A Plant Design Heuristic Considering the Eventual Measurement of Currently Unknown Variables

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ABSTRACT

It is common practice for chemical plants to be sized using estimated parameter values that are uncertain at the design stage, but whose true values will be known once the plant is in operation. Moreover, not all design decisions are fixed once the plant is built, as some may be adjusted during operation. In this paper, we present a heuristic method for plant design under uncertainty that takes these characteristics into account. The problem is framed as selecting the best from a set of candidate designs, where each candidate design results from optimizing the plant for a set of possible values of the uncertain variables. Decision trees are used to select the best-performing alternative given the probability distribution of the uncertainties. A working example is presented that relates to the design of a heat-integrated reactor with uncertainty in the plant inlet composition. Candidate designs and optimal operation for different compositions are found by using the Solver add-in of MS Excel. It is concluded that decision trees allow post-construction operational adjustments and parameter uncertainties to be easily and clearly incorporated into the design process.

Keywords-uncertainty; chemical plant design; optimization; decision trees

I. INTRODUCTION

When designing a chemical process plant, it is often the case that the values of several important parameters are not known precisely, so engineers must rely on typical values justified by accumulated experience [1]. While the literature provides methods for optimal plant design under uncertainty, most of which maximize the expected profit of the plant, the resulting problem is mathematically very difficult to solve [2]. For plant design purposes, the uncertain parameters can be divided into two types: those related to inherently uncertain variables, and those related to variables whose true value will not be known until the plant is in operation. A robust design will perform well for the first type, whereas a flexible design can be adjusted later, when the values of the relevant variables are known. This differentiation has not been addressed in the literature on stochastic plant design.

This paper proposes a method for designing robust and flexible plants, using decision trees [3] to select a design from a set of candidates that are optimal for a set of possible values of the uncertainties. To select a flexible design, the heuristic method represents the problem as a tree with two decisions, one before and one after the relevant parameters are known. The heuristic method is demonstrated using the design of a heat integrated reactor with an uncertain inlet composition. The optimal designs for different parameter sets were obtained using the Solver add-in of MS Excel.

II. LITURATURE REVIEW

Research on plant design under uncertainty can be broadly categorized by the type of process being studied.

A. Research on Power Generating Plants

Martin [4] investigated the uncertainties in power plant design and developed a mixed integer linear programming model for the design of processes that convert solar and wind energy into methanol and hydrogen. Salman et al. [5] proposed a waste-to-energy conversion plant design through stochastic optimization and simulation, whereas Previtali et al. [6] considered the variability of the inlet stream composition in the design of combined heat and power plants. Teichgraeber and Brandt [7] used scenario reduction and stochastic optimization to account for utility price uncertainty in the design of electricity intensive processes, and Ahmad et al. [8] presented an exergy analysis of a cumene plant.

B. Research on Chemical and Petrochemical Processes

Examples of studies that have considered the effect of parameter uncertainty on process controllability include the work of Palazoglu and Arkun [9], who used multi-objective semi-infinite dynamic programming to design a system of serial stirred reactors; Bahakim and Ricardez-Sandoval [10], who used stochastic programming to design processes to be regulated by model predictive control; and Hauptmanns [11], who used simulation to study the effect of uncertainty on the safe operation of an acetic anhydride reactor. Stochastic optimization of industrial wastewater treatment systems is considered by Lemita et al. [12] and Sun and Lou [13], who developed a multi-objective optimization method for the design of the treatment section of an ammonia process, whereas Bahakim and Ricardez-Sandoval [14] approached the design of a carbon dioxide capture plant through a power series expansion model. Ramin et al. [15] and Li et al. [16] identified the preferred activated sludge plant configuration under inlet stream uncertainty using sensitivity analysis through a metamodel and simulation, respectively. Carnio et al. [17] investigated the effect of parameter uncertainty on emissions from a biogas-to-methanol processing plant.

