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Early Phase Process Evaluation: Industrial Practices

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A B S T R A C T

Process route evaluation is a part of research and development (R&D) works in an industrial chemical project life cycle. In this early phase, good process evaluation, including process synthesis and designs, provide guidance's on the R&D project. The paper aimed to collect practical methods used in this early phase process route evaluation from author's 10 years of industrial experiences. The collected methods range from forward-backward process synthesis, functional process design, use of cost estimation, and applications of Monte Carlo simulation. Led by a good project management (*e.g.* via a stage-gate approach) use of these methods have shown beneficial results. Some important results are strong arguments on whether or not the project will continue, as well as relevant technical and economic issues identified during this early phase process synthesis and design. Later on, these issues become guidance's to the follow-up project, if it is continued.

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1. INTRODUCTION

As the world keeps on changing, chemical industries nowadays faces challenges that never happened few decades ago. (Repenning & Sterman, 2001) Some of these challenges are due to diminishing raw materials and resources, stricter regulations, new products' requirements, issues on sustainability, and competing process technologies. (Kemp & Soete, 1992) These challenges cannot be solved by using the old methods of simply trial and error. Considering their high risks and problem complexities, companies have been trying to put together systematic way of solving problems. (Putra, 2016)

In an industrial chemical project life-cycle, research and development (R&D) projects play a very important role. (Souder, 1988) This includes, among others, defining what product, which production route, and which technology to use. (Utterback & Abernathy, 1975) The R&D department of a company is also often asked about directions regarding current or future issues that are faced by the company. (Ruekert & Walker, 1987) All of these are done in the very early phase of the cycle and often with relatively limited budgets. (Kline & Rosenberg, 1986) Hence, such projects have to be executed in a systematic manner, as well as supported by industrially accepted tools.

In this article, some information that have been applied in industrial practices are described. They have been used to answer the above questions, as well as to give insights on the questions themselves. Along with a good project management, via a stage-gate approach, ideas are generated with the help of forward-backward process synthesis. Some of the routes are then selected, designed, and compared to each other, technically and economically. Sensitivity analysis such as Monte Carlo simulation is done to account for uncertainties as a whole. And during this whole process of early phase process evaluation, insights on both technical and economic issues are found.

2. INDUSTRIAL PROBLEMS

Some of the abovementioned problems that are faced by chemical industries can be seen in **Figure 1**. These are typical questions asked to the R & D department of companies. And the answers require thorough understanding on related subjects. This is where researches are being done.

In industries, a research project can be simplified into several smaller projects. (Cooper, 1979) Like any other project in general, a research project has three constraints, namely budget, human resource, and time. (Hartmann & Briskorn, 2010) The result of such research project(s) should be able to give a solution or a direction on where to go. It should also form a strong foundation for the next phase of a project, if it is to be continued. For example, it could be a selected process route to be worked on in greater details and accuracy in the next phase. This information transfer to the next phase imply for the well-known stage-gate approach1 to smoothen the workflow of the project.

3. STAGE GATE APPROACH

The stage-gate approach is a systematic way in which a project is divided into several stages with company specific requirements to fulfill in each stage. When the requirements are fulfilled, a meeting of that stage is held, which is called a gate. Depending on the outcomes, this gate meeting will then decide whether or not the project will go to the next stage. This approach has been proven to increase the output of the R&D processes.

