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An approach for reduction of computational complexity of a two-stage stochastic optimization problem for capturing parameters uncertainty in an ATAD system

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An approach for reduction of the computational complexity of a two-stage stochastic optimization problem for capturing parameters uncertainty in a conventional ATAD system is proposed in this study. The main aim is to find the boundary values of the variables of the first stage of the approach which will result in solutions into the boundaries of the stochastic space. The boundaries of variation of the first stage variables determine the variation of the parameters of the main equipment (heat exchangers surfaces and operating volumes of heat storage tank) which are affected by the change in stochastic parameters. The computational complexity is reduced as in any scenario vertex in the stochastic space a deterministic optimization problem is formulated and solved. As an optimization criterion, the minimum capital costs for purchase of heat exchangers and heat storage tank are used. For the purpose of the study, data from measurements in a real ATAD system were used. As a result of the deterministic optimization problems solution, the values of the parameters of main equipment corresponding to the minimum capital costs are determined. Based on these values the lower and the upper boundaries of the variables of the first stage of the approach are determined.

Keywords: ATAD system, Stochasticoptimization, Uncertainties

INTRODUCTION

Optimization is the heart of the decision-making process in chemical engineering, and other fields of the economy and business. It provides the opportunity to formulate a wide range of problems in a concise manner, using the combination goals and constraints of the process. In some cases, there are uncertainties in the data or model parameters. In these cases, optimization problems are considered as stochastic optimization problems. In their solution the influence of the uncertain parameters should be taken into consideration. This influence can take the process out of the optimum operating conditions and to constraints violation. The most common approach to deal with uncertainties in chemical engineering problems is two-stage stochastic programming.

In general, the two-stage stochastic optimization problems, for each possible scenario include a separate set of second-stage variables. Thus, the problem can be presented as a multi-dimensional problem of deterministic mathematical programming.

Thus, the task can be presented as a multidimensional task of the determined mathematical programming. Assuming the independence of the scenarios, the coefficients of the constraints form a huge block-diagonal matrix in which each block describes the corresponding structures of the constraints with the specific to the given scenario parameters, Figure 1.

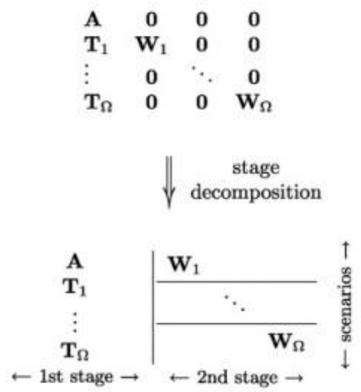

Fig. 1. Decomposition of the two-stage optimization problem [1].

The decomposition approach is the most widely used one to solve such optimization problems. The strategy of the process of obtaining the solution is the following: firstly, the values of the first stage parameters are determined, such as the probability objective function to be optimized. This stage of the process of obtaining the solution is called formulation of Master problem. The first stage variables represent the solutions which need to be taken into account before the uncertainty data are known (for example investment for equipment). While the second stage variables are solutions in which the uncertain parameters have already been found and additional solutions are obtained such as the constraints to be satisfied. The main aim of the

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optimization is to select these values of the first and the second stages variables (costs) so that their total amount to be minimal.

Assuming that the uncertainty parameters are with a certain probability, assign sets of known discrete values, postulate a final number of points (scenarios) in the stochastic space, then the two-stage stochastic optimization problem can be formulated as an equivalent deterministic multi-scenario optimization problem. The latter is well known as a multi-scenario model of the two-stage stochastic programming:

$$\min_{\bar{d},\bar{w}_s} Z = C'(\bar{d}) + \sum_s p_s C''_s(\overline{w_s}, \overline{\theta_s}),$$

Subject to:

$$h_{i,s}(\bar{d}, \overline{w_s}, \theta_s) = 0 \quad \forall i \in I,$$

$$g_{j,s}(\bar{d}, \overline{w_s}, \theta_s) \le 0 \quad \forall j \in J,$$

$$\bar{d} \in D, \quad \overline{w_s} \in W, \quad \theta_s \in \Theta, \quad \forall s \in S.$$

$$\sum_{s=1}^{S} p_s = 1$$

where $\bar{d}$ is the vector of the first stage variables (design variables), and $\overline{w_s}$ is the vector of the second stage variables in scenario *s* (state variables). Θ_s is the vector of the uncertain parameters in scenario *s*, and p_s is the probability of the occurrence of scenario *s*. The scenarios number in the model is *S*. There are equality and inequality constraints for each scenario. In addition, the objective function, conditionally called cost function, includes the costs for the first stage (design variables) and the total amount of costs expected for the second stage $\sum_s p_s C''_s(\overline{w_s}, \overline{\theta_s})$, calculated based on the costs for "system operation" for all scenarios with the respective probabilities p_s. The latter largely depend on the choice of the first-stage variables. However, the great number of scenarios leads to an increase in the computational complexity of the problem, even with the use of decomposition techniques. In order reasonable computational time to be reached it is necessary to determine the boundaries of the values of the first-stage variables that lead to solutions within the stochastic space.