Other reported applications of process stochastic optimization include those of Marques et al. [18], who coupled linear programming and Monte Carlo simulation to consider uncertainties in the launch of a pharmaceutical product; Chen et al. [19, 20], who applied the generalized disjunctive programming method for the synthesis of chemical processes, the latter demonstrating its application to methanol and toluene hydrodealkylation plants; Duong et al. [21], who used the polynomial chaos expansion method and process simulation to assess the performance sensitivity of complex processes hindered by multiple uncertainties; and Ali et al. [22], who applied these tools to assess the reliability of a natural gas plant. Finally, Lotz et al. [23] studied the optimization of a plant under uncertainty through a two-stage model coupling simulation and an evolutionary strategy, distinguishing between design decisions that are fixed and those that can be changed later.

C. Discussion

Except for the work of Lotz et al. [23], there are no reports on stochastic methods that explicitly distinguish between fixed and adjustable design decisions. In addition, the aforementioned work does not take a decision analytic approach like the one presented in this study. Decision analysis provides tools to account for changes in the decision maker's knowledge as previously unavailable new information becomes known.

III. DESCRIPTION OF THE HEURISTIC METHOD

The factors that determine the plant profit G are divided into three vectors: D includes permanent decisions (e.g., the equipment type and size), q denotes adjustable operating conditions (e.g., controller setpoints), and y groups non-controllable variables:

$$G = G(\mathrm{D}, \mathrm{q}, \mathrm{y}) \tag{1}$$

For a known y, the optimal design $[\mathrm{D}, \mathrm{q}]$ that maximizes G is called $[\mathrm{D}, \mathrm{q}]_{\mathrm{OPT}}(\mathrm{y})$, and is the solution of (2):

$$[\mathrm{D}, \mathrm{q}]_{\mathrm{OPT}}(\mathrm{y}) = \{[\mathrm{D}, \mathrm{q}] | \max_{\mathrm{D},\mathrm{q}}(G(\mathrm{D}, \mathrm{q}, \mathrm{y}))\} \tag{2}$$

For y uncertain, the optimal design that maximizes the expected value of G, $E[G]$, is the solution of (3):

$$[\mathrm{D}, \mathrm{q}]_{\mathrm{OPT}} = \{[\mathrm{D}, \mathrm{q}] | \max_{\mathrm{D},\mathrm{q}}(E[G(\mathrm{D}, \mathrm{q}, \mathrm{y})])\} \tag{3}$$

If the conditions q can be adjusted depending on y, the optimal design is found by solving (4):

$$\mathrm{D}_{\mathrm{OPT}} = \{\mathrm{D} | \max_{\mathrm{D}}(E[G(\mathrm{D}, \mathrm{q}(\mathrm{y}), \mathrm{y})])\} \tag{4}$$

If D, q, and y are continuous variables, finding the solution of (3) and (4) is mathematically very complex. To avoid this complexity, this paper proposes a heuristic method to find a design that performs acceptably. The heuristic method consists of the following steps:

1. Assume that y is a single discrete random variable y with n possibilities $y_0, y_1, \dots, y_n$ and probabilities $p_i = p(y = y_i)$ for $i = 0,1, \dots n$. If y is continuous, it can be discretized.
2. For each value of y_i, an optimal design $[\mathrm{D}, \mathrm{q}]_{\mathrm{OPT}}(y_i)$ is found by solving the problem stated in (5). The resulting n designs make up the set of "candidate designs".

$$[\mathrm{D}, \mathrm{q}]_{\mathrm{OPT}}(y_i) = \{[\mathrm{D}, \mathrm{q}] | \max_{\mathrm{D},\mathrm{q}}(G(\mathrm{D}, \mathrm{q}, y_i))\} \tag{5}$$

3. If y is not measured, the problem reduces to selecting, among the n designs $[\mathrm{D}, \mathrm{q}]_{\mathrm{OPT}}(y_i)$, the one with the best performance for the distribution of y. If $\mathrm{D}_{\mathrm{OPT}}(y_i)$ and $\mathrm{q}_{\mathrm{OPT}}[\mathrm{D}_{\mathrm{OPT}}(y_i), y_i]$are the values of D and q, respectively, resulting from solving (5), then the selection is shown in Figure 1. The performance of the selected design is likely to be worse than that of the solution of the stochastic optimization (3). However, the selected design will be competitive as it is optimal for one possibility of y and is selected by considering the degradation in performance caused by other values of y, weighted by the probability of those values.