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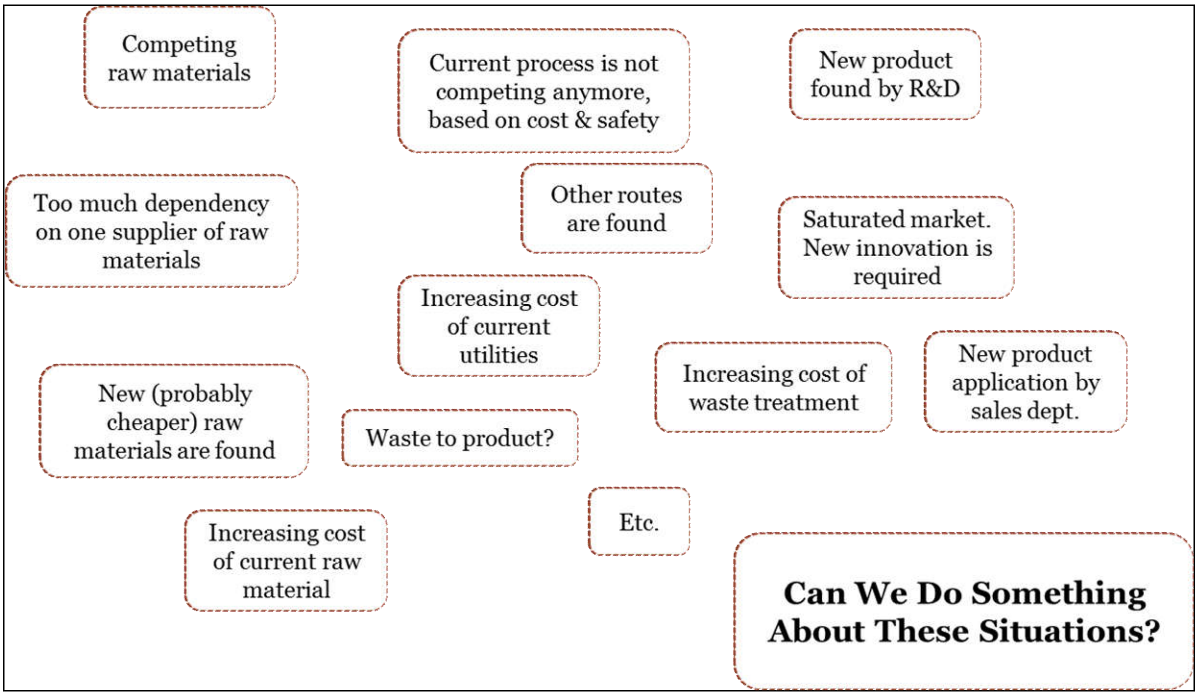

Figure 1. Industrial problems faced by chemical industries nowadays

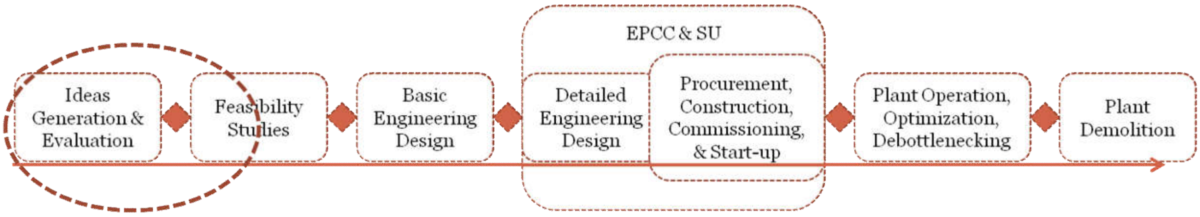

Figure 2. Stage-gate approach in chemical project life-cycles

In an industrial chemical project life-cycle is important. **Figure 2** shows the overview of stage-gate approach in chemical project life-cycles. Each box represents the stage, while each diamond represents the gate.

The research project is at the very early the cycle, shown by the red dotted circle in **Figure 2**. By zooming in the circle in this figure, we obtained that for a certain problem, ideas need to be generated first.

Based on rough and qualitative comparison, few of them are selected. These are then worked on further to be able to make more accurate comparisons.

Figure 3 shows stage-gate approach in process evaluation, along with the tasks involved. The whole concept and tasks in this phase of a project is what forms the early phase process synthesis and design tasks.

