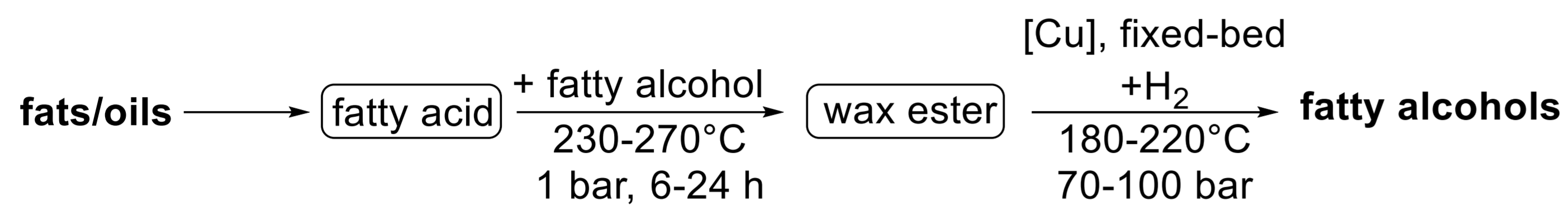


The Alternative Lurgi Process: Connection of Biocatalysis and Chemocatalysis to Synthesize Fatty Alcohols

Motivation

Industrial process for fatty alcohol synthesis: Lurgi process [1]



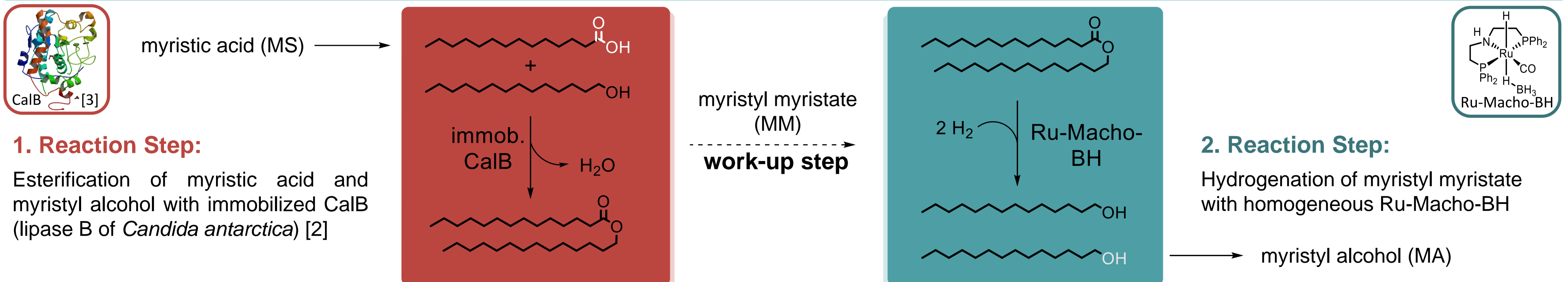
Disadvantages: Long reaction time, high temperatures and pressure

