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# Synergistic Effects of Performing Process Synthesis with Heat, Electricity, Shaft work and Mass Integration

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Process system engineering applying the system thinking approach leads to a tremendously improved process design that considers many conflicting objectives. These conflicting objectives lead to interesting trade-offs that could hardly have been predicted since the processes are operating under many complex interactions taking place between their subsystems. Studying these interactions can reveal new insights into and rules for better process design. An example of such insight was proposed by Lang et al. (1988), showing that performing heat integration simultaneously with process optimisation leads not only to a reduction of utility consumption but also to decreased raw material usage due to higher overall conversion. This observation was made for processes with recycling steps performing heat integration within the recycle loops. However, the processes generally consist of several steps: the raw material preparation step, the central reaction/separation step with or without recycling, and the final product purification, conditioning step. Different synergistic effects are expected when the integration is performed only partly within a recycle. Moreover, different types of integration can lead to diverse solutions. In this study, the following scenarios were studied: i) no integration, ii) heat integration, iii) power (shaft work) integration, and iv) heat and electricity (shaft work) integration. The solutions obtained enable us to provide some valuable insights about exploiting the synergistic effects of various types of integration, their effects on the design, conversion, and selectivity of the processes and, nevertheless, also the effects among different processes via Mass Integration.

## 1. Introduction

In the field of process flowsheet synthesis, despite some attempts of simultaneous process synthesis (Ryu et al, 2020), most of the computational tools continue to be sequential, based on the hierarchical decomposition approach, considering five decision levels: a) batch versus continuous, b) input-output structure, c) recycle structure and reactors, d) separation system, e) heat exchanger network (Chen and Grossmann, 2017). Considerable attention was dedicated to combine heat and power system e.g. for Total Site (Lee et al, 2020). There are also many detailed studies considering e.g. practical operating constraints (Pavao et al., 2020). There is only a limited studies for innovative process synthesis. Although hierarchical decomposition enables division of complex decision making into a set of simpler subproblems, many interactions are lost, leading to suboptimal solutions. All the complex interactions can only be exploited by performing the simultaneous optimisation approach, as in the previously mentioned case of simultaneous heat integration and process optimisation (Lang, 1988), which showed the relation between heat integration and process synthesis/optimisation, when considering the recycle loop. This synergistic relationship shifts the trade-off between raw-material and utility consumption towards higher overall conversion and lower raw material consumption. This is a highly relevant insight, gathering the understanding of one of the basic principles of process synthesis.

### 1.1 Aim/Novelty

In this study, this assessment of the relationship between process synthesis and simultaneous heat integration was extended by studying various trade-offs, while performing process synthesis/optimisation and simultaneously considering both power integration and heat integration. Particular attention was paid to the location of integration places, whether they were inside or outside the recycle loop, and to the mutual sequence of heat and power integration places, since these can have a significant impact on the general assessment.

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## 2. Theoretical background

To gather a general understanding of process synthesis, a simple linear model, as presented by Biegler et al. (1997), was extended in order to include the effects of power integration. The cost of the presented flowsheet is modelled as follows. A simple reaction is assumed, where A is converted to B, in the presence of inert component C. The net feedstock cost $C_{NF}$ is determined as the cost of feedstock $C_F$ reduced by the purge income $I_P$. Both depend on the flowrates of component A and C $f_0^A + f_0^C$ for feedstock and $f_6^A + f_6^C$ for the purge. The flows are multiplied by the price of feedstock $c_f$ and purge $c_p$.

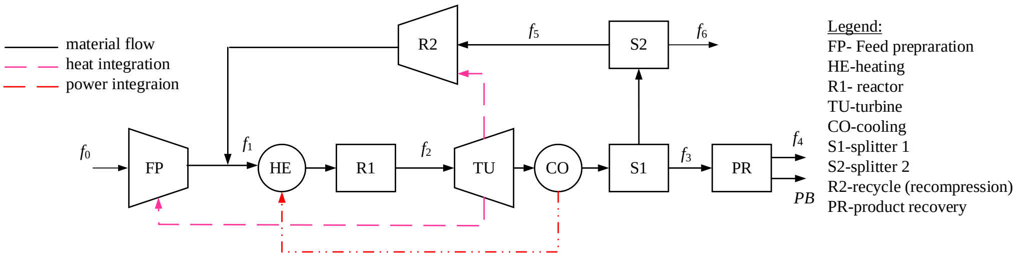


*Figure 1: General flowsheet of the process with recycling considering Heat and Power Integration*

$$\begin{aligned} C_{NF} &= C_F - I_P \\ C_F &= c_f\left(f_0^A + f_0^C\right) \\ I_P &= c_p\left(f_6^A + f_6^C\right) \end{aligned} \tag{1}$$