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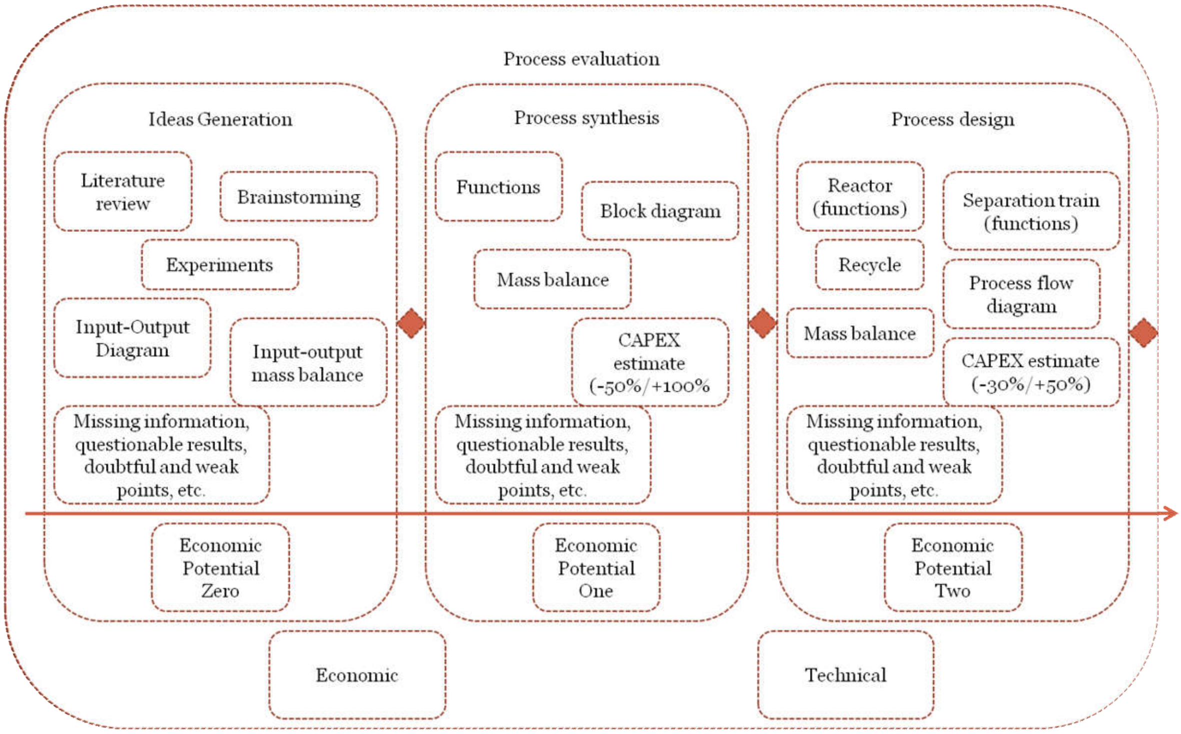

Figure 3. Stage-gate approach in process evaluation, along with the tasks involved

In the ideas generation part, with rough information, qualitative information, and maybe very rough mass balance, some process options can be selected or discarded. The next part of process synthesis is built on the idea generation part. More information is obtained in this part, and hence, more accurate comparison can be done. Fewer options can then be selected and designed to the extent of major process equipment in the next part of process design. At the end of this process, few options will emerge with their inherent technical and economic issues.

2. FORWARD-BACKWARD PROCESS SYNTHESIS

Forward-backward process synthesis is chosen in this idea generation part. The concept of this forward-backward process synthesis is elaborated in a quite recent literature[2]. Assume on the left side that there is a (new) raw material, while on the right side there are some products. Based on the information obtained from literatures and/or experiments, a brainstorming session can be conducted to synthesize a chemical route from both directions (raw material and products). Synthesizing route from the raw material part is called the forward synthesis, while from the product part is called backward synthesis. Hence, the name is formed.

From the generated routes, several promising routes can be selected. In this example, the green routes are the selected ones. Apart from the raw material and product data that are already obtained, other considerations can be used to discard or select fewer ideas. This may include; whether this is a known or novel route, how mature is the technology, how short is the route, how easy it is to control/achieve the operating condition, if other raw materials are involved and how much, if all the products are known, if there are foreseeable difficult separation, and other related questions. The answers can be qualitatively used in screening the options. Hence, several options can be selected from this step.

3. INPUT – OUTPUT DIAGRAM

From the selected routes, a more detailed information has to be obtained to further compare them in more details. Questions like all raw materials involved, selectivity's, conversions (that leads to recycles), known and unknown compositions, or number of required steps need to be accounted. Based on this information, an input-output diagram is made (see **Figure 4**). With additional data, input-output mass balance is then created.