Approach

Fatty alcohol synthesis by chemo- and biocatalytic two-step reaction

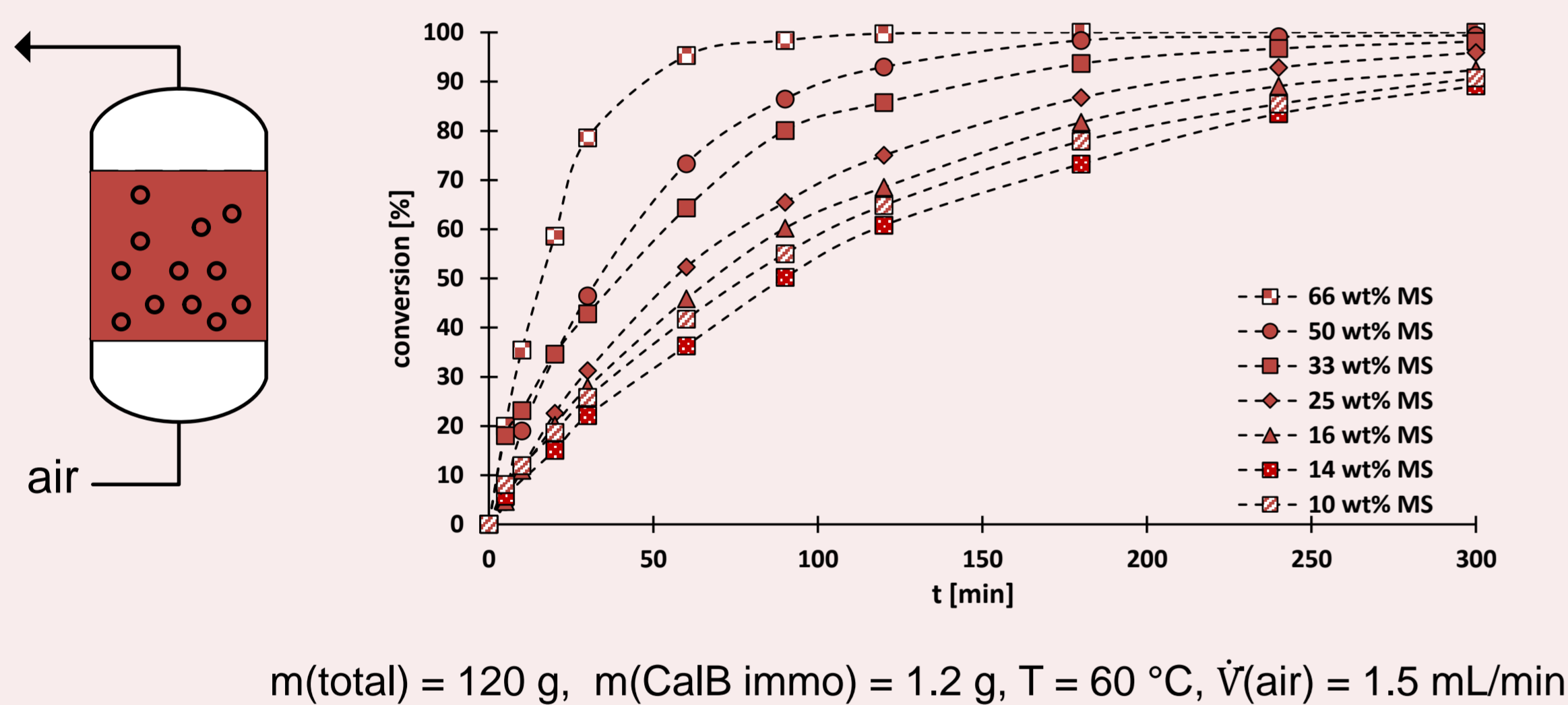
- A **solvent-free** and a **highly atom economic** reaction will be developed
- Minimization of the downstream process:
 - 1) Filtration of CalB immo, 2) Crystallization of fatty alcohol
