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Target-Oriented Robust Optimization of Polygeneration Systems

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Polygeneration systems offer the possibility of efficient, low-carbon production of different product streams from a single facility. Such systems take advantage of opportunities for integrating processes to achieve effective recovery of waste energy and material streams. Mathematical programming methods have proven to be valuable for the optimal synthesis of such polygeneration systems. However, in practice, numerical parameters used in optimization models may be subject to uncertainties. Examples include cost coefficients in volatile markets, and technical or thermodynamic coefficients in new process technologies. In such cases, it is necessary for the uncertainties to be incorporated into the optimization procedure. The target-oriented robust optimization (TORO) is a new methodology that is inspired by robust optimization. The use of this methodology leads to the development of a mathematical model that maximizes robustness against uncertainty, subject to the achievement of system targets. Its properties allow us to preserve computational tractability and obtain solutions to realistic-sized problems. To this end, we propose a methodology for the synthesis of polygeneration systems using TORO. We illustrate this new approach with an industrial polygeneration case study.

1. Introduction

Energy generation is a major contributor to global carbon dioxide (CO_2) emission. Because of this, research in this area has focused on the development of strategies for improving the efficiency and environmental performance of power generating facilities. These include techno-economic assessments such as the work of Cormos (2014) for a hydrogen and power co-generation plant and process modelling methods for their design and optimization such as the work of Pan et al. (2014) for integrated combined cycle gas turbine plants. In addition, polygeneration systems have been introduced since these provide an opportunity for maximizing the utility of fuels by integrating process units for generating several types of products. As a result, such systems have higher thermodynamic efficiency and lower emissions than equivalent stand-alone systems (Serra et al., 2009). On the other hand, systematic design of polygeneration plants requires the simultaneous consideration of interdependent process units. Various process systems engineering (PSE) techniques have thus been proposed for computer-aided synthesis of polygeneration plants, including linear programming (LP) (Lozano et al., 2009), mixed integer linear programming (MILP), multi-criterion optimization (Carvalho et al., 2012), fuzzy optimization (Ubando et al., 2013) and P-graphs (Varbanov and Friedler, 2008). In addition to design problems, optimization models (Kasivisvanathan et al. 2013) and P-graphs (Tan et al., 2014) have also been used for determining operational strategies under abnormal conditions.

There has also been significant interest in optimal design under uncertainty in PSE. Different approaches exist, the most basic of which is sensitivity analysis (Seferlis and Hrymak, 1996). A review by Sahinidis (2004) surveyed various approaches used in PSE, such as fuzzy programming, stochastic programming, chance-constrained programming, etc. A robust optimization approach was proposed for polygeneration systems, based on the principle of separating design and operational decisions within the model (Kasisvisvanthan et al., 2014).

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Consequently, a target-oriented robust optimization (TORO) method has been proposed by Ng and Sy (2014a) as an approach which determines a robust system design that is able to absorb uncertainties in key model parameters. The TORO approach has been used for such applications as transmission network planning (Ng and Sy, 2014a) and workforce inventory (Ng and Sy, 2014b).
In this paper, we propose a TORO model for the synthesis of polygeneration systems. The approach is concerned in particular with managing the risk associated with over-investing in capacity when demand for a product fails to materialize as anticipated. The rest of the paper is organized as follows. Section 2 provides the formal problem statement while Section 3 discusses the development of the optimization model utilizing the target-oriented robust optimization (TORO) methodology. Section 4 then presents a case study to demonstrate how the model works. Finally, conclusions and recommendations for future work are provided.

2. Problem Statement

The formal problem statement can be stated as follows: given a polygeneration system with *m* process units, utilizing fuel to generate *n* types of product output, how should the system be designed to maximize its profit while satisfying the required demand for each product type in consideration of the risks brought by market fluctuations. The market fluctuations are modelled by providing a range for the product demands with the upper and lower limits considered as the most optimistic and the most pessimistic scenario.