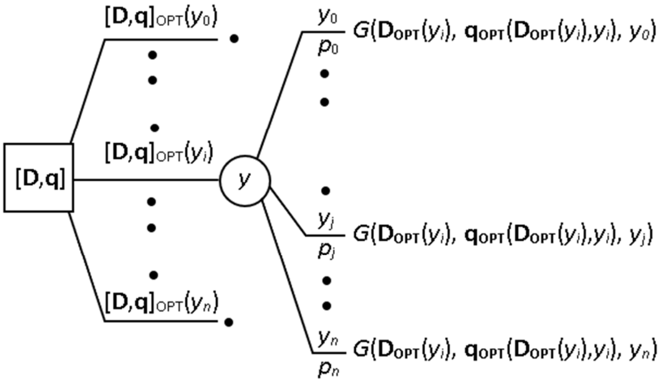

Fig. 1. Decision tree for unmeasured y.

4. In the more general case, the plant's permanent design items D are set to $\mathrm{D_{OPT}}(y_i)$, whereas the operating parameters q are changed once y becomes known. The optimal q, for D equal to $\mathrm{D_{OPT}}(y_i)$ and $y = y_j$, is given by (6):

$$\mathrm{q_{OPT}}\left(\mathrm{D_{OPT}}(y_i), y_j\right) = \left\{\mathrm{q} \mid \max_{\mathrm{q}} \left(G\left(\mathrm{D_{OPT}}(y_i), \mathrm{q}, y_j\right)\right)\right\} \quad (6)$$

Equation (6) indicates that if the design permanent items are set to $\mathrm{D_{OPT}}(y_i)$, which is optimal for y_i, but the value of y happens to be y_j instead of y_i, the operating parameters q would be changed to $\mathrm{q_{OPT}}\left(\mathrm{D_{OPT}}(y_i), y_j\right)$ to increase the profit. The decision tree with this variation is shown in Figure 2.

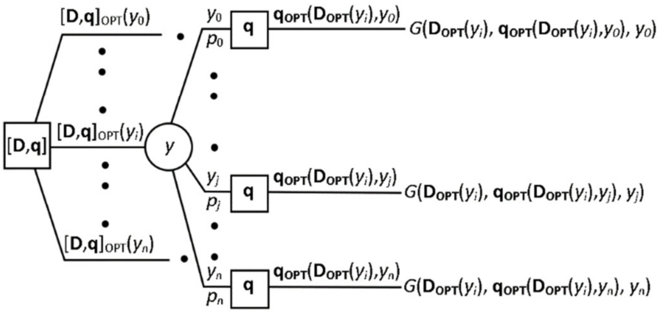

Fig. 2. Decision tree with adjustable operation.

In decision trees, squares represent decisions and circles represent uncertainties. The lines starting from a square are alternatives, while those starting from circles are possibilities. If a decision is to the right of an uncertainty, it means that the former was made knowing which possibility occurred in the latter (as decision q with respect to uncertainty y in Figure 2). If the decision is to the left of the uncertainty, it means that it was made without knowing what happened for the latter (as decisions $[\mathrm{D}, \mathrm{q}]$ with respect to y in Figure 1).

IV. CASE STUDY EXAMPLE

Figure 3 shows a numerical example, where the reaction A→B occurs in a catalytic reactor with W kg of catalyst. A feed of molar flow F_0 and temperature T_0 containing A and inert I, with mole fractions $y_{A,0}$ and $y_{I,0}$, respectively, passes through two heat exchangers before entering the reactor. The recovery exchanger (HX-R) raises the inlet stream temperature to T_1, whereas the service exchanger (HX-S) uses a utility stream of flow q_S, specific heat capacity cp_S, and temperature T_{SE} to further raise the feed temperature to T_2. The reactor outlet, with mole fractions of A, B, and I, y_A, y_B, and y_I, respectively, and temperature T_3 leaves the HX-R exchanger at temperature T_4. The thermodynamic parameters of the system are given in Table I.

