Process System Engineering for Sustainable Product-Process Engineering, Evaluation and Design

Simultaneous optimization and heat integration

http://www.pseforspeed.com/

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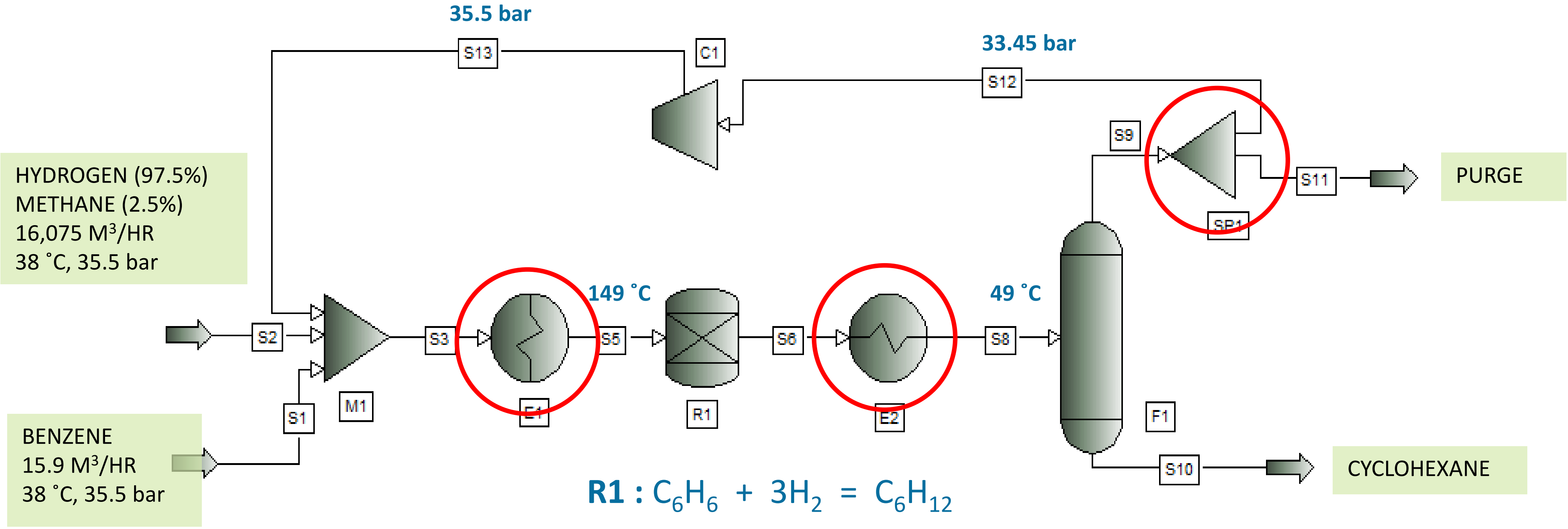
Case study : Cyclohexane plant

- Cyclohexane is produced by **benzene hydrogenation**, a conversion reactor has been used to model **R1**.
  - Exothermic reaction : **C_6H_6 + $3H_2$ = C_6H_{12}**
  - Vapor phase
  - Reactor is jacketed and controlled to **224^{o}C**, thus steam is produced
  - **98 % conversion (ξ)** of benzene to cyclohexane
  - Heat of reaction (at 25 ^{o}C) **= -202,400 kJ**/kmol benzene

- **SRK thermodynamics with API liquid** density was used.
- All heat exchangers have a **0.35 bar pressure drop**.
- **E1** is modeled as a **counter current** heat exchanger with U = 0.568 kW/m^{2}K and Area = 60.4 m^2.



HYDROGEN (97.5%)
METHANE (2.5%)
16,075 M^3/HR
38 ˚C, 35.5 bar

BENZENE
15.9 M^3/HR
38 ˚C, 35.5 bar

R1 : C_6H_6 + $3H_2$ = C_6H_{12}

$\xi = 0.98$

Case study : Cyclohexane plant

In order to emphasize the simultaneous optimization and heat integration the **four steps** have been followed

Step 1 : *Simulation **without heat integration** of the initial design*

***Step 2 : Cost optimization of the plant** to determine the optimal design*

Step 3 : *Simulation of the **optimum operating point with "intuitive"** heat integration*

Step 4 : Simultaneous cost optimization and heat integration

Case study : Cyclohexane plant

Objective Function

- A function representing the profit has been used for the optimization problem

f = **revenue** - **costs**

Where: **revenue** = cyclohexane (S10) + generated steam in reactor

costs = feed + purge + compressor work + Flash duty + HX utilities

Revenue = Cyclohexane (S10) + Generate Steam in the reactor
= C1*P1+C4 *ABS(P2)
Costs = feed + purge + compressor work + Flash duty + HX utilities
= C3*P3 + C2*P4 + C8*P5 + C5*P7 +C6*ABS(P6) + C7*ABS(P8) + C6*ABS(P9)
Profit = Revenue - Cost

