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CONCEPTUAL DESIGN OF PROPYLENE PRODUCTION BY METATHESIS OF 2-BUTENE

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As the demand for propylene is increasing, viable solutions for conversion of low-value raw materials to high-value olefins are of interest. This article investigates the economic feasibility of a process for propylene production by metathesis of 2-butene (a by-product of fluid catalytic cracking). Process synthesis by hierarchical approach is applied for several process alternatives, with the goal of determining the best economical process flowsheet which returns the highest revenue for a fixed flow rate of raw material.

Keywords: olefin metathesis, conceptual design, hierarchical approach, economic analysis

1. Introduction

The demand of olefins, especially propylene, increased in the chemical and petrochemical industries for applications such as polypropylene, acrylonitrile, cumene, propylene oxide and other valuable products. Alternative technologies for production of propylene have been applied such as propane dehydrogenation, olefin metathesis, methanol to propylene, and cracking low-value olefins [1]. Currently the largest producers of propylene are fluid catalytic cracking units (FCCU) and naphtha steam cracking units. Although extensive research is being done for increasing the propylene yield in these units, alternative technologies should be considered for on-purpose propylene production.

In this article, the process synthesis by hierarchical approach of 2-butene olefin metathesis for propylene production will be considered, with the goal of identifying the most cost-effective process alternative from several different flowsheets. The metathesis reaction of 2-butene is carried out in the presence of tungsten oxide catalyst which converts the butenes to valuable olefin products ranging from C_2 to C_6, particularly propylene. The low-cost feedstock for olefin metathesis is a by-product of fluid catalytic cracking unit (FCC), containing 70 mole % 2-butene (reactant, denoted by A) and 30 mole % n-butane (inert, denoted by I), which is typically used in the liquified petroleum gas (LPG) pool. A fixed feed flow rate of 5.7 t/h was considered for all process alternatives evaluated.

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Firstly, the stoichiometry and kinetics of the reaction system is presented. Then, the economic analysis is applied for the process synthesis by hierarchical approach [2, 3], using Aspen Plus as efficient computer-aided design tool. Sensitivity studies were performed, at several decision levels and for different unit configurations, to reveal the best process flowsheet solution which has the highest economic potential for the given feed flow rate.

2. Reaction system

The metathesis reactions of 2-butene can be performed in the presence of tungsten oxide mesoporous silica catalyst [1]. The reactions take place in gas phase and are slightly endothermic. The reaction mechanism includes three reversible reactions (isomerization, cross-metathesis and self-metathesis) and one irreversible reaction (cracking) in which propylene is produced via two main alternatives routes: cross metathesis of 1-butene and 2-butene and cracking of 2-butene. In the following, the components will be referred as: A (2-butene), B (1-butene), C (propylene), D (2-pentene), E (ethylene), and F (3-hexene). The stoichiometry of metathesis process is well described by the following reactions:

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} B \tag{1}$$

$$A + B \underset{k_{-2}}{\overset{k_2}{\rightleftarrows}} C + D \tag{2}$$

$$2B \underset{k_{-3}}{\overset{k_3}{\rightleftarrows}} E + F \tag{3}$$

$$2A \xrightarrow{k_4} E + 2C \tag{4}$$

The kinetic model was developed [1] based on the following assumptions:

a) isomerization, cross-metathesis and self-metathesis are reversible, while cracking is irreversible

b) The pentene isomers are considered as 2-pentene (D), and the hexene isomers as 3-hentene (F)

c) All paraffin, isobutene and aromatic products are negligible

d) Contribution of secondary metathesis in propylene production is negligible

e) No oligomerization reactions are considered

The reaction rates are described by the following expressions [1]:

$$r_1 = k_1 \cdot (C_A - \frac{1}{K_{eq,1}} \cdot C_B) \tag{5}$$

$$r_2 = k_2 \cdot (C_A \cdot C_B - \frac{1}{K_{eq,2}} \cdot C_C \cdot C_D) \tag{6}$$

$$r_3 = k_3 \cdot (C_B{}^2 - \frac{1}{K_{eq,3}} \cdot C_E \cdot C_F) \tag{7}$$

$$r_4 = k_4 \cdot C_E \cdot C_C \tag{8}$$

where: r_i = reaction rate, kmol/m^3/s

$k_i = k_{0,i} \cdot \exp(-E_{a,i}/R/T)$ - rate constants, m^3/kmol/s

$K_{eq,i} = \exp(A_i + B_i/T)$ – equilibrium constants at various temperatures T

C_A, C_B, C_C, C_D, C_E, C_F = molar concentrations of components, kmol/m^3

The kinetic parameters $k_{0,i}$ and $E_{a,i}$ presented in Table 1 were numerically determined by fitting the experimental data of 2-butene metathesis obtained from reference [1] to the model of an isothermal plug-flow reactor, as shown in Fig 1. The expressions for $K_{eq,i}$ were taken from the same reference [1].