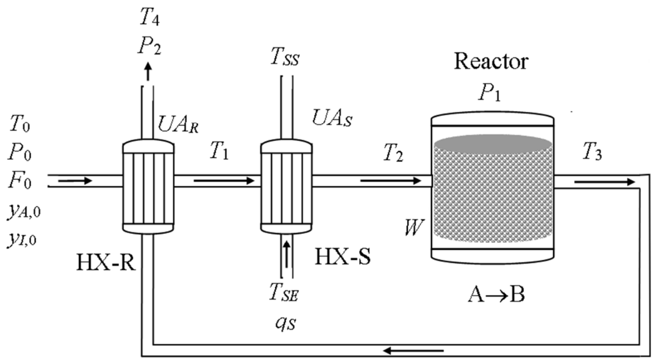

Fig. 3. Numerical case study.

TABLE I. THERMODYNAMIC PARAMETERS

Variable	Symbol	Value
Heat capacity of *A*	cp_A	90 kCal/kmol °C
Heat capacity of *B*	cp_B	90 kCal/kmol °C
Heat capacity of *I*	cp_I	90 kCal/kmol °C
Kinetic preexponential factor	A_0	1×10^{-2} kmol/(kg×min×atm)
Activation energy	E_A	8,000 kCal/kmol
Heat of reaction	ΔH	-20,000 kCal/kmol

The net profit of the system (G) is calculated as

$$G = G_B \times F_0 \times y_B - C_{CAT} \times W - C_{HX} \times (UA_R + UA_S) - C_{QS} \times q_S \quad (7)$$

Table II shows the definition and values of the economic parameters in (7). The permanent design decisions, D, are the heat exchanger sizes (UA_R and UA_S) and the catalyst weight (W). The adjustable operating parameter vector, q, has only one entry, the flow of utility to the service exchanger (q_S). The inlet composition ($y_{A,0}$) is considered an uncertain parameter at the time the process is designed. Figure 4 shows the numerical values of the system parameters.

TABLE II. ECONOMIC PARAMETERS

Variable	Symbol	Value
Net profit per *B* produced	G_B	\$3/kmol
Catalyst cost	C_{CAT}	\$0.5/kg
Heat exchangers cost (per unit of *UA*)	C_{HX}	\$0.02/(kCal×°C)
Utility stream cost	C_{QS}	\$2/(kg/min)

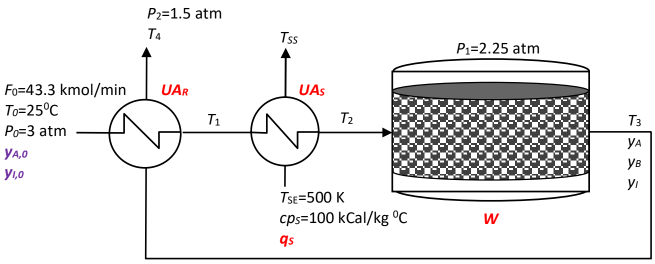

Fig. 4. Design variables (red), uncertainties (purple), and parameters that are either constant or set by material and energy balances (black).

The value of $y_{A,0}$ is uncertain, but is known to be in the range 0.72-0.80, as represented by the distribution in Table III.

TABLE III. INLET COMPOSITION PROBABILITY DISTRIBUTION

$y_{A,0}^i$	$p(y_{A,0} = y_{A,0}^i)$
0.80	$p(y_{A,0} = 0.8)$
0.75	$p(y_{A,0} = 0.75)$
0.72	$p(y_{A,0} = 0.75)$

The alternative designs presented in Table IV are $[\mathrm{D,q}]_{\mathrm{OPT}}(0.72)$, $[\mathrm{D,q}]_{\mathrm{OPT}}(0.75)$, and $[\mathrm{D,q}]_{\mathrm{OPT}}(0.80)$, each of which is the optimal design for one possibility of $y_{A,0}$. The optimizations were performed using the Solver add-in of MS Excel.

TABLE IV. ALTERNATIVE DESIGNS

Design	UA_R	UA_S	W	q_S	G
$[\mathrm{D,q}]_{\mathrm{OPT}}(0.8)$	839.9	434.3	62.6	3.7	20.6
$[\mathrm{D,q}]_{\mathrm{OPT}}(0.75)$	698.6	599.8	62.9	5.1	10.1
$[\mathrm{D,q}]_{\mathrm{OPT}}(0.72)$	616.1	697.5	63.0	5.9	3.9

A. *Design without Measurement of $y_{A,0}$*

In the case of a design without measurement of $y_{A,0}$, q_S remains fixed, as shown in Figure 5.