- Decrease of reaction temperature, pressure and reaction time

Investigation of Esterification and Hydrogenation of Myristic Acid



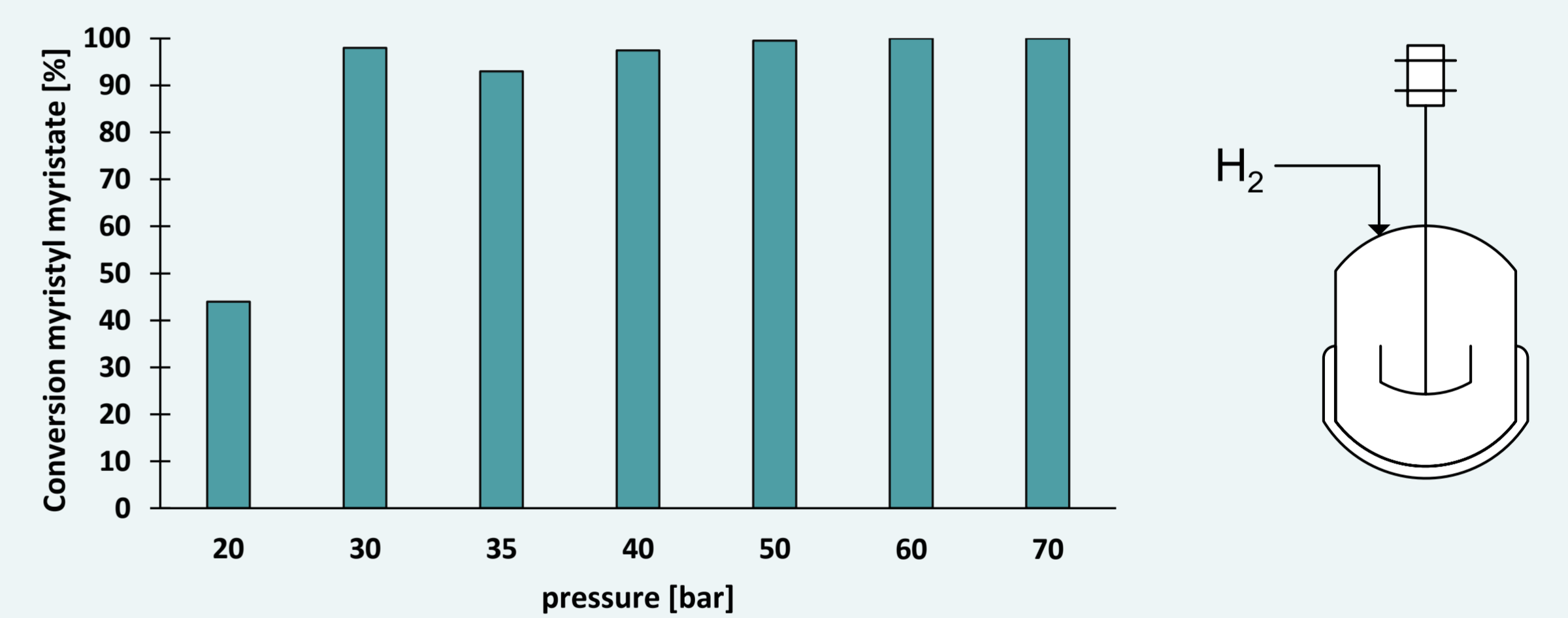
Substrate ratio variation for the esterification in a bubble column