The maintenance and capital cost $C_{OC}$ consist of the electricity and compressor cost for feed preparation, $C_{FP}$, reactor capital cost ($C_{R1}$), including the cost of heating and the heater (HE), cooling and the cooler (CO) and turbine (TU)(Figure 1). The $C_{R2}$ represents the cost of the recycle stream, considering recompression. $C_{PR}$ represents the cost of product recovery or downstream processes still required after the reaction and separation.

$$\begin{aligned} C_{FP} &= c_{fp}\left(f_0^A + f_0^C\right) \\ C_{R1} &= c_{R1}\left(f_2^A + f_2^C\right) \\ C_{R2} &= c_{R2}\left(f_5^A + f_5^B\right) \\ C_{PR} &= c_{PR}\frac{P_B}{\beta} \\ C_{OC} &= C_{FC} + C_{R1} + C_{R2} + C_{PR} \end{aligned} \tag{2}$$

When simultaneous heat integration is performed within the recycle loop, the cost of heating and $C_{R1}$ is decreased, resulting in a higher recycle rate and a higher overall conversion. Consequently, raw material consumption and cost are decreased. In the case of power integration, this is not the case. Although power integration reduces the cost of $C_{R2}$, which favours a higher overall conversion, this favourable effect is more than outweighed by even more significant cost reductions achieved in the feed preparation $C_{FP}$ outside the loop, which favours a solution with a lower overall conversion and higher raw material consumption. Figure 2 presents the case when a) only heat integration is applied and b) when only power integration is performed. We can see from the above insight that performing only heat integration does change the trade-off towards higher overall conversion and lower raw material consumption, while performing only power integration shifts the trade-off in process synthesis towards lower overall conversion and higher raw material consumption. Since those two effects are contradictory, it is hard to predict which effect will be dominant when both heat and power integration are performed simultaneously.

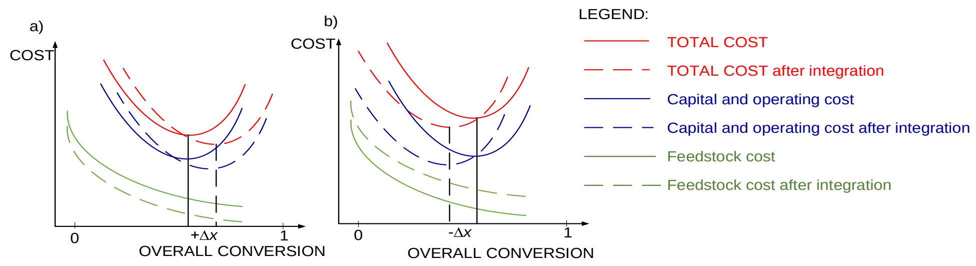


*Figure 2: Process cost versus overall conversion when a) Heat and b) Power Integration is performed*

## 3. Method

A flowsheet synthesis was performed by mixed-integer nonlinear programming (MINLP) in the MipSyn process synthesiser (Kravanja, 2010) for cases i) without Heat and Power Integration, ii) with simultaneous Heat Integration, iii) with simultaneous Power Integration, and iv) with simultaneous Heat and Power Integration.

## 4. Case study

The case of methanol production was used as a case study, which was described in greater detail by Srinivasan et al. (2019). The original superstructure consists of two possible feed utilisation, one- or two-step compression of intermediate materials, two types of reactor, and one- or two-step recompression of the recycled stream. To enable Power Integration, the utilisation of a turbine (TURB) instead of a valve was introduced (Figure 3). The input data for process synthesis is presented in Table 1.

