

Removal of benzaldehyde from a water/ethanol mixture by applying scavenging techniques



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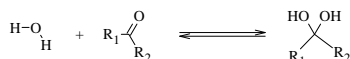
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1. Introduction

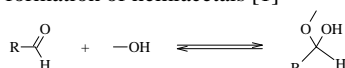
- High reactivity of carbonyl compounds causes formation of undesired impurities in reaction systems
- Removal of the carbonyl compounds could be performed in two ways:
 - physical approaches – adsorption, extraction, absorption...;
 - chemical approaches – derivatization into new products.
- Main focus of this work: remove benzaldehyde from the water/ethanol mixture (70:30, v/v) by applying derivatization agents

2. Theory

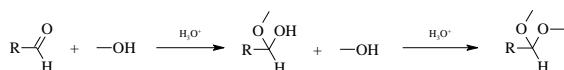
- Chemical reactions of carbonyl compounds with water
 - formation of hydrates [1]



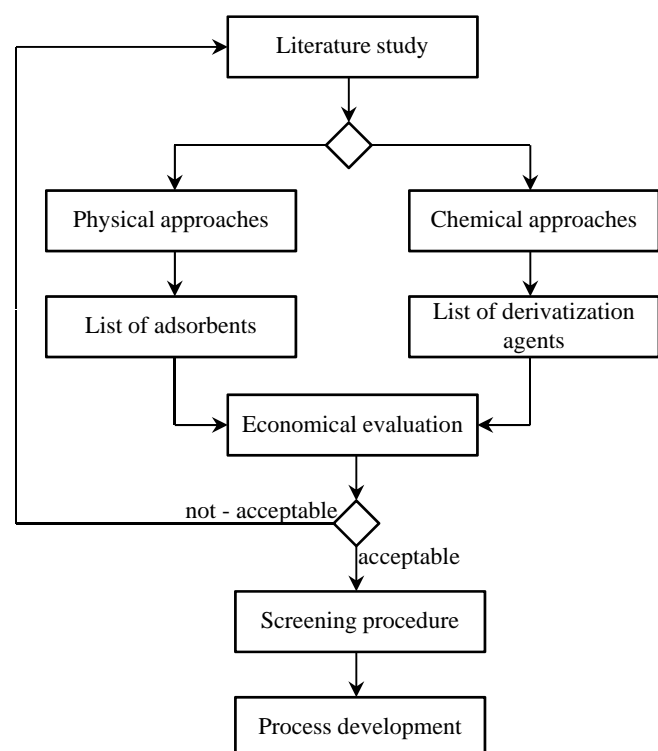
- Chemical reactions of carbonyl compounds with alcohols
 - formation of hemiacetals [1]



- formation of acetals [1]



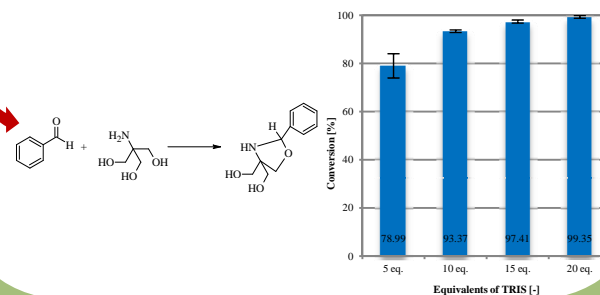
3. Methodology



4. Results

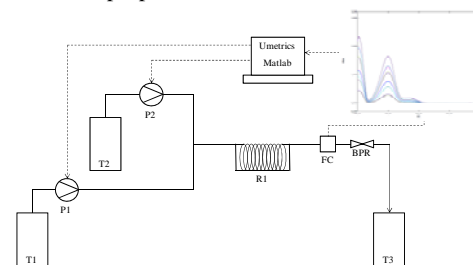
- Screening procedure resulted with good conversions [2-3]

No.	Scavenger	Conversion [%]
1	n-butylamine/isatoc anhydride	58.2
2	ammonium-acetate	14
3	tris(hydroxymethyl)aminomethane	99.35
4	sodium-bisulphite	88.96
5	triethanol amine	16.7



5. Current Status

- Process design for continuous derivatization
- Implementation of in-line UV-VIS real time monitoring
- Applications of multivariate/univariate data calibration for process control purposes



T1, T2, T3 – tanks; P1 and P2 – pumps; T – thermometer, FC – flow cell, BPR – back pressure regulator

6. Conclusions

- Removal of benzaldehyde could be successfully performed by using scavengers
 - tris(hydroxymethyl)aminomethane showed best results
- Applications of continuous removal of benzaldehyde in a tubular laminar reactor is about to be performed
- Real-time monitoring and control with UV-VIS spectroscopy and MATLAB® is a future work

References:

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- Bubb, W. A. et al., *Bioorganic Chemistry*, **1995**, 2, 119
- Sharma, R. et al., *Synlett*, **2012**, 15, 2209

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