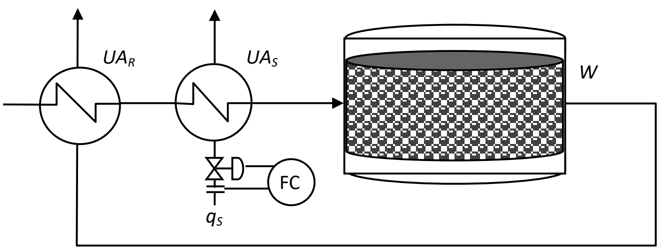

Fig. 5. Operation without composition gauge.

To select the best design, G is evaluated for each design alternative and possibility of $y_{A,0}$. The results are presented in Table V. The evaluation is performed using the decision tree shown in Figure 6. Uncertainty nodes are resolved by calculating the expected value of the gain of the branches originating from them. The design that leads to the uncertainty node with the highest expected value is selected.

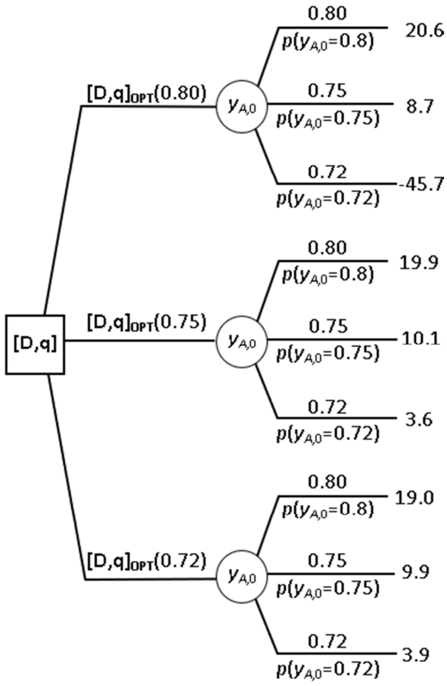

Fig. 6. Decision tree when $y_{A,0}$ is not measured.

TABLE V. NET PROFIT G FOR ALTERNATIVE DESIGNS AND INLET COMPOSITION POSSIBILITIES

Design	$y_{A,0} = 0.80$	$y_{A,0} = 0.75$	$y_{A,0} = 0.72$
$[\mathrm{D,q}]_{\mathrm{OPT}}(0.80)$	20.6	8.7	-45.7
$[\mathrm{D,q}]_{\mathrm{OPT}}(0.75)$	19.9	10.1	3.6
$[\mathrm{D,q}]_{\mathrm{OPT}}(0.72)$	19.0	9.9	3.9

The recommended design for different values of $p(y_{A,0} = 0.8)$ and $p(y_{A,0} = 0.72)$, with $p(y_{A,0} = 0.75)$ being their complement to one, is shown in Figure 7. While the exact value of $y_{A,0}$ is not known, the user is expected to be able to provide estimates of these probabilities, with the recommended design given by the region of Figure 7 in which these values lie.

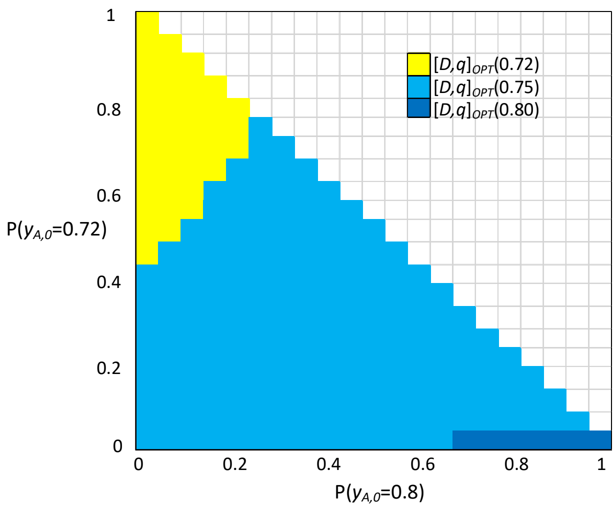

Fig. 7. Selected design when $y_{A,0}$ is not measured.