Table 1

Estimated kinetic parameters

Reaction	Pre-exponential factor k_0 / [m^3/kmol/s]	Activation energy E_a / [kJ/kmol]	A	B / [K]	Heat of reaction / [kJ/mol]
1: Isomerization	0.0287	25.12821	4.662791	-1154.68	6.87
2: Cross-metathesis	6.802	102.0203	5.480296	-144.335	-0.54
3: Self-metathesis	3.815	187.0776	9.544931	-3139.28	2.47
4: Cracking	0.123	84.56967	-	-	53.61

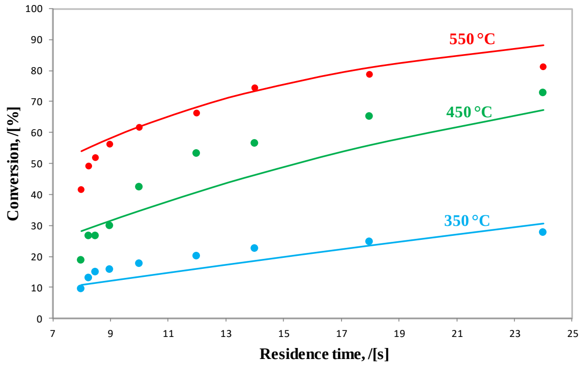

Fig. 1. Conversion of 2-butene vs. residence time, at different values of the reaction temperature: markers - experimental data [1]; lines – calculated values.

3. Process analysis by hierarchical approach

In conceptual design, one of the most important aspects is hierarchical pre-screening the most promising solutions from a bulk of process alternatives. A rule of thumb in process design says that it is favorable to recover more than 99% of all valuable materials [2,3]. Thus, unit structures US1 include the recycle of un-reacted raw material but differ in the way the inert is removed. Analysis of the structure US1a showed that high purge fraction lead to higher revenues. For this reason, process alternatives US2 without recycle were also investigated. In the following figures, the stream denoted as PRODUCTS consists of valuable components that can be sold: ethylene, propylene, pentene, hexene; the stream denoted as INERT consists mainly of n-butane. The stream PURGE contains a mixture of butenes and n-butane; the stream BY-PRODUCTS represents a C_4 fraction containing butenes without or with inert (Fig. 5 and Fig. 6, respectively).

Flowsheets with recycle (US1)

i. US1a: Typical Reactor – Separation - Recycle structure. The inert is removed from the system by means a purge (Fig. 2).

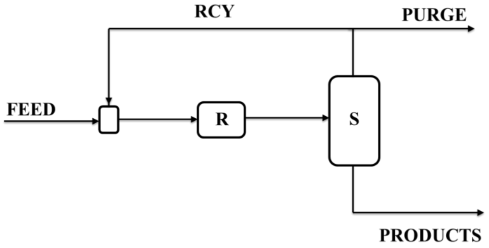

Fig. 2. US1a: Reactor – Separation – Recycle (A+B+I), with purge.

ii. US1b: Reactor – Separation - Recycle structure which uses an additional separation unit to remove the inert from the system (Fig. 3).

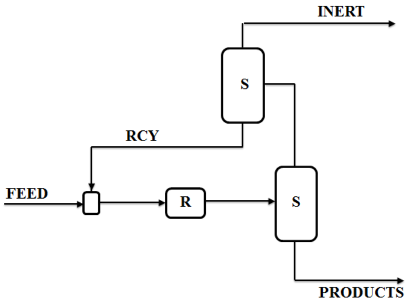

Fig. 3. US1b: Reactor – Separation – Recycle (A+B). The inert (I) is separated and removed downstream of reactor

iii. US1c: Reactor – Separation - Recycle structure where the inert is removed before entering the plant (Fig. 4). In this way, both inert accumulation and recycle are avoided.

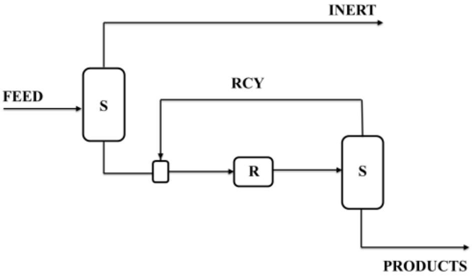

Fig. 4. US1c: Reactor – Separation - Recycle (A+B). The inert (I) is separated and removed upstream of reactor

Flowsheets without recycle (US2)

i. US2a: Reactor – Separation, where the inert is removed before entering the reactor (Fig 5), to avoid overloading the reactor and separation sections.