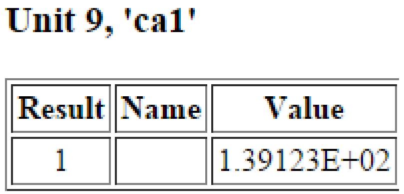
The prices of the chemical and costs of the utilities are given below

C	Item	Price or Cost
1	Product	3.81 $\$ / \text{kmol of } S_{10}$
2	Feedstocks	0.20 $\$ / \text{kmol of } S_2$
3		0.40 $\$ / \text{kmol of } S_1$
4	Generated Steam	18.537 \$ / MkJ
5	Electricity	0.025 \$ / kWh
6	Cooling Utility	2.4642 \$ / MkJ
7	Heating Utility	55.613 \$ / MkJ
8	Purge Penalty	0.1 $\$ / \text{kmol of } S_{11}$

P		
1	**S10**	Stream S10 Flowrate of all components on a wet basis in kg-mol/hr
2	**R1**	Conversion R1 duty in x 10^6 kJ/hr
3	**S1**	Stream S1 Flowrate of all components on a wet basis in kg-mol/hr
4	**S2**	Stream S2 Flowrate of all components on a wet basis in kg-mol/hr
5	**S11**	Stream S11 Flowrate of all components on a wet basis in kg-mol/hr
6	**F1**	Flash F1 Duty in x 10^6 kJ/hr
7	**C1**	Compressor C1 Actual work in kW
8	**E1**	Heat Exchanger E1 Duty in x 10^6 kJ/hr
9	**E2**	Heat Exchanger E2 Duty in x 10^6 kJ/hr

