

Robust Resource Targeting in Continuous and Batch Process

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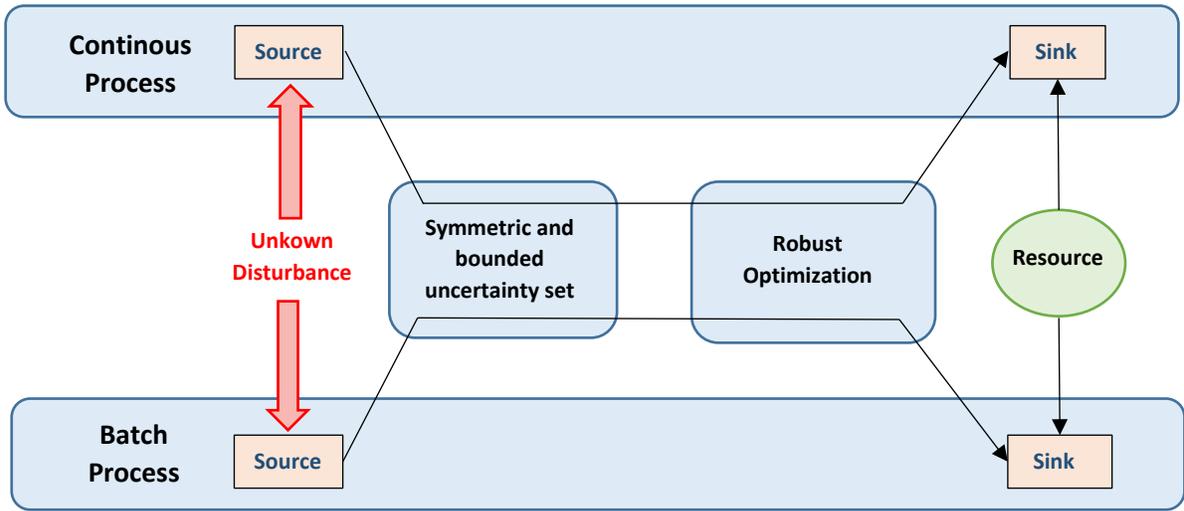
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ABSTRACT

Water is considered a significant resource in process industries. It is essential for planners to target and optimize the use of water as an external resource for industrial operations. Such optimization problems account for uncertainties related to internal resources and must be handled to provide solutions for real plants of industrial relevance. In this paper, these parametric uncertainties are addressed, while targeting resources for continuous and flexible schedule batch process. The proposed robust counterpart formulations include resource minimization constraints for continuous and batch processes to satisfy the demand. Three different robust optimization methodologies are adapted and extended to handle parametric uncertainties associated with internal resources. Assuming bounded and known uncertainty, the resultant formulations are then implemented to literature examples and the results are compared with the deterministic formulation. The results show that the formulation proposed by Bertsimas and Sim is the most appropriate model for the defined problem because it preserves the linearity and provides a mechanism to control the degree of conservatism, guaranteeing feasibility. This model will assist the planner to decide the resource requirement under uncertain conditions. Thus, immune the process against uncertainties to satisfy demands.

Keywords: Robust Optimization, Water conservation, Resource Conservation, Batch Process, Continuous process.

Graphical Abstract



Nomenclature

Sets

N_{sr}	number of sources
N_{sk}	number of sinks
$s \in S$	any state
$s_{sr} \in S_{sr}$	source state ($S_{sr} \subset S$)
$s_{sk} \in S_{sk}$	sink state ($S_{sk} \subset S$)
$i \in I$	unit
$k \in K$	event point

Continuous process variables

R	external resource requirement for continuous process
$f(s_{sr}, s_{sk})$	flow supplied from source 's _{sr} ' to demand related to sink 's _{sk} '
$f_w(s_{sr})$	flow supplied from source 's _{sr} ' to waste
$f_r(s_{sk})$	flow supplied from external resource R to demand related to sink 's _{sr} '
$u_c(s_{sr}, s_{sk}),$ $v_c(s_{sr}, s_{sk})$	additional variables associated with RO 2 for continuous process formulation
$z_f^c, q_f^c(s_{sk}),$ $z_c^c, q_f^c(s_{sr}, s_{sk})$	additional variables associated with RO 3 for continuous process formulation

Continuous process parameters

$F_{sr}(s_{sr})$	flow available from source related to 's _{sr} '
$\overline{F}_{sr}(s_{sr})$	nominal value of flow available from source related to 's _{sr} '
$\widehat{F}_{sr}(s_{sr})$	variation amplitude from $\overline{F}_{sr}(s_{sr})$

$c_{sr}(s_{sr})$	contaminant concentration of source related to 's _{sr} '
$\overline{c}_{sr}(s_{sr})$	nominal value of contaminant concentration of source related to 's _{sr} '
$\widehat{c}_{sr}(s_{sr})$	variation amplitude from $\overline{c}_{sr}(s_{sr})$
$F_{sk}(s_{sk})$	flow demand related to sink 's _{sk} '
$c_{sk}(s_{sk})$	concentration demand related to sink 's _{sk} '
Ω_f^c, Ω_c^c	additional parameters associated with RO 2 for continuous process formulation
Γ_f^c, Γ_c^c	budget parameter associated with RO 3 for continuous process formulation

Batch process variables

$R(s_{sk}, i', k')$	resource requirement for demand related to (s _{sk} , i', k')
$T_p(s, i, k)$	time at which state 's' appears in unit 'i' at event point 'k'
$T_{sr,s}(s_{sr}, i, k)$	time at which source related to state 's _{sr} ' starts in unit 'i' at event point 'k'.
$T_{sr,e}(s_{sr}, i, k)$	time at which source related to state 's _{sr} ' ends in unit 'i' at event point 'k'.
$T_{sk,s}(s_{sk}, i, k)$	time at which sink's demand related to state 's _{sk} ' starts in unit 'i' at event point 'k'
$T_{sr,e}(s_{sr}, i, k)$	time at which sink's demand related to state 's _{sk} ' ends in unit 'i' at event point 'k'
$X(s_{sk}, s_{sr}, i, i', k, k')$	fraction of time when the source related to (s _{sr} , i, k) to supply the sink's demand related to (s _{sk} , i', n') to the total duration of the source, where $i' \in I, n' \in N$
$f_{av}(s_{sk}, s_{sr}, i, i', k, k')$	flow available from a source related to (s _{sr} , i, k) to supply the sink's demand related to (s _{sk} , i', n'), where $i' \in I, n' \in N$
$f_{sup}(s_{sk}, s_{sr}, i, i', k, k')$	flow supplied from a source related to (s _{sr} , i, k) to the sink's demand

related to (s_{sk}, i', n') , where $i' \in I, n' \in N$

$y_w(s_{sk}, s_{sr}, i, i', k, k')$ binary variable denoting availability of source related to (s_{sr}, i, k) related to sink's demand related to (s_{sk}, i', n') , where $i' \in I, n' \in N$