After 90 min 66 wt% myristic acid reached 100% conversion, whereas the use of 16 wt% myristic acid just gives 60% conversion. An excess of myristyl alcohol lowers the activity of CalB.



Pressure screening for hydrogenation of myristyl myristate

Nearly identical conversions (93-100%) were reached after 18 h for pressures of 30 bar and higher. The applied pressure can be reduced to 30 bar hydrogen

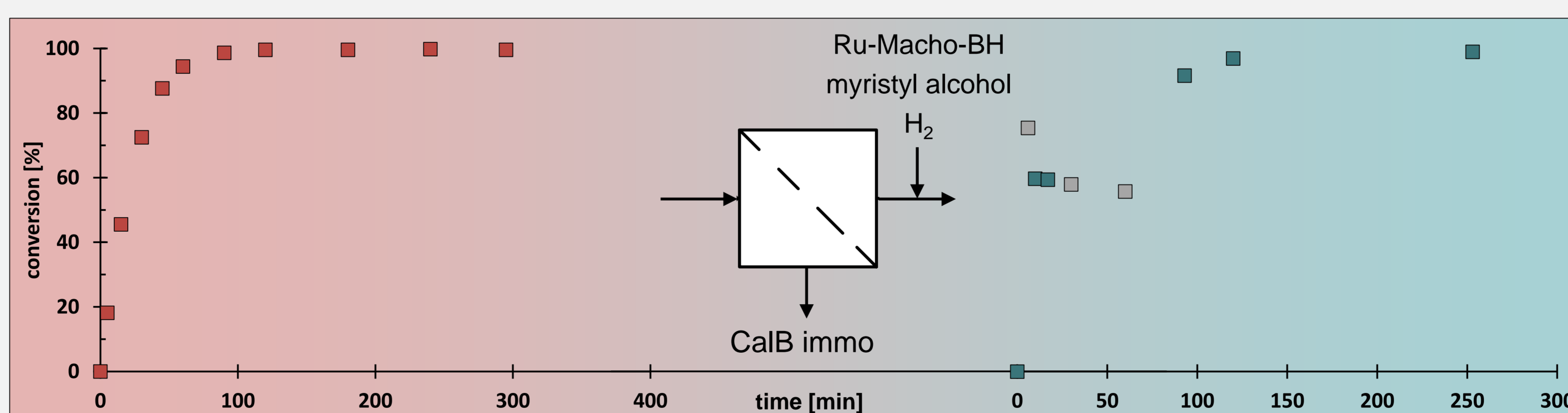
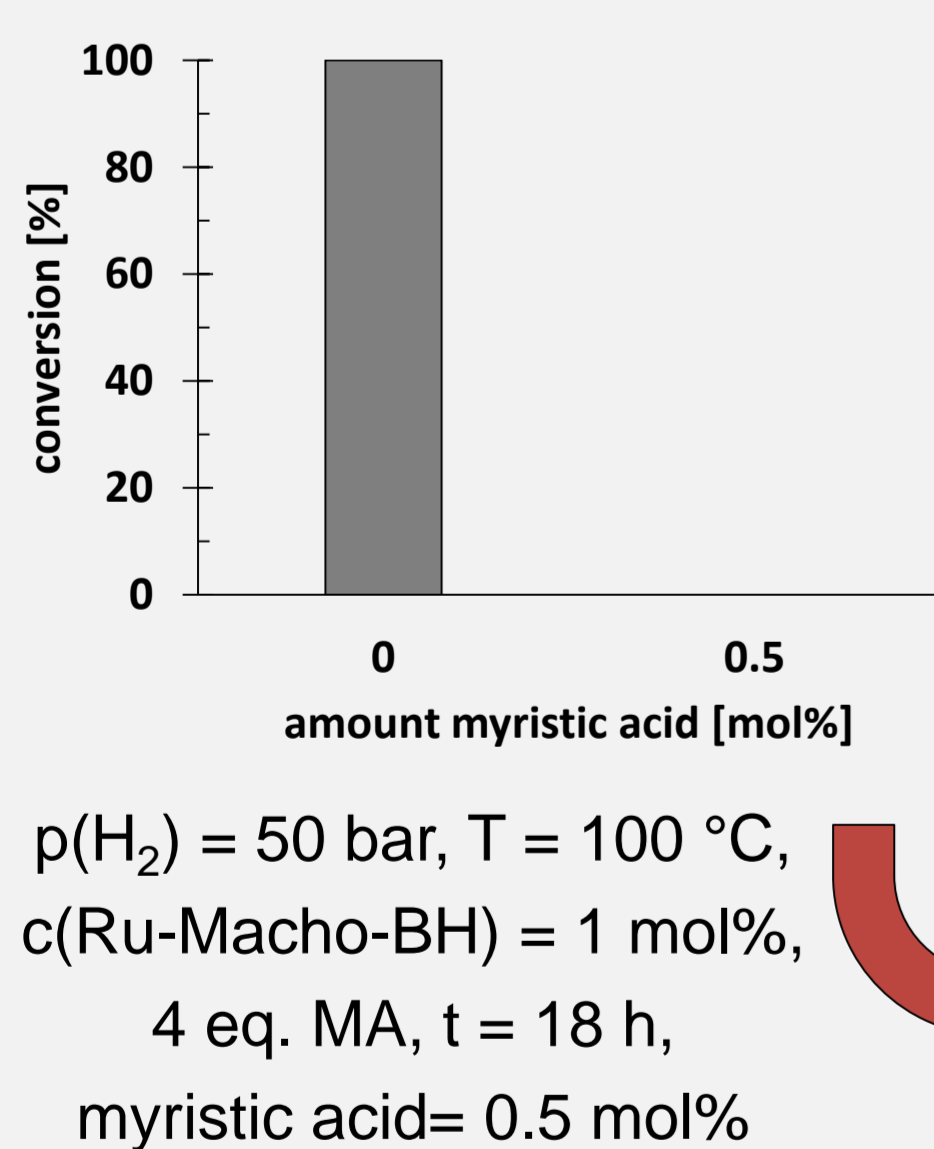


Combination of esterification and hydrogenation in a two step reaction sequence

With residues of myristic acid or CalB immo after esterification, hydrogenation shows **no or low conversion**. Consequently the challenge is to find a compromise to realize both reaction steps.