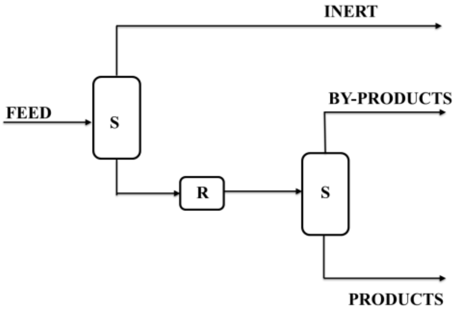

Fig. 5. US2a: Reactor – Separation, the inert is removed upstream of the reactor

ii. US2b: Reactor - Separation, where the inert is passed through the reactor (Fig. 6). This is the simplest process alternative.

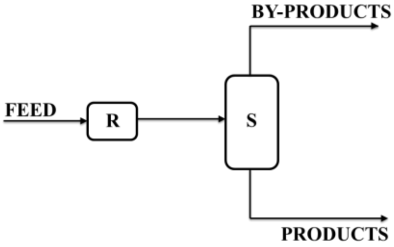

Fig. 6. US2b: Reactor - Separation

Economic evaluation

The flowsheet alternatives were assessed in a hierarchical approach, with the goal of determining the most cost-effective solution. Typically, the raw materials cost represents between 35 - 85% of the total processing costs. Therefore, prior complicating the design, an initial step is calculating the economic potential (*EP1*) as if the unit cost would be zero [3]. Thus, the process alternatives were evaluated from an Input / Output point of view, being considered black boxes, and taking into account only the cost of raw materials and the value of products and by-products.

EP1= {value of products} – {cost of raw materials}

The feed, containing 2-butene (A) and n-butane (I), is usually sent to the LPG pool and has a cost of 388.8 $ / ton. The same value is assigned to the C_4 mix purged (containing 2-butene, 1-butene, n-butene), as it can be sent to the same LPG pool. Table 2 also lists the prices considered in this study for products (C, D, E, F) and for the high purity n-butane (I).

Table 2

Prices of raw material and products (99% purity)

Component	Feed	C_4 mix	C	D	E	F	I
Prices / [$/tonne]	388.8	388.8	648	486	540	486	452

At the second level, more details are added to the analysis by including the reactor and the catalyst costs and determining the new economic potential (*EP2)*. The balance between reactor size and recycle flowrate which ensures the optimum economic potential is established by analyzing Reactor – Separation - Recycle configurations, where the separation is considered as a “black-box” and the reactor model incorporates the reaction kinetics [4].

EP2 = {value of products} – {cost of raw materials} – {reactor cost} – {catalyst cost}

The capital cost estimation used in the article correspond to the simplified version of Guthrie’s correlations [5] with the value for Marshall and Swift Index *M&S = 1536.5* corresponding to year 2011. A typical payback time of 3 years is considered with plant operation of 8000 hours/year. The catalyst price considered is 20 $/kg and the equation cost for reactor mentioned below is applicable for any pressure vessels (e.g. reflux vessels, columns, separators):

$$Installed\,Cost(\$) = (M\,\&\,S/280)\cdot(957.9\cdot D^{1.066}\cdot H^{0.82})\cdot(2.18+F_c) \qquad (9)$$

with both D diameter and H height expressed in meters. The factor F_c takes into account the material (F_m) and the operating pressure (F_p).

$$F_p = 1+0.0074\cdot(P-3.48)+0.00023\cdot(P-3.48)^2 \qquad (10)$$

with P in bar. The material factor F_m can be determined from Table 3.

Table 3

Material factor for different types of material

Shell material	Carbon steel	Stainless steel	Monel	Titanium
F_m clad	1.00	2.25	3.89	4.25
F_m solid	1.00	3.67	6.34	7.89

The reactor diameter was determined considering a maximum pressure drop of 0.005 bar / m. Further, the reactor length was varied for establishing the optimum conversion with the highest benefit.

The third level of analysis adds the separation and recycle costs, leading to the economic potential (*EP3*). The cost associated with a distillation column is comprised of several items such as pressure vessels (column and reflux vessel), heat exchangers (condenser and reboiler) and column internals (trays/ packing).

EP3 = {value of products} – {cost of raw materials} – {reactor cost} – {catalyst cost} – {distillation column cost}

Cost equations for column internal (e.g. trays):

$$Installed\,Cost\,(\$) = (M\,\&\,S/280)\cdot 97.2\cdot D^{1.55}\cdot F_c\cdot NTT \qquad (11)$$

For standard 24-inch tray spacing the overall correction factor is:

$$F_c = F_m + F_t \qquad (12)$$

where tray factor F_t is 0 for sieve trays, 1.8 for bubble cap, and 3 for more complicated trays as two-pass or three-pass glitch trays. Material factor F_m is 1 for carbon steel, 1.7 for stainless steel, with considerable higher values for other alloys.

The cost equation for heat exchangers (shell and tube) is:

$$Installed\,Cost\,(\$) = (M\,\&\,S/280)\cdot 474.7\cdot A^{0.65}\cdot (F_c + 2.29) \qquad (13)$$

where heat exchanger area (A) is expressed in m^2 and is applicable for heat transfer surfaces between $20<A<500$ m^2/shell.

$$F_c = F_m\cdot (F_d + F_p) \qquad (14)$$

where corrections for material, design type and pressure are included in Table 4.

