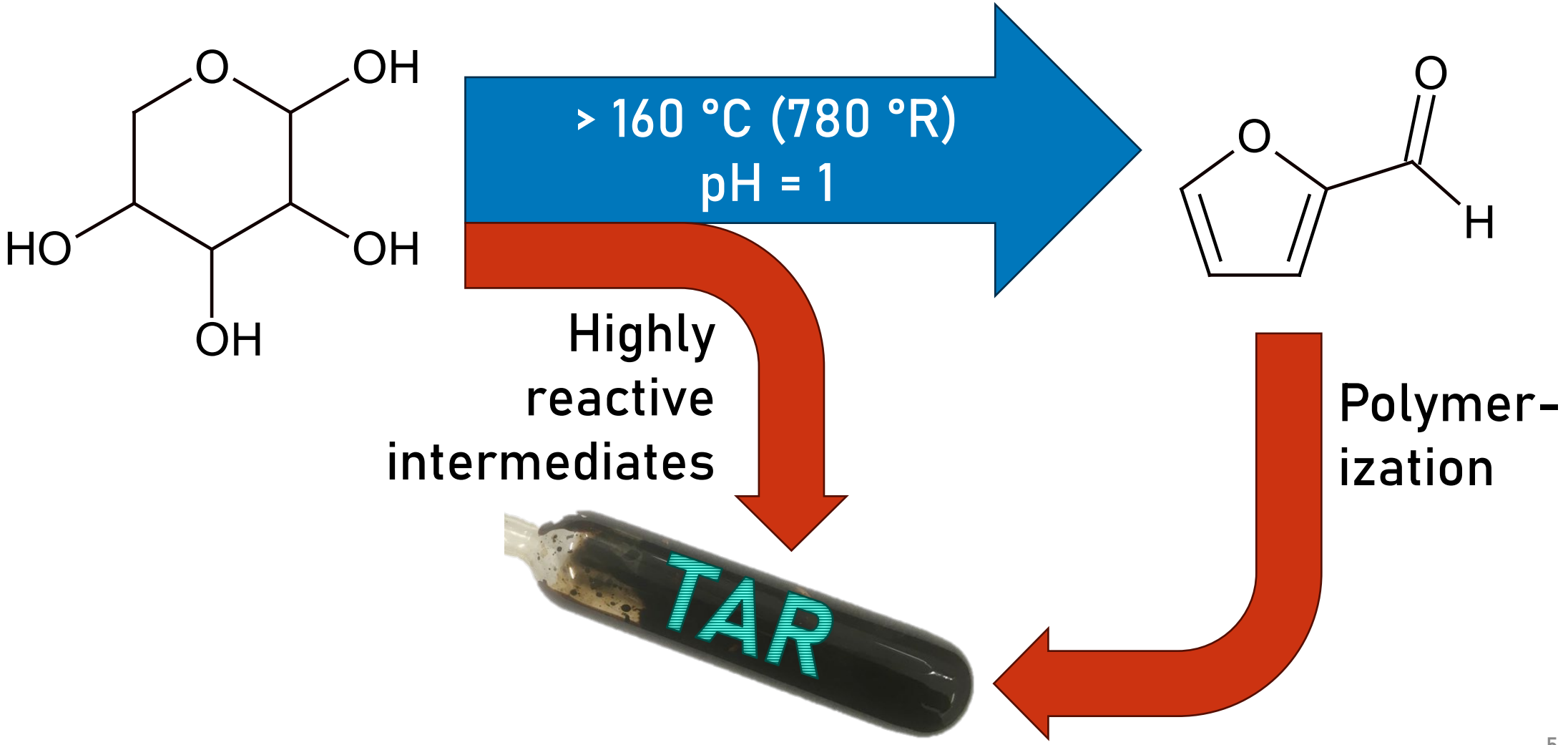
Sam Houston
Tollway
EXIT 2 MILES

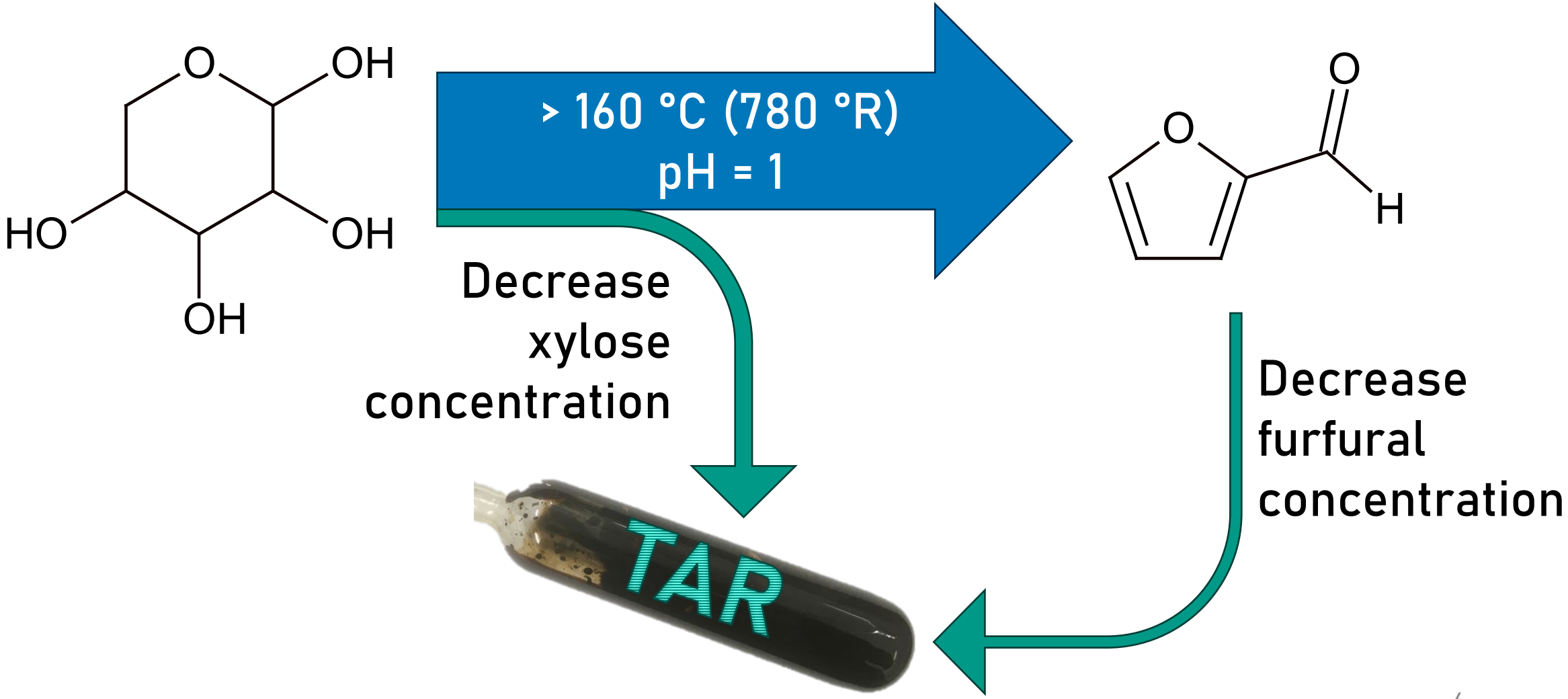
From by-product to platform chemical



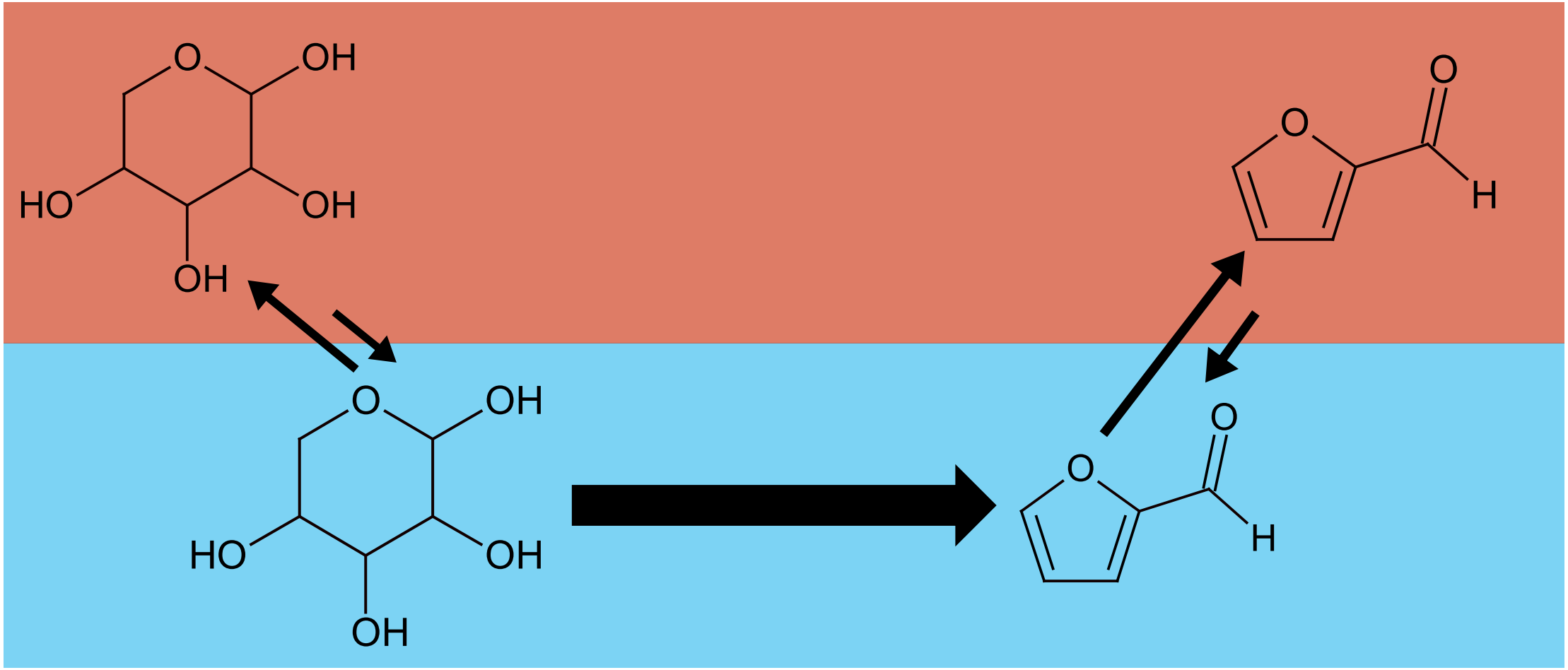
Current practice



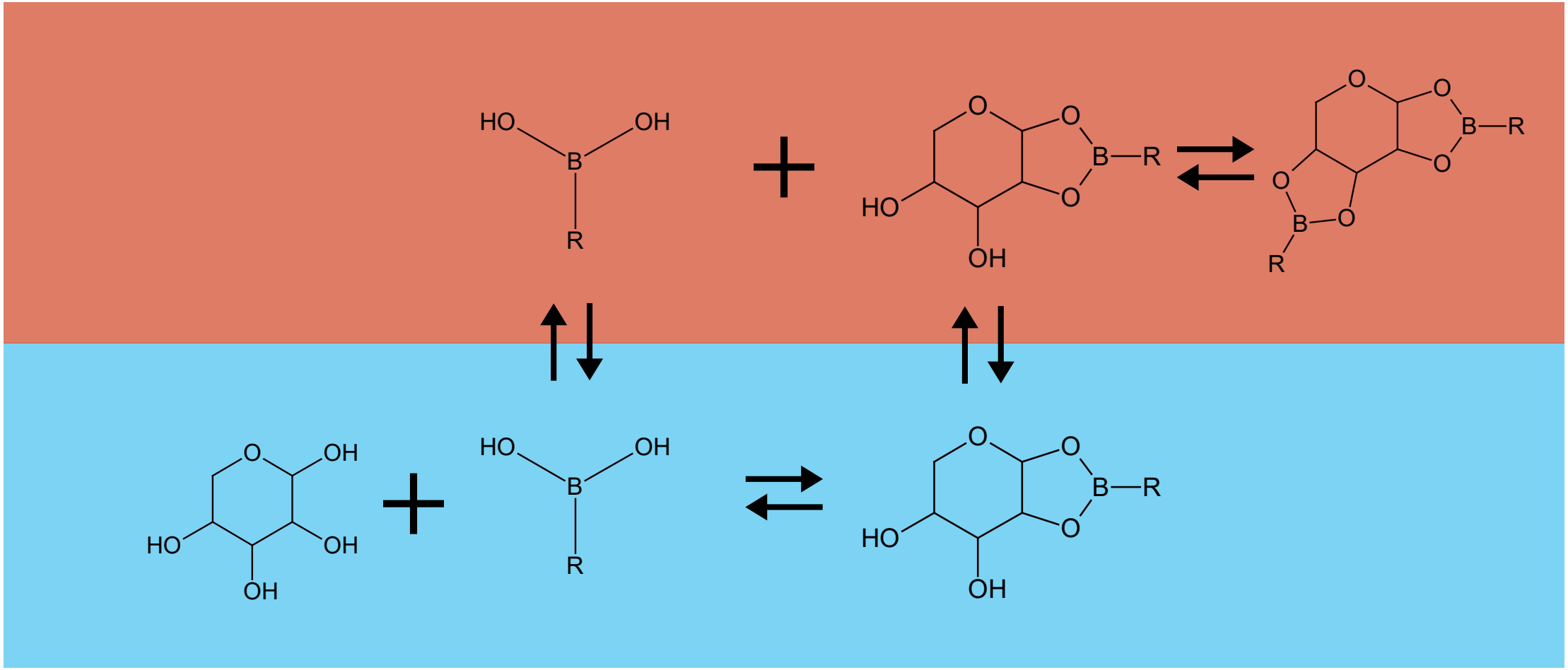
Alternatively



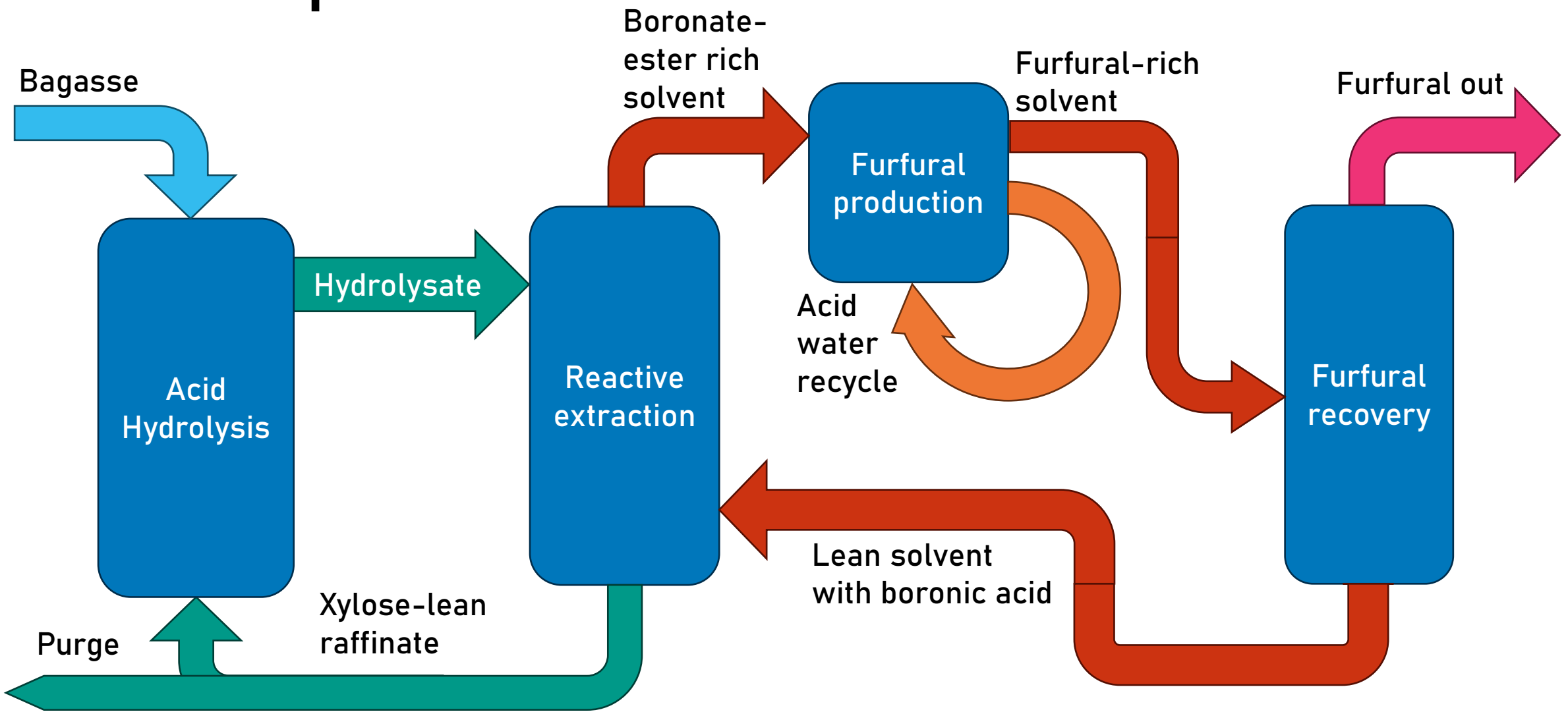
Realizing low concentrations



“Dissolving water into oil”



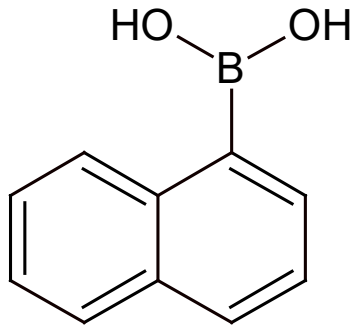
Overall process



Choice of chemicals

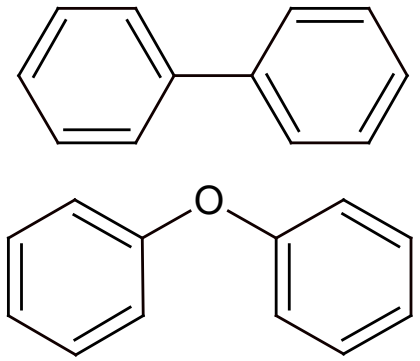
Boronic acid

- Apolar side group
  - High partition of ester to organic phase
  - Low solubility in water
- High reaction rate in esterification
- Aromatic