Notably, the alternative design $[\mathrm{D},\mathrm{q}]_{\mathrm{OPT}}(0.8)$ is only recommended for a very limited range of probabilities. This is because its performance deteriorates sharply for the values of $y_{A,0}$ other than 0.8, especially for $y_{A,0}=0.72$, for which it yields a profit of -45.7. Thus, $[\mathrm{D},\mathrm{q}]_{\mathrm{OPT}}(0.8)$ is only recommended if a $y_{A,0}$ value of 0.72 cannot occur, $p(y_{A,0}=0.72)=0$, and there is a high confidence that $y_{A,0}$ is 0.8, $p(y_{A,0}=0.8)>0.7$.

B. Design with Measurement of $y_{A,0}$

In the case of a design with measurement of $y_{A,0}$, once the plant is running, a gauge will measure the composition $y_{A,0}$, allowing the adjustment of the utility flow to the service exchanger q_S, as shown in Figure 8.

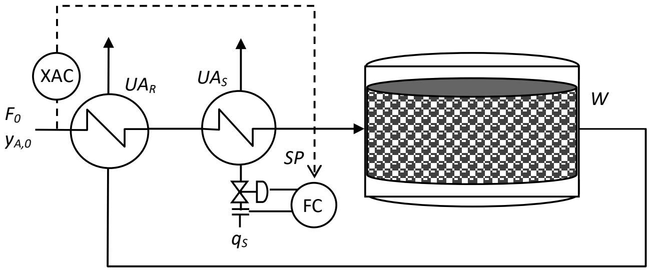

Fig. 8. Operation with composition gauge.

Let $\mathrm{D}_{\mathrm{OPT}}(y^i_{A,0})$ refer to the fixed elements (UA_R, UA_S, and W) of the design $[\mathrm{D},\mathrm{q}]_{\mathrm{OPT}}(y^i_{A,0})$. Given a possibility $y^j_{A,0}$ other than $y^i_{A,0}$, $q_{S,\mathrm{OPT}}(\mathrm{D}_{\mathrm{OPT}}(y^i_{A,0}),y^j_{A,0})$ is the value of q_S that maximizes G, provided that UA_R, UA_S, and W are those optimal for $y^i_{A,0}$ and the value of $y_{A,0}$ is $y^j_{A,0}$. As before, the optimal value of q_S was determined using the Solver add-in of MS Excel. The optimization results are shown in Table VI, where the optimal values of q_S are listed in the $q_{S,\mathrm{OPT}}$ columns.

TABLE VI. VALUES OF q_S MAXIMIZING G FOR DIFFERENT $\mathrm{D}_{\mathrm{OPT}}(y^i_{A,0})$ AND $y_{A,0}=y^j_{A,0}$

Design	UA_R	UA_S	W	$y_{A,0}=0.8$		$y_{A,0}=0.75$		$y_{A,0}=0.72$	
				$q_{S,\mathrm{OPT}}$	G	$q_{S,\mathrm{OPT}}$	G	$q_{S,\mathrm{OPT}}$	G
$\mathrm{D}_{\mathrm{OPT}}(0.8)$	839.9	434.3	62.6	3.7	20.6	4.7	9.4	5.4	1.9
$\mathrm{D}_{\mathrm{OPT}}(0.75)$	698.6	599.8	62.9	4.3	20.2	5.1	10.1	5.7	3.8
$\mathrm{D}_{\mathrm{OPT}}(0.72)$	616.1	697.5	63.0	4.7	19.6	5.4	10.0	5.9	3.9

The decision tree for this scenario is shown in Figure 9. It has two decisions, the initial selection of $\mathrm{D}_{\mathrm{OPT}}(y^i_{A,0})$ and the change of q_S to its optimal value given $\mathrm{D}_{\mathrm{OPT}}(y^i_{A,0})$ and the observed $y_{A,0}$.