Table 4

Correction factors for material, design type and pressure

Shell	CS	CS	CS	CS	SS	Monel	CS
Tubes	CS	Brass	Monel	SS	SS	Monel	Titanium
F_m	1.0	1.3	2.15	2.81	3.75	4.25	8.95

Correction factor for shell & tubes heat exchangers:			
Design type	F_d	Design pressure, bar	F_p
Kettle reboiler	1.35	<10	0
Floating head	1.00	20	0.1
U-tube	0.85	30	0.25
Fixed-tubesheet	0.8	60	0.52

In order to fine-tune the process alternatives, in the last level of analysis the costs associated to utilities (e.g. steam, cooling water, electricity, refrigerant etc.) and other major equipment (e.g. furnace, compressor) are included, for finding the new economic potential (*EP4*). The utilities considered for olefin metathesis process are low- and medium-pressure steam, (LPS, MPS), electricity

(E), cooling water (CW), refrigerant (R134a) and fuel gas (FG). Typical prices for utilities are listed in Table 5.

EP4 = {EP3} – {furnace cost} – {compressor cost} – {preheat train cost} – {pumps cost}-{utilities}

Table 5

Prices for plant utilities

Utility	LPS / [$/GJ]	MPS / [$/GJ]	R134a / [$/GJ]	CW / [$/GJ]	E / [$/kWh]	FG / [$/GJ]
Price	8	12	10	0.8	0.08	7.5

Equation costs for equipment associated with olefin metathesis process include cost of compressor, furnace, preheat train and pumps.

Cost of the furnace:

$$Installed\,Cost\,(\$) = (M\,\&\,S/280)\cdot(15668\cdot Q^{0.85})\cdot(F_c + 1.27) \qquad (15)$$

where Q is the duty expressed in MW, with $20<Q<300$. The correction factor is given in Table 6.

$$F_c = F_m + F_d + F_p \qquad (16)$$

Table 6

Correction factor for different type of heaters

Design type	F_d	Radiant tube material	F_m	Design pressure, bar	F_p
Process heater	1	Carbon steel	0	<40	0
Pyrolysis	1.1	Chrome/Molibden	0.35	100	0.15
Reformer (no catalyst)	1.35	Stainless	0.75	150	0.30

Purchased cost for gas compressor is mentioned in the following equation:

$$\text{Purchased Cost }(\$) = (M\,\&\,S/280)\cdot(664.1\cdot P^{0.82}\cdot F_c) \qquad (17)$$

where P is brake power in kW, with $25<P<750$ kW. The correction factor F_c is given in Table 7:

Table 7

Correction factor for different types of compressor

Design type	F_C
Centrifugal compressor / driven by motor	1.00
Reciprocating compressor/ driven by steam	1.07
Centrifugal compressor/ driven by turbine	1.15
Reciprocating compressor/ driven by motor	1.29
Reciprocating compressor/ driven by gas engine	1.82

The number of pumps was determined considering a sparing philosophy of one active pump and one spare pump (1+1). The cost of pumps was considered 4% of total CAPEX.

4. Results of economic evaluation of flowsheet alternatives

Economic analysis was applied to identify the most profitable process alternative in the early design, for different unit structures of the olefin metathesis process.

Flowsheets with recycle

US1a: Typical Reactor – Separation - Recycle (A + B + I)

Sensitivity cases were performed for a fixed reactor temperature of 550°C and a pressure 1 bar with a constant reactor diameter of 3 meters. A variable purge fraction, denoted as *P*, was introduced to establish the optimum design with respect to economic potential. Results show, that at given reactor length, higher reactant conversion is obtained by increasing the purge fraction (Fig. 7). This can be explained by the fact that the recycle (containing large amounts of inert) decreases both the reactor residence time and reactant concentration.

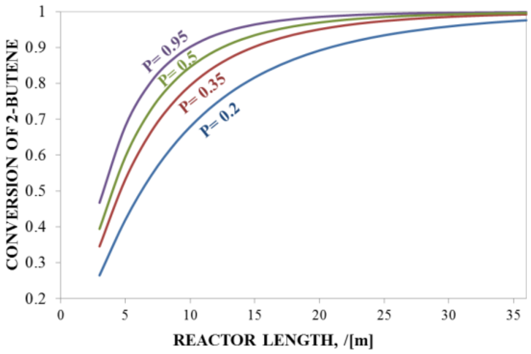

Fig. 7. Conversion of 2-butene vs reactor length (D = 3 m), for different values of the purge fraction P

As a result, bigger reactors are necessary to obtain a certain conversion, with negative effect on capital expenditures (CAPEX) and operating expenditures (OPEX). The results from Fig. 8 reveal that as purge fraction is increased the unit is more profitable. Note that decision levels 3 and 4 lower the economic potential by more than 200% of the initial *EP1*.