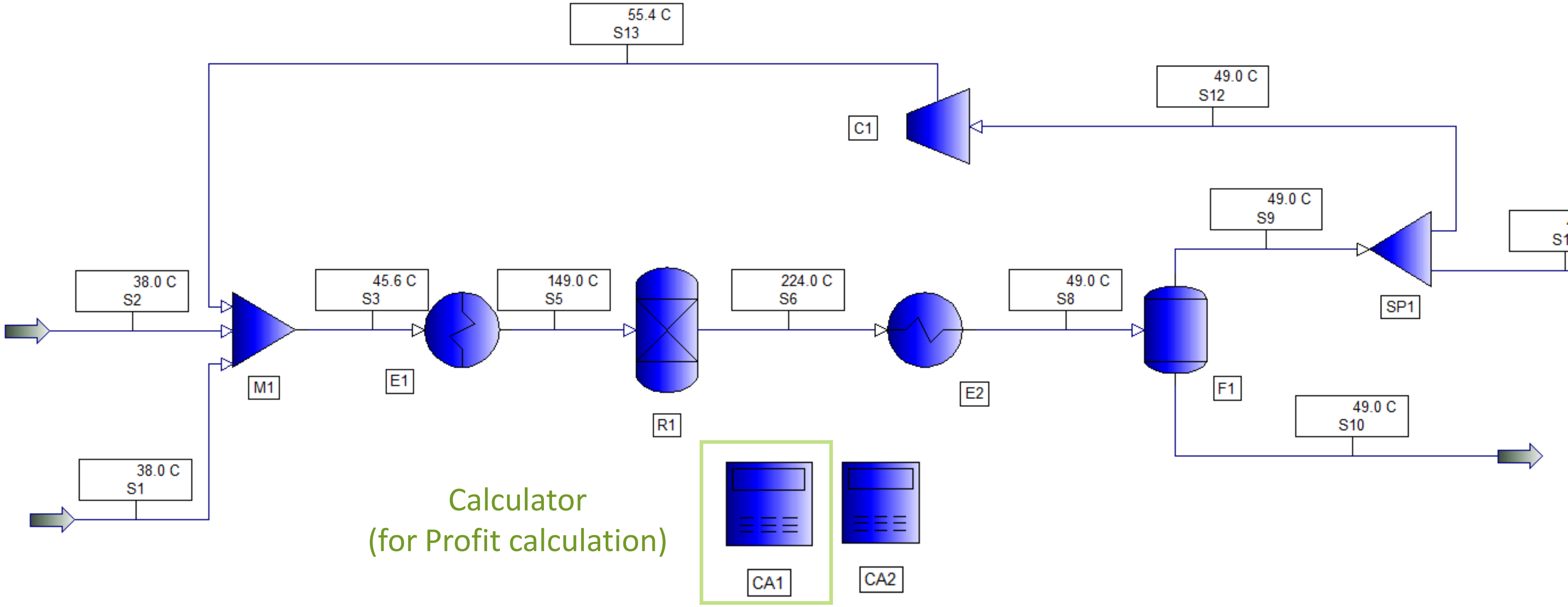
Case study : Cyclohexane plant

Step 1: Simulation without heat integration

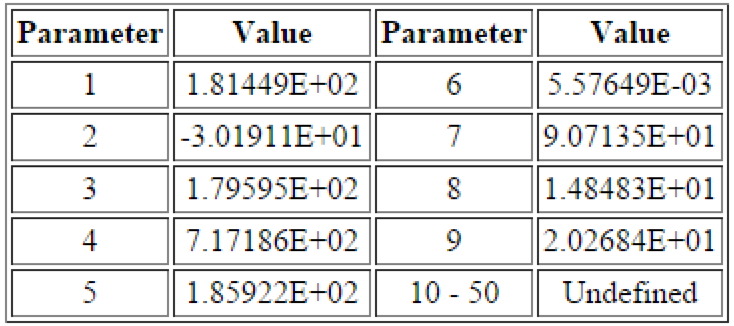


Unit 9, 'ca1'

Result	Name	Value
1		1.39123E+02



Calculator
(for Profit calculation)



Parameter	Value	Parameter	Value
1	1.81449E+02	6	5.57649E-03
2	-3.01911E+01	7	9.07135E+01
3	1.79595E+02	8	1.48483E+01
4	7.17186E+02	9	2.02684E+01
5	1.85922E+02	10 - 50	Undefined

Stream Name		S1	S2	S10	S11	S13
		Benzene	Hydrogen+ Methane	**Cyclohexnae**	Purge	Recycle
Temperature	C	38	38	49	49	55.54
Pressure	BAR	35.5	35.5	33.45	33.45	35.5
Flowrate	KG-MOL/HR	179.6	717.2	181.45	185.92	1602.67

The simulation of the initial design of the process ***without heat integration*** indicates that the ***profit*** is ***139.12 $/h***

Case study : Cyclohexane plant

Step 2. : **Cost optimization of the plant to determine the optimal design**

- The configuration of flowsheet in step 1 is **unchanged** and a better design is investigated in order to maximize the **profit** by solving the following optimization problem :

