HUNGARIAN JOURNAL
OF INDUSTRIAL CHEMISTRY
VESZPRÉM
Vol. 37(2) pp. 139-143 (2009)

DIFFERENCES BETWEEN OPTIMUM FLOW SHEET SOLUTIONS OBTAINED BY DIFFERENT ECONOMIC OBJECTIVE FUNCTIONS

M. KASAŠ, Z. KRAVANJA, Z. NOVAK PINTARIČ✉

University of Maribor, Faculty of Chemistry and Chemical Engineering
Smetanova 17, SI 2000 Maribor, Slovenia
✉E-mail: zorka.novak@uni-mb.si

This paper discusses the shapes of cash flow functions obtained by modelling chemical processes at different levels of complexity, and the influence of these shapes on optimal solutions obtained by different economic objective functions. Cash flow functions can be unimodal (with maximum) or monotonically increasing (concave) with respect to capital investment. This depends on the quality of major trade-offs established in the model. Unimodal shape is common for modelling with simple and aggregated models, where increasing the investment above certain level causes loss to a project, which indicates improper or insufficient trade-offs in the model. Monotonically increasing concave cash flow functions are usually obtained by using more detailed models. This implies better trade-offs in the model as increasing the investment always brings some benefit (higher or lower). Example of methanol process synthesis presented in the paper indicate that models with monotonic cash flow functions produce significantly different optimal solutions when optimizing different economic criteria, e. g. the net present value, the profit and the internal rate of return. On the other side, the optimal solutions of models with unimodal functions are similar. These results suggest that models should be formulated at the level of complexity which produces monotonically increasing cash flow functions.

Keywords: cash flow, investment, unimodal, concave function, trade-off, optimization, mathematical programming, objective function, chemical process, flow sheet

Introduction

The engineering community uses different measures for assessing the economic attractiveness of investment projects. The most common are the total annual cost, annual profit before taxes, the payback time, the net present value and the internal rate of return. Buskies [1] established that optimal values of process parameters obtained during the optimization of chemical processes depend on the objective function used in the optimization. Novak Pintarič and Kravanja [2] discussed the differences between optimal process designs obtained by means of qualitative, quantitative and compromise economic criteria. Faria and Bagajewicz [3] performed MINLP design of water utilization systems by maximizing the net present value and internal rate of return and also observed different optimal solutions. The origin and characteristics of these differences have not been explained sufficiently in the open literature.

The main intention of this paper is to discuss the characteristics of optimal process flow sheets obtained by synthesis and optimization with different economic criteria. It was observed that in some cases, significantly different optimal designs are obtained, while in other cases, differences are negligible. It will be shown in this paper that differences between optimal solutions depend on the slope of the cash flow derivative function, while its slope depends on the shape of the cash flow function with respect to capital investment. Unimodal shapes (with maximum) are obtained by using simple, aggregated models. More detailed models produce monotonically increasing concave functions of cash flow. The example in our paper shows that different economic criteria lead to optimal solutions that are significantly different in the term of conversion, level of heat integration, investment, cash flow, and even in the term of topology.

The important simplification in this paper is that investment costs are represented as simple continuous nonlinear functions of process size. In general, complex cost functions are discontinuous in terms of size and other factors, e.g. pressure and temperature, and require special modelling techniques in order to be included in optimization models, as shown by Turkay and Grossmann [4].

Optimality conditions

Optimality conditions for different economic criteria are well known. Maximum net present value (NPV) is obtained at the investment level where the marginal (incremental) NPV is equal to zero and marginal internal rate of return (IRR) equals to discount rate used for

NPV maximization. In practice this means that process units should be enlarged only as long as the incremental increase has positive marginal NPV and the incremental IRR is greater than the minimum acceptable rate of return (MARR). Maximum profit before taxes (PB) and IRR are obtained at the investment levels where the marginal profit and IRR, respectively, equalize to 0. It could therefore be expected that applying different criteria in the objective function by designing, optimizing and synthesizing process flow sheets would not lead to the same optimal results.