$u_b(s_{sk}, s_{sr}, i, i', k, k')$,
 $v_b(s_{sk}, s_{sr}, i, i', k, k')$ additional variables associated with RO 2 for batch process formulation

$z_f^b(s_{sr}, i, k)$,
 $z_c^b(s_{sk}, i', k')$ additional variables associated with RO 3 for batch process formulation

$q_f^b(s_{sr}, i, k)$,

$q_c^b(s_{sk}, s_{sr}, i, i', k, k')$

Batch process parameters

MM any large number

$\tau_{sr}(s_{sr}, i)$ duration of source related to state ' s_{sr} ' and unit ' i '

$\tau_{sk}(s_{sk}, i)$ duration of sink's demand related to state ' s_{sk} ' in unit ' i '

$F_{sr}(s_{sr}, i, k)$ flow available from source related to state ' s_{sr} ' and unit ' i '

$\overline{F}_{sr}(s_{sr}, i, k)$ nominal value of flow available from source related to state ' s_{sr} ' and unit ' i ', for deterministic case $F_{sr}(s_{sr}, i, k) = \overline{F}_{sr}(s_{sr}, i, k)$

$\widehat{F}_{sr}(s_{sr}, i, k)$ variation amplitude from $\overline{F}_{sr}(s_{sr}, i, k)$

$F_{sk}(s_{sk}, i', k')$ flow demand of sink related to state ' s_{sk} ' in unit ' i '

$c_{sr}(s_{sr}, i)$ contaminant concentration available from source related to state ' s_{sr} ' in unit ' i '

$\overline{c}_{sr}(s_{sr}, i)$ nominal value of contaminant concentration available from source related to state ' s_{sr} ' in unit ' i ', for deterministic case $c_{sr}(s_{sr}, i) = \overline{c}_{sr}(s_{sr}, i)$

$\widehat{c}_{sr}(s_{sr}, i)$ variation amplitude from $\overline{c}_{sr}(s_{sr}, i)$

$c_{sk}(s_{sk}, i)$ maximum contaminant concentration limit accepted by sink related to state ' s_{sk} ' in unit ' i '

Ω_f^b, Ω_c^b additional parameters associated with RO 2 for batch process

formulation

Γ_f^b, Γ_c^b

budget parameter associated with RO 3 for batch process formulation

1. Introduction

Water is one of the essential commodities in process industries and can be conserved via modifying process behaviour, optimization, proper scheduling in order to decrease overall water usage and improving internal reuse (Klemeš 2013). One of the essential facets of cleaner manufacturing practices is the effective consumption of resource and consequently the reduction of waste. Optimum use of resource and water footprint elimination leads to greater profitability with a reduced burden on the climate (Hanjra and Qureshi 2010). Gleeson et al. (2012) estimated that about 20% of the aquifers in the globe are subjected to exploitation, causing severe outcomes including flood hazard compounded by the sea-level rise and land subsidence. Weerasooriya et al. (2021) presented a review of sustainable development goals and industrial water conservation by water footprint. This climate change may cause water supply problems or worsen the water scarcity problem in some parts of the world; such resource constraints will then create the need for more systematic water conservation initiatives to be implemented.

Process industries are one of the major consumers of water, in India, the water demand for the industrial sector is on a rise and will account for 8.5% and 10.1% of the total freshwater abstraction in 2025 and 2050 respectively (FICCI 2011). Nevertheless, with sustainable design through process integration and mathematical modelling, a significant amount of water can be conserved (Foo 2012). Process industries operations are broadly based on continuous and batch processes and aim to produce finished products with judicious use of water as a resource. It is necessary to evaluate existing water usage and set targets to assure strategies that minimize water and hence associated costs. With increasing concern over water savings and utilization, it is important to target the optimum water requirement more accurately in these processes. In a continuous process, the goal of minimizing the use of external resources can be attained by

assigning flow from different internal sources to demands (or sinks) in the overall network with the major constraint for wastewater recovery (Wang and Smith 1994). Significant research attempts have been made for continuous processes to minimize external use of water using various approaches such as heuristic-based algorithm (Gomes et al. 2007), hybrid approach, i.e. involving insight-based techniques and mathematical programming (Statyukha et al. 2008), graphical methods (Chwan and Foo 2009), game theory approach (Mei et al. 2009) etc.

In process industries, batch processing is popular, particularly when specialized productions with discrete tasks are required. In a batch process, water is not always needed or produced because the process units are not always active during the time horizon of interest (Gouws et al. 2010). Compared to continuous processes, the inclusion of time constraints makes it more challenging to evaluate water conservation opportunities in batch processes (Majozi 2010). Methodologies developed for resource conservation in batch processes are classified into two categories; fixed schedule and flexible schedule. In a fixed schedule operation, time is treated as a parameter whereas, in the flexible schedule, resource minimization is carried out by determining an optimal schedule of operations. Gouws et al. (2010) presented a review of the methodologies proposed to minimize water consumption in batch processes. Further, Chaturvedi and Bandyopadhyay (2014), focused to minimize resource requirements without any impact on production. Recently, Lee and Foo (2017) presented a methodology to determine the optimum production schedule that achieves maximum profit along with minimum resource consumption.

Although the deterministic model leads to the optimum value, it is not immune to data uncertainty due to a lack of reliable process models and process parameter variability. Therefore, it is important to establish systematic approaches to solve the issue of uncertainty in order to build accurate and consistent water networks. Methodologies have been developed to target

minimum resource requirement with uncertainties in parameters. In an important work, Alredhwan et al. (2005) developed an approach based on stochastic programming and sensitivity analysis to develop flexible and resilient process water networks. Further, Zhang et al. (2009) proposed numerical indices to quantify the flexibility of water network designs. Tan (2011) presented a fuzzy mathematical programming model for the synthesis of water networks when the model parameters exhibit fuzzy uncertainties. Arya et al. (2018) proposed a stochastic pinch analysis approach to handle uncertainties associated with source qualities and flows while targeting resource requirement in a continuous process. Rodriguez-perez et al. (2018), presented a stochastic model to control quality in sequencing batch reactors under uncertainty. Bandyopadhyay (2020) developed interval pinch analysis using the fuzzy approach to handle epistemic uncertainties. Kumawat and Chaturvedi (2020) presented a robust optimization approach to target resource based on the level of uncertainty with the capability of adjusting the level of risk. Poplewski and Foo (2021) developed a flexible water network to handle parametric variations using the extended corner point method. The works of literature are restricted to minimizing resource requirement with uncertainties in the continuous process only. Therefore, a mathematical formulation is required to handle parametric uncertainties while targeting resource requirement in the flexible schedule batch process. This work provides formulations encompassing such uncertainties, to ensure robustness and feasibility of an optimization problem for the entire given uncertainty space.

