Energy and operating cost analysis of the smart-scaled flow route directly to adipic acid

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Abstract title	ENERGY AND OPERATING COST ANALYSIS OF THE SMART-SCALED FLOW ROUTE DIRECTLY TO ADIPIC ACID
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1.Background:Process intensification through micro-process technology allows to reach processing far from state of the art. It is based mainly on transport intensification. A second emerging chemical intensification uses harsh process conditions to boost micro-processing. Beyond these, a third process-design intensification heads for integrated and simplified flow process design [1]. The latter two constitute Novel Process Windows.

2.Aims:The first-hour demonstration example is the direct oxidation of cyclohexene with hydrogen peroxide for synthesis of adipic acid which is an important intermediate for nylon manufacture. This direct route provides an innovative alternative to the industrial technologies that are carried out in 2-stages and it is aimed to investigate its potential for process simplification in a holistic picture in terms of cost, energy and eco-efficiency.

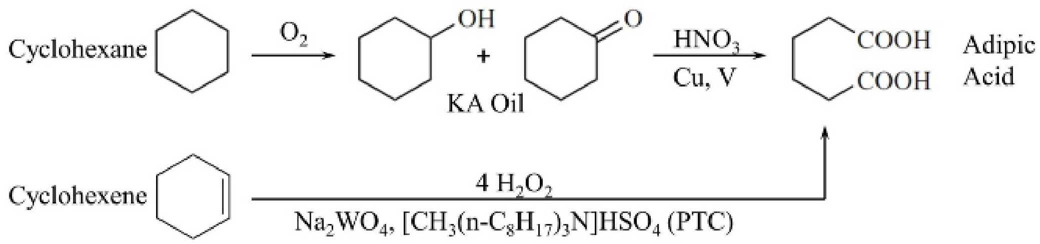
3.Methods:In order to be able to make comparison of this new direct route with the commercial route (2-step air/nitric acid oxidation of cyclohexane) process models are needed(see Fig.1). This direct oxidation is only demonstrated in lab [2] so process scheme is not available. The characteristics of the reaction and the flow diagram of the commercial nitric acid oxidation are used to propose the design including downstream equipment and process conditions for this process. Process simulations are done using Aspen for commercial route with data from literature and for direct route following the proposed design at capacity of 400 kton/day. For comparison of the routes in terms of capital cost, purchased cost of equipment is estimated using sizing information from simulation. Also, operating cost comparison is searched where energy consumption is considered. The heating and cooling requirements are determined using simulation. Pinch analysis is carried out to propose an energy efficient heat exchanger network maximizing process-to-process heat recovery. The utility requirement is found accordingly. Also, in our group environmental impact of the routes is analyzed using Life Cycle Assessment(LCA).

4.Results:Process flowsheets of the two routes(see Fig.2) reveal that the direct route leads to a more compact plant design. The reduction in number of steps in synthesis leads to requirement of only one reactor and fewer number of downstream units. Accordingly, we recently demonstrated that use of the direct route in flow cuts the total purchase cost of equipment approximately in half. However, there is an increase in cost for the more advanced flow reactor shifting the plant footprint from separation dominated to reaction dominated(see Fig.3). H_2O_2 is clean oxidant however considering cradle to grave with LCA it is found not entirely green(Anthaquinone process). Energy analysis is now in focus. After the application of pinch analysis, it reveals that utility requirement can be 75% lower with the direct route enabling major operating cost saving(see Fig.4).