In our previous work [2] it was shown, that optimization of qualitative criteria, such as payback time and internal rate of return, stimulate smaller process designs and fast (re)investment of capital which results in high profitable solutions. Quantitative criteria, such as profit or total costs, produce large processes and higher cash flows, but also require higher capital investments, and achieve lower profitabilities. Criteria, such as the net present value and equivalent annual cost, result in intermediate size of the process. These are compromise criteria as they establish a compromise between the investment costs, profitability of invested money, and dynamics of investing [5].

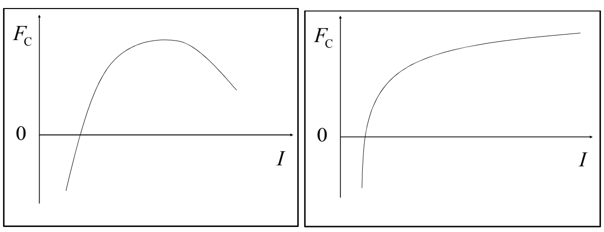
Cash flow functions

Cash flow, F_C, is defined by the following equation:

$$F_C = (1 - r_t)(R - E) + r_t \frac{I}{t_D} \tag{1}$$

where r_t represents the tax rate, R the revenues or incomes, E the expenditures, I the investment and t_D the depreciation period. The term $(R - E)$ in the right-hand side of Eq. (1) is the surplus of the revenues over the expenses and actually represents a benefit resulting from invested money. The second part is a tax credit of depreciation originating directly from investment.

Two shapes of cash flow function with respect to the level of capital investment are mostly obtained when optimizing process flow sheet models: unimodal function with maximum, and monotonically increasing concave function (*Fig. 1*). Convex functions of cash flow vs. investment are very rare in the flow sheet optimization.



a) b)

Figure 1: Cash flow functions, a) unimodal, b) concave

Unimodal cash flow functions

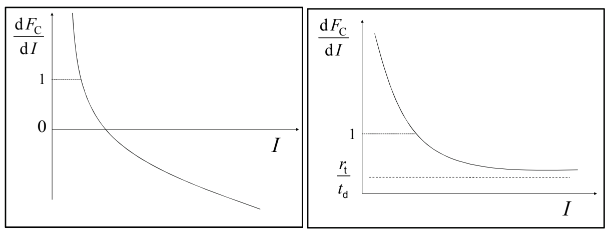
Unimodal cash flow function is common for flow sheet modeling with simple and aggregated models at early stages of process development, e.g. by stoichiometric reactor with fixed conversion per pass or simple component splitter. In such models, the trade-offs between the revenues, operating costs and investment are often established only through the recycle flow rate.

In the case of unimodal cash flow function a mode (maximum) exists and derivative thus changes the sign (*Fig. 2a*). Stationary point for maximum cash flow is obtained at:

$$\frac{dF_C}{dI} = (1 - r_t)\frac{d(R - E)}{dI} + \frac{r_t}{t_D} = 0 \tag{2}$$

$$\frac{d(R - E)}{dI} = -\frac{r_t}{(1 - r_t) \cdot t_D} \tag{3}$$

From the upper equation it follows, that maximum cash flow of unimodal function occurs at the level where increasing the investment would reduce benefit to a project, as the right hand side of Eq. (3) is a constant negative value. This result leads to the assumption that flow sheet optimization model with unimodal cash flow function indicates improper or insufficient trade-offs. In practice, increased investment should result in increased benefit. The benefit growth rate is lower and lower as investment grows, but should not change to a loss, as in the case of unimodal cash flow function, though there are some exceptions in engineering applications. E.g. adding insulation (increasing investment) to circular tubes whose outside radius is smaller than the critical radius increases heat losses up to the value of critical thickness [6]. Note that the shape of the benefit function $(R - E)$ vs. investment I would be very similar to the shape of the unimodal cash flow function shown in Fig. 1a.



a) b)

Figure 2: Derivative of unimodal (a) and concave (b) cash flow function

Concave monotonic cash flow functions

Monotonic concave cash flow functions are obtained by more detailed modeling, where more precise tradeoffs are present, e.g. by kinetic reactor or distillation column. These trade-offs reflect as direct benefit resulting from invested money, e.g. longer catalyst bed in the reactor enables higher conversion of reactants per pass, larger exchanger area enables more heat transferred between process streams and thus lower utility costs etc.