Robust optimization is a systematic approach focused to immune the model for any realization of uncertainty and determining flexible solutions with a viable option to conserve the optimality. The evidence on uncertainty is believed to be unknown but constrained assuming the uncertainty space is convex. The optimization problem is reformulated into its robust counterpart

optimization problem with uncertain parameters without any historical knowledge of parametric behaviour. Applications of such formulations are evident in various aspects related to process systems engineering, in the context of process systems engineering, Grossmann et al. (2017) presented the review of such mathematical programming techniques for optimization under uncertainty.

The primary introduction to handle coefficient uncertainty was presented by Soyster (1973). The ideology was to convert the uncertain optimization problem into a deterministic counterpart model such that any viable solution within their predefined uncertainty sets could be feasible with all realizations of uncertain parameters. This approach is considered to be valuable because no knowledge on the possibility of unknown parameters is required and the decision against ambiguity on all possible parameter values is immunized. However, this approach mostly attains over-conservative solutions and loses optimality. This eventually means that a robust solution can be guaranteed at the cost of losing optimality.

Further, the framework of robust optimization is extended, Ben-tal and Nemirovski (2000) proposed the robust counterpart formulation which is enormously conservative and is highly desirable with the flexibility to allow a tradeoff between performance and robustness. In this formulation, uncertainties in linear programming are addressed using nonlinear constraints with a mechanism to control the degree of solution conservatism through the constraint violation probability. The limitation of this formulation is that it introduces nonlinearity to the formulation, which increases the problem size and computational efforts. The framework was adopted by Lin et al. (2004), they presented a robust formulation to schedule production for the multipurpose batch process with uncertain processing times, market demands, and prices of products.

To avoid the complexity associated with nonlinearity, Bertsimas and Sim (2004) proposed robust linear programming (LP) with coefficient uncertainty. They stated that it is improbable that all of the uncertain coefficient parameters would attain the worst-case value at the same time. Therefore, a budget parameter is introduced to control the conservatism of the solution. This formulation is capable to control those parameters that are allowed to get their worst-case value and to tradeoff with an upper bound of probability violation (Thiele 2007). Implementation of this methodology is evident in aspects of process systems engineering, Li and Ierapetritou (2008), presented the robust counterpart mixed-integer linear programming (MILP) formulation to target uncertainties while scheduling production in a batch process. Sabouni and Mardani (2013), used this methodology to manage agricultural water resources under uncertainty.

In this paper, robust optimization formulations are implemented to target the minimum resource requirement under uncertainty. Applicability of the robust counterpart is explained for continuous and batch processes as they possess similar uncertainties associated with internal source parameters (flow rate and contaminant concentration). Significant contributions of this work are:

- Handling parametric uncertainties in internal sources of batch and continuous processes and presenting them concurrently.
- Solving the robust optimization techniques using three broadly adopted methodologies that do not require historical information of parameters related to uncertainty or their behaviour.
- Comparison of deterministic model with different robust optimization models and evaluating the best of them.
- Demonstrating applicability of the formulations proposed via illustrative examples

Further, the paper is structured as follows: In section 2, the deterministic LP model for continuous and MILP model for flexible schedule process is presented, along with defining the problem statement of parametric uncertainties. In section 3, robust counterpart formulations for both processes are proposed based on three robust optimization methods. One of the three robust optimization methods is the traditional one proposed by Soyster (1973), for brevity, this method is denoted as RO 1. Ben-tal and Nemirovski (2000) and Bertsimas and Sim (2004) methodologies are denoted as RO 2 and RO 3. The applicability of the proposed formulation is illustrated via examples in section 4 and compared with the deterministic model on the basis of the objective value, size, and nature of the formulated problem. Finally, the paper is concluded, emphasizing the importance of the proposed work and other prospects for future work.

2. Problem Statement and Optimization Model

Given a source-sink problem where water is used as a resource/ utility for intermediate steps. With a constraint to satisfy the demand, the optimization problem's objective is to minimize the use of the external resource. Deterministic optimization models are available to target resource in continuous and batch processes. The internal source parameters (flow rate and contaminant concentration) are uncertain and can vary in their respective bounded region.

The objective is to create a robust counterpart formulation to handle such parametric uncertainties and produce feasible results to unknown realizations of the parameters. The deterministic model to target minimum resource in continuous and batch processes are as follows:

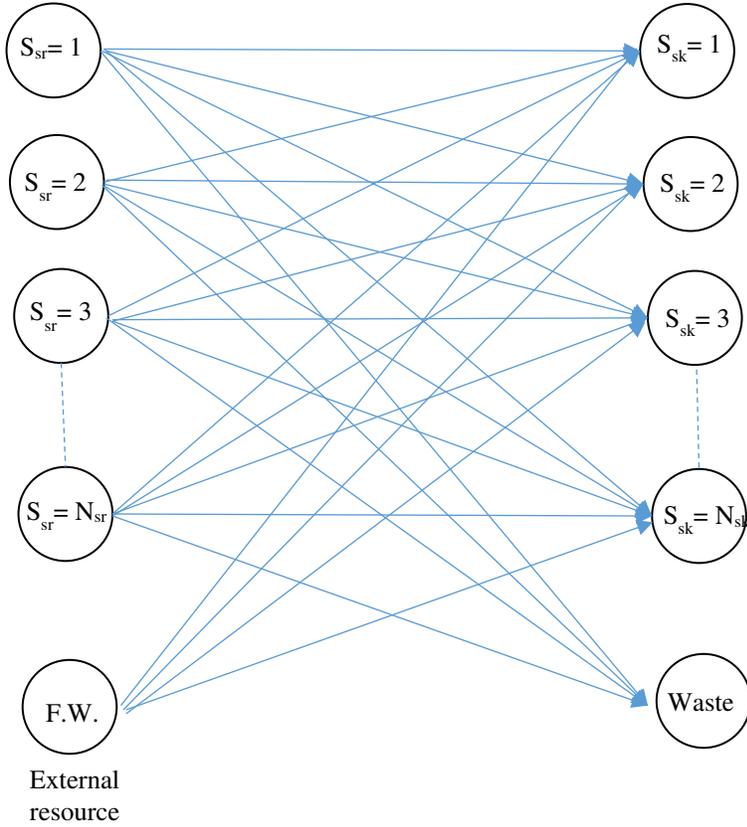


Fig. 1 Schematic representation of continuous water network

2.1 Continuous Process

Given a set S_{sr} consisting N_{sr} internal sources, each internal source produces a flow $F_{sr}(s_{sr})$ having a contaminant concentration $c_{sr}(s_{sr})$. N_{sk} internal demands need to be satisfied such that each demand accepts a flow $F_{sk}(s_{sk})$ with a quality $c_{sk}(s_{sk})$. The unused flow from the internal sources is sent to waste, without any quality or flow limits. The objective is to minimize the resource requirement (R) in the resource allocation network (RAN) to satisfy demand. A schematic representation is presented in Fig. 1.