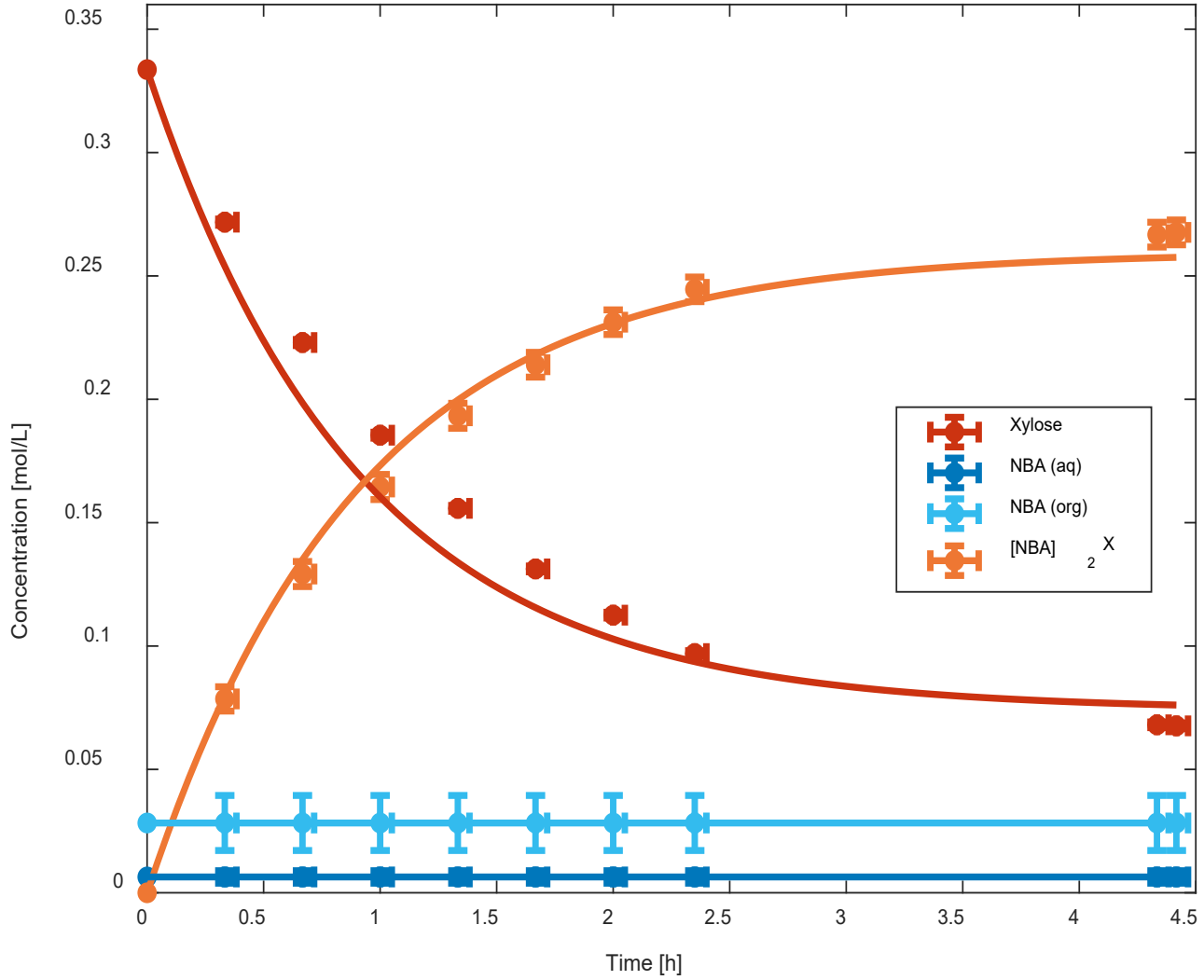
Solvent

- Aromatic
- Boiling point above furfural (162 °C)



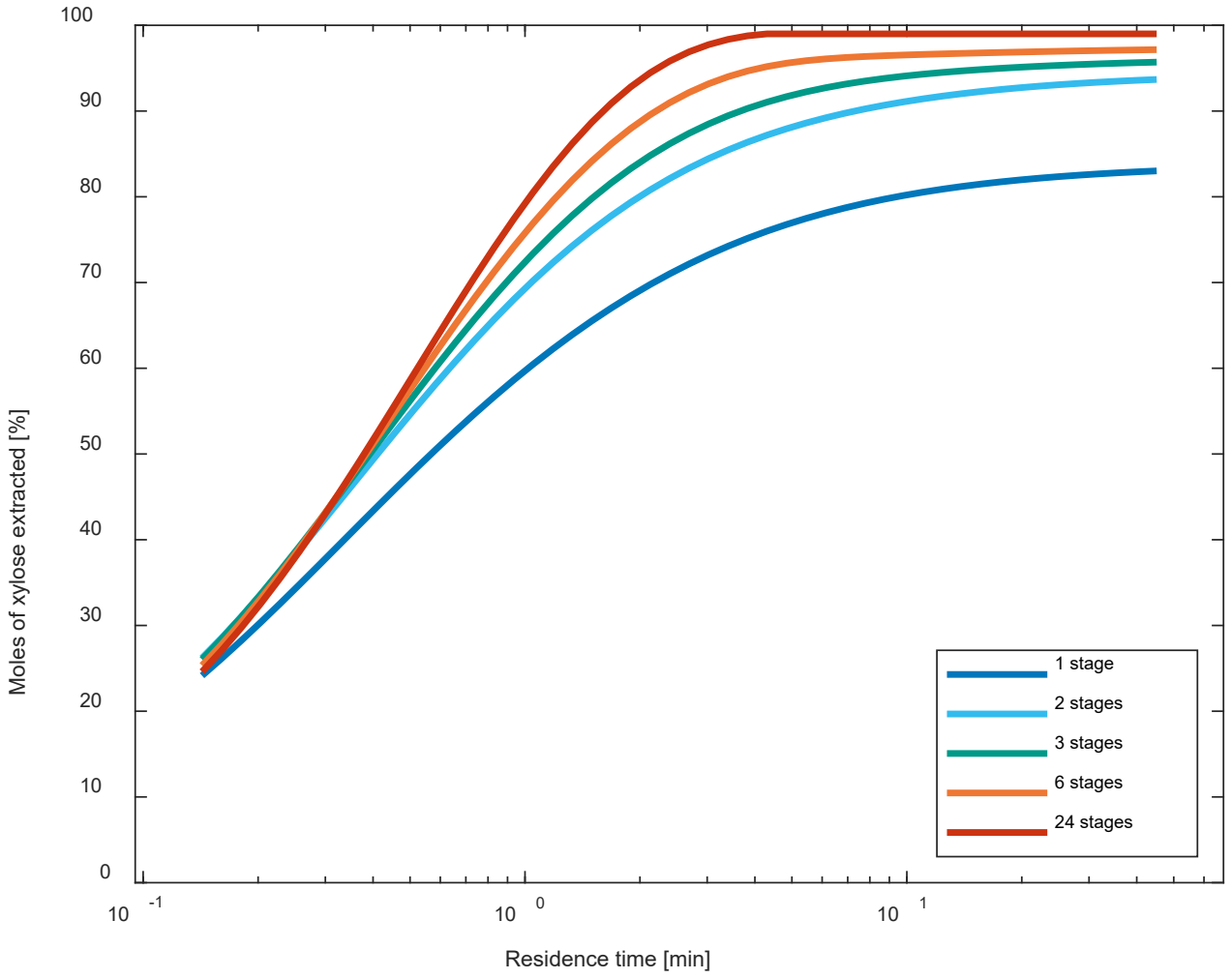
Extraction experiments

- Measured kinetics and equilibria from 20 to 90 °C
- Higher T favors kinetics and equilibrium
  - >80 % extracted in a few minutes at 90 °C