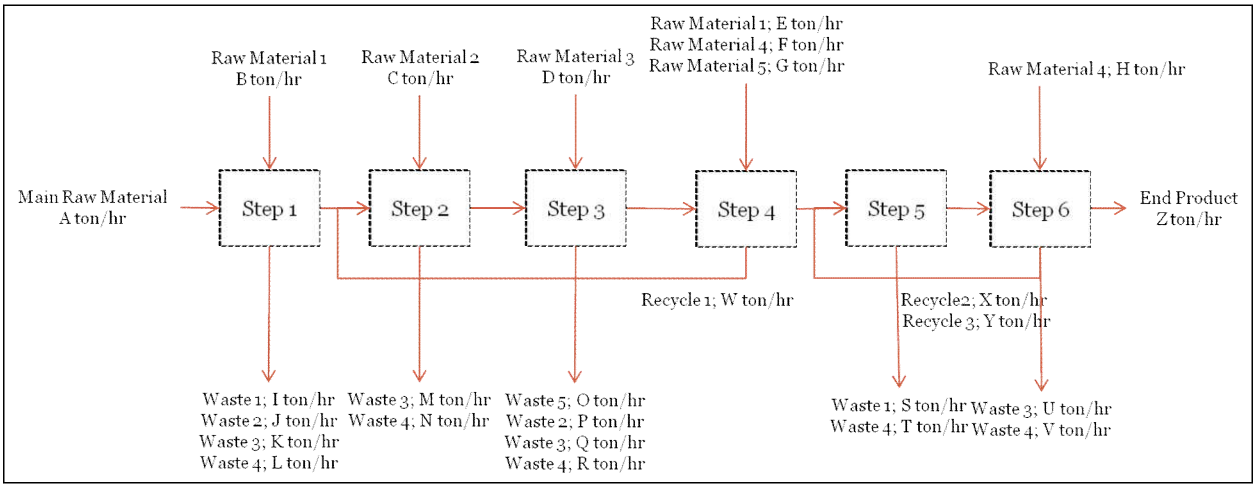

Figure 4. Input-output diagram tasks involved

From this step, a sense of feeling on how big the material streams can be obtained. Whether one route produces high amount of waste, or too much byproducts, or whether there are quite many recycles involved are among the questions need to be asked in the comparison. Additional information from basic cost figures (raw materials, products, byproducts, waste) is also useful.

With the raw materials, products, and byproducts cost figures, the economics of those routes can be evaluated roughly, which is normally called as Economic Potential Zero (EP^0). Estimated capital investment figures can be searched by comparing similar steps in the routes with literatures. These numbers can also be then compared with capital investment estimated from the EP^0 with an acceptable payback period. These are of course ballpark numbers. Nonetheless, with this information, some routes can probably be discarded.

4. BLOCK DIAGRAM

One step further is to synthesize a functional block diagram for each step of each selected route. The block diagram is developed based on functionality. This includes functions like reaction, separation, mixing, change of phase, change of temperature, and change of pressure. It is also important to assign destinations for all output streams. They should be economically attractive, if possible. The idea is to visualize what the consequences are to the whole process. With this in mind, the developed block diagram, and the subsequent developed process, is basically an effective process.

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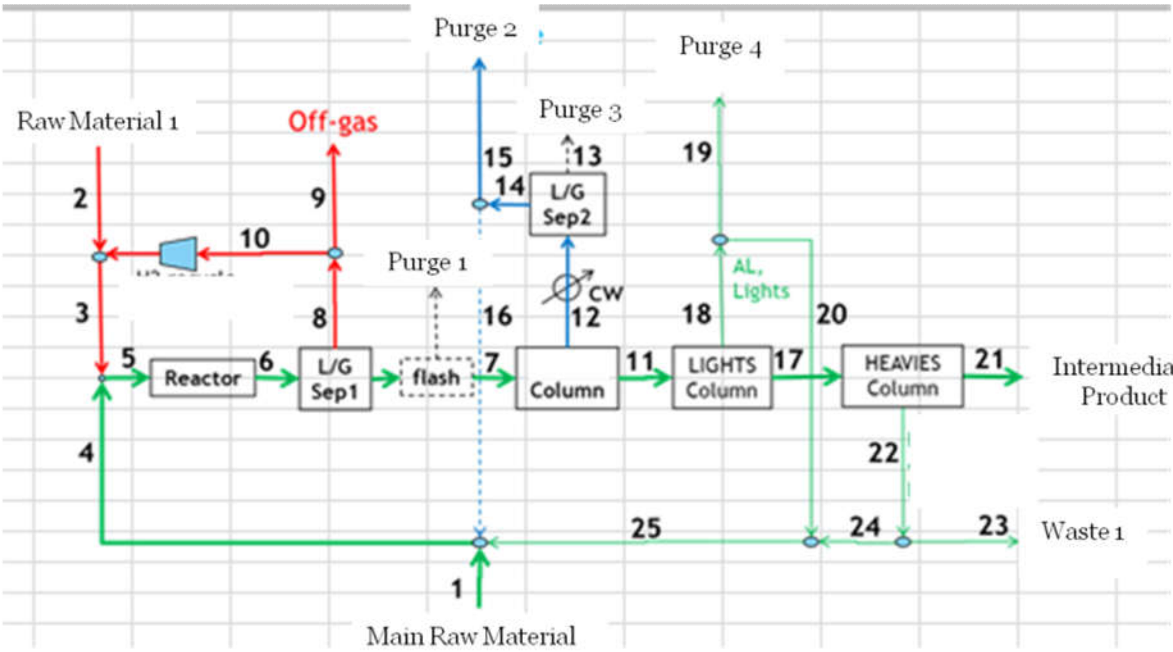

Figure 5. Block diagram

Another thing to keep in mind is that during this process synthesis, due to limited information, or doubtful source, or unknown parameters, there will be technical challenges. This may include what sort of separation process that is required, if there is any chemical compatibility issue, if it is easy to bring the raw material to the required place and operating condition, materials of construction, if there is a technology already available to do the job, and many more. All of these technical issues need to be listed down to work on in the next step or phase of the project.