Maximize f subject to : x_{C6H12} **in S10** $\in [0.97 , 1]$

$\left(\dot{m}_{H_2} / \dot{m}_{C_6H_6}\right)$ **in S3** $\in [10 , 14]$

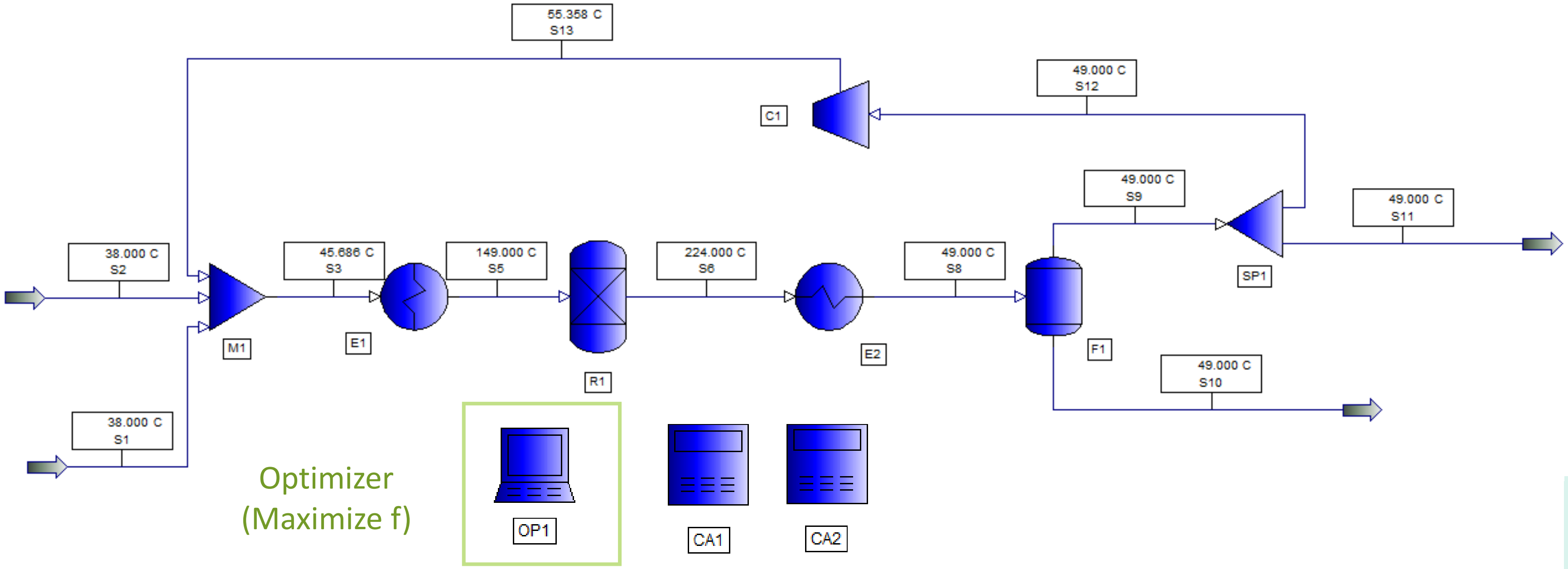
varying : $\xi \in [0.9 , 0.99999]$

$\dot{m}_{C_6H_6}$ **of S1** $\in [0 , 300]$

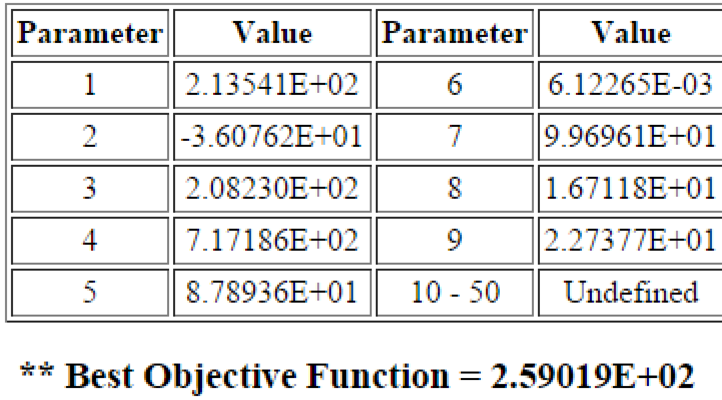
- Choosing these variables, we assume that new technologies have been developed allowing to obtain a ***better conversion*** with ***a smaller ratio between the reactants in the feed***. Also we permit the ***feed flowrate to be bigger*** and a ***better purity of cyclohexane is asked.***

Case study : Cyclohexane plant

Step 2 : Cost optimization of the plant to determine the optimal design



Optimizer
(Maximize f)



Parameter	Value	Parameter	Value
1	2.13541E+02	6	6.12265E-03
2	-3.60762E+01	7	9.96961E+01
3	2.08230E+02	8	1.67118E+01
4	7.17186E+02	9	2.27377E+01
5	8.78936E+01	10 - 50	Undefined

** **Best Objective Function = 2.59019E+02**

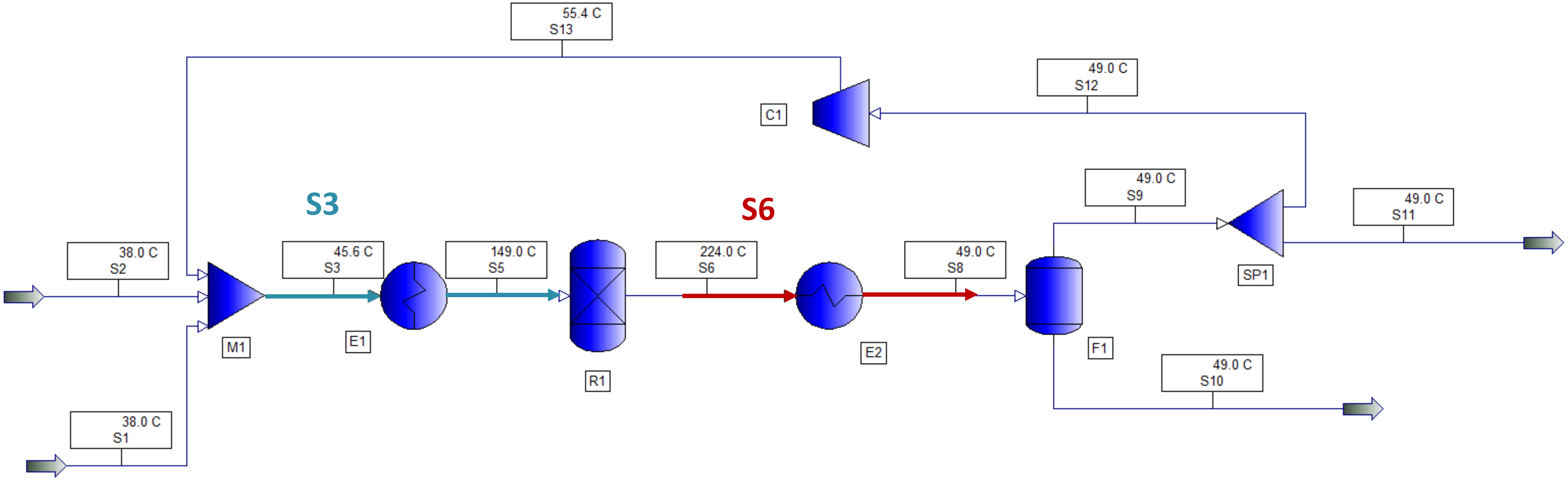
With this penalizing constraint a better profit of 259.01 $/h is obtained