3. Optimization Model

The over-all objective function for the polygeneration system is to maximize the profit as shown in Eq(1). The profit is obtained from the net stream value (total sales of the products less the costs incurred by the purchase of raw materials) less the annualized capital cost as shown in Eq(2) where **p** is the price vector for the materials, **y** is the demand for products/raw materials, **v** the variable cost vector and **x** is the capacity vector of the process units. It must be noted that appropriate conversion factors should be used to ensure that the units are consistent.

$$\text{Maximize Profit} \tag{1}$$
$$\text{Profit} = \mathbf{py} - \mathbf{vx} \tag{2}$$

The model constraints include, material balances for the required input and output streams as defined by Eq(3) where **A** is the technical coefficient's matrix, containing the elements a_{ij} to represent the amount of material *i* that flows into (negative flow) or out of (positive flow) process *j.* Furthermore, the capacity or sizing vector should be non-negative as shown in Eq(4). Eqs(1) to (4) describe the optimization model for the polygeneration system which does not consider uncertainties.

$$\mathbf{Ax} = \mathbf{y} \tag{3}$$
$$\mathbf{x} \geq 0 \tag{4}$$

However, in the design of polygeneration systems, there is a need to consider uncertainties which may arise due to seasonal changes or fluctuations in product demand. This uncertainty can greatly affect the feasibility and profitability of investments and thus it is important that the implemented design is that which remains feasible at the highest possible degree of uncertainty. The basic optimization model is thus modified in this work to account for uncertainties particularly in product demand (**y**). This affects the objective function and the demand constraints in the formulation. Once uncertainties are considered, the revised formulation is given by Eqs(5) and (6) where, $\tilde{\mathbf{y}}$ denotes the uncertain demand.

$$\max_{\mathbf{x} \geq \mathbf{0}} \mathbf{p}\tilde{\mathbf{y}} - \mathbf{vx} \tag{5}$$
$$\mathbf{Ax} \leq \tilde{\mathbf{y}} \tag{6}$$

We attempt to integrate this uncertainty through the Target-Oriented Robust Optimization or TORO methodology proposed by Ng and Sy (2014a). TORO facilitates process synthesis through the achievement of targets derived under uncertainty. The primary objective is to identify appropriate settings for the decision variables so that system constraints are feasible for as large a range of uncertain parameters as possible. In line with this, the uncertain vector $\tilde{\mathbf{y}}$ could then be defined as follows (Eq(7)):

$$\tilde{\mathbf{y}} = \bar{\mathbf{y}} - \mathbf{y} \tag{7}$$

where $\bar{\mathbf{y}}$ represents the nominal values of demand and the perturbations $\mathbf{y}$ are such that as given in Eq(8):

$$\mathcal{Y}_\theta = \{\mathbf{y} \in \Re^N \mid 0 \leq y_i \leq \hat{y}_i(\theta), \forall\, i = 1, \ldots, N\} \tag{8}$$

The largest perturbations would take on the values $y_i = \hat{y}_i$, for all $i = 1, \ldots, N$. This also assumes that under the most favorable case, $\tilde{\mathbf{y}}$ would be at the maximum $(\mathbf{y} = 0)$. This follows since profit is directly proportional to the number of units sold by the system. It can also be seen that these perturbations are parameterized by the robustness index, $\theta \in [0,1]$. A higher value of θ implies a larger degree of perturbations for the demand. This has practical implications in describing the attitude of a decision maker. A more uncertainty averse attitude would prefer a higher θ, while a risk seeking attitude would lean towards a lower θ.

TORO hinges on the integration of the robust optimization framework and target-oriented decision making. As mentioned, we want to ensure that process synthesis remains feasible for as large a range of uncertain parameters as possible. Meanwhile, target-oriented decision making is reflected in the model by transforming the original objective function into a constraint through its assignment as a system target. Using this perspective primarily allows us to solve our uncertain problem in an efficient and effective manner, which would be discussed below.

The succeeding model reflects the modification to the original uncertain model such that the objective function now maximizes the robustness index Eq(9) subject to achieving the profit target (τ) as given by Eq(10). This is in conjunction to the other functional constraints of the system such as the set of demand constraints defined earlier Eq(11) and Eq(12).

$$\max_{\boldsymbol{\theta} \in [\mathbf{0},\mathbf{1}]} \theta \tag{9}$$

$$\mathbf{p}\tilde{\mathbf{y}} - \mathbf{v}\mathbf{x} \geq \tau \qquad \forall\, \tilde{\mathbf{y}} \in \mathcal{Y}_\theta \tag{10}$$

$$\mathbf{A}\mathbf{x} \leq \tilde{\mathbf{y}} \qquad \forall\, \tilde{\mathbf{y}} \in \mathcal{Y}_\theta \tag{11}$$

$$\mathbf{x} \geq 0 \tag{12}$$

As discussed by Ng and Sy (2014a), the robust model as it is formulated above would require evaluating an infinitely large number of constraints. This is because the uncertain constraints would lead us to create individual constraints for each possible realization of the uncertain demand. Hence, there is a need to convert this into an equivalent formulation, which would be amenable to solve using traditional linear programming techniques. Using the property of duality, an equivalent formulation is obtained below Eqs(13) to (19):