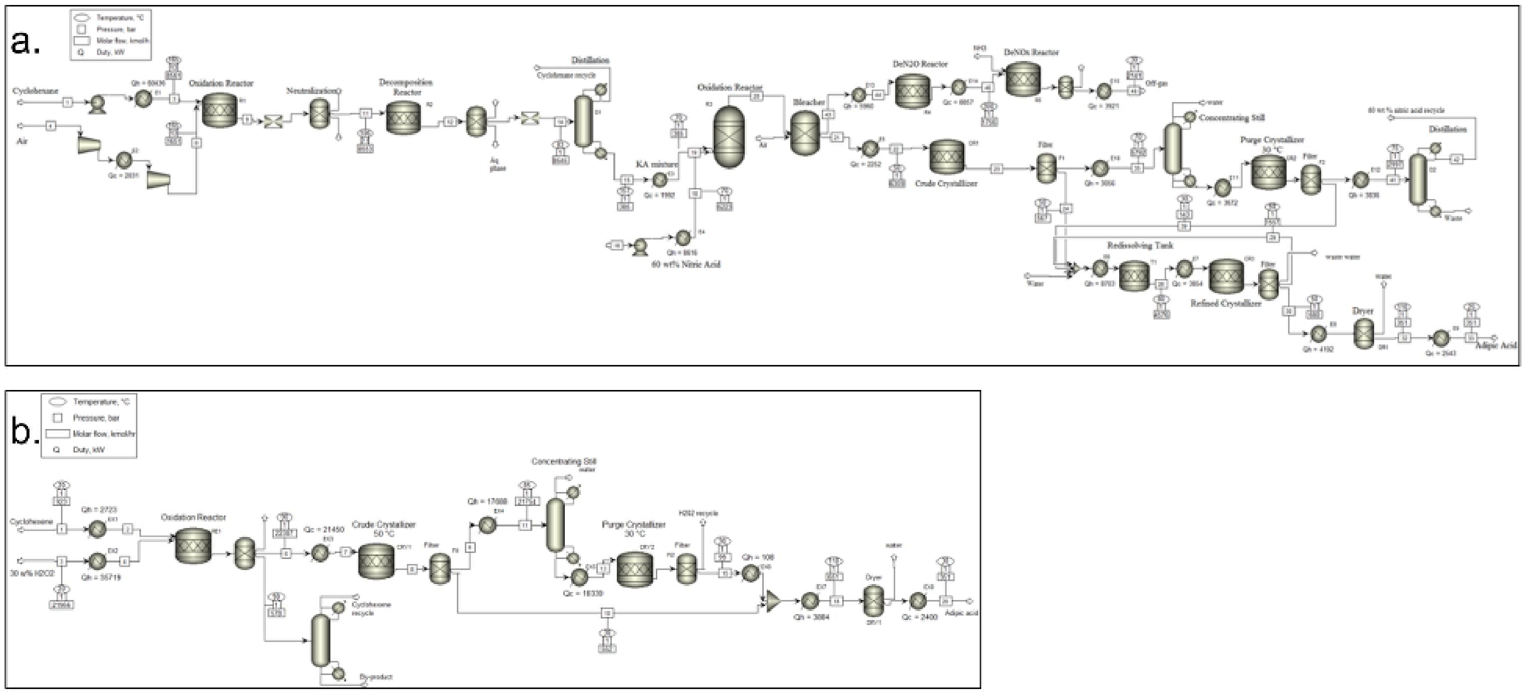
5.Conclusions:It is demonstrated that a massive theoretical potential is given for process simplification when choosing the direct route. The use of micro-process or other smart-scaled technology can achieve considerable capital cost and energy consumption reduction through process-design intensification lowering the management's main decision barrier towards new technologies. Yet, considerable challenges are expected when releasing the theoretical potential into industrial practice.

[1]Hessel,Vural-Gursel,Wang,Noel,Lang. Chem.Eng.Tech. 35(7),1184(2012).

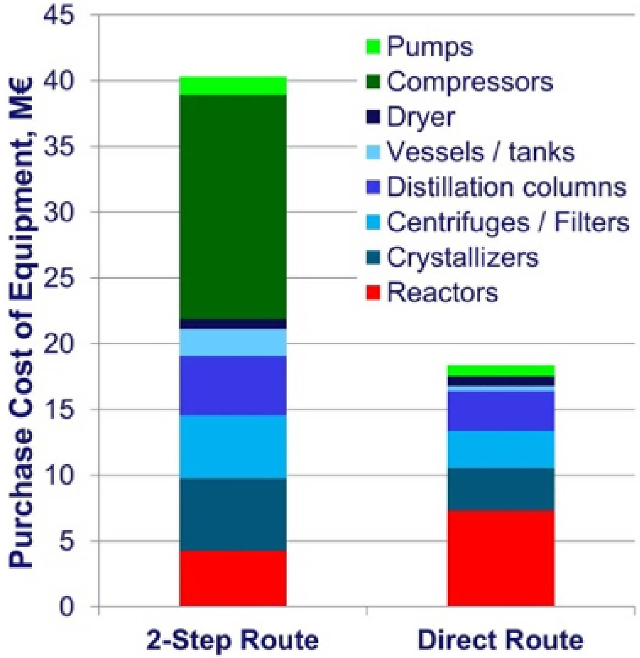
[2]Sato,Aoki,Noyori. Science 281,1646(1998).