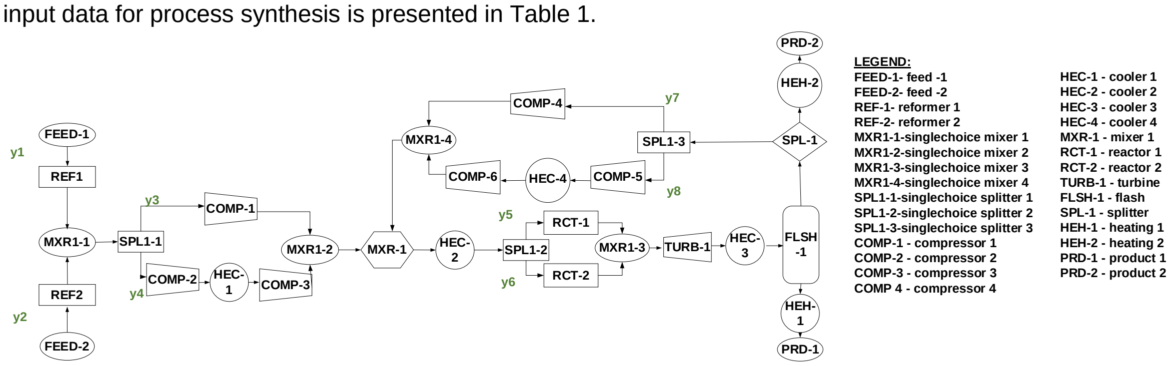


*Figure 3: Superstructure of methanol production*

*Table 1: Input data for process synthesis*

| *Feed* | *Composition* | *Cost* k\$ s kmol$^{-1}$y | *Process Unit* | *Fixed cost* k\$/y | *Variable cost* k\$ (y×m$^3$)$^{-1}$ |
|---|---|---|---|---|---|
| FEED-1 | 0.15 CO | 77 903 | RCT-1 | 500 | 25 |
| composition | 0.85 $CH_4$ | | RCT-2 | 650 | 30 |
| FEED-2 | 0.4 $H_2$ | 129 219 | REF-1 | 500 | 25 |
| composition | 0.3 CO | | | | |
| | 0.235 $CH_4$ | | REF-2 | 1,000 | 50 |
| | 0.065 $C_2H_4$ | | | | |
| *Product* | *Composition* | *Cost* k\$ s kmol$^{-1}$y | compressor | 50 | 87.5 |
| PRD-1 | 0.9 methanol | 294 127 | FEED-1-storage | 91.8 | 308.3 |
| PRD-2 | purge | 18 383 | FEED-2-storage | 46 | 140.14 |
| *Utilities* | *Temperature limits* | *Cost* k\$ (MW y)$^{-1}$ | MXR, SPL, ICOMP | 10 | - |
| Hot utility-steam | 177 °C | 165 | PRD-1-storage | 91.8 | 308.3 |
| Cold utility-water | inlet: 10 °C outlet: 22 °C | 20.65 | PRD-2-storage | 91.8 | 308.3 |
| Electricity | | 1275 | FLSH | 25 | |
| *Heat exchanger type* | *Fixed cost k\$/y* | *Variable cost k\$ (y.m$^3$)$^{-1}$* | *Area limits m$^2$* | | *Temperature limits / °C* |
| Double pipe | 3.06 | 0.1828 | $A^{LO}$ = 0.25, $A^{UP}$ = 200 | | $T^{LO}$=-101, $T^{UP}$=600 |
| Shell and tube | 8.093 | 0.01287 | $A^{LO}$ = 10, $A^{UP}$=1000 | | $T^{LO}$=-200, $T^{UP}$=850 |
| U-tube HE | 6.726 | 0.01813 | $A^{LO}$=10, $A^{UP}$=1000 | | $T^{LO}$=-200, $T^{UP}$=850 |
| Plate and frame | 8.653 | 0.0231 | $A^{LO}$= 1, $A^{UP}$=1000 | | $T^{LO}$=-25, $T^{UP}$=250 |