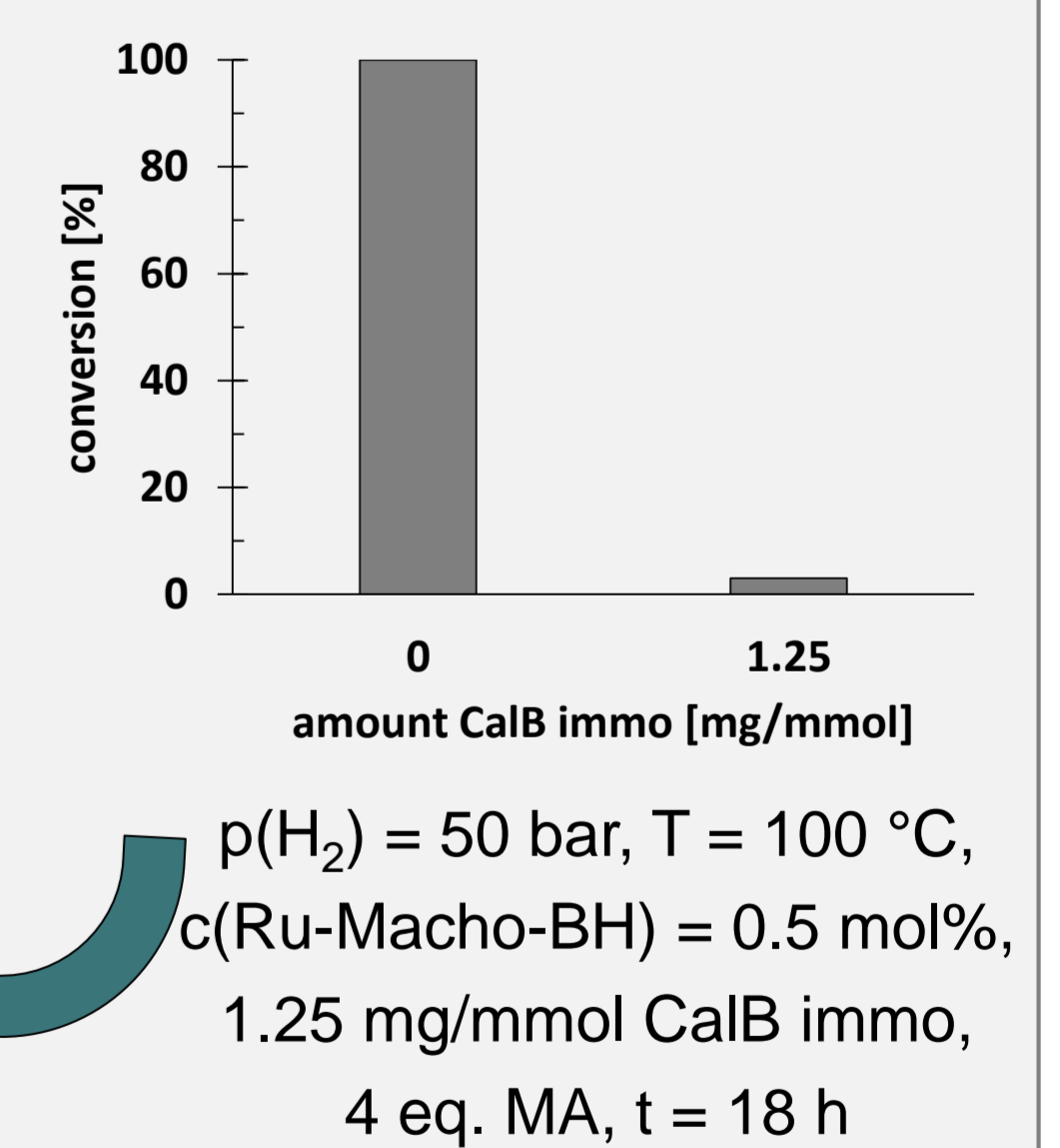
➔ **Two step process was realized successfully by carrying out esterification in equimolar ratio and a fine mesh filtration for separation of immobilized enzyme**

Acid residues in hydrogenation



bubble column: $m(\text{total}) = 120 \text{ g}$, $\text{MA:MS} = 1:1$, $\dot{V}(\text{air}) = 1.5 \text{ L/min}$, $T = 60^\circ\text{C}$, $m(\text{CalB immo}) = 1 \text{ wt\%}$, $t = 300 \text{ min}$
autoclave: $m(\text{total}) = 100 \text{ g}$, $\text{MA:MS} = 3:1$, $p(\text{H}_2) = 36 \text{ bar}$, $c(\text{Ru-Macho-BH}) = 0.5 \text{ mol\%}$, $t = 18 \text{ h}$, $U = 600 \text{ rpm}$

CalB immo residues in hydrogenation



Summary

- **Lower activity** was found with increasing myristyl alcohol mole fractions.
- Hydrogenation was possible with **20 bar** and higher. **Full conversion** was reached after 18 h with 30 bar hydrogen and higher pressures.
- **Two step process was successfully implemented** by the reduction of the reaction temperature, pressure and time compared to the Lurgi process.

Outlook

- Detailed **optimization of parameters** for both reactions in view of the two step process.
- Transfer to fatty acids with a **longer chain length** and scale-up.
- **Separation and reusability of Ru-Macho-BH** via crystallization of myristyl alcohol.