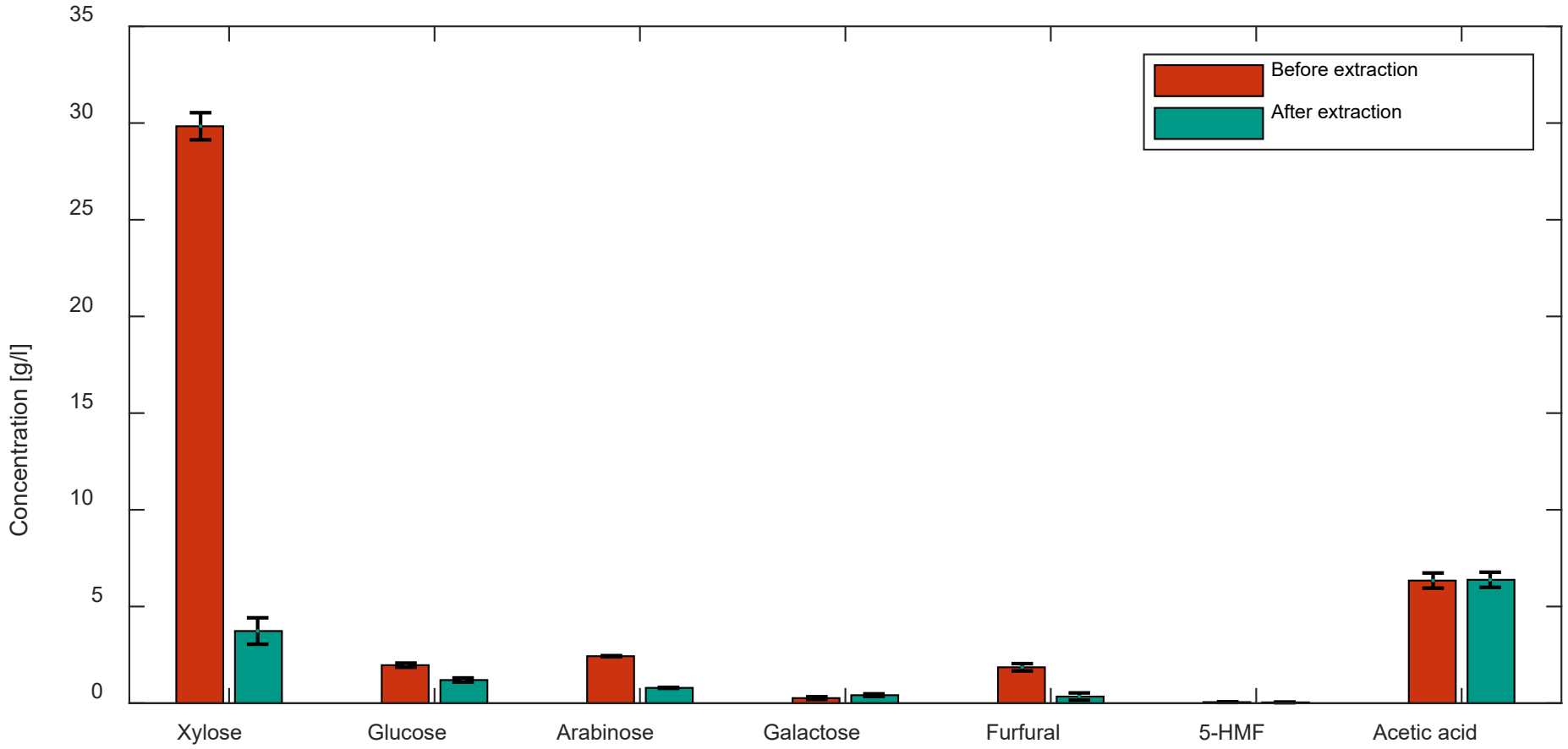


Extraction model

- CSTR model using measured kinetics and equilibria
- Designed a mixer-settler cascade for 90 % xylose recovery
  - Need three stages and 4 minutes
- Need to crystallize NBA out from raffinate

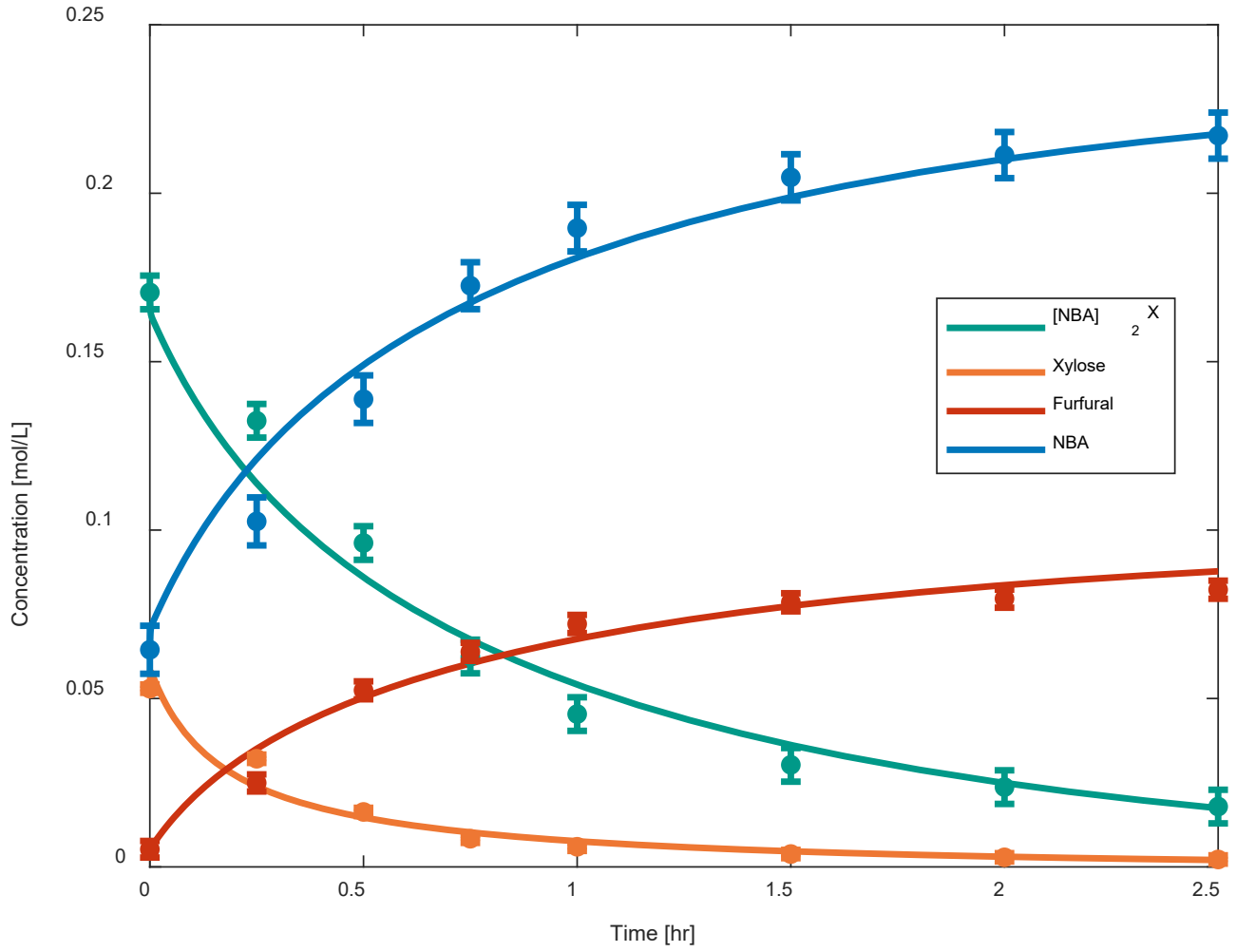


What about real (TC)biomass?



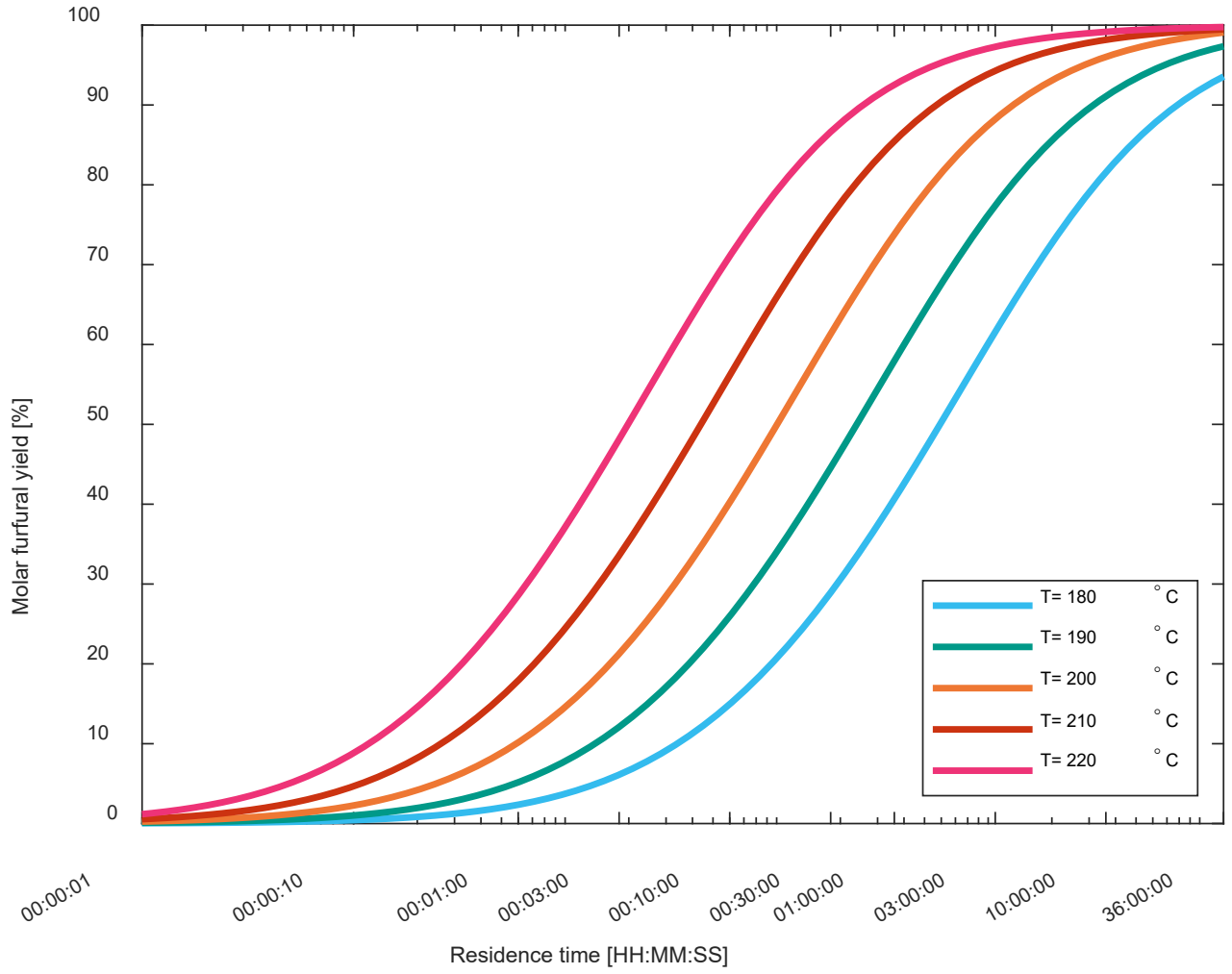
Furfural production experiments

- Successful production of furfural
- Also proven for hydrolysate
- >70 % molar selectivity batch-wise
- Selectivity varies little with temperature