The optimum 2-butene conversion is X_A= 90% for a reactor length of L_R = 9 m and a high value of the purge fraction (e.g. above 95%). Note that considering the purge fraction of *P*=0.2, the profit decreases from an initial *EP1*=4500 k$/year at the first level of decision to *EP4*=500 k$/year at the 4th level. In other words, the process alternative went from an economical solution to a barely-profitable design by recycling the reactants back to the reactor.

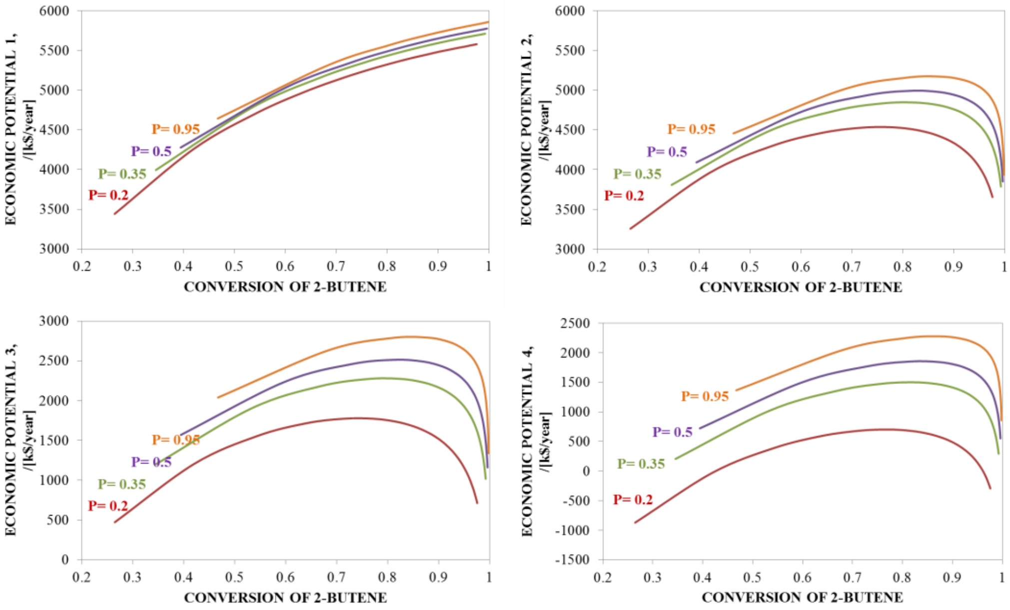

Fig. 8. Economic potential plotted against conversion, at different purge fractions, for US1a

US1b: Reactor – Separation - Recycle (A+B) with inert separation downstream of reactor

The second alternative considers the separation of the inert (n-butane) from the reactants in a distillation column downstream of the reaction section. Additional costs for OPEX and CAPEX are expected for this distillation column because the volatilities of the key components are very close. Although the n-butane separation is very difficult, the product with high purity can be the raw material of an isomerization process producing isobutane, which can be used in alkylation units for obtaining high gasoline additives with high octane number. Results are presented in Fig. 9 (left).

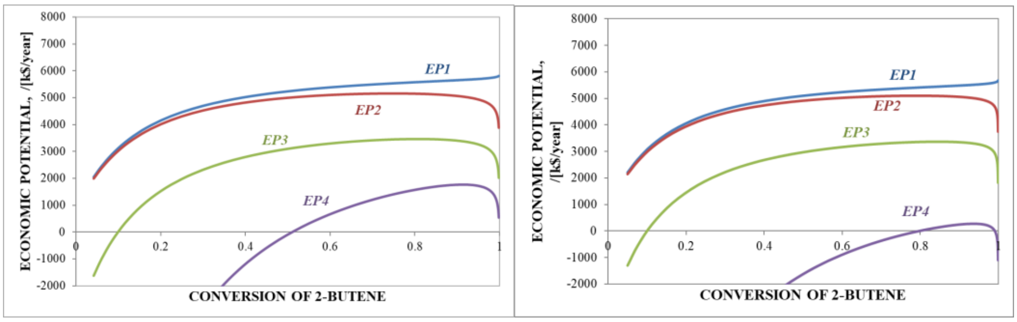

Fig. 9. Economical potential vs. conversion of 2-butene for US1b (left) and US1c(right)

The sensitivity analysis reveals that the addition of another distillation column requires higher costs and affects the final economic potential *EP4*. The separation of inert (I) and recycling only A and B components does not have a positive effect on overall plant cost, compared to the previous alternative US1a. For reactor length of L_R = 9 m and conversion of X_R = 87% the maximum economic potential is *EP4* = 1773 k$/year.