$$\max_{\boldsymbol{\theta} \in [\mathbf{0},\mathbf{1}]} \theta \tag{13}$$

$$\mathbf{p}(\bar{\mathbf{y}} - \theta\hat{\mathbf{y}}\mathbf{z_1}) - \mathbf{v}\mathbf{x} \geq \tau \tag{14}$$

$$\mathrm{A}\mathbf{x} \leq (\bar{\mathbf{y}} - \theta\hat{\mathbf{y}}\mathbf{z_2}) \tag{15}$$

$$\mathbf{z_1} \geq \mathbf{p} \tag{16}$$

$$\mathbf{z_2} \geq \mathbf{1} \tag{18}$$

$$\mathbf{x}, \mathbf{z_1}, \mathbf{z_2} \geq 0 \tag{19}$$

where $\mathbf{z_1}$ and $\mathbf{z_2}$ are the dual variables obtained during the translation of the constraints. We briefly discuss how these sets of constraints were obtained. To ensure robustness, it suffices that we maximize the degree of perturbation in $\tilde{\boldsymbol{y}}$ as shown in Eq(20).

$$\mathbf{p}\bar{\mathbf{y}} - \max(\mathbf{p}\mathbf{y}) - \mathbf{v}\mathbf{x} \geq \tau \qquad \forall\, \mathbf{y} \in \mathcal{Y}_\theta \tag{20}$$

We could then express this as a maximization problem as shown in Eqs21) and Eq(22):

$$\max(\mathbf{p}\mathbf{y}) \tag{21}$$

$$0 \leq y \leq \theta\, \hat{\mathbf{y}} \tag{22}$$

which would then have a dual counterpart in the form of Eqs(23) and (24):

$$\min(\theta\hat{\mathbf{y}})\mathbf{z_1} \tag{23}$$

$$\mathbf{z_1} \geq \mathbf{p} \tag{24}$$

The translation of the demand constraints follows a similar procedure. We refer readers to Bertsimas and Sim (2003) for a more in depth discussion on the properties of strong and weak duality that proves the equivalence of the two models. Consequently, it is also through these properties that we are able to reduce each of the uncertain set of constraints into a single one- one constraint each for the profit target and demand requirements.

Furthermore, we see that $\mathcal{Y}_{\theta'} \subseteq \mathcal{Y}_{\theta}$ whenever $\theta \geq \theta'$. If a process synthesis is feasible for an uncertainty set defined by θ, then it will be feasible for all perturbations that would fall within this range. In addition, given a fixed value of θ, the model is linear with respect to the decision variables. The model could thus be solved for the maximum robustness index by performing a line search on $\theta \in [0,1]$. We could utilize well-known search algorithms like the bisection or golden search methods in this regard. The following case study demonstrates how the bisection search could be used in identifying the best value of θ that would satisfy a profit target set for the system.

4. Case Study

The case study considers a hypothetical trigeneration system with five main process units namely: a generator (G), a combined heat and power plant (CHP), a boiler (B), an electric chiller (EC) and an absorption chiller (AC). A trigeneration system is a polygeneration system which produces three products. In this case, the products are electricity (E), heat (H) and cooling or refrigeration (R). The generator utilizes fuel (F) to generate electricity at an efficiency of 0.4. The CHP uses fuel to co-generate electricity and heat at an efficiency of 0.3 and 0.5. The boiler unit utilizes fuel to generate heat at an efficiency of 0.8. The electric chiller requires electricity to provide refrigeration and has a coefficient of performance (COP) of 5.0. Finally, the absorption chiller utilizes heat to generate refrigeration with COP of 0.7.

The information can be organized into a technology matrix (**A**), which is shown in Table 1 where negative entries indicate that a material is an input to the process unit as defined in the column heading while a positive entry indicates an output. The uncertainties in the demand for products are shown in the last column of Table 1.

*Table 1: Technology coefficient matrix (**A**) and product price and demand vectors*

	Process unit					Unit Price (USD/MWh)	Demand (y)
Stream	G	CHP	B	EC	AC		
F (1)	- 2.50	-3.33	- 1.25	0.00	0.00	0.02	n/a
E (2)	+ 1.00	+ 1.00	0.00	-0.20	0.00	0.07	3 - 4 MW
H (3)	0.00	+ 1.67	+ 1.00	0.00	-1.40	0.03	4 - 5 MW
R (4)	0.00	0.00	0.00	+ 1.00	+ 1.00	0.04	5 - 6 MW

The variable capital cost for the process units are given in Table 2. The trigeneration system operates for 8,000 h/y and has a service life of 10 y. It is assumed that the process units have no salvage value at the end of their service life and that process units follow straight line depreciation.