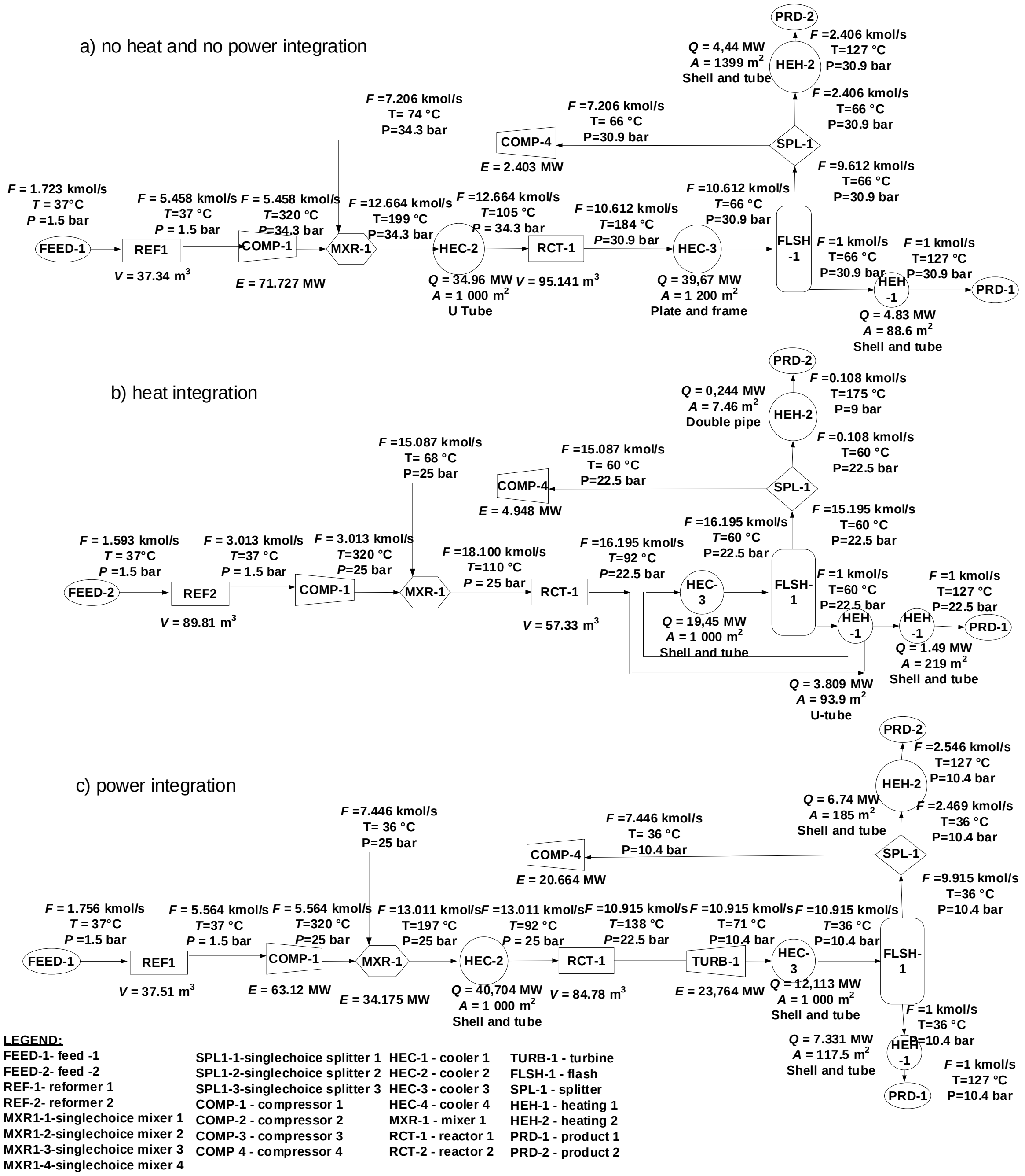


*Figure 4: Optimal process design when a) no heat and no Power Integration, b) Heat Integration and c) Power Integration was carried out*

As a reference solution, process synthesis with no heat and power integration was performed. The net present value of the obtained solution was 95,184 k€, with an overall conversion of 0.466 (Figure 4a). Considering heat integration simultaneously with process synthesis resulted in a solution with a net present value of 96,636 k€ (Figure 4b). In line with the previous general assessments, the overall conversion of the process increased to 0.824, owing to the more than doubled recycle rate and to the more than doubled number of reaction passes. Consequently, raw material consumption was reduced. It should be noted that feed 2 with lower methane consumption was selected. The flowrate reduction is not as significant as expected. More notable is the flowrate reduction after the reformer. When performing only power integration (Figure 4c), better economic viability was achieved, with a 108,704 k€ net present value. The process conditions changed quite significantly, as the power integration enabled recompression of the recycle loop with a significantly higher compression ratio. The flash now operated at much lower pressure 10.4 bar, while in the reference case, it was 30.9 bar.