At this point, a more accurate cost comparison can be made. Apart from the material balance figures, investment cost can also be approximated in a more accurate way. Hence, it is taken into account in the cost calculation. It is then called Economic Potential One (EP^1). From here, there maybe 2 or 3 routes left.

5. BLOCK DIAGRAM WITH MAJOR EQUIPMENT

Block diagrams of the selected route are then detailed more during the process design part (See **Figure 6**). Major equipment is added to the diagrams, which are also done based on functions. Guidance on process design can be found in literatures 3,4. Questions like what the required operating conditions are in the reactor and in the separation units, if properties data in those conditions are available, if we encounter problems with azeotropes, and many others are some of the questions that need to be addressed in this part.

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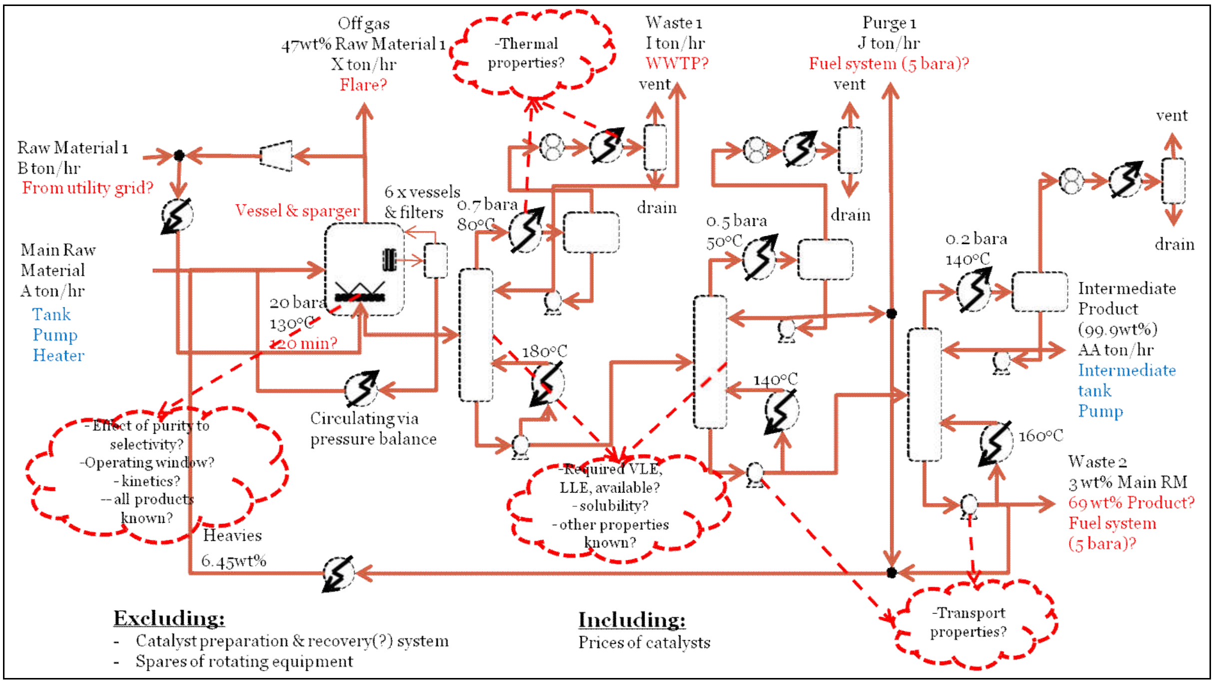