Furfural production model

- Modelled a CSTR
- >90 % selectivity possible
- Construction is ongoing for experimental validation



Conclusion

- State-of-art yield of furfural is low
- Boronate ester improvement
- Proven reactive extraction
- Promising conversion

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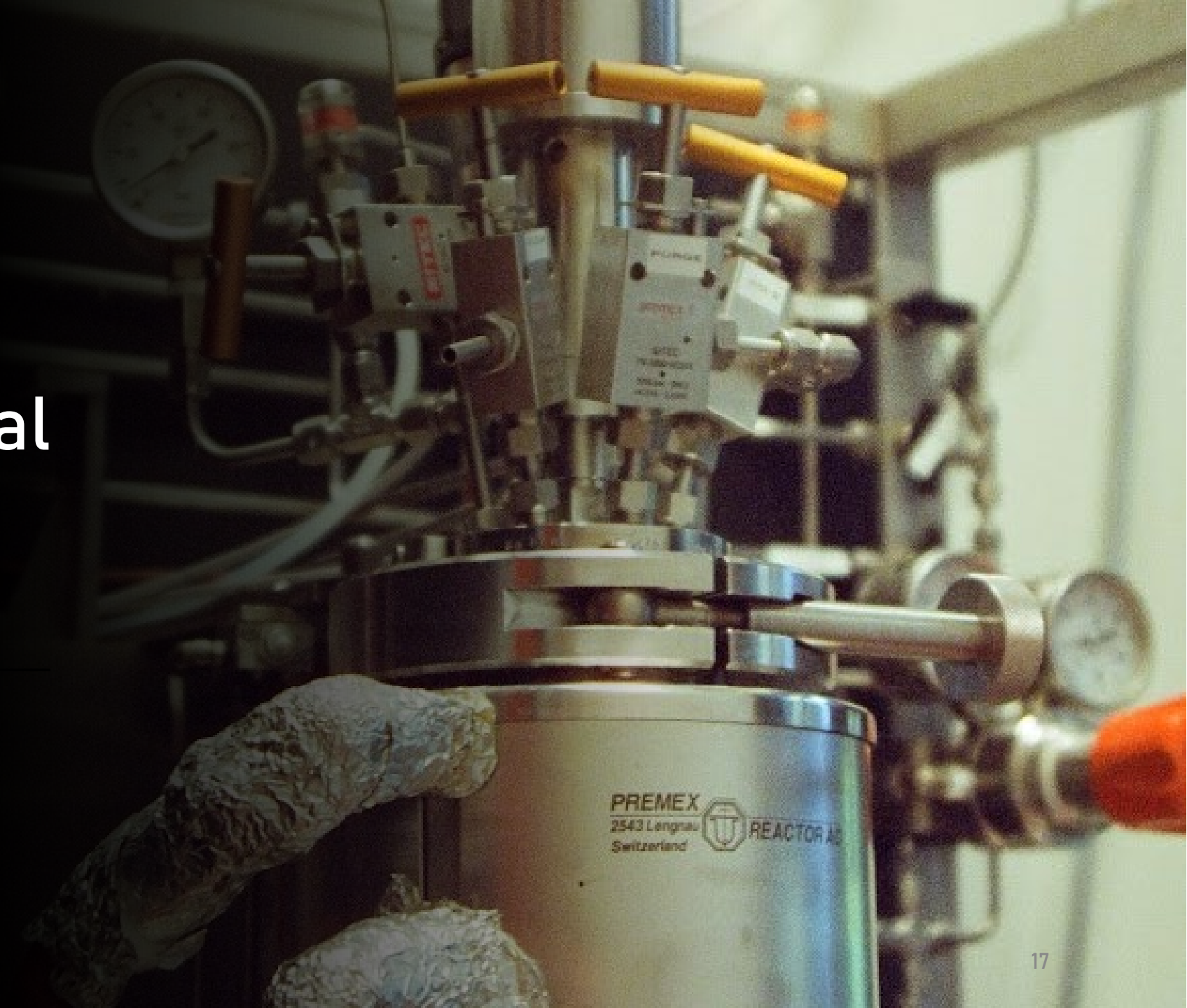
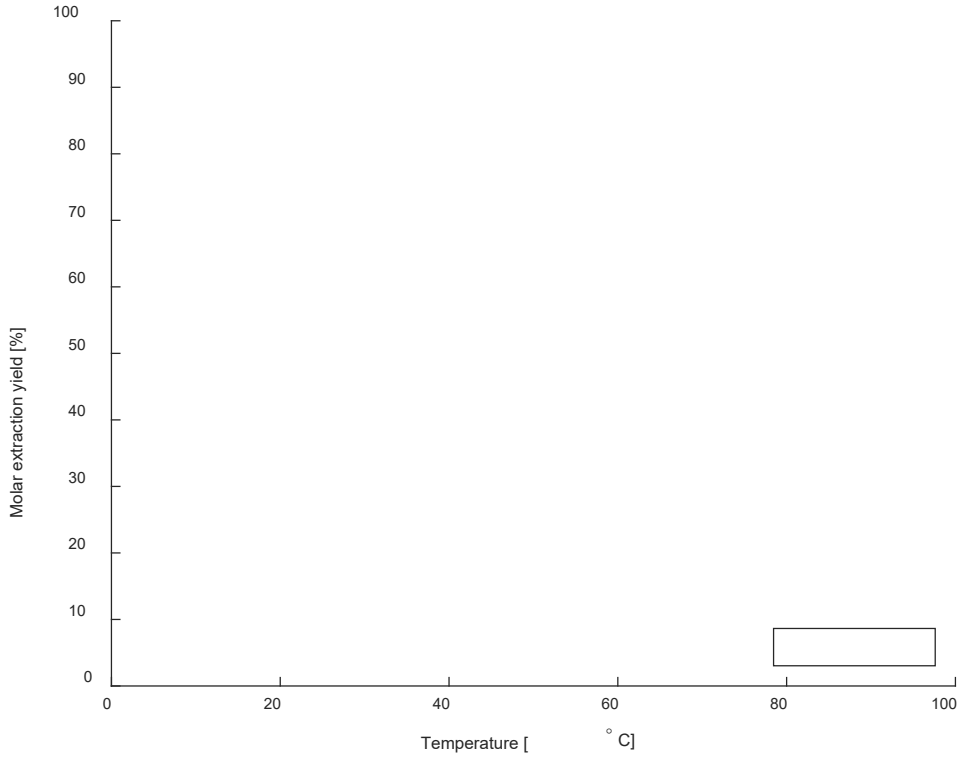


What about real (TC)biomass?

	Initial amount (g/L)	Extracted per pass (wt.%)
Xylose	29.83±0.70	87.5±2.3
Glucose	1.97±0.11	39.0±6.4
Arabinose	2.43±0.03	67.4±1.1
Galactose	0.26±0.07	No significant change
Furfural	1.87±0.19	81.5±10.3
5-HMF	0.06±0.02	No significant change
Acetic acid	6.34±0.39	No significant change