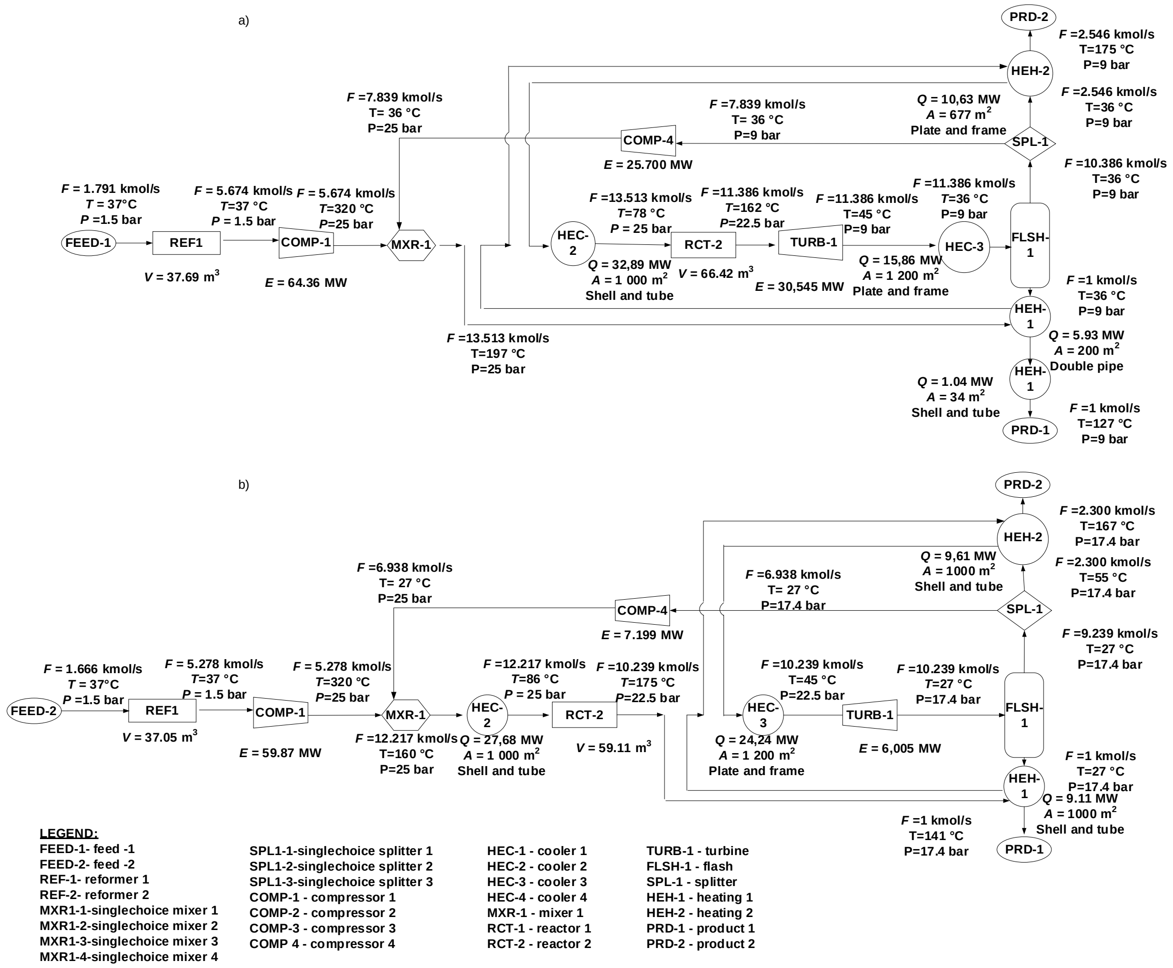


*Figure 5: Optimal process design when a) the turbine is positioned first after the reactor and b) when the heat exchanger is positioned first after the reactor*