Table 2. Associated variable cost to process units

Process Unit		**Variable cost (x 1,000 USD/MW capacity)**
1	G	175
2	CHP	350
3	B	70
4	EC	250
5	AC	200

We defined an allowable change for each demand to be equal to one unit. Aside from this, we likewise need to consider the manner by which to set targets. Setting a very high target might result in risk of shortfalls while setting a very low target might lead to significant opportunity loss due to being very conservative. Hence, we apply a simple method that would allow decision makers to identify the appropriate target that should be set as shown in Eq(25):

$$\tau = \alpha\tau_1 + (1 - \alpha)\,\tau_0 \qquad (25)$$

where $\alpha \in [0,1]$, τ_0 reflects the highest possible profit under the most favorable conditions (demand at the maximum), and τ_1 reflects the lowest possible profit under the most pessimistic conditions (demand at the minimum).

In the succeeding computational experiments, we considered $\alpha \in [0,1]$ under 0.1 increments, leading to 11 profit targets. We obtained a corresponding design solution for each of these targets through a bisection search on θ to identify the best robustness index for each profit target. The computations were performed using MATLAB, with the application of the modeling toolbox ROME version 1.0.9, designed for robust optimization problems in the MATLAB environment. In addition, the solver engine CPLEX Studio 12.5 was called to solve the underlying linear optimization problems. The average computer solution time of the algorithm is around 0.348 s on a Windows 7 Intel Core i5 @2.50 GHz, 8.00 GB and 64-bit operating system.

Out-of-sample testing has also been performed using 1000 realizations of the demand under a uniform distribution. This was done in order to gauge the performance of each design solution under different scenarios. Tables 3 and 4 present the performance of the TORO model in terms of expected profit and probabilities concerning the two sets of constraints in the model. Specifically, these refer to the probability of achieving the profit target and the probability of staying within the demand restrictions.

Table 3 Results for 0.50 ≤ θ ≤ 1.0

Target (x 1,000 USD/y)	**8,122**	**8,318**	**8,514**	**8,710**	**8,906**	**9,102**
Robustness Index, θ	1.0000	0.9000	0.8000	0.7000	0.6000	0.5001
Expected Profit (x 1,000 USD/y)	10,158	9,814	9,563	9,371	9,232	9,114
P (Profit ≥ τ)	1.0000	0.9930	0.9540	0.8590	0.7140	0.5200
P (Ax ≤ y)	1.0000	0.7640	0.6180	0.5260	0.4810	0.4890

Table 4 Results for 0≤ θ ≤ 0.40

Target (x 1,000 USD/y)	**9,298**	**9,494**	**9,690**	**9,889**	**10,083**
Robustness Index, θ	0.4001	0.3001	0.2001	0.1001	0.0001
Expected Profit (x 1,000 USD/y)	9,008	8,951	8,922	8,967	9,111
P (Profit ≥ τ)	0.3210	0.1480	0.0360	0.0080	0.0000
P (Ax ≤ y)	0.5060	0.4800	0.4100	0.2610	0.0000

Note that during instances where the constraint $\mathbf{Ax} \le \mathbf{y}$ gets violated during out of sample testing, the model is subjected to re-optimize and adjust the design solution. The results stated in Tables 3 and 4 allow a decision maker to consider multiple tradeoffs between multiple performance measures. For instance, a decision maker might want to compare a design solution with respect to how well it achieves the target or other functional constraints and its expected profit.

In the computational experiments, one could observe that the expected profit increases from a robustness index of 0.20 to 1.0 and declines between 0 to 0.20. Furthermore, it is interesting to note that the expected profit at the highest target ($\theta = 0$) is only at par with the expected profit under a θ of 0.50. It could also be seen that at the higher robustness indices, the expected profits are generally higher than their respective profit targets. This suggests that the system is able to adjust and adapt to more favorable conditions than what was initially planned for. These observations imply that it might be better off that a mid-range target is considered, rather than be too aggressive in setting a profit target for the system.

Using the highest target is equivalent to stating that one would not consider any degree of uncertainty. As a result, the corresponding design solution will always underperform with regards to the benchmark profit it should be able to achieve. The same is true for the demand restriction constraint. These observations are consistent with the fact that higher targets can only be achieved at the expense of greater risks.

On the other hand, the lowest target level likewise resulted in the lowest expected profit. But the design solution resulted in 100 % target and demand constraint achievement. In some cases, a decision maker might not need to be this conservative. He could instead pick either design solutions under θ of 0.9 or 0.8 that would allow him to achieve higher levels of profit while not sacrificing much with regards to achievement probabilities.