A closer look at the equilibrium



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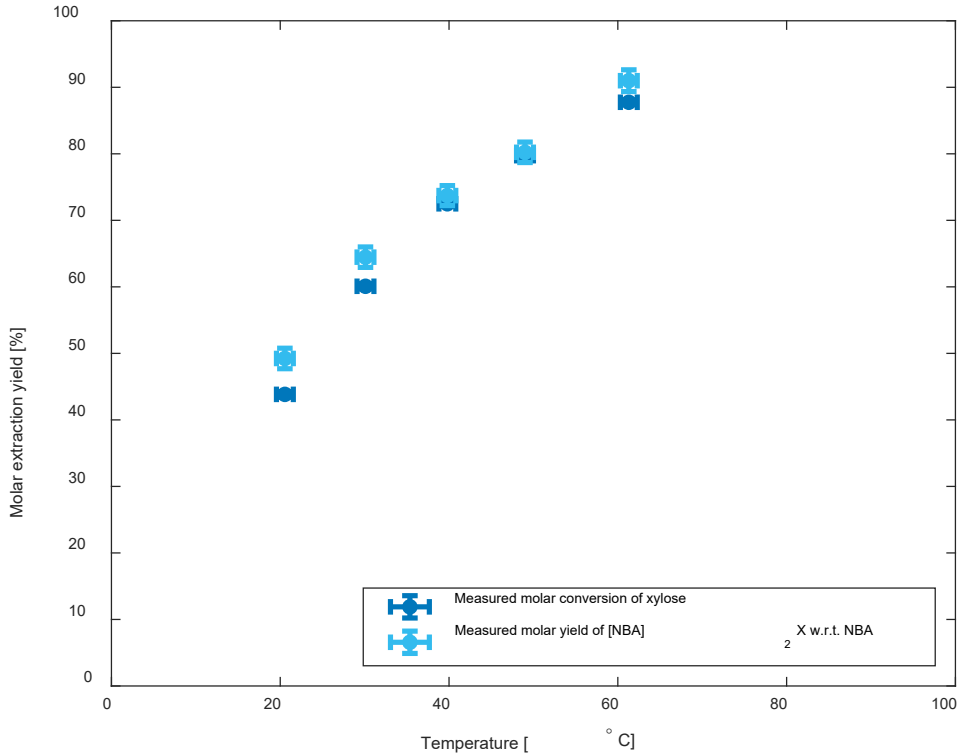
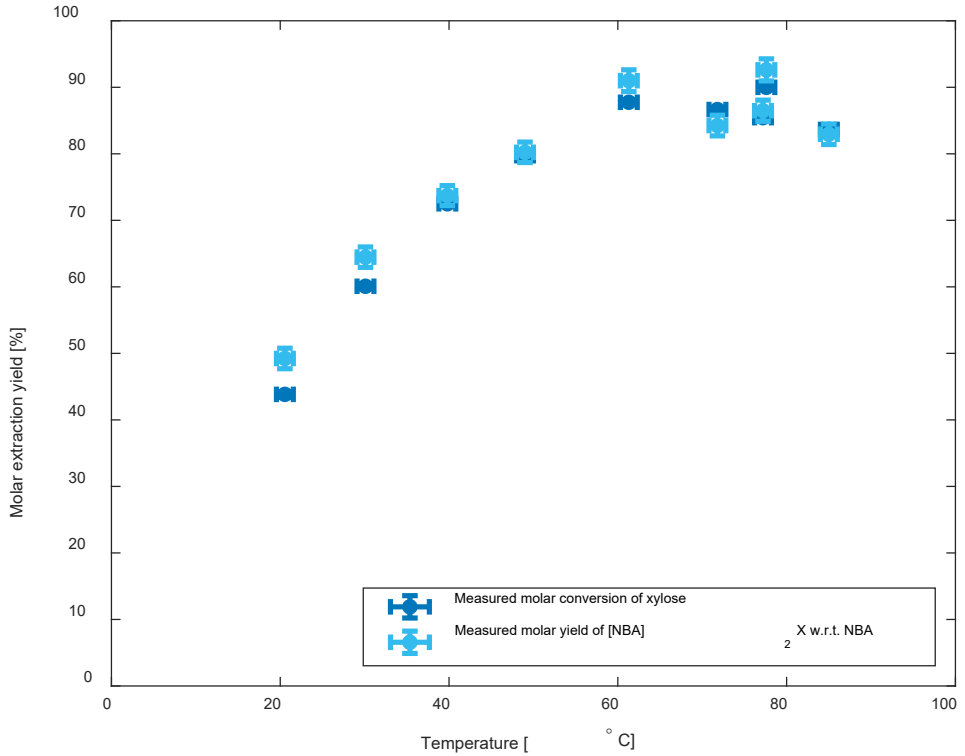


A closer look at the equilibrium

- $K = \frac{c^{org}_{[NBA]_2X}}{c^{aq}_{X} c^{aq}_{NBA} c^{org}_{NBA}}$



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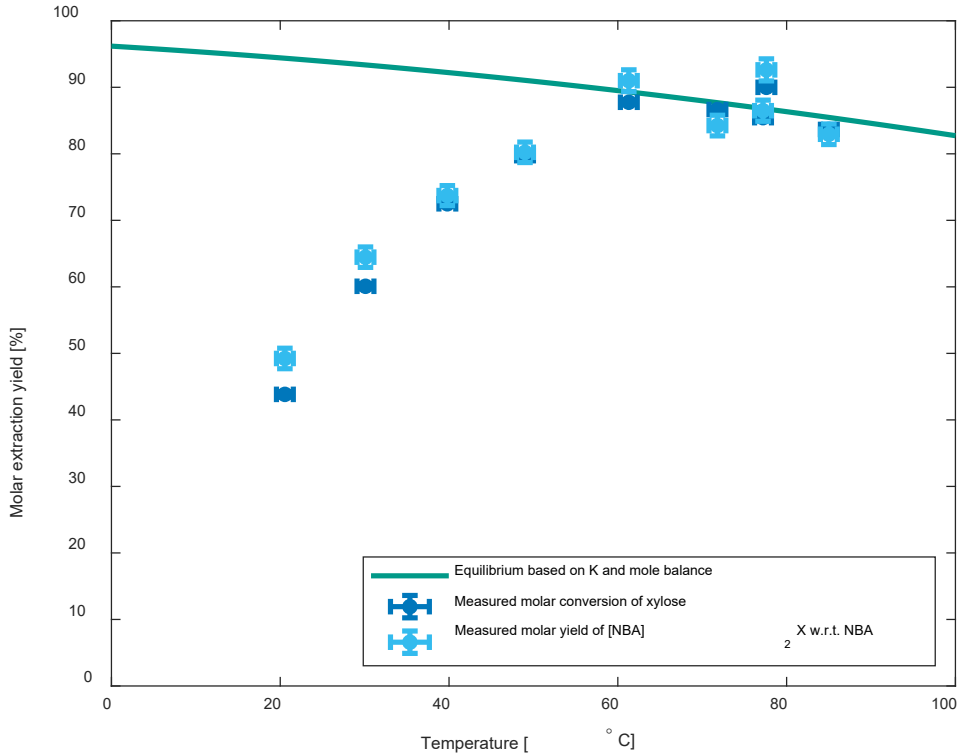

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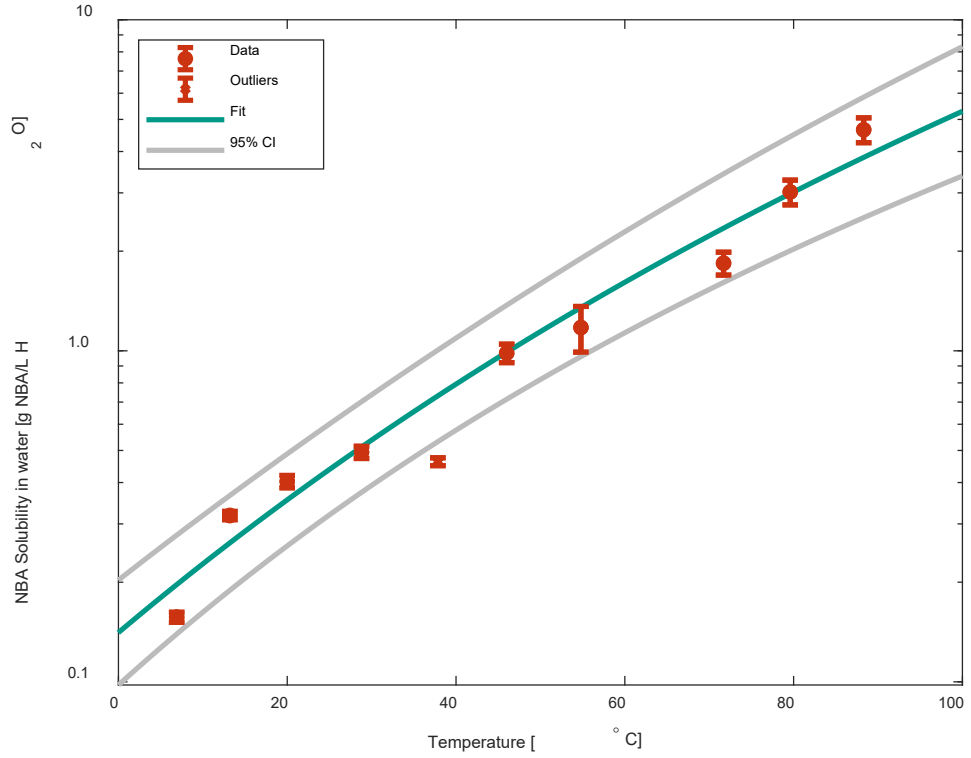