Note that, although the higher compression ratio led to almost 10 times higher power consumption for the recompression, the net power consumption on the recycle and on the feed stream was, because of the Power Integration, significantly lower. The overall conversion did not change significantly and was 0.468. When performing both heat and power integration (Figure 5a) with the turbine on the reactor outlet stream being positioned before the cooler, the net present value was 109,050 k€, which is a result quite similar to the one obtained by Power Integration. From this comparison, we can conclude that in this case, power integration had a much greater effect than Heat Integration. In fact, the current sequence of the turbine and the cooler prevented heat integration. Observation of process conditions revealed even lower operating pressure of flash at 9 bar compared to the reference solution, leading to a much lower temperature in the turbine outlet stream, which caused the operation of the cooler at even lower temperature, so that the heat released from the cooler could no longer be recuperated for preheating the reactor inlet stream. An additional solution was obtained, where the order of power production and cooling on the reactor outlet stream was reversed. It enabled to perform the heat integration first and the power generation later. The result obtained was significantly better than the previous one, since the net present value increased to 116,853 k€. Compared to the reference solution, this result was 22.8% better in economic performance. The operating pressure of flash was at 17.4 bar, compared to 9.4 bar when the turbine was positioned first.

Although everybody is aware of the link between pressure and temperature, there is still a lack of simultaneous heat and power integration in practice. This case study shows how important it is to perform both at the same time, since the properties are connected, and they affect the heat and power demand significantly. The correct order of the pressure and temperature changing units does have a tremendous effect. The order should not be predetermined, but rather taken as an optimisation variable, given the complex trade-offs involved.

Table 1 presents a comparison of solution i) without heat and power integration (No I), ii) only Heat Integration (HI), iii) only Power Integration (PI), iv) both heat and power integration (HI+PI) with the turbine positioned before the cooler, and v) both heat and power integration (HI+PI2) in the reverse order of the turbine and the cooler. The highest net present value occurred in the case of HI+PI2. The conversion of the first part (REF-1 or REF-2) was always 0.850, despite a different type of reactor and feed being selected in the case with heat integration alone. The solutions with higher recycle rate have lower conversion per pass of the reactor in the second part (RCT-2); however, there was a higher overall conversion of the second part. The overall conversion is determined by multiplication of the conversion of the first part and the overall conversion of the second part.

*Table 2: Net present value and conversion of solutions obtained*

| Solution | No I | HI | PI | HI+PI | HI+PI2 |
|---|---|---|---|---|---|
| Net present value | 95,184 | 96,636 | 108,704 | 109,050 | 116,853 |
| Conversion of the first reaction part (REF1 or REF2) | 0.850 | 0.850 | 0.850 | 0.850 | 0.850 |
| Conversion per pass of the second reactor part (RCT-1 or RCT-2) | 0.415 | 0.250 | 0.352 | 0.345 | 0.350 |
| Overall conversion of the second part | 0.549 | 0.970 | 0.550 | 0.547 | 0.548 |
| Overall conversion of process | 0.466 | 0.824 | 0.468 | 0.465 | 0.466 |

## 5. Conclusions

In this study, the synergistic effects of performing process synthesis/optimisation simultaneously with heat and power integration considering reactions with recycle was studied to derive novel insights and more detailed interpretation of already known insights. These insights are as follows:

- When Heat Integration is performed within the recycle loop, it results in a higher overall conversion rate and lower raw material consumption.
- When Power Integration is performed, there is integration within the recycle loop, resulting in higher overall conversion, as well as between the feed stream and the stream within the recycle loop, leading to lower overall conversion. Since the feed stream flowrate is higher, it is reasonable to expect the overall conversion to shift towards lower conversion.
- Neglecting the synergistic effects between heating, cooling, compression, and expansion can lead to poor Heat and Power Integration. When on a segment of process streams, both pressure and temperature change units appear, the superstructure of different orders of those units should be considered to achieve the appropriate trade-offs between raw-material usage, and utility and power consumption.

### Acknowledgements

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