US1c: Reactor – Separation – Recycle (A+B), with inert separation upstream of reactor

Compared to the other two options presented above (with recycle streams), this case is interesting because the initial separation of inert upstream of reactor could have a positive effect, relieving the following equipment of useless circulation of inert. However, it is also challenging because the separation n-butane / 2-butene is very difficult due to their similar volatilities.

The economic potential was determined against the reactor conversion by sensitivity cases in Aspen Plus. The results (Fig. 9 right) show that the structure US1c returns a maximum economic potential (*EP4*) of only 273 k$/year.

Flowsheets without recycle

US2a: Reactor - Separation with inert removal upstream of reactor

For process alternative US2a, no major difference in the economic optimum is seen compared to US1c. This happens because in US1c the optimum design corresponds to a rather large value of the conversion, therefore a small recycle which has a low impact on the revenue. The results for the decision levels are presented below (Fig. 11 left) and are very similar with the process alternative US1c. The economic potential for this process alternative is *EP4* = 288 k$/year.

US2b: Reactor - Separation

For the once-through configuration without recycle, the economic potential at different decision levels was plotted on a single graph to reveal the economic impact to the unit. At the first level (Fig 11 right) the *EP1* increases with conversion, as the products value and raw materials costs are included.

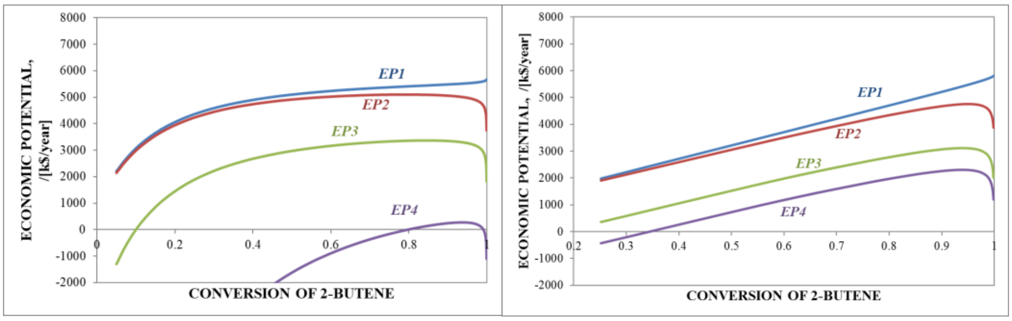

Fig. 11. Economic potential vs conversion of 2-butene for US2a (left) and US2b (right)

As the next layer of complexity is added, the economic potential *EP2* is slightly lower, mostly because the cost of reactor and catalyst has low impact on fixed capital expenditures. The economic potential *EP*3 is dramatically modified, by more than 100%, when the separation equipment is included. The decision level 4 impacts the OPEX by further decreasing the economic potential *EP4*. The summary with the optimum points from the economic analysis for the five different flowsheet alternatives studied is presented in Table 8.

Table 8

Results of the optimal flowsheet solutions for the olefin metathesis process

	US1a	US1b	US1c	US2a	US2b
Optimal conversion X_A	90%	87%	92%	96%	93%
Economic potential *EP4* / [k$/year]	500	1773	273	288	2300
Return of Investment *ROI*	17%	26%	4%	4%	35%

The rate of return of investment (ROI) was calculated to express the annual profit generated by the capital invested.

$$\%ROI = \frac{Annual\ net\ profit}{Invested\ capital} \cdot 100\% = \frac{EP4}{CAPEX} \cdot 100\% \tag{18}$$

Considering the highest %ROI, the flowsheet US2b was selected for further investigation and detailed equipment sizing.

5. Details of the Reactor – Separation flowsheet

The simplified process flow diagram (Fig. 13) for the most economical solution US2b reveals the major equipment considered in the process synthesis. A preliminary sizing was performed for the main equipment considering process guidelines and technical literature. The unit mass balance is reported in Table 9.