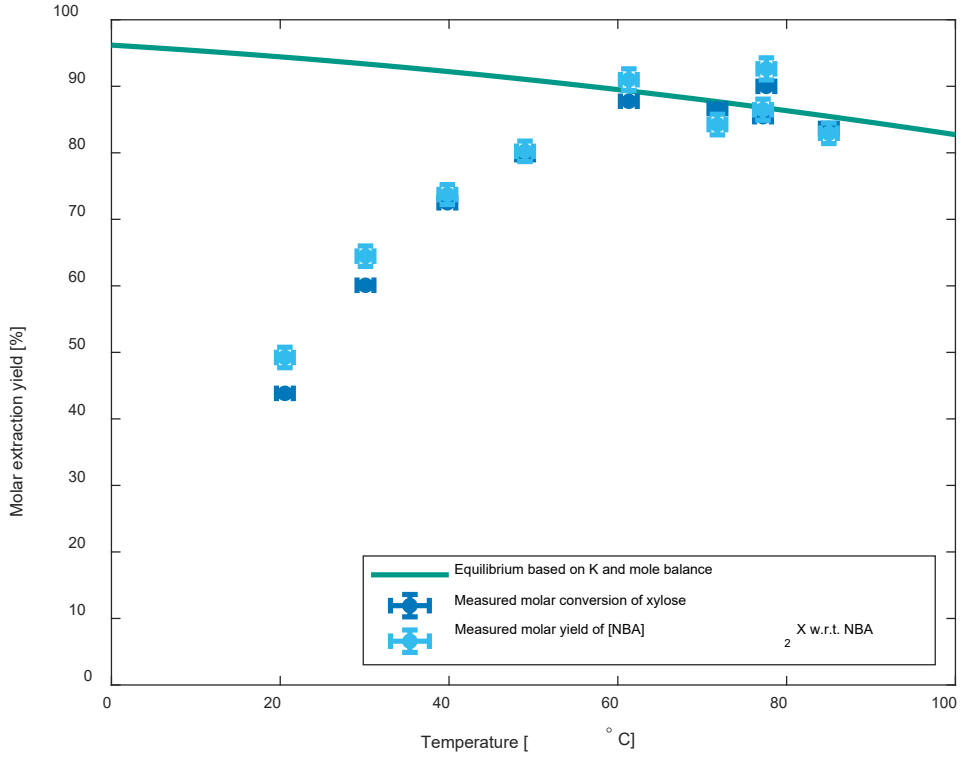

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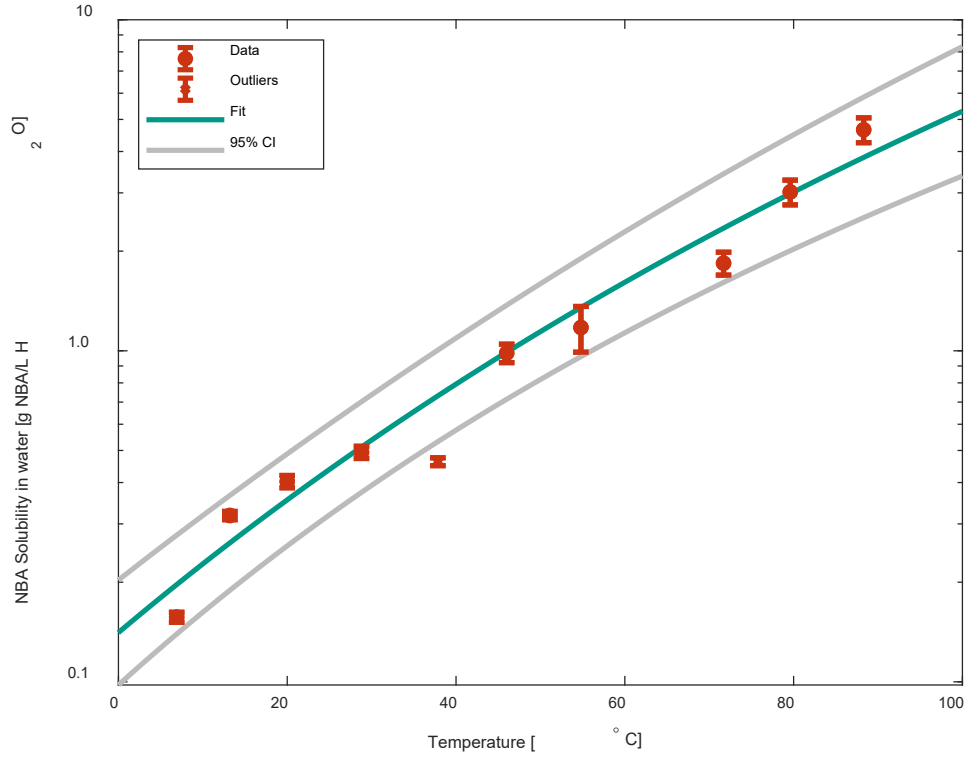

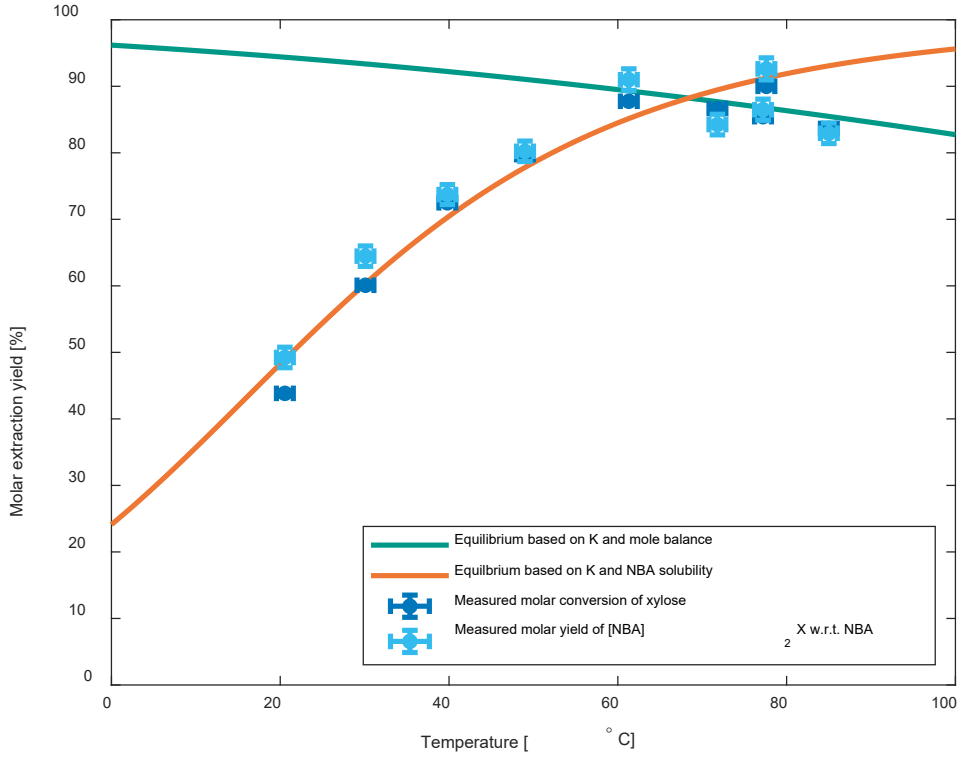

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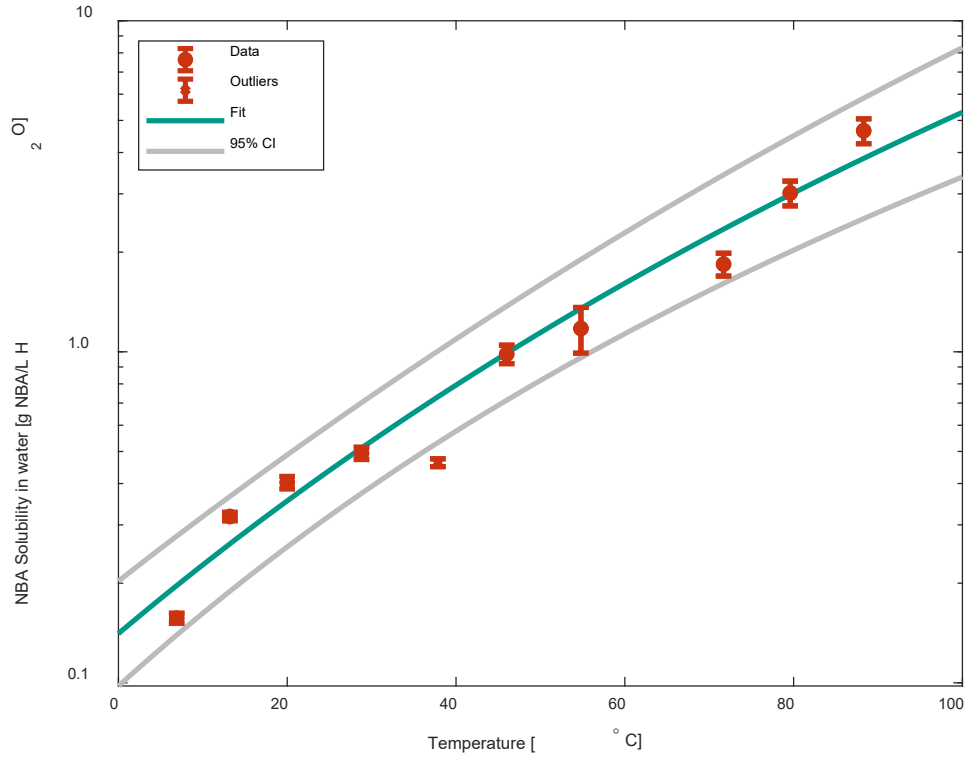