The deterministic optimization problem to minimize external resource supplied to (Eq. 1) subject to constraints (Eqs. 2-4) is presented as follows:

$$\text{minimize } R = \sum_{s_{sk} \in S_{sk}} f(s_{sr}, s_{sk}), \quad s. t. \quad (1)$$

$$\sum_{s_{sk} \in S_{sk}} f(s_{sr}, s_{sk}) + f_w(s_{sr}) = F_{sr}(s_{sr}) \quad \forall s_{sr} \in S_{sr} \quad (2)$$

$$\sum_{s_{sr} \in S_{sr}} f(s_{sr}, s_{sk}) + f_r(s_{sk}) = F_{sk}(s_{sk}) \quad \forall s_{sk} \in S_{sk} \quad (3)$$

$$\sum_{s_{sr} \in S_{sr}} f(s_{sr}, s_{sk}) c_{sr}(s_{sr}) + f_r(s_{sk}) c_r - F_{sk}(s_{sk}) c_{sk}(s_{sk}) \leq 0 \quad \forall s_{sk} \in S_{sk} \quad (4)$$

Eq. (2) states that the total available flow $F_{sr}(s_{sr})$ should be supplied to sink and remaining to the waste. The demand associated with the sink should be satisfied with internal and external resources (Eq. 3). Eq. (4) expresses the material balance to meet demand quality. Targeting minimum resource for the real process could be different due to perturbation in source parameters. In uncertain framework, from the available N_{sr} internal sources, each produces an uncertain flow with uncertain quality in a bounded region with a known deviation from its nominal value.

$$F_{sr}(s_{sr}) \in [\overline{F_{sr}}(s_{sr}) - \widehat{F_{sr}}(s_{sr}), \overline{F_{sr}}(s_{sr}) + \widehat{F_{sr}}(s_{sr})]$$

$$c_{sr}(s_{sr}) \in [\overline{c_{sr}}(s_{sr}) - \widehat{c_{sr}}(s_{sr}), \overline{c_{sr}}(s_{sr}) + \widehat{c_{sr}}(s_{sr})]$$

The robust counterparts for this are explored in section 3.

2.2 Batch Process

For the general purpose of resource targeting problem in the batch process, deterministic formulation proposed by Chaturvedi and Bandyopadhyay (2014) is used. The formulation comprises two class of constraints related to the production (task durations, product recipes, equipment capacities, time horizon) and resource minimizing constraints (time mapping, flow balance, contaminant balance). The mathematical model to target production for a flexible

schedule process can be adapted from literature. The deterministic formulation to minimize the resource requirement is as follows:

$$\text{Minimize } \sum_{s_{sk} \in S_{sk}} \sum_{i' \in I} \sum_{k' \in K} R(s_{sk}, i', k') \quad (5)$$

$$T_{sk,e}(s_{sk}, i, k) = T_p(s_{sk}, i, k) \quad \forall i \in I, k \in K, s_{sk} \in S_{sk} \quad (6)$$

$$T_{sr,e}(s_{sr}, i, k) = T_p(s_{sr}, i, k) \quad \forall i \in I, k \in K, s_{sr} \in S_{sr} \quad (7)$$

$$T_{sk,s}(s_{sk}, i, k) = T_{sk,e}(s_{sk}, i, k) - \tau_{sk}(s_{sk}, i)y(s_{sk}, i, k) \quad \forall s_{sk} \in S_{sk}, i \in I, k \in K \quad (8)$$

$$T_{sr,s}(s_{sr}, i, k) = T_{sr,e}(s_{sr}, i, k) - \tau_{sr}(s_{sr}, i)y(s_{sr}, i, k) \quad \forall s_{sr} \in S_{sr}, i \in I, k \in K \quad (9)$$

$$\begin{aligned} & X(s_{sk}, s_{sr}, i, i', k, k') \\ & \leq \frac{(T_{sk,e}(s_{sk}, i', k') - T_{sr,s}(s_{sr}, i, k)) + MM(1 - \gamma_w(s_{sk}, s_{sr}, i, i', k, k'))}{\tau(s, i)} \end{aligned} \quad (10)$$

$$\forall s_{sr} \in S_{sr}, s_{sk} \in S_{sk}, i, i' \in I, k, k' \in K$$

$$X(s_{sk}, s_{sr}, i, i', k, k') \leq \gamma_w(s_{sk}, s_{sr}, i, i', k, k') \quad \forall s_{sr} \in S_{sr}, s_{sk} \in S_{sk}, i, i' \in I, k, k' \in K \quad (11)$$

$$0 \leq X(s_{sk}, s_{sr}, i, i', k, k') \leq 1 \quad \forall s_{sr} \in S_{sr}, s_{sk} \in S_{sk}, i, i' \in I, k, k' \in K \quad (12)$$

$$\begin{aligned} & f_{av}(s_{sk}, s_{sr}, i, i', k, k') \\ & = F_{sr}(s_{sr}, i, k)X(s_{sk}, s_{sr}, i, i', k, k') \quad \forall s_{sr} \in S_{sr}, s_{sk} \in S_{sk}, i, i' \in I, k, k' \in K \end{aligned} \quad (13)$$

$$\begin{aligned} & f_{sup}(s_{sk}, s_{sr}, i, i', k, k') \\ & = f_{av}(s_{sk}, s_{sr}, i, i', k, k') \quad \forall s_{sr} \in S_{sr}, s_{sk} \in S_{sk}, i, i' \in I, k, k' \in K \end{aligned} \quad (14)$$

$$\begin{aligned} F_{sk}(s_{sk}, i', k') & = \sum_{s_{sr} \in S_{sr}} \sum_{j \in J} \sum_{n \in N} f_{sup}(s_{sk}, s_{sr}, i, i', k, k') \\ & + R(s_{sk}, i', k') \quad \forall s_{sk} \in S_{sk}, i' \in I, k' \in K \end{aligned} \quad (15)$$

$$\sum_{s_{sk} \in S_{sk}} \sum_{i' \in I} \sum_{k' \in K} f_{sup}(s_{sk}, s_{sr}, i, i', k, k') - F_{sr}(s_{sr}, i, k) \leq 0 \quad \forall s_{sr} \in S_{sr}, i \in I, k \in K \quad (16)$$

$$\sum_{s_{sk} \in S_{sk}} \sum_{i \in I} \sum_{k \in K} f_{sup}(s_{sk}, s_{sr}, i, i', k, k') c_{sr}(s_{sr}, i) + R(s_{sk}, i', k') c_r - F_{sk}(s_{sk}, i', k') c_{sk}(s_{sk}, i') \leq 0 \quad \forall s_{sk} \in S_{sk}, i' \in I, k' \in K \quad (17)$$