Stream Name		S1	S2	S10	S11	S13
Temperature	C	38	38	49	49	55.4
Pressure	BAR	35.5	35.5	33.45	33.45	35.5
Flowrate	KG-MOL/HR	208.23	717.13	213.54	87.90	1766.5

Case study : Cyclohexane plant

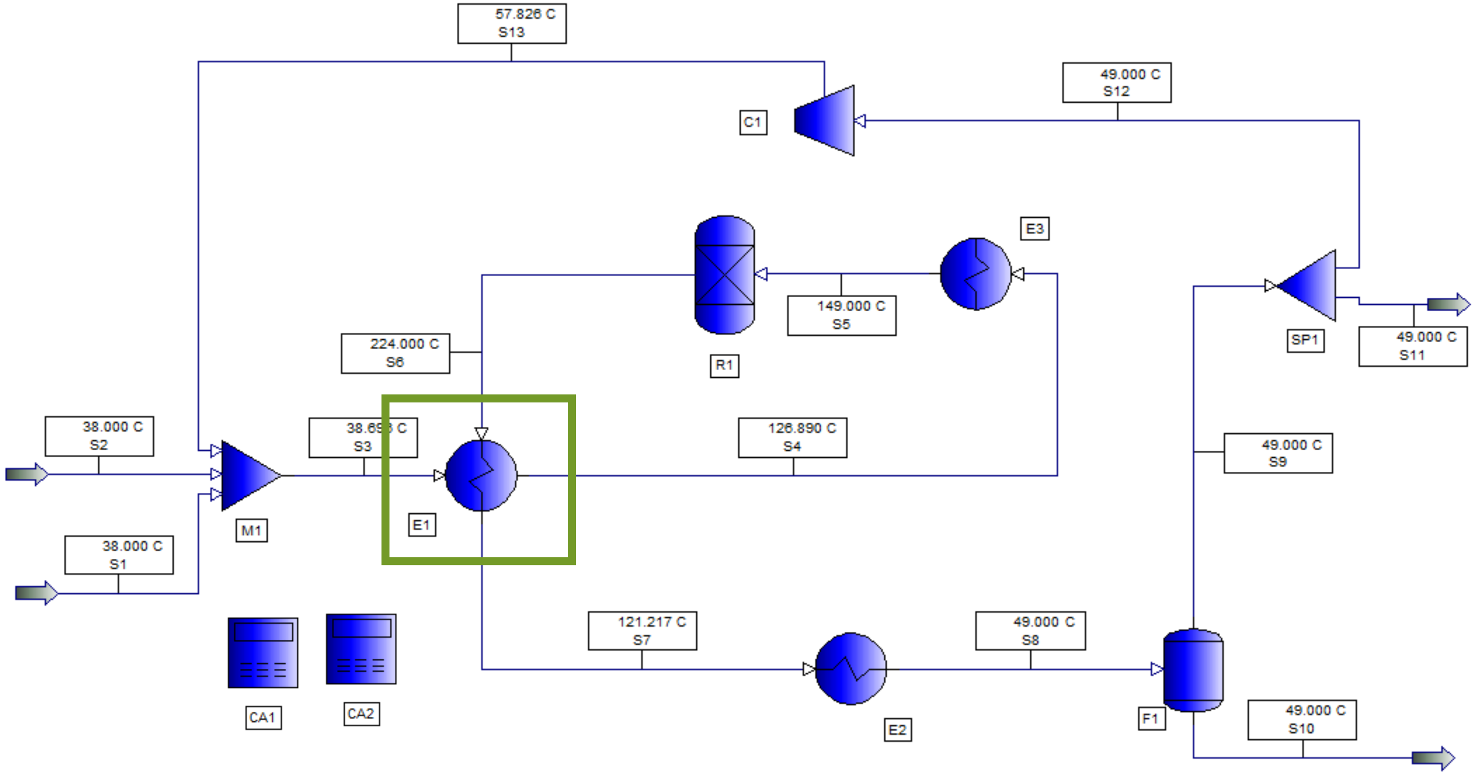
Step 3 : **Incorporation of “intuitive” heat integration**

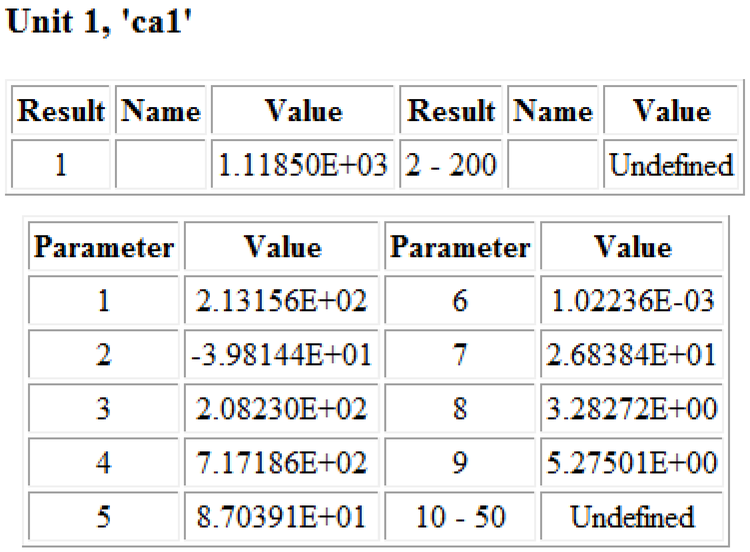
- ✓ Observing the temperature at different places in the flowsheet. it is not difficult to see that a more economical design can be achieved using **heat integration**.