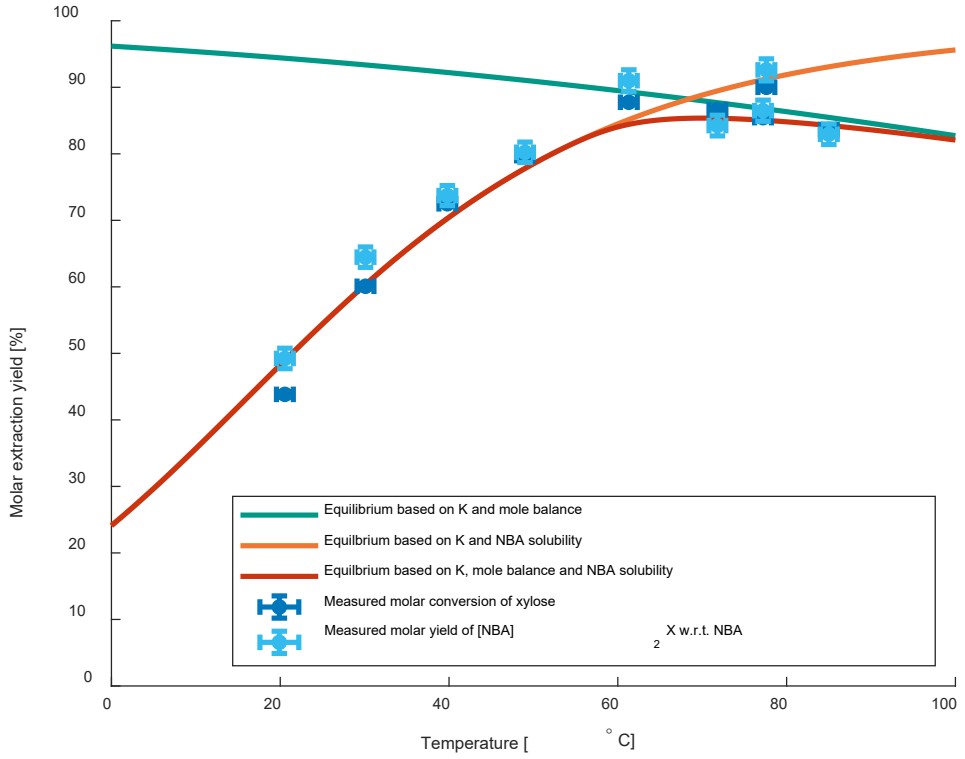

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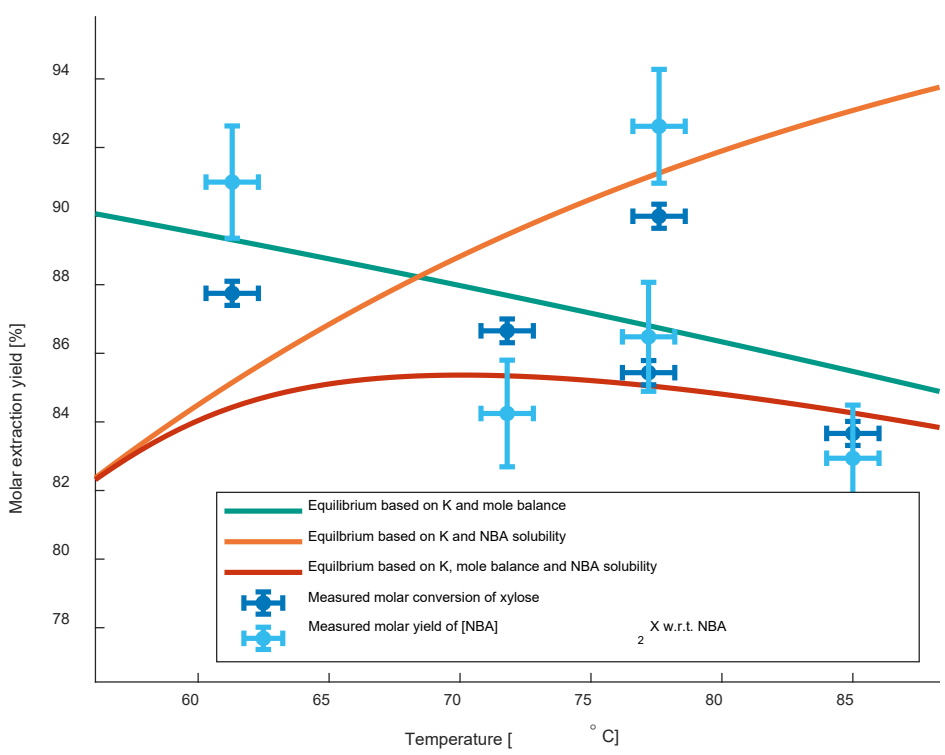
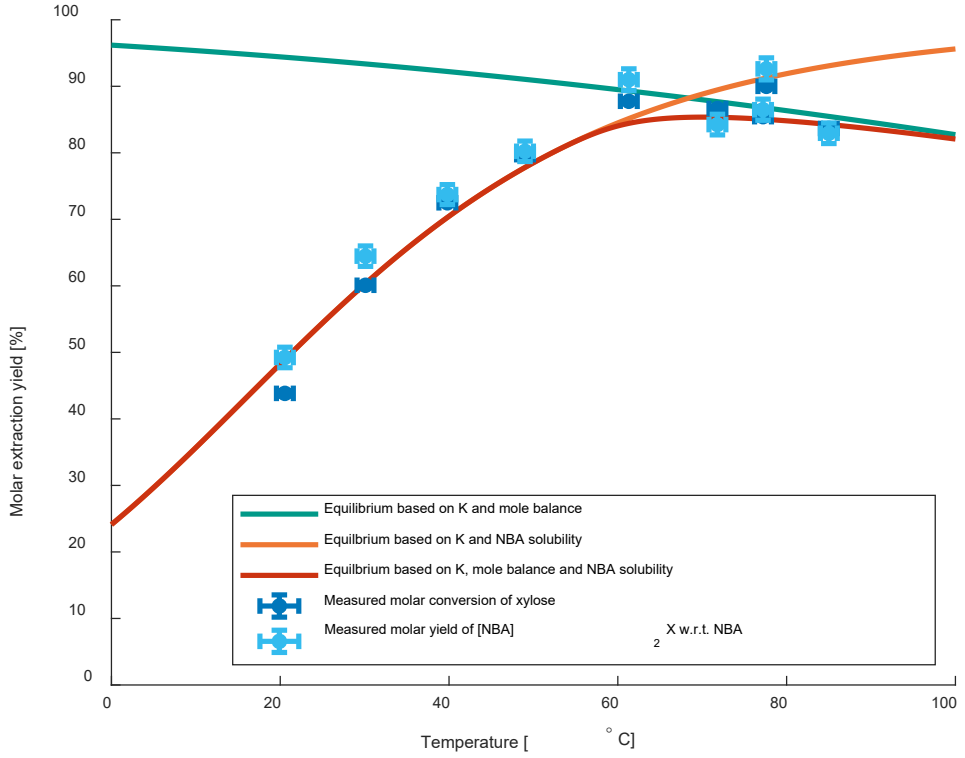
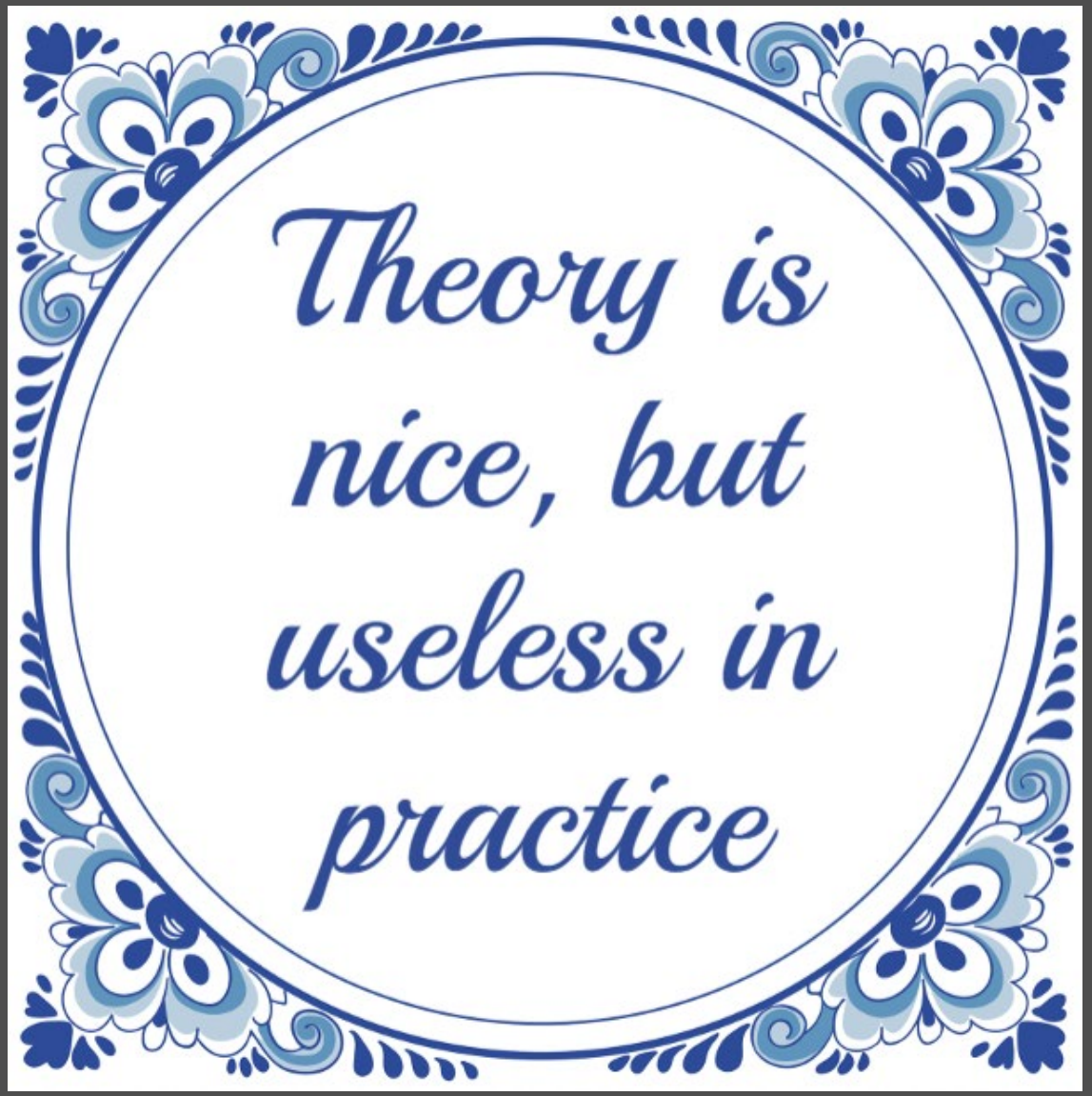





Theorie is mooi,
maar in de praktijk
heb je er niets aan


Theory is
nice, but
useless in
practice