In the formulation mentioned above, the objective is to minimize the total external resource requirement (Eq. 5). Eqs. (6-9) map time of source and sink with respective process units. It should be noted that a source might be partially available for demand. The limit of flow $X(s_{sk}, s_{sr}, i, i', k, k')$ available from a source (s_{sr}, i, k) for a demand (s_{sk}, i', k') can be calculated as the fraction of time when the source is available to supply the sink to the total duration of source directed by Eq. (10) and (11). It should be noted that this fraction (X) must be between zero and one (Eq. 12). Eq. (13) expresses the flow of a source available to the sink. Eq. (14) imposes the source flow limitation where $f_{sup}(s_{sk}, s_{sr}, i, i', k, k')$ is the flow supplied from $f_{av}(s_{sk}, s_{sr}, i, i', k, k')$ to a sink related to (s_{sr}, i', k') . Eqs. (15-16) expresses the flow balance for demand and the limit of source supplied as per the availability. Eq. (17) expresses the maximum limit on the contaminant level of demands.

In uncertain framework, the internal source flows ($F_{sr}(s_{sr}, i, k)$) and contaminant concentration ($c_{sr}(s_{sr}, i)$) are uncertain and can take values in the following symmetric region.

$$F_{sr}(s_{sr}, i, k) \in [\overline{F}_{sr}(s_{sr}, i, k) - \widehat{F}_{sr}(s_{sr}, i, k), \overline{F}_{sr}(s_{sr}, i, k) + \widehat{F}_{sr}(s_{sr}, i, k)].$$

$$c_{sr}(s_{sr}, i) \in [\overline{c}_{sr}(s_{sr}, i) - \widehat{c}_{sr}(s_{sr}, i), \overline{c}_{sr}(s_{sr}, i) + \widehat{c}_{sr}(s_{sr}, i)]$$

The robust counterparts are explained in the next section.

3. Robust optimization model for targeting minimum resource requirement

The optimization problem defined in the previous section with uncertain parameters is reformulated into a robust counterpart optimization problem. The uncertainty in internal sources

parameters (flow and concentration) is known and considered to minimize resource requirement for continuous and batch process. These counterpart formulations aim to choose a solution that satisfies the various realizations of uncertain but bounded data. The worst-case scenario corresponds to the minimum flow and maximum contaminant concentration available from internal sources in order to minimize external resource requirements. Modified constraints for robust counterpart formulation are as follows:

3.1. Soyester's Formulation (RO 1)

The formulation considers coefficient uncertainty and shows that such uncertainty in source parameters can be handled by an equivalent LP model without increasing the overall size of the problem. It constructs uncertainty sets as boxes and uses them for robust optimization. The objective value is calculated taking the boundary values of the interval to ensure that solution remains feasible for every realization of the uncertain coefficient. The major disadvantages are that it loses optimality and have no control over the degree of conservatism. However, the results would be valuable if the immunity of the model is essential then objective value.

Continuous Process: The worst-case formulation, considering uncertain flow and contaminant concentration can be transformed by replacing Eq. (2) and (4) with Eq. (18) and (19) respectively in the formulation presented in section 2.1.

$$\sum_{s_{sk} \in S_{sk}} f(s_{sr}, s_{sk}) + f_w(s_{sr}) - F_{sr}(s_{sr}) + \widehat{F}_{sr}(s_{sr}) = 0 \quad \forall s_{sr} \in S_{sr} \quad (18)$$

$$\sum_{s_{sr} \in S_{sr}} f(s_{sr}, s_{sk}) c_s(s_{sr}) + f_r(s_{sk}) c_r - F_{sk}(s_{sk}) c_{sk}(s_{sk}) + \sum_{s_{sr} \in S_{sr}} f(s_{sr}, s_{sk}) \widehat{c}_s(s_{sr}) \leq 0 \quad \forall s_{sk} \in S_{sk} \quad (19)$$

In the above equations, the first three terms are related to flow balance (Eq. 18) and contaminant balance (Eq. 19) with the additional fourth term to handle uncertainty as per the formulation

proposed by Soyester (1973).

Batch Process: Similarly, the deterministic MILP model for the flexible schedule batch process is transformed into its robust counterpart and can be obtained by substituting constraints (Eq. 16 and 17) with the following equations in the batch process model presented in section 2.2.

$$\sum_{s_{sk} \in S_{sk}} \sum_{i' \in I} \sum_{k' \in K} f_{sup}(s_{sk}, s_{sr}, i, i', k, k') - F_{sr}(s_{sr}, i, k) + \widehat{F}_{sr}(s_{sr}, i, k) \leq 0 \quad \forall s_{sr} \in S_{sr}, i \in I, k \in K \quad (20)$$

$$\begin{aligned} \sum_{s_{sr} \in S_{sr}} \sum_{i \in I} \sum_{k \in K} f_{sup}(s_{sk}, s_{sr}, i, i', k, k') c_{sr}(s_{sr}, i) + R(s_{sk}, i', k') c_r \\ - F_{sk}(s_{sk}, i', k') c_{sk}(s_{sk}, i') \\ + \sum_{s_{sr} \in S_{sr}} \sum_{i \in I} \sum_{k \in K} f_{sup}(s_{sk}, s_{sr}, i, i', k, k') \widehat{c}_{sr}(s_{sr}, i) \\ \leq 0 \quad \forall s_{sk} \in S_{sk}, i' \in I, k' \in K \end{aligned} \quad (21)$$

In Eq. (20) first, two terms represent flow balance with an additional third term to handle flow uncertainty. Similarly, with the mass balance in Eq. 21, the fourth term corresponds to handle concentration uncertainty.

3.2 Ben-Tal and Nemirovski's Formulation (RO 2): This formulation provides a mechanism to tradeoff between robustness and solution conservatism towards uncertainty. It provides flexibility to control the model to tradeoff between optimization value and reliability level. Even though providing the ease of controlling the problem, the main drawback is that it corresponds to the nonlinear formulation, which significantly increases the size of the problem. An additional parameter positive parameter (Ω) is introduced in the formulation to calculate the probability of constraint reliability using $e^{-\Omega^2/2}$.