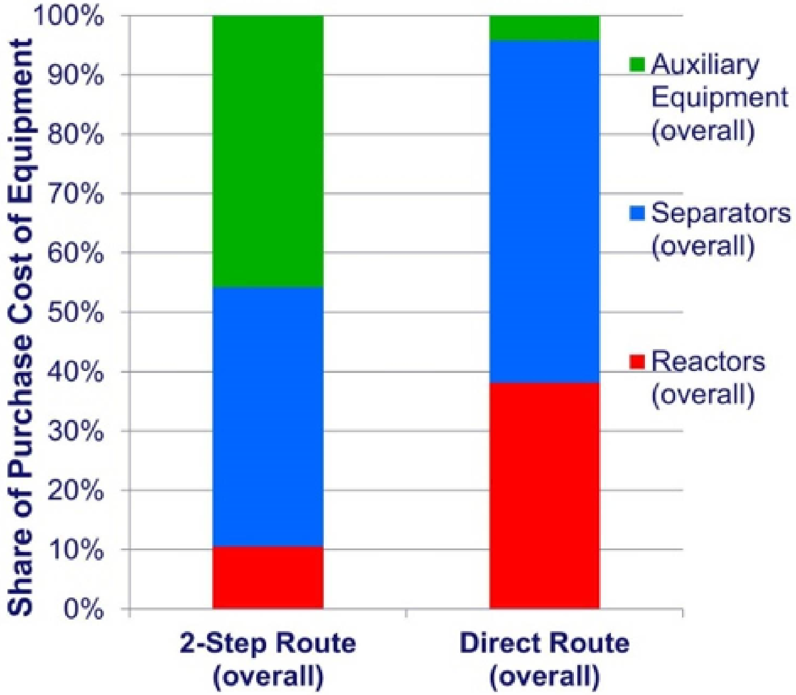


Cyclohexane
O_2
OH
+
KA Oil
O
HNO_3
Cu, V
COOH
COOH
Adipic
Acid
Cyclohexene
$4\ H_2O_2$
Na_2WO_4, $[CH_3(n\text{-}C_8H_{17})_3N]HSO_4$ (PTC)



a.
Temperature, °C
Pressure, bar
Molar flow, kmol/h
Duty, kW
Cyclohexane
Air
Oxidation Reactor
Neutralization
Decomposition Reactor
Distillation
Cyclohexane recycle
Aq. phase
KA mixture
Oxidation Reactor
60 wt% Nitric Acid
Bleacher
DeN2O Reactor
DeNOx Reactor
Off-gas
Crude Crystallizer
Filter
Concentrating Still
Purge Crystallizer
Distillation
Water
Redissolving Tank
Refined Crystallizer
Dryer
Adipic Acid
b.
Temperature, °C
Pressure, bar
Molar flow, kmol/hr
Duty, kW
Cyclohexene
30 wt% H2O2
Oxidation Reactor
Crude Crystallizer
50 °C
Filter
Concentrating Still
Purge Crystallizer
30 °C
H2O2 recycle
Cyclohexene recycle
By-product
Dryer
Adipic acid





2-step Route	Before Pinch (kW)	After Pinch (kW)	Cost (10^6 €/yr)	Saving (10^6 €/yr)
Hot utility (LP steam)	65,804	51,491	16.668	4.633
Hot utility (MP steam)	23,035	23,035	7.871	0.000
Cold utility (Cooling water)	14,313	0	0.000	0.115
Total	103,153	74,526	24.539	4.748

Direct Route	Before Pinch (kW)	After Pinch (kW)	Cost (10^6 €/yr)	Saving (10^6 €/yr)
Hot utility (LP steam)	60,105	18,516	5.995	13.463
Cold utility (Cooling water)	42,189	600	0.005	0.335
Total	102,294	19,116	6.000	13.798