Figure 6. Block diagram with major equipment

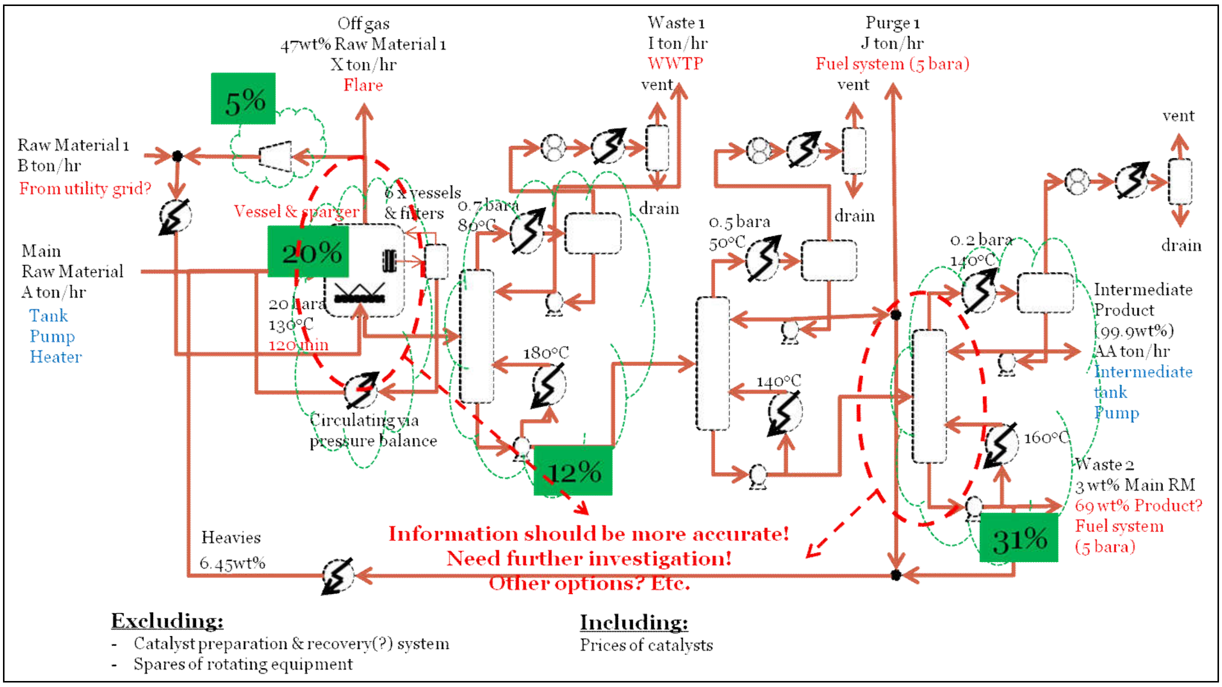

Figure 7. Insights from economic estimation

It is obvious that at this very early phase, there are many unknowns and uncertainties. Hence, keeping this list of questions alive is very important. Later on, knowing what the knowns and the unknowns of the selected process will bring confident to the project team, give focus on what to do next, and ease the project transitions.

At this step, capital investment can be estimated more accurately. In-house estimation tool, text book literatures[5], or commercial software's can be used for the cost estimation. The cost estimate gives beneficial insights into the process. Some of which are which part of the process controls the cost, which part needs to be optimized, which parameters need to be very accurately defined, and which information needs to be dig deeper. The bottom line is that cost estimate gives guidance on how to optimize R&D resources so that the next step in the project will be an efficient one. The example **Figure 7** shows that the last distillation column and the reactor consume half of the capital investment. Any improvement in this two area will significantly reduce the cost. Hence, further investigation in these two sections are recommended in the next step of the project.

8. ROUTE SELECTION

At the end of this whole early phase process synthesis and design, one might still be faced with two or three remaining routes. These routes carry their own uncertainties and unknowns. **Figure 8** shows schematically an example of two competing processes to make the same product. The next questions arise are then which route to take under which circumstances, how sure the results are, and what the backup plans are.