Continuous Process: A robust counterpart formulation can be generated by substituting Eq. (2) and (4) with Eqs. (22-24) in the continuous process model discussed in section 2.1. Note that the formulation is a convex nonlinear programming (NLP) problem with auxiliary variables

$v_c(s_{sr}, s_{sk})$ and $u_c(s_{sr}, s_{sk})$.

$$\sum_{s_{sk}} f(s_{sr}, s_{sk}) + f_w(s_{sr}) - F_s(s_{sr}) + \widehat{F}_s(s_{sr}) + \Omega_f^c \widehat{F}_s(s_{sr}) = 0 \quad \forall s_{sr} \in S_{sr} \quad (22)$$

$$\begin{aligned} & \sum_{s_{sr} \in S_{sr}} f(s_{sr}, s_{sk}) c_s(s_{sr}) + \sum_{s_{sr} \in S_{sr}} u_c(s_{sr}, s_{sk}) \widehat{c}_s(s_{sr}) \\ & + \Omega_c^c \sqrt{\sum_{s_{sr} \in S_{sr}} v_c^2(s_{sr}, s_{sk}) \widehat{c}_s^2(s_{sr}) + f_r(s_{sk}) c_r - F_{sk}(s_{sk}) c_{sk}(s_{sk})} \\ & \leq 0 \quad \forall s_{sk} \in S_{sk} \end{aligned} \quad (23)$$

$$-u_c(s_{sr}, s_{sk}) \leq f(s_{sr}, s_{sk}) - v_c(s_{sr}, s_{sk}) \leq u_c(s_{sr}, s_{sk}) \quad \forall s_{sr} \in S_{sr}, s_{sk} \in S_{sk} \quad (24)$$

In Eq. (22) last two terms are introduced to handle the right-hand side (R.H.S.) uncertainties (free parameter) in available internal flows. Similarly, the second and third (non-linear) term in Eq. (23) are added to handle concentration uncertainty.

Batch Process: Similarly, the following constraints (Eqs. 25-27) are used in place of Eq. (16) and (17) in the formulation presented in section 2.2, to obtain a mixed-integer nonlinear programming (MINLP) formulation with additional variables.

$$\begin{aligned} & \sum_{s_{sk} \in S_{sk}} \sum_{i' \in I} \sum_{k' \in K} f_{sup}(s_{sk}, s_{sr}, i, i', k, k') - F_{sr}(s_{sr}, i, k) + \widehat{F}_{sr}(s_{sr}, i, k) + \Omega_f^b \widehat{F}_{sr}(s_{sr}, i, k) \\ & \leq 0 \quad \forall s_{sr} \in S_{sr}, i \in I, k \in K \end{aligned} \quad (25)$$

$$\begin{aligned} & \sum_{s_{sr} \in S_{sr}} \sum_{i \in I} \sum_{k \in K} f_{sup}(s_{sk}, s_{sr}, i, i', k, k') c_{sr}(s_{sr}, i) + R(s_{sk}, i', k') c_r \\ & - F_{sk}(s_{sk}, i', k') c_{sk}(s_{sk}, i') \\ & + \sum_{s_{sr} \in S_{sr}} \sum_{i \in I} \sum_{k \in K} u_b(s_{sk}, s_{sr}, i, i', k, k') \widehat{c}_s(s_{sr}, i) \\ & + \Omega_c^b \sqrt{\sum_{s_{sr} \in S_{sr}} \sum_{i \in I} \sum_{k \in K} v_b^2(s_{sk}, s_{sr}, i, i', k, k') \widehat{c}_s^2(s_{sr}, i)} \leq 0 \end{aligned} \quad (26)$$

$$\forall s_{sk} \in S_{sk}, i' \in I, k' \in K$$

$$\begin{aligned} -u_b(s_{sk}, s_{sr}, i, i', k, k') &\leq f_{sup}(s_{sk}, s_{sr}, i, i', k, k') - v_b(s_{sk}, s_{sr}, i, i', k, k') \leq \\ u_b(s_{sk}, s_{sr}, i, i', k, k') &\forall s_{sr} \in S_{sr}, s_{sk} \in S_{sk}, i, i' \in I, k, k' \in K \end{aligned} \quad (27)$$

3.3 Bertsimas and Sims Formulation (RO 3)

The ideology for this formulation is the assumption that all the uncertain coefficient parameters will not get the worst-case value simultaneously. This approach aims to establish a reasonable tradeoff between the robustness of the solution and conserving the optimality. Despite the worst-case approach, in this method, the violation of constraints is allowed and the method seeks a relatively robust solution based on the behaviour of the process and planner's choice. The resultant solution is feasible and close to optimal for most of the possible values of uncertain parameters. For each set of constraints having coefficient uncertainty, a budget parameter is introduced to control the degree of conservatism and the level of uncertainty in source parameters linked with that particular set of constraint. Few auxiliary variables are also introduced to convert the primal form of the optimization problem to dual form (Thiele 2007). Due to this, the overall size of the problem increases, but it preserves the linearity of the optimization model. Propositions to calculate the upper bound of probability violation can also be adapted from the literature.

Continuous Process

The formulation for the continuous process has been proposed by Kumawat and Chaturvedi (2020). The robust counterpart is obtained by eliminating Eq. (2) and (4) and using the set of following constraints (Eqs. 28-32) in the model presented in section 2.1.

$$\sum_{s_{sk} \in S_{sk}} f(s_{sr}, s_{sk}) + f_w(s_{sr}) - F_{sr}(s_{sr}) + \Gamma_f^c z_f^c + q_f^c(s_{sr}) = 0 \quad \forall s_{sr} \in S_{sr} \quad (28)$$

$$\sum_{S_{Sr} \in S_{Sr}} f(S_{Sr}, S_{Sk}) c_{Sr}(S_{Sr}) + f_r(S_{Sk}) c_r - F_{Sk}(S_{Sk}) c_{Sk}(S_{Sk}) + \Gamma_c^c z_c^c + \sum_{S_{Sr}} q_f^c(S_{Sr}, S_{Sk}) \quad (29)$$

$$\leq 0, \quad \forall S_{Sk} \in S_{Sk}$$

$$z_f^c + q_f^c(S_{Sk}) \geq \widehat{F}_{Sr}(S_{Sk}) \quad \forall S_{Sr} \in S_{Sr} \quad (30)$$

$$z_c^c + q_f^c(S_{Sr}, S_{Sk}) \geq \widehat{c}_{Sr}(S_{Sr}) f(S_{Sr}, S_{Sk}) \quad \forall S_{Sr} \in S_{Sr}, S_{Sk} \in S_{Sk} \quad (31)$$

$$z_f^c, q_f^c(S_{Sk}), z_c^c, q_f^c(S_{Sr}, S_{Sk}) \geq 0 \quad (32)$$

In Eq. (28) and (29), the first three terms are related to flow balance and contaminant balance with the fourth term with parameter Γ_f^c and Γ_c^c . These additional parameters are introduced to control the degree of conservatism and level of uncertainty in source flow and contaminant concentration respectively. The formulation also includes four positive auxiliary variables (Eq. 32) introduced by the duality theorem.