The considered optimization approach is applied to a conventional Autothermal Thermophilic Aerobic Digestion (ATAD) system for municipal wastewater treatment operating under uncertainty. The ATAD process is conducted by the help of thermophilic microorganisms in two consecutively connected bioreactors operating in batch and semi-batch mode. As a final product Class A biosolidsare produced which are used as fertilizers in agriculture.

One of the main problems for the sustainable operation of the ATAD systems is the presence of uncertainty with regard to the main parameters of the ATAD systems such as temperature, quantity and composition of the raw sludge incoming into the ATAD system and the temperature of "product" flows outgoing from the ATAD system. This causes a lack of sustainability to the operating temperatures in the first-stage bioreactors and temperatures fluctuation in the whole system, as well as the presence of thermal shock on the thermophilic microorganisms resulting in prolongation of stabilization and pasteurization processes.

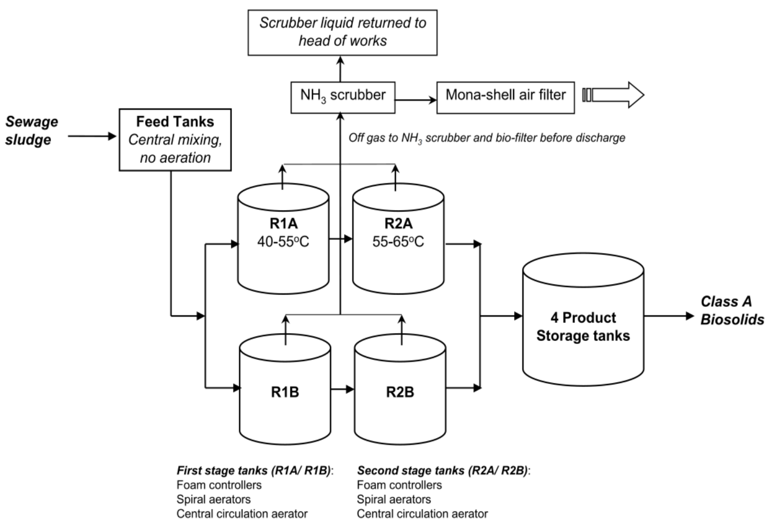

Fig. 2. Two-stage ATAD wastewater treatment system [2].

In order to increase the operating temperatures in the first bioreactor stages and to reduce the thermal shock on the thermophilic microorganisms, a mathematical model of heat integration with two heat exchangers (hot and cold) and one heat storage tank can be applied [3]. This model can be used as to utilize the waste heat from the second stage bioreactors for preheating of the sludge in the first-stage bioreactors, as well as to capture uncertain parameters of the flows incoming and outgoing from the ATAD system. For this purpose this model is modified in such a way to be involved in a two-stage stochastic optimization problem which involves variables of the first and the second stage [4]. However, the solution of this problem is hampered by the large stochastic space formed by the values of the uncertainty parameters.

This study proposes an approach for reduction of the stochastic space mentioned above by determination of reasonable boundary values of the variables of the first stage (design variables) of the two-stage stochastic optimization problem [4]. The latter leads to solutions obtained in the boundaries of the stochastic space, as well as to reduction of the needed calculation time for stochastic optimization problem solution.

In order to determine these boundaries, deterministic optimization problems should be formulated and solved in the boundaries of the stochastic space. The stochastic space can be conditionally interpreted as hyper-rectangular with vertices, determined from all possible combinations of lower and upper boundary values of the uncertainty parameters. Their number is equal to 2^N, where N in the number of the uncertainty parameters. The boundary values of the variables of the first stage should determine these regions of variation of the characteristics of the main equipment (heat exchangers surfaces and operating volume of the heat storage tank) which are affected by the change of the uncertainty parameters. For the ATAD system under consideration, the main uncertain parameters affecting the application of the heat integration model and their boundary values are as follows:

Volumes of loaded/treateddaily sludge: 12 [m^3] – 20 [m^3];

Temperatures of loaded sludge: 5.6 °C – 20.2 °C;

Temperatures of outgoing treated sludge: 54.5 °C – 68.1 °C.