In addition, the recommended design for different values of $p(y^i_{A,0})$ is shown in Figure 10. From this figure, it is apparent that the area where the $\mathrm{D}_{\mathrm{OPT}}(0.8)$ design is selected grows considerably compared to that in Figure 7. This is because the adjustment of q_S when $y_{A,0}$ takes the value of 0.72 avoids a negative profit for this design and $y_{A,0}$ value.

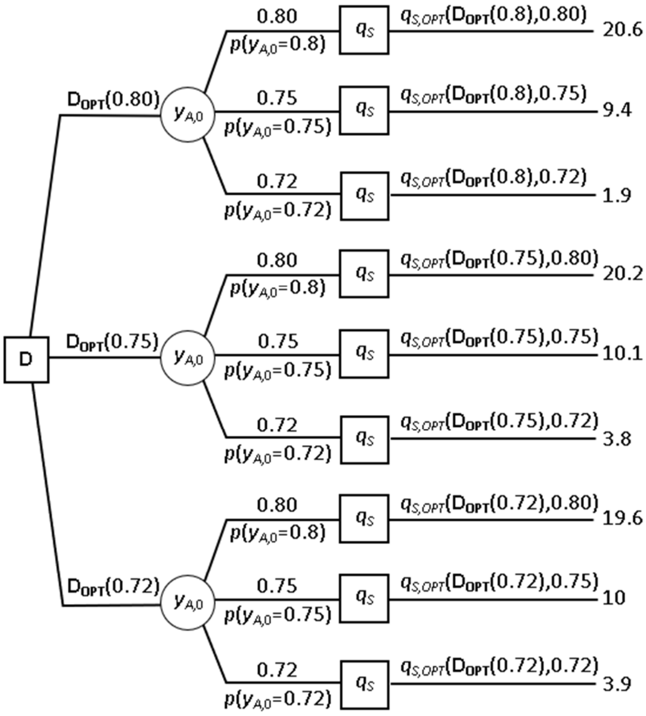

Fig. 9. Decision tree when $y_{A,0}$ is measured.

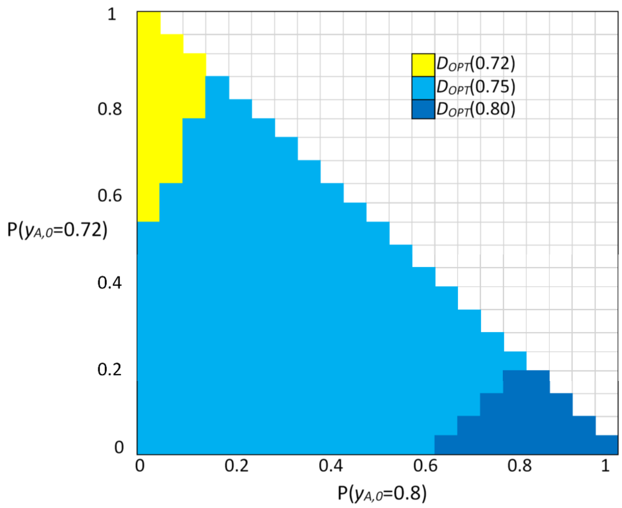

Fig. 10. Selected design when $y_{A,0}$ is measured.

V. CONCLUSIONS

This paper presents a method for plant design under uncertainty that incorporates two common characteristics of chemical plant design: the fact that some uncertain variables will eventually be known, and that some design decisions are adjustable. These aspects, which have been ignored in the previous literature on plant design under uncertainty, are addressed by decision trees. The method selects the best design from a set of candidates that result from optimizing the system for the possibilities of the uncertain variables. The problem structure is represented by decision trees that have two decisions for the case of adjustable parameters, one for the decisions made before the plant is built and the other for the decisions made after the plant is in operation. Once the heuristic method is described, it is applied to the design of a heat integrated reactor system hindered by uncertainty in feed composition. The results are presented as regions of the composition probability space for which a given alternative design is recommended.

Decision trees provide a clear, neat representation of the decision structure (the temporal entanglement of decisions and uncertainties). However, tackling more complex problems than the one worked on here, with more uncertain variables, possibilities, or decisions, would be hindered by an exponential growth in the size of the trees needed to represent the problem. To limit the growth of the trees, the engineer would need to group variables that are likely to occur simultaneously or have a similar effect on the process.

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