Case study : Cyclohexane plant

Step 3 : Incorporation of “intuitive” heat integration





Unit 1, 'ca1'

Result	Name	Value	Result	Name	Value
1		1.11850E+03	2 - 200		Undefined

Parameter	Value	Parameter	Value
1	2.13156E+02	6	1.02236E-03
2	-3.98144E+01	7	2.68384E+01
3	2.08230E+02	8	3.28272E+00
4	7.17186E+02	9	5.27501E+00
5	8.70391E+01	10 - 50	Undefined

The simulation of the flowsheet with the optimized values found previously show that ***the profit is drastically increased to 1,118.5 $/h.***

Stream Name		S1	S2	S10	S11	S12
Temperature	C	38	38	49	49	49
Pressure	BAR	35.5	35.5	32.75	32.75	32.75
Flowrate	KG-MOL/HR	208.23	717.19	213.16	87.04	349.69

Case study : Cyclohexane plant

Step 4 : Simultaneous optimization and heat integration

- ✓ Now, the previous results are left apart and the newly ***PSE for SPEED heat integration module of Pro/II based on is incorporated*** to the input file in order to perform **a simultaneous cost optimization** and heat integration.

PSE for SPEED Heat Integration module based on [1] [2]

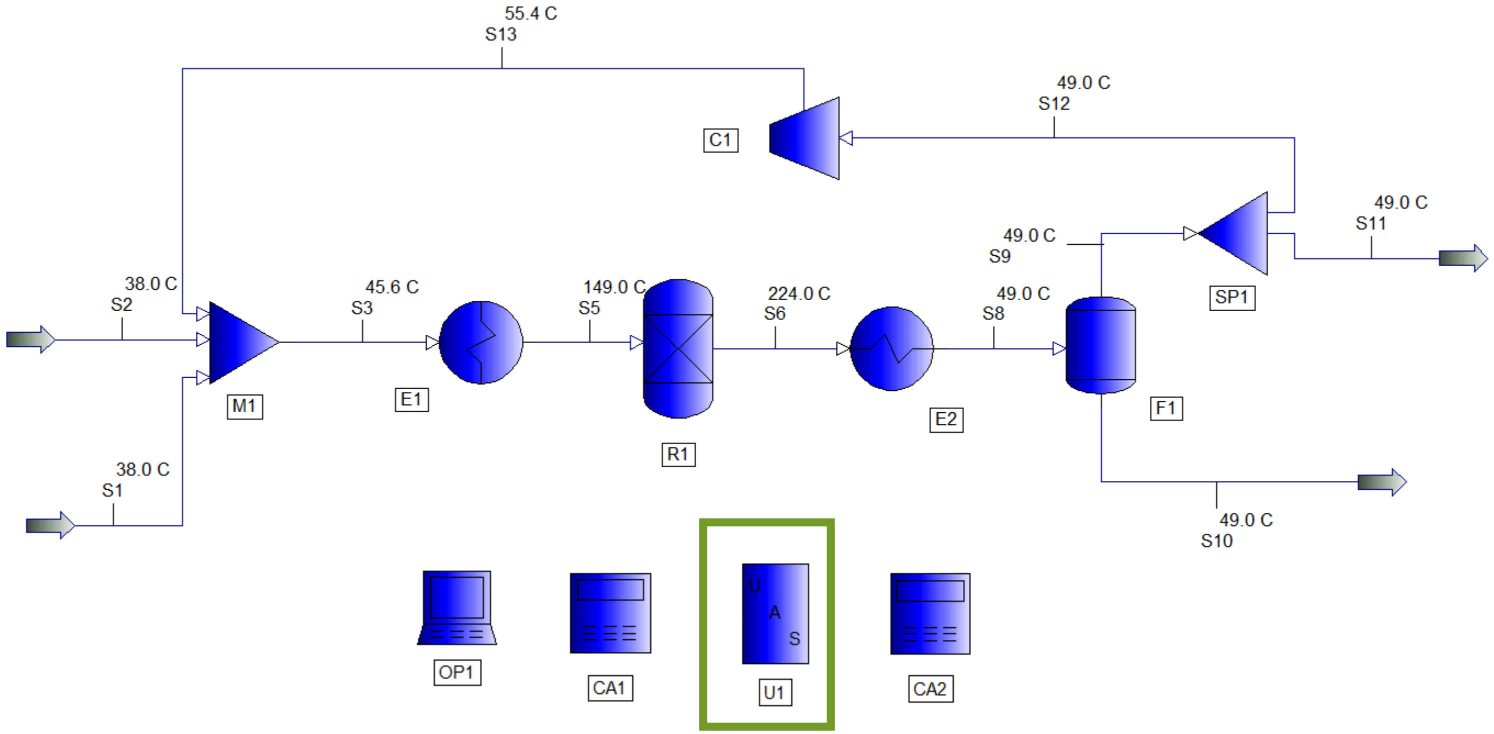
Integer vector elementes			Real Vector elements		
1	1	number hot streams	1	10	HRAT
2	1	number of cold streams	2	55.613	heating utility cost $/MkJ
3	1	number of hot utilities	3	2.4642	cooling utility cost $/MkJ
4	1	number of cold utilities	4	400	hot utility temperature C
5	6	Stream number of hot inlet stream	5	20	cold utility temperature C
7	8	Stream number of hot outlet stream	OUTPUT (heat loads)		
8	3	Stream number of cold inlet stream	6		
9	5	Stream number of cold outlet stream	7		