For the purpose, for each scenario vertex in the stochastic space, a deterministic optimization problem is formulated. It results in formulation of 2^N deterministic optimization problems. They include the already used model of heat integration of the ATAD process [4], the constraints for feasibility of the heat exchange, as well as the constraints for efficiency of the heat integration.

Formulation of deterministic optimization problem

Data needed:

To formulate the deterministic optimization problem the following data should be known:

$M^c = V\rho$ - mass of the fluid subject to heating/cooling [kg];

cp^c - specific heat capacity of the fluid subject to heating [J/(kg.°C)];

T^{c0} - temperature of the cold sludge subject to heating [°C];

cp^h - specific heat capacity of the fluid subject to cooling [J/(kg.°C)];

T^{h0} - temperature of the fluid subject to cooling [°C];

U^c - heat transfer coefficient in heat exchanger *HE-c* [W/(m^2°C)];

U^h - heat transfer coefficient in heat exchanger *HE-h* [W/(m^2°C)].

$\Delta T^{\min}$ - admissible minimum temperature difference at the end of the heat exchangers [°C];

cp^m - specific heat capacity of the fluid in the heat storage tank [J/(kg.°C)];

T^{ef} - lower boundary of the efficiency of the heat integration scheme [°C].

Control variables

The following independent control variables are introduced – heat exchangers surfaces A^c and A^h of the two heat exchangers *HE-c* and *HE-h*, the operating volume of the heat storage tank V^m, $M^m = V^m.\ \rho^m$, as well as the times τ^c and τ^h for heating and cooling fluids in the heat exchangers.

The independent variables are continuous variables which vary within the following boundaries:

$$A\min^c \le A^c \le A\max^c, \quad (1)$$

$$A\min^h \le A^h \le A\max^h, \quad (2)$$

$$V\min^m \le V^m \le V\max^m, \quad (3)$$

$$\tau\min^c \le \tau^c \le \tau\max^c, \quad (4)$$

$$\tau\min^h \le \tau^h \le \tau\max^h, \quad (5)$$

Mathematical description of the heat exchange

The mathematical description [3] includes equations determining the temperatures at the inputs and the outputs of both heat exchangers at the end of the heat integration of the processes in the ATAD system. In addition, the model includes the equations determining initial temperatures in the heat storage tank, from which it begins to perform the functions of hot and cold respectively, as follows:

$$T^{c1}\left(\tau^c\right)=T^{c0}+\left[T^{mh}\left(\tau^c\right)-T^{c0}\right]R\Phi e^c, \quad (6)$$

$$T^{mh1}\left(\tau^c\right)=T^{mh}\left(\tau^c\right)-\left[T^{mh}\left(\tau^c\right)-T^{c0}\right]R\Phi e^c, \quad (7)$$

$$T^{mh}\left(\tau^c\right)=T^{c0}+\left(T^{mh0}-T^{c0}\right)\exp\left(-G^{mh}\Phi e^c\tau^c\right), \quad (8)$$

where: $R^c=\dfrac{w^{mh}.cp^m}{w^c.cp^c}$, $w^c=\dfrac{M}{\tau^c}$ [kg/s], $w^{mh}=\dfrac{M^m}{\tau^c}$ [kg/s], $G^{mh}=\dfrac{w^{mh}}{M^m}$ [s^{-1}],

$$\Phi e^c=\frac{1-\exp\left(-y^c.U^c.A^c\right)}{1-R^c.\exp\left(-y^c.U^c.A^c\right)}, \text{ and}$$

$$y^c=\frac{1}{w^{mh}.cp^m}-\frac{1}{w^c.cp^c};$$

$$T^{h1}\left(\tau^h\right)=T^{h0}-\left(T^{h0}-T^{mc}\left(\tau^h\right)\right)\Phi e^h, \quad (9)$$

$$T^{mc1}\left(\tau^h\right)=T^{mc}\left(\tau^h\right)+\left(T^{h0}-T^{mc}\left(\tau^h\right)\right)R^h\Phi e^h, \quad (10)$$

$$T^{mc}\left(\tau^h\right)=T^{h0}+\left(T^{mc0}-T^{h0}\right)\exp\left(-R^h\Phi e^h G^{mc}\tau^h\right), \quad (11)$$