Batch Process: Similarly, the formulation presented in section 2.2 can be modified by replacing Eq. (16) and (17) with the following set of equations (Eqs. 33-37), comprising two additional parameters (Γ_f^b and Γ_c^b) and four positive variables (Eq. 37).

$$\sum_{S_{Sk} \in S_{Sk}} \sum_{i' \in I} \sum_{k' \in K} f_{sup}(S_{Sk}, S_{Sr}, i, i', k, k') - F_{Sr}(S_{Sr}, i, k) + \Gamma_f^b z_f^b(S_{Sr}, i, k) + q_f^b(S_{Sr}, i, k) \quad (33)$$

$$\leq 0 \quad \forall S_{Sr} \in S_{Sr}, i \in I, k \in K$$

$$\sum_{S_{Sr} \in S_{Sr}} \sum_{i \in I} \sum_{k \in K} f_{sup}(S_{Sk}, S_{Sr}, i, i', k, k') c_{Sr}(S_{Sr}, i) + R(S_{Sk}, i', k') c_r$$

$$- F_{Sk}(S_{Sk}, i', k') c_d(S_{Sk}, i') + \Gamma_c^b z_c^b(S_{Sk}, i', k') \quad (34)$$

$$+ \sum_{S_{Sr} \in S_{Sr}} \sum_{i \in I} \sum_{k \in K} q_c^b(S_{Sk}, S_{Sr}, i, i', k, k') \leq 0 \quad \forall S_{Sk} \in S_{Sk}, i' \in I, k' \in K$$

$$z_f^b(S_{Sr}, i, k) + q_f^b(S_{Sr}, i, k) \geq \widehat{F}_{Sr}(S_{Sr}, i, k) \quad \forall S_{Sr} \in S_{Sr}, i \in I, k \in K \quad (35)$$

$$z_c^b(s_{sk}, i', k') + q_c^b(s_{sk}, s_{sr}, i, i', k, k') \geq \widehat{c}_{sr}(s_{sr}, i) f_{sup}(s_{sk}, s_{sr}, i, i', k, k') \quad \forall s_{sr} \in S_{sr}, s_{sk} \in S_{sk}, i, i' \in I, k, k' \in K \quad (36)$$

$$z_f^b(s_{sr}, i, k), z_c^b(s_{sk}, i', k'), q_f^b(s_{sr}, i, k), q_c^b(s_{sk}, s_{sr}, i, i', k, k') \geq 0 \quad (37)$$

4. Illustrative Examples

To understand the applicability of the proposed robust formulation, two examples are presented, the first example is of continuous process and the second example is of batch process. The uncertainty is modelled and explored with three different scenarios; (i) flow uncertainty, (ii) concentration uncertainty and (iii) both flow and concentration uncertainty. Considering bounded and symmetric uncertainty in flowrate and contaminant concentration of each internal resource, a detailed comparison of all three robust optimization formulations is presented via the following examples. The optimization problems are solved with GAMS 24.8.2 using a system having configuration: Intel (R) Core (TM) i5-2400 CPU @ 3.10 GHz and 8 GB RAM. The computational results for both examples are evaluated and were obtained in a few seconds.

4.1 Illustrative Example 1: Robust targeting in continuous process

Data for the continuous process is given in Table 1 (Kumawat and Chaturvedi 2020). Here, the external resource is available at a contaminant concentration of 5 ppm. For deterministic case, the external resource is required at the flow rate of 375.27 t/h producing 185.27t/h of waste, a possible RAN is presented in Table 3(a). The availability of each internal source parameters has ± 20 t/h variability in flowrate and $\pm 10\%$ fluctuation in concentration.

Table 1. Source-sink data for Example 1

Source		Sink	
Flow (t/h)	Contaminant concentration (ppm)	Flow (t/h)	Contaminant concentration (ppm)
150 ± 20	80 ± 8	200	20

200 ± 20	60 ± 6	300	70
100 ± 20	55 ± 5.5	100	15
140 ± 20	75 ± 7.5	180	12

With the objective to minimize the use of the external resource under uncertainty, the worst-case scenario corresponds to the minimum value of all flow rates available (130, 180, 80, 120) and the maximum value of the contaminant concentration (88, 66, 62.5, 82.5). The resulting objective values obtained from worst-case formulation (RO 1) for three different scenarios are 377.1 t/h, 389.55t/h and 399.51 t/h respectively. This formulation provides the maximum protection against uncertainty and would be optimum for worst-case, but the objective value is overestimated for other realizations of parameters. The resultant RAN for scenario (iii) is presented in Table 3 (b).

Table 2. Model and solution statistics of Example 1

<i>Flow uncertainty</i>	nominal	RO 1	RO 2	RO 3 (Γ_f^c)					
				Budget Parameter					
				0	0.25	0.5	0.75	1	
Objective (t/hr)	375.27	377.1	398.9	406.7	375.27	375.72	376.18	376.63	377.1
Const. violation prob.			0.8	0.20	0.75	0.682	0.625	0.562	0.5
Single equations	13	13	13	13	17	17	17	17	17
Single variables	25	25	25	25	30	30	30	30	30
<i>Concentration uncertainty</i>				Budget Parameter (Γ_c^c)					
				0	1	2	3	4	
Objective (t/hr)	375.27	389.55	385.8	388.3	375.27	385.02	388.4	389.35	389.55
Const. violation prob.			0.80	0.20	0.71	0.452	0.295	0.13	0.062
Single equations	13	13	48	48	29	29	29	29	29
Single variables	25	25	58	58	42	42	42	42	42
<i>Flow and Concentration uncertainty</i>				Budget Parameter (Γ_f^c, Γ_c^c)					
				0,0	0.25, 1	0.5, 2	0.75, 3	1, 4	
Objective (t/hr)	375.27	399.51	404	414.3	375.27	386.65	392.36	396.59	399.51
Single equations	13	13	49	49	33	33	33	33	33
Single variables	25	25	58	58	47	47	47	47	47
Type	LP	LP	NLP		LP				
Solver	CPLEX	CPLEX	DCOPT		CPLEX				

Providing flexibility to the model, RO 2 formulation is solved with 20% and 80% reliability. For scenario (i), extremely conservative results are obtained and the use of the external resource is comparatively more than the result obtained from RO 1. Here the subsequent model nature is LP because the uncertain parameter is free form variable. For scenario (ii) the objective value for the mentioned reliability is calculated to be 385.8 t/h and 388.3 t/h respectively. Due to the formulation's nonlinearity, the size of the problem is increased and solved using DICOPT solver. Considering both the uncertainties in scenario (iii) with a 20% probability of constraint violation, the objective value shoots by 11.8%, the resultant RAN is shown in Table 3 (c).