Furthermore, the design of the trigeneration system with respect to the robustness index is shown in Table 5. It can be seen that at all levels of robustness, the chosen units are processes 1, 2 and 4 which correspond to the generator, CHP and electric chiller.

Table 5. Size factors of process units in trigeneration system for $0 \leq \theta \leq 1.0$

θ	X1 (MW of E)	X2 (MW of E)	X3 (MW of H)	X4 (MW of R)	X5 (MW of R)
1.0000	1.6048	2.3952	0	5.0000	0
0.9000	1.6649	2.4551	0	5.1000	0
0.8000	1.7250	2.5150	0	5.2000	0
0.7000	1.7851	2.5748	0	5.3000	0
0.6000	1.8452	2.6347	0	5.4000	0
0.5001	1.9054	2.6946	0	5.4999	0
0.4001	1.9655	2.7545	0	5.5999	0
0.3001	2.0256	2.8143	0	5.6999	0
0.2001	2.0857	2.8742	0	5.7999	0
0.1001	2.1458	2.9341	0	5.8999	0
0.0001	2.2059	2.9939	0	5.9999	0

5. Conclusions

A target oriented robust optimization model has been developed for the design of a trigeneration system, which can be easily extended for other polygeneration systems, in consideration of product demand uncertainties. Results show that it is important to evaluate the different design alternatives in consideration of different robustness indices. The selection of the final design will depend on the simultaneous consideration of expected profit, system robustness and the probability of meeting targets. Future work can thus focus on the implementation of multi-objective decision analysis methods and the consideration of the presence of uncertainties for other system parameters.

References

Bertsimas D., Sim M., 2003. Robust discrete optimization and network flows. Mathematical Programming, 98, 49-71.

Carvalho M., Lozano M.A., Serra L.M., 2012. Multicriteria synthesis of trigeneration systems considering economic and environmental aspects. Applied Energy, 91, 245-254.

Cormos C.C., 2014. Techno-economic and Environmental Analysis of Hydrogen and Power Co-generation based on Co-gasification of Coal and Biomass/Solid Wastes with Carbon Capture. Chemical Engineering Transactions, 37, 139 - 144.

Kasivisvanathan H., Barilea I.D.U., Ng D.K.S., Tan R.R., 2013. Optimal operational adjustment in multi-functional energy systems in response to process inoperability. Applied Energy, 102, 492-500.

Kasivisvanathan H., Ubando A.T., Ng D.K.S., Tan R.R., 2014. Robust optimisation for process synthesis and design of multi-functional energy systems with uncertainties. Ind.Eng. Chem. Res., 53, 3196–3209.

Lozano M.A., Carvalho M., Serra L.M., 2009. Operational strategy and marginal costs in simple trigeneration systems. Energy, 34, 2001-2008.

Ng T.S., Sy C., 2014a. An affine adjustable robust model for generation and transmission network planning. Electrical Power and Energy Systems, 60, 141-152.

Ng T.S., Sy C.L. 2014b. A resilience optimization approach for workforce-inventory control dynamics under uncertainty. Journal of Scheduling, 17, 427-444.

Pan M., Agulonu A., Gharaie M., Perry S., Zhang N., Bulatov I., Smith R., 2014. Optimal Design Technologies for Integration of Combined Cycle Gas Turbine Power Plant with CO_2 Capture. Chemical Engineering Transactions, 39, 1441 – 1446.

Sahinidis N.V., 2004. Optimization under uncertainty: state-of-the-art and opportunities. Computers & Chemical Engineering, 28, 971-983.

Seferlis P., Hrymak A.N., 1996. Sensitivity analysis for chemical process optimization. Computers & Chemical Engineering, 20, 1177-1200.

Serra L.M., Lozano M.A., Ramos J., Ensinas A.V., Nebra S.A., 2009. Polygeneration and efficient use of natural resources. Energy, 34, 575-586.

Tan R.R., Cayamanda C.D., Aviso K.B., 2014. P-graph approach to optimal operational adjustment in polygeneration plants under conditions of process inoperability. Applied Energy, 135, 402-406.

Ubando A.T., Culaba A.B., Aviso K.B., Tan R.R., 2013. Simultaneous carbon footprint allocation and design of trigeneration plants using fuzzy fractional programming. Clean Technologies and Environmental Policy, 15, 823-832.

Varbanov P., Friedler F., 2008. P-graph methodology for cost-effective reduction of carbon emissions involving fuel cell combined cycles. Applied Thermal Engineering, 28, 2020-2029.