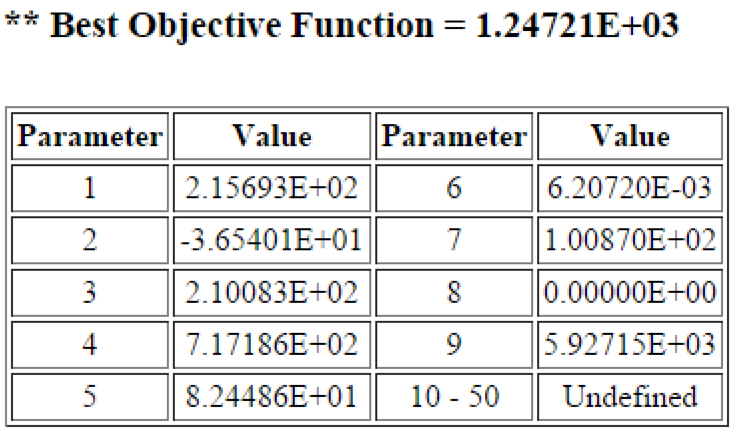
[1] Duran, M A, & Grossmann I E, (1986) Simultaneous optimization and heat integration of chemical processes. AIChE J, 32, 123 (disjunctive programming)

[2] Chapter 18 (Simultaneous optimization and heat integration) of Biegler, Grossmann Westerberg book on Systematic Methods of Chemical Process Design.

Case study : Cyclohexane plant

Step 4 : Simultaneous optimization and heat integration





** Best Objective Function = 1.24721E+03

Parameter	Value	Parameter	Value
1	2.15693E+02	6	6.20720E-03
2	-3.65401E+01	7	1.00870E+02
3	2.10083E+02	8	0.00000E+00
4	7.17186E+02	9	5.92715E+03
5	8.24486E+01	10 - 50	Undefined

The profit would then reach 1,247.21 $/ h

Stream Name		S1	S2	S10	S11	S13
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Temperature	C	38	38	49	49	55.41
Pressure	BAR	35.5	35.5	33.45	33.45	35.5
Flowrate	KG-MOL/HR	210.1	717.2	215.7	82.45	1787.47

Case study : Cyclohexane plant

Step 4 : **Simultaneous optimization and heat integration**

- This run indicates that all the heating utilities can be provided within the process itself and not via external utilities.
- An important remark to give here is that because the dimension of heat exchanger E1 is fixed, the total heat needed to bring S_3 to 149^{o}C could not be obtained with this exchanger.
- An alternative which was not found intuitively would be to use the hot stream leaving the reactor to finish the heating of the reactor feed in our constrained heat exchanger E1 (called E2 in Figure 3) and start the heating of this stream with the hot side output stream.