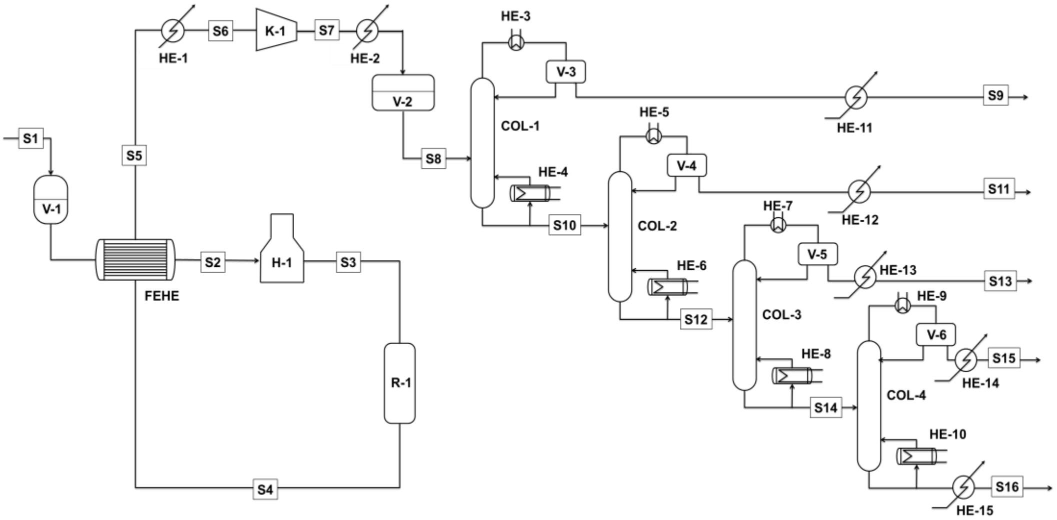

Fig. 13. Simplified process flowsheet for US2b

Table 9

Mass balance for "best" process alternative US2b

OLEFIN METATHESIS PROCESS – MASS BALANCE									
Stream	U.M	S1	S2	S3	S4	S5	S6	S7	S8
Temperature	°C	40	450	550	511.7	149.7	50	207.8	50
Pressure	bar	7	6.5	1.2	1.15	1.05	1.05	31	31
Vapor Frac		0	1	1	1	1	1	1	0
Mole Flow	kmol/hr	100	100	100	102.5	102.5	102.5	102.5	102.5
Mass Flow	kg/hr	5671	5671	5671	5671	5671	5671	5671	5671
Mole Fractions									
A		0.7	0.7	0.7	0.065	0.065	0.065	0.065	0.065
B					0.042	0.021	0.021	0.042	0.042
C					0.242	0.259	0.259	0.242	0.242
D					0.191	0.209	0.209	0.191	0.191
E					0.1	0.117	0.117	0.1	0.1
F					0.07	0.092	0.092	0.07	0.07
I		0.3	0.3	0.3	0.29	0.29	0.29	0.29	0.29

OLEFIN METATHESIS PROCESS – MASS BALANCE									
Stream	U.M	S9	S10	S11	S12	S13	S14	S15	S16
Temperature	°C	-15	140	40	154	40	112.7	40	40
Pressure	bar	32	34.2	25.5	25.5	6.5	7.5	2.5	3.5
Vapor Frac		0	0	0	0	0	0	0	0
Mole Flow	kmol/hr	12.0	90.5	26.5	64	32.8	31.2	21.74	9.42
Mass Flow	kg/hr	337	5334	1118.2	4215.3	1901.3	2314	1520.9	793.1
Mole Frac									
A		<0.01	0.01	<0.01	0.014	0.019	<0.01	<0.01	<0.01
B		<0.01	0.024	<0.01	0.034	0.067	<0.01	<0.01	<0.01
C		<0.01	0.294	0.99	<0.01	<0.01	<0.01	<0.01	<0.01
D		<0.01	0.236	<0.01	0.335	<0.01	0.687	0.985	<0.01
E		0.99	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
F		<0.01	0.104	<0.01	0.147	<0.01	0.303	<0.01	0.99
I		<0.01	0.331	<0.01	0.469	0.913	0.01	0.014	<0.01

Reactor sizing

For the olefin metathesis process, an adiabatic tubular reactor was considered with the tungsten oxide catalyst supported on silica. The reactor is operated at 1 bar and 550°C. The reaction is conducted in vapor phase. The sizing of the reactor vessel is presented in Table 10:

Table 10

Reactor design results

Diameter / [m]	Length / [m]	Volume / [m^3]	Residence time, /[sec]
3	9	81	34

Column sizing

The operating pressure for distillation columns was determined to allow using cooling water in the condenser (except the de-ethanizer, where refrigerant is used). For all columns, the recoveries of the key components were set to 99.9%.

The number of actual stages, feed tray and reflux ratio were determined by using Winn-Underwood-Gilliland method. These were used as input data for calculating the tray diameter with RADFRAC model from Aspen Plus, which uses the flooding velocity to ensure proper pressure drop between trays and minimum liquid entrainment. The equation that estimates the column diameter is Souder and Brown equation which determines the maximum vapor velocity:

$$v = (-0.171s^2 + 0.27s - 0.047)\cdot[\frac{\rho_l - \rho_v}{\rho_v}]^{0.5} \tag{19}$$

where v is the vapor velocity in m/s, s represents tray spacing in m; ρ_l and ρ_v represents the liquid and vapor densities in kg/m^3. Typical value of tray spacing is $s = 0.61$ m with sieve tray type being the most common used in the industry. The column diameter is calculated using the following relation:

$$D_C = \sqrt{\frac{4\cdot G_m}{v\cdot\pi\cdot\rho_v}} \tag{20}$$

where D_C – column diameter / [m] and G_m – vapor mass flow rate / [kg/hr]

The results from the columns design are presented in Table 11 and Table 12. Column height was determined considering the number of actual stages calculated with the 0.6 m as typical value of tray spacing and allowing enough vapor disengaging at top of the column equal with 4 trays and sufficient residence time in the bottom of the column equal with 3 trays. The vessels were sized based on a residence time of minimum 5 minutes to reject process perturbation and to ensure enough Net Positive Suction Head for reflux pump (Table 13).