Table 3. RAN for each formulation (flowrate given in t/h)

	Sink 1	Sink 2	Sink 3	Sink 4	Waste
(a) Deterministic case					
Source 1		45			105
Source 2		115	4.727		80.273
Source 3	60		14.8	25.2	
Source 4		140			
External Resource	140	80.473			
(b) RO 1					
Source 1		0.482			129.518
Source 2		163.607	16.393		
Source 3	54.054	3.243		22.703	
Source 4		120			
External Resource	145.946	12.668	83.607	157.297	
(c) RO 2					
Source 1	21.16	35.895	0.33	3.95	43.47
Source 2	5.5	137.66	6.29	5.35	
Source 3	9.923	29.83	9.18	5.86	
Source 4	5.23	84.06	1.25	4.226	
External Resource	158.2	12.55	82.9	160.6	
(d) RO3					
Source 1	4.41	5.323			130.27
Source 2	7.1	168.710	7.1	7.1	
Source 3	33.134	41.382	7.742	7.742	
Source 4	5.677	84.586	1.963	5.677	32.1

The RO 3 formulation is solved using the budget parameter providing flexibility to make a tradeoff with objective value and upper bound of probability violation. Here the subsequent model is LP with an increase in problem size having a negligible impact over computational time. For scenario (i) budget parameter (Γ_f^c) takes a value between [0, 1] and for scenario (ii) budget parameter (Γ_c^c) takes a value between [0, 4]. With the upper bound of the budget parameter, maximum protection against uncertainty is guaranteed and the solution will be equivalent to RO 1. For scenario (iii), combinations of different budget parameters are used to solve the problem and target resource requirement based on uncertainty level. A correlation between the objective and budget parameter with an upper probability of constraint violation was observed; a higher budget parameter results in a more conservative solution with larger feasibility and higher resource requirement. For the budget parameters to be $\Gamma_f^c = 0.5$, $\Gamma_c^c = 2$, which consequently means the corresponding flow and concentration constraints may be violated with the maximum probability of 62.5 % and 29.5 % respectively, with the minimum resource requirement of 392.36 t/h is calculated. This objective value is 4.5 % higher than the requirement for the deterministic case. A possible RAN for this case is presented in Table 3(d). Table 2 comprises the result comparing the deterministic model with the other three robust optimization models. It also includes model statics and objective values obtained using RO 1, RO 2, RO 3 with probability bound stating the reliability of the obtained solution.

It is been observed from Table 2 that out of the three formulations presented, RO 3 provides flexible and conservative solutions using a linear optimization model. The performance of the robust solution as a function of the budget parameter for the continuous process is illustrated in Fig. 4. Considering both uncertainties, it demonstrates how optimality is affected as the budget

parameter increases. It's also worth noting that, in this case, increasing the protection level above $(\Gamma_C^c) = 3.4$ has a negligible impact on objective value, showing that 85% of the uncertain parameters in a continuous water network greatly influence the optimal solution.

4.2 Illustrative Example 2: Robust targeting in batch process

This case study comprises a literature example for simultaneously optimizing maximum production and resource requirement in a batch process proposed by Chaturvedi and Bandyopadhyay (2014). Using three raw material feed, two products can be produced according to the state task network as shown in Fig. 2 through three reactions, heating and separation task. In order to maintain the purity of products and multipurpose use of equipment, freshwater is used as an external resource and required for washing of reactors (RR1 and RR2) at the end of any reaction.

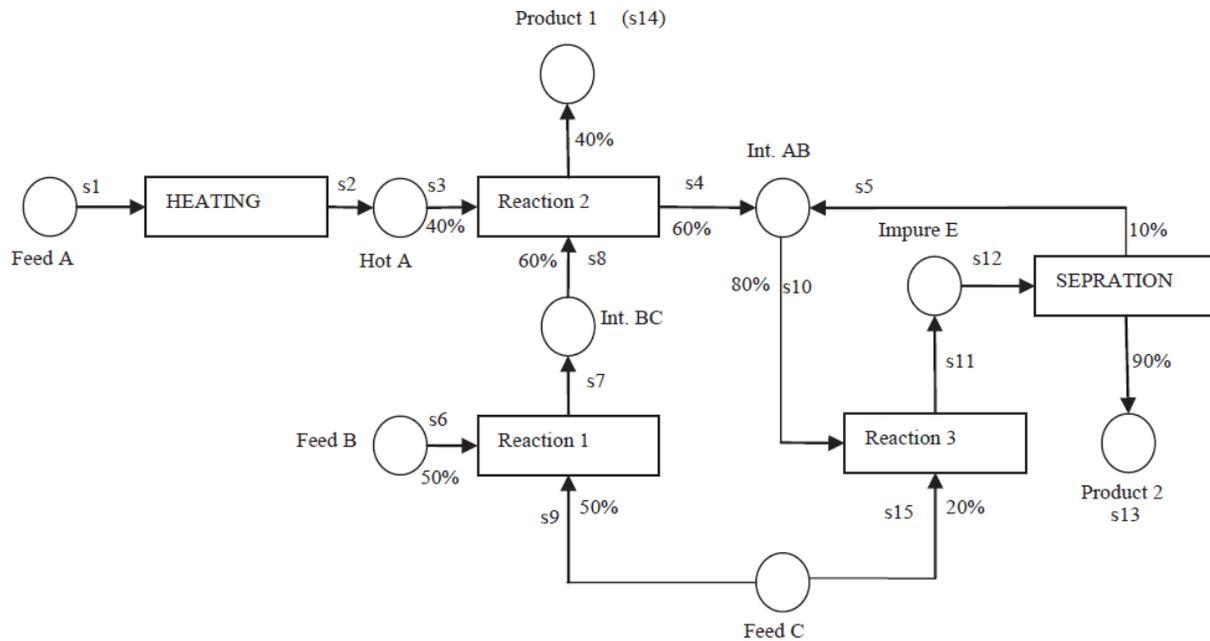


Fig. 2 State Task Network (STN) representation of the two product batch process

At first, the example was initially solved with nominal parameters. The minimum water requirement is determined to be 280 kg to produce 149.86 kg of aggregate product (1 and 2) in 8

hours (time horizon), the production schedule is shown in Fig.3. The water minimization data for the process are tabulated in Table 4. Similar to the previous example, flow and contaminant concentration can vary $\pm 20\text{kg}$ and 10% from nominal values respectively. It should be noted that for any realization of flow parameters, the production schedule does not change in this example, only external resource stream (RS1, RS2.....RS7) supplied to RR1 and RR2 are affected.

Table 4. Water/resource minimization data for Example 2

Task	