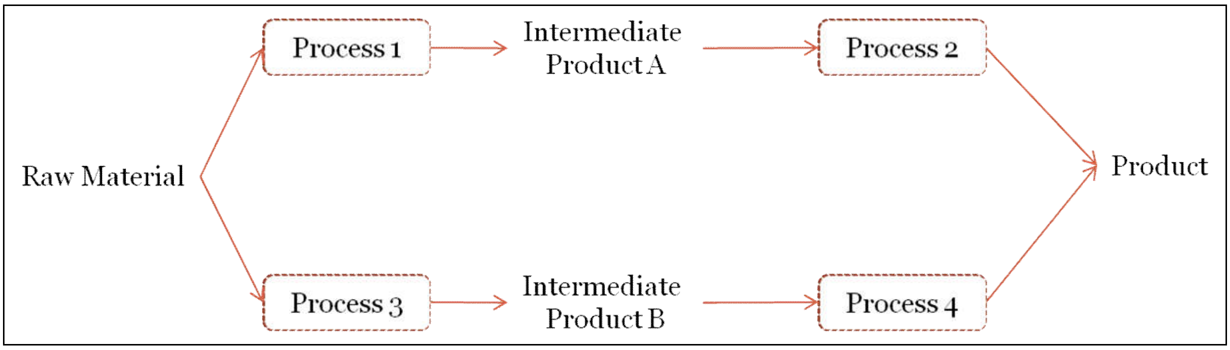

Figure 8. Insights from economic estimation.

To approach this problem, sensitivity analysis is done on major economic terms such as capital investment (CAPEX) and operational expense (OPEX). In addition, total annual cost (TAC) that combines both CAPEX and OPEX on yearly basis is also compared. However, since there are many parameters with their own uncertainties, having all of those parameters in graphs will be tremendously difficult to digest. One solution is to utilize Monte Carlo analysis. This type of analysis has been done in engineering field6. The analysis includes all parameters with their uncertainties. An example of the result is shown in **Figures 9-11**.

From **Figures 9-11**, Route 1 is cheaper in CAPEX but more expensive in OPEX. The total annual cost is almost the same for the two routes. From this observation, one may conclude that any of these two routes can be the chosen one, while the other serves as the backup route.

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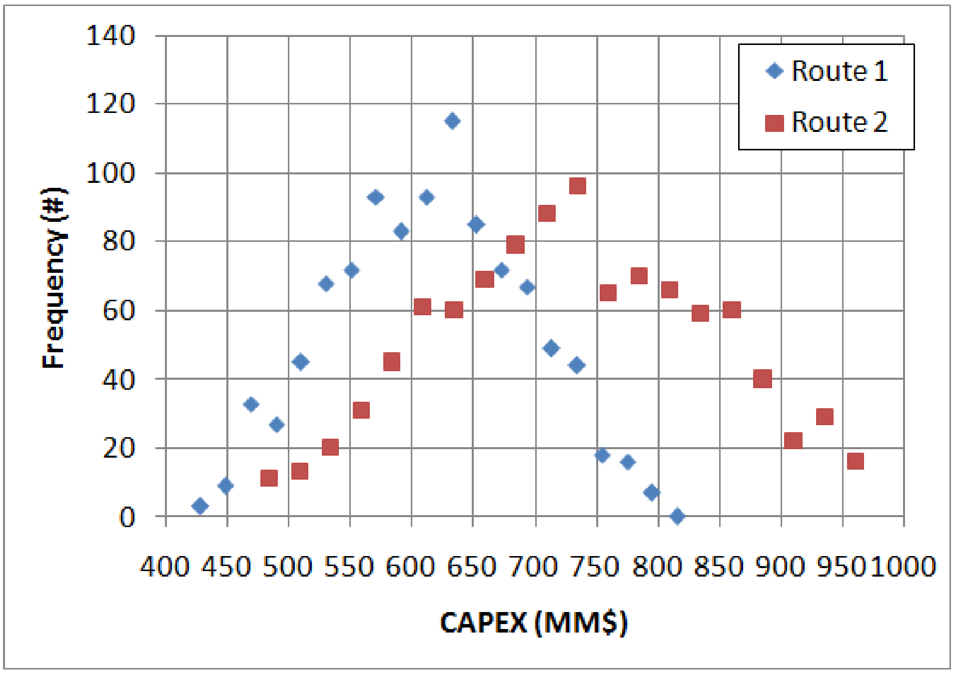