In the case of concave monotonic cash flow functions, the slope of the cash flow curve is always positive and decreases monotonically (*Fig. 2b*). The term (R – E) in Eq. (1) becomes constant at high investment values and its derivative approaches to zero. The shape of the (R – E) function vs. investment I would be similar to that shown in Fig. 1b, with the exception that (R – E) curve would remain constant at higher values of investment while cash flow curve increases linearly due to depreciation term in Eq. (1).

Cash flow derivative thus approaches asymptotically to a constant nonnegative value as investment approaches infinity:

$$\lim_{I \to \infty} \frac{\mathrm{d}F_{\mathrm{C}}}{\mathrm{d}I} = \frac{r_{\mathrm{t}}}{t_{\mathrm{D}}} \tag{4}$$

From the above equation, it can be seen that asymptotic constant value depends only on the tax rate, and depreciation period. Cash flow at high investment values increases linearly only because of depreciation term in Eq. (1). Further increase of investment does not increase benefit, but at least does not cause any loss.

Differences in optimal solutions

It could be shown by deriving stationary conditions for optimum economic criteria that the investment levels of optimal solutions increase in the direction from IRR over NPV to PB criterion [7]. The magnitude of these differences depends on the steepness of cash flow derivative function. The steeper this function is, more similar are the optimal solutions.

The derivative function of monotonic cash flow is more flat because it approaches asymptotically to a constant positive value (Fig. 2b). Optimum NPV and PB solutions are thus more apart. Besides, models with monotonic cash flow functions comprise more precise trade-offs that enable to find the solutions with higher profitabilities. This forces investment level of optimum IRR solution below investment levels of the other two optimum solutions. Models with unimodal functions comprise only rough trade-offs which do not allow high profitable solutions. Optimization of such models often results in similar optimal solutions.

Methanol process synthesis

MINLP synthesis of methanol process flow sheet from synthesis gas is considered in this section. The example was taken from the literature [8] and the prices were updated. Superstructure of the process involves four topological selections: 1) two feed streams from which the first one (FEED-1) is cheaper as it contains less hydrogen, 2) one-stage or two-stage compression of the feed stream, 3) two reactors from which the second one (RCT-2) is more expensive and allows higher conversion, and 4) one-stage or two-stage compression of the recycle stream. Kinetic model is used for both reactors. Flow sheet comprises 4 hot streams and 2 cold streams. MINLP model for heat integration [9] with 4 stages is added to the mathematical model of superstructure for simultaneous heat integration and heat exchanger network (HEN) synthesis. Design variables for assessment of capital investment are the reactor's volume, compressors power, and heat exchangers area. The composed MINLP model comprises about 600 constraints and 600 variables from which 46 are binary (8 for process topology and 38 for heat matches).

The MINLP synthesis is performed by means of automated MINLP Process Synthesizer MIPSYN [10]. Three economic objective functions are optimized: IRR, NPV and PB. The second feed stream is selected in all optimal solutions together with the two-stage compression of feed stream, and one-stage compression of recycle stream (*Fig. 3*). The cheaper reactor (RCT-1) with lower conversion is selected by maximizing IRR and NPV, while more expensive reactor (RCT-2) with higher conversion is obtained by maximizing PB (dotted line on Fig. 3). Optimal heat integration scheme is equal in all three cases.