where $R^h=\dfrac{w^h.cp^h}{w^{mc}.cp^m}$, $w^h=\dfrac{M}{\tau^h}$, [kg/s], $w^{mc}=\dfrac{M^m}{\tau^h}$ [kg/s],

$$\Phi e^h=\frac{1-\exp\left(-y^h.U^h.A^h\right)}{1-R^h.\exp\left(-y^h.U^h.A^h\right)}$$

$$y^h=\frac{1}{w^h.cp^h}-\frac{1}{w^{mc}.cp^m} \text{ and } G^{mc}=\frac{w^{mc}}{M^m} \text{ [s}^{-1}\text{]};$$

$$T^{mh0}=\frac{b^{22}+b^{12}b^{21}}{1-b^{11}b^{21}}; \quad T^{mc0}=\frac{b^{12}-b^{11}b^{22}}{1-b^{11}b^{21}}, \quad (12)$$

where:

$b^{11}=\exp(-G^{mh}\Phi e^c\tau^c)$; $b^{12}=\left[1-\exp\left(-G^{mh}\Phi e^c\tau^c\right)\right]T^{c0}$

$b^{21}=\exp(-R^h\Phi e^h G^{mc}\tau^h)$; $b^{22}=\left[1-\exp\left(-R^h\Phi e^h G^{mc}\tau^h\right)\right]T^{h0}$.

Constraints

The model should be supplied with constraints for the feasibility of the heat exchange in the heat exchangers:

$$\Delta T^c\geq\Delta T^{\min} \quad (13)$$

$$\Delta T^h\geq\Delta T^{\min}, \quad (14)$$

where ΔT^c and ΔT^h are minimum temperature differences at the ends of the heat exchangers *HE-c* and *HE-h*. The values obtained of the temperatures allow ΔT^c and ΔT^h to be determined. They are equal to the smaller of the two temperature differences at the end of each of the heat exchangers:

$$\Delta T^c=\min\left\{\left(T^{mh1}\left(\tau^c\right)-T^{c0}\right),\left(T^{mh}\left(\tau^c\right)-T^{c1}\left(\tau^c\right)\right)\right\}, \quad (15)$$

$$\Delta T^h=\min\left\{\left(T^{h0}-T^{mc1}\left(\tau^h\right)\right),\left(T^{h1}\left(\tau^h\right)-T^{mc}\left(\tau^h\right)\right)\right\}, \quad (16)$$

In order the proposed model of heat integrated ATAD system to operate efficiently, the temperature of the pre-heated raw sludge incoming into the first bioreactors stage, should be higher or equal to T^{ef} [3].

$$T^{c1}\geq T^{ef} \quad (17)$$

Optimization criterion

The aim of each scenario vertex is to determine the minimum costs for the main equipment for the purpose of the heat integration:

$$Cost=\alpha_{HE}\left(A^c\right)^{\beta_{HE}}+\alpha_{HE}\left(A^h\right)^{\beta_{HE}}+\alpha_{HS}\left(V^m\right)^{\beta_{HS}},$$

$$\underset{A^c,A^h,V^m}{MIN}\left(Cost\right)\cdot \quad (18)$$

Determination of the boundaries of the first-stage variables. Results

Data used:

1. Characteristic data of the heating/cooling flows for the different scenario vertices, Table 1.
2. The specific heat capacity of the fluid in the heat storage tank. Water is used as an intermediate heating/cooling agent in the heat exchangers: cp^m = 4.186 [kJ/(kg. °C)].
3. Heat transfer coefficient in the heat exchanger U^c =657 [W/(m^2°C)] – heat transfer coefficient in the heatexchanger *HE-c*.
4. U^h =657 [W/(m^2°C)] - heat transfer coefficient in the heat exchanger *HE-h.*
5. Admissible minimum temperature difference at the end of the heatexchangers: ΔT^{min}= [°C].
6. Lower boundary of the efficiency of the heat integration scheme: T^{ef}= 18[°C].
7. Price correlation coefficients, [5] for the heat exchangers *HE-c* and *HE-h*: α_{HE} = 3.078.10^3 [CU/m^2] and β_{HE} = *0.62*; for the heat storage tank α_{HS} = 3=247.10^2 [CU/m^3] and β_{HS}=0.68.

Table 1. Data for each scenario vertex.

Number of hyper-rectangle vertices	V^c, V^h [m³]	ρ^c, ρ^h [kg/m³]	cp^c, cp^h [kJ/(kg °C)]	T^{c0} [°C]	T^{h0} [°C]
1	12	1025	4	5.6	54.5
2	12	1025	4	5.6	68.1
3	12	1025	4	20.2	54.5
4	12	1025	4	20.2	68.1
5	20	1025	4	5.6	54.5
6	20	1025	4	5.6	68.1
7	20	1025	4	20.2	54.5
8	20	1025	4	20.2	68.1

Table 2. Solutions obtained for the scenarios vertices.