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 heat integration module
  SimSci International LTD.
              Carnegie-Mellon University
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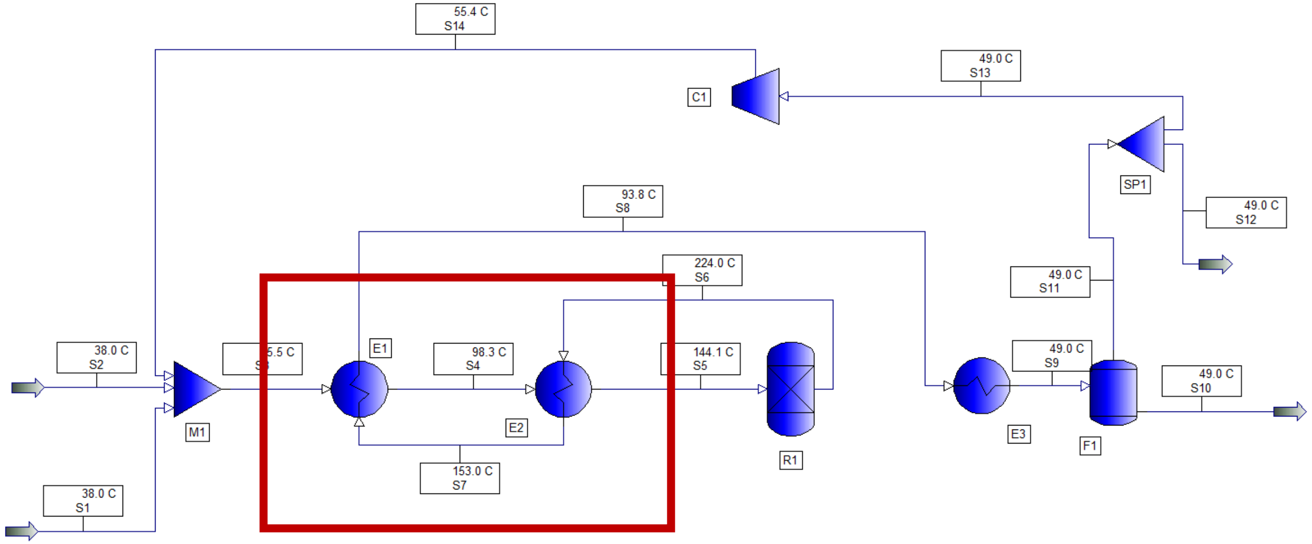
HOT STREAM  S6        INLET TEMPERATURE          224.0000
HOT STREAM  S6        INLET ENTHALPY             32385.70
HOT STREAM  S8        OUTLET TEMPERATURE         49.00000
HOT STREAM  S8        OUTLET ENTHALPY            9538.313
COLD STREAM  S3         INLET TEMPERATURE        45.62626
COLD STREAM  S3         INLET ENTHALPY           11481.43
COLD STREAM  S5         OUTLET TEMPERATURE       149.0000
COLD STREAM  S5         OUTLET ENTHALPY          28261.34

HEAT INTEGRATION - RESULTS
HOT  UTILITY N%       1       HEAT LOAD    0.000000000000000E+000
COLD UTILITY N%       1       HEAT LOAD    6067.48437500000
```



Case study : Cyclohexane plant

Summary of 4 step results

Variables	Units	Cyclo1	Cyclo2	Cyclo3	Cyclo4
Duty (E1)	MkJ / h	14.867	16.994	11.398	0^{*}
Duty (E2)	MkJ / h	20.292	23.164	11.624	6.147^{**}
Duty (E3)	MkJ / h	-	-	5.393	-
Work (C1)	kW	90.75	101.93	137.2	101.59
Duty (R1)	MkJ / h	30.247	36.544	36.609	36.451
$\dot{m}$ of S_{10}	kmol / h	181.78	217.10	216.76	216.45
ξ	%	98	99.943	99.943	99.943
$\dot{m}$ of S_1	kmol / h	179.92	211.33	211.33	210.77
x_{C6H12} in S_{10}	%	96	96.902	96.96	96.93
$\left(\dot{m}_{H2}/\dot{m}_{C6H6}\right)$ in S_3	none	11.864	10.126	10.127	10.154
f	\$ / h	140.27	269.97	936.75	1247.93

* Hot heat load ** Cold heat load

Stream Name	S_1	S_2	S_{10}	S_{11}	S_{13}	S_3
	Benzene	Hydrogen	Cyclohexane	Purge Gas	Recycle	
Phase	Liquid	Vapor	Liquid	Vapor	Vapor	Mixed
Temperature C	38.00	38.00	49.00	49.00	55.54	45.38
Pressure (Bar)	35.50	35.50	33.45	33.45	35.50	35.50
Flowrate (Kmol / hr)	179.92	717.19	181.78	184.99	1603.84	2501.0
Composition						
Hydrogen	0.0000	0.9750	0.0146	0.8985	0.8985	0.8558
Methane	0.0000	0.0250	0.0085	0.0888	0.0888	0.0641
Benzene	1.0000	0.0000	0.0169	0.0003	0.0003	0.0721
Cyclohexane	0.0000	0.0000	0.9600	0.0124	0.0124	0.0079

Cyclo1 = Original simulation

Cyclo2 = Optimization

Cyclo3 = Optimization + Heat integration sequentially

Cyclo4 = Optimization and Heat integration simultaneous (with PSE for SPEED heat integration module)

- **Objective of sustainable process design has been achieved through the Optimization and Heat integration simultaneous (with PSE for SPEED heat integration module)**
- **Further improvement is possible through process intensification but we have not studied it.**