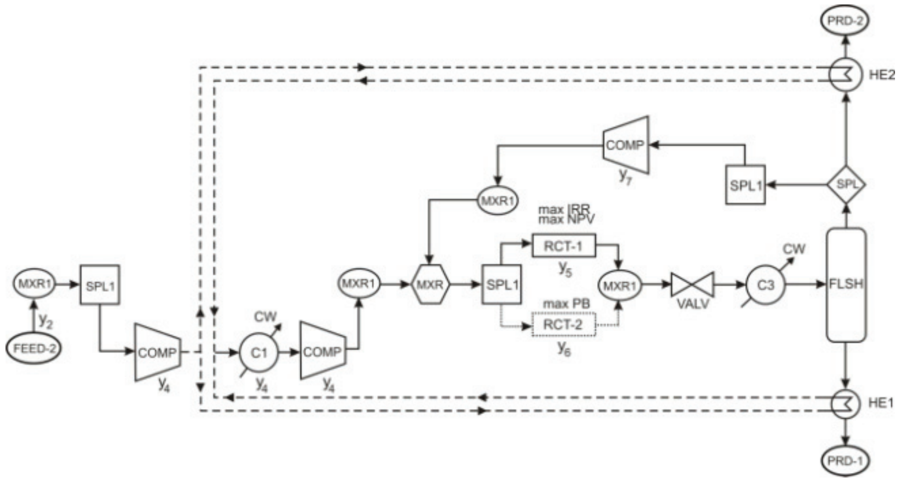


Figure 3: Optimal structures of methanol synthesis

The solution with highest capital investment and cash flow is obtained in the case of PB maximization (*Table 1*), while the lowest values are observed in the case of maximum IRR solution.

Table 1: Optimal solutions of methanol synthesis

	max r_{IRR}	max W_{NP}	max P_B
I (MEUR)	82.63	85.24	89.12
F_C (MEUR/yr)	34.63	35.13	35.50
F_C/I	0.419	0.412	0.398
R (MEUR/yr)	83.98	83.80	83.69
c_{rm} (MEUR/yr)	28.59	28.17	27.90
c_{ut} (MEUR/yr)	11.04	10.68	10.43
W_{NP} (MEUR)	180.80	181.98	180.92
P_B (MEUR/yr)	38.83	39.26	39.41
r_{IRR} (%)	41.69	40.97	39.57
X_{RCT} (%)	16.20	18.19	19.56
X_O (%)	79.93	80.31	80.54
A_{HEN} (m^2)	2769	3285	3783
V_{RCT} (m^3)	24.60*	31.70*	29.37**
P_{comp} (MW)	40.30	38.78	37.87
I (A_{HEN}) (MEUR)	10.77	12.71	14.57
I (V_{RCT}) (MEUR)	16.72	19.38	22.60
I (P_{comp}) (MEUR)	55.14	53.15	51.95

* RCT-1, ** RCT-2

Although some economic figures do not differentiate substantially, the optimal designs are significantly different. The cheaper reactor (RCT-1) is selected by IRR and NPV criteria and, as expected, the reactor is significantly larger in the case of max NPV. The reactor of PB solution is medium-sized because more expensive option (RCT-2) with higher conversion and capital investment is selected. The total area of heat exchanger network (A_{HEN}) is significantly different in all three cases. The investment levels of reactor and HEN increase from IRR to PB, while on the contrary, the total power of compressors (P_{comp}) decreases and is the smallest in the case of PB solution. This is because the highest conversion is obtained by PB criterion, and consequently, the amounts of feed and recycle streams are the smallest. The largest revenue is achieved in the case of optimum IRR solution, however, the consumptions of raw materials and utilities are also the highest. High profitability is achieved on the account of higher input of reactants and utilities, but not with increased level of heat integration and conversion of reactants. The latter increases from IRR over NPV to PB optimum solution.

Fig. 4 represents the concave shape of cash flow functions of both optimal process structures obtained by IRR and NPV criteria, as well as by PB criterion. Increased investment is used for increasing the reactor volume and the conversion, as well as for increasing heat exchangers area and thus heat transfer between process streams. *Fig. 5* represents the derivative functions of both optimal structures.