Heat exchanger sizing

The heat exchanger sizing was determined considering a minimum temperature approach of 15°C for shell and tube exchangers and a typical value of 200 W/m^2/K for global heat transfer coefficient. The log mean temperature difference (LMTD) was calculated and hence the heat transfer area (A).

The cost analysis performed for US2b is detailed in Table 14 for illustrating the contribution of main equipment to the overall CAPEX. The cost associated with distillation columns are the highest followed by catalyst and feed preheat exchangers costs.

Table 11

Operating parameters for distillation columns from US2b

Column TAG	COL-1	COL-2	COL-3	COL-4	
Column description	De-ethanizer	De-propanizer	De-butanizer	De-pentanizer	
Top Pressure, bar	32	25.5	6.5	2.5	
Top Temperature, °C	-10.2	60.3	60.2	65.3	
Bottom Temperature, °C	140	154.4	119.4	111.9	
Reflux ratio	2.8	5.54	10.27	1.6	
Distillate rate, kmol/hr	12	26.57	32.8	21.7	
Component mole fraction	C2 Product	C3 Product	C4 Product	C5 Product	C6 Product
C2	0.99	-	-	-	
C3	0.01	0.99	-	-	
INERT	-	0.01	0.913	0.016	
1-C4	-	-	0.019	-	
2-C4	-	-	0.068	-	
C5	-	-	-	0.984	0.01
C6	-	-	-	-	0.99

Table 12

Results of column sizing

Column TAG	COL-1	COL-2	COL-3	COL-4
Column description	De-ethanizer	De-propanizer	De-butanizer	De-pentanizer
Number of actual stages	47	45	44	48
Column diameter / [m]	0.58	0.520	0.51	0.43
Column height / [m]	31	29	29.5	32
Stage pressure drop / [bar]	0.01	0.01	0.01	0.01
Reboiler duty / [Gcal/hr]	0.4	0.38	0.29	0.24
Condenser duty / [Gcal/hr]	-0.07	-0.42	-0.49	-0.28

Table 13

Results of vessel sizing

Equip. TAG	V-1	V-2	V-3	V-4	V-5	V-6
Equip. description	Feed vessel	Buffer vessel	Reflux drum COL-1	Reflux drum COL-2	Reflux drum COL-3	Reflux drum COL-4
Diameter / [m]	0.8	0.8	0.6	0.825	0.93	0.75
Length / [m]	3.1	3.1	1.5	1.65	1.85	1.5
Volume / [m^3]	1.6	1.6	0.43	0.88	1.25	0.67
Residence time / [min]	10	10	5	5	5	5

Table 14

Equipment cost and contribution to total fixed cost

Nr.crt	Equipment	Pcs	Installed Cost / [k$]	Percentage of CAPEX / [%]
1	Reactor	1	548	9%
2	Catalyst	1	1017	16%

3	Distillation columns	4	2309	37%
4	FEHE	1	689	11%
5	Furnace	1	141	2%
6	Compressor	1	635	10%
7	Vessels	2	133	2%
8	Pumps	8	266	4%
9	Contingency		534	9%
TOTAL			6272	100%

The operating expenses for each utility are illustrated in Table 15.

Table 15

Utility cost and contribution to Operating Expenditures (OPEX)

Nr.crt	Utility	Cost / [k$/year]	Percentage of OPEX / %
1	Gas	111	14.5 %
2	Steam	339	44 %
3	Cooling Water	31	4.1 %
4	Electricity	259	33.8 %
5	Refrigerant	26	3.6 %
TOTAL		766	100%

Steam used in reboilers has the largest contribution, followed by power necessary to compress the reaction mixture before the ethylene separation.

6. Conclusions

The metathesis reaction of 2-butene over mesoporous tungsten catalyst is a viable opportunity to produce more valuable olefins (such as propylene) from less desired ones (as 2-butene). Sensitivity cases were performed for two configurations, with and without recycle. The results revealed that recycling keeps important amounts of inert (I) inside the unit, therefore increasing the CAPEX and OPEX. Moreover, the separation of inert (I) from reactants A and B implies the cost of additional expensive distillation column. The most economical solution is US2b (Reactor – Separation, without recycle) with the highest profitability *EP4*=2300 [k$/year]. For a feed rate consisting of 2-butene (70 %molar) and n-butane (30 % molar), the investment and operating costs are 6272 k$ and 766 k$/year, respectively, giving a return of investment of *ROI* =35%

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