Figure 9. Sensitivity of economic

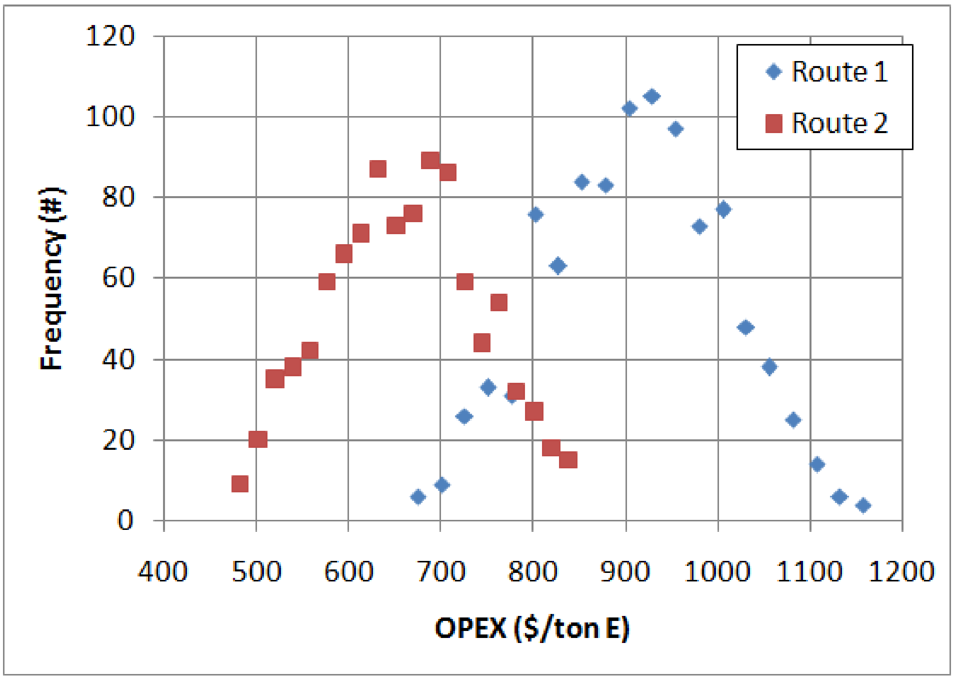

Figure 10. Sensitivity of economic evaluations (OPEX).

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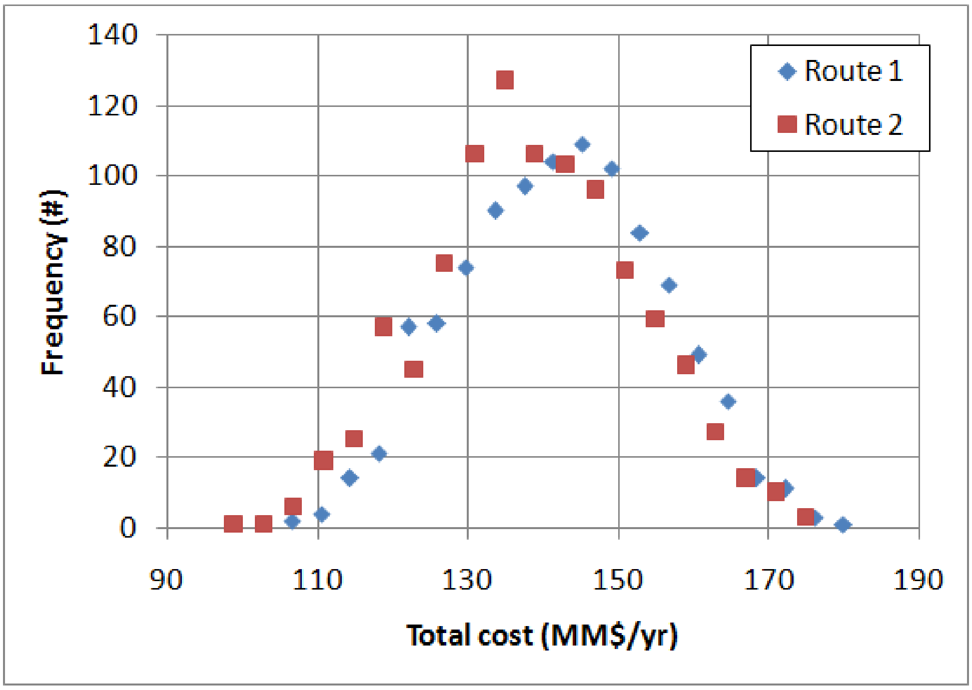

Figure 11. Sensitivity of economic evaluations (Total Annual Cost).

6. CONCLUSIONS

The described steps in early phase process route evaluation via process synthesis and design have shown that tangible results can be obtained. Options can be weighed and compared, technical issues are listed down, and cost estimate can show where the next R&D focus will be. Sensitivity analysis with Monte Carlo has shown that comparison can be made with relatively confident, even with a lot of uncertainties in this early phase. This whole process is, nonetheless, an iterative process. It requires a lot of communications, weighs options, takes calculated risks, make decisions, and then moves forward. By following the described steps systematically, the risk of having a failure project is expected to be reduced.

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8. AUTHOR'S NOTES

The author(s) declare(s) that there is no conflict of interest regarding the publication of this article. Authors confirmed that the data and the paper are free of plagiarism.

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