Vertex No	1	2	3	4	5	6	7	8
Cost[CU]	16272.4	16968.0	11538.5	16604.0	19215.8	21453.2	15094.4	18877.4
A^c[m²]	24.72	32.11	**13.64**	24.79	41.17	**53.77**	22.96	39.35
A^h[m²]	51.88	64.19	**26.39**	57.99	82.42	**105.63**	45.61	76.34
V^m[m³]	**75.39**	63.3	**31.02**	65.79	62.48	70.49	45.75	64.94
τ^c [s]	2640	2640	2640	2640	2640	2640	264	2640
τ^h [s]	1320	1320	1320	1320	1320	1320	1320	1320

The values used for the boundaries of the control variables in formulated deterministic optimization problem (1)-(18) are as follows:

$0 \le A^c \le 200$;

$0 \le A^h \le 250$;

$0.239 \le V^m \le 100$;

$900 \le \tau^c \le 2640$;

$900 \le \tau^h \le 1320$.

The obtained optimization problem solutions (1)-(18) for the scenarios vertices from 1 to 8 (Table 1) are listed in Table 2. As can be seen from Table 2, the capital costs for heat exchange equipment and heat storage tank range from 11538.5 [CU] to 21453.2 [CU]. They are defined by different values of the variables A^c, A^h, and V^m, while the times for heating/cooling the fluids in the respective heat exchangers have values defined by their upper limits.

Determining the minimum and maximum values with respect to A^c, A^h, and V^m for the scenarios vertices, the boundaries of the first stage variables are determined. They are presented in Table 3. The lower boundaries of the variables A^c, A^h, and V^m represent solutions of scenario vertex 3, while the mentioned above solutions correspond to scenario vertex 6.

Table 3. Boundaries of the first stage variables.

Heat exchanger*HE-c*,[m²]*;*	Heat exchanger*HE-h*,[m²]*;*	Heat storage tank -*HS*[m³]*;*
$13.65 \le A^c \le 53.77$	$26.39 \le A^h \le 105.63$	$31.02 \le V^m \le 75.39$

CONCLUSION

The approach proposed in this study can be used to reduce the stochastic space for solutions of ATAD system operating under uncertainties. It is based on determination of the boundary values of the first-stage variables. It is realized through deterministic optimization problems formulation and solution in different combinations of the boundary values of the uncertain parameters which effect the sustainable operation of the ATAD system. Determination of the boundaries of the stochastic space allow to choose the size of the main equipment whereby the optimization problem has a solution and the capital costs for redesign of the ATAD system will be minimal. The combination of the boundary values reduces the solution space, decreasing the computational complexity of the two-stage stochastic optimization problem under consideration.

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ПОДХОД ЗА НАМАЛЯВАНЕ НА ИЗЧИСЛИТЕЛНАТА СЛОЖНОСТ НА ДВУСТАДИЙНА СТОХАСТИЧНА ОПТИМИЗАЦИОННА ЗАДАЧА ЗА ДЕФИНИРАНЕ НА НЕСИГУРНОСТИТЕ В ПАРАМЕТРИТЕ В АТАD СИСТЕМА

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(Резюме)

В това изслеване се предлага подход, чрез който да бъде намалена изчислителната сложност на двустадийна стохастична оптимизационна задача, приложен за ограничаване въздействието на несигурните параметри върху конвенционална ATAD система. Методът цели да бъдат намерени границите на стойностите на променливите за първия стадий, които водят до решения в границите на стохастичното пространство. Границите, в които се изменят променливите на първия стадий определят изменението на характеристиките на основното оборудване (топлообменни повърхности и работен обем на топлинния резервоар), които се влияят от изменението на стохастичните параметри. Изчислителната сложност е намалена като за всеки сценариенвръх на стохастичното пространство, е формулирана и решена детерминирана оптимизационна задача. Използваният оптимизационен критерий са минималните капиталовите разходи за топлообменното оборудване и топлинния резервоар. За целите на изследването са използвани данни от измервания в реална ATAD система. В резултат на решаването на оптимизационните задачи са определени стойностите на основното оборудаване с най-ниски капиталови разходи. Въз основа на тези стойности саопределени и долната и горната граници, в които се изменят променливите на първия стадий.