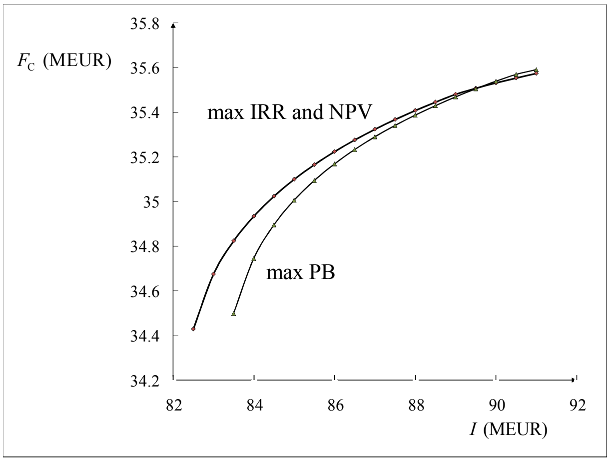


Figure 4: Cash flow functions of optimal methanol structures

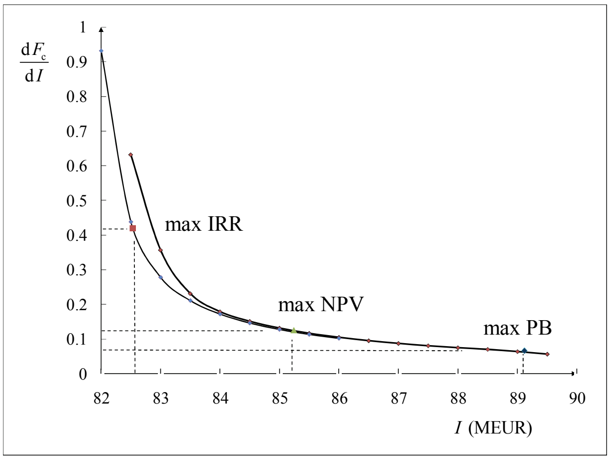


Figure 5: Cash flow derivative functions of optimal methanol processes

Conclusion

The differences between optimal solutions obtained by using different economic criteria depend on the slope of cash flow derivative function. The derivative curve of concave cash flow function often has a gentle slope as it asymptotically approaches positive constant value. For this reason, different economic criteria lead to optimal solutions that are significantly different in the term of design variables, and/or economic figures or even in the term of topology if process synthesis is performed. On the other side, the derivative of unimodal cash flow function is very steep leading to similar optimal designs.

It was shown that optimum IRR solution is obtained at the lowest investment level, optimum NPV solution at intermediate level, and optimum PB solution at the highest investment level. Conversion of reactants increases from IRR to PB, while raw material and utility consumptions decrease. Qualitative criteria, like IRR and payback time, produce highly profitable optimal solutions with low capital investment. Quick return on investment is of top priority, while the effective resource utilization is less important. Quantitative criteria, like

PB and total annual cost, foster the generation of more efficient solutions with lower operating costs which are achieved by e.g. higher conversion, better separation and/or higher level of heat integration. These solutions are, despite of higher investment level, oriented towards long-term, more sustainable flow sheets. The return to investors is slower, however, this is compensated with higher cash flows. Compromise criteria, like NPV and equivalent annual cost, establish a balance between quick return on investment and long-term steady generation of benefit.

It could be concluded that flow sheet models should be formulated at the level of complexity which produces monotonically increasing cash flow functions.

REFERENCES

1. BUSKIES U.: *Economic process optimization strategies.* Chemical Engineering & Technology (1997) 20, 63–70
2. NOVAK PINTARIČ Z., KRAVANJA Z.: *Selection of the economic objective function for the optimization of process flow sheets.* Industrial & Engineering Chemistry Research (2006) 45, 4222–4232
3. FARIA D. C., BAGAJEWICZ M. J.: *Profit-based grassroots design, retrofit of water networks in process plants.* Computers & Chemical Engineering (2009) 33, 436–453
4. TURKAY M., GROSSMANN I. E.: *Structural flowsheet optimization with complex investment cost functions.* Computers & Chemical Engineering (1998) 22, 673–686
5. NOVAK PINTARIČ Z., KRAVANJA Z.: *Multiperiod investment models for the gradual reconstruction of chemical processes.* Chemical Engineering & Technology (2007) 30, 1622–1632
6. ECKERT E. R. G., DRAKE R. M. J.: *Analysis of Heat and Mass Transfer*. 1972, New York: McGraw-Hill.
7. KASAŠ M., KRAVANJA Z. in Novak Pintarič Z.: Cash flow functions and optimal solutions of flow sheet models at different levels of complexity. *CAPE Forum* (2009) Limerick.
8. KRAVANJA Z., GROSSMANN I. E.: *Prosyn - an MINLP process synthesizer.* Computers & Chemical Engineering (1990) 14, 1363–1378
9. YEE T. F., GROSSMANN I. E.: *Simultaneous optimization models for heat integration-II. Heat exchanger network synthesis.* Computers & Chemical Engineering (1990) 14, 1165–1184
10. KRAVANJA Z., GROSSMANN I. E.: *New developments and capabilities in Prosyn-an automated topology and parameter process synthesizer.* Computers & Chemical Engineering (1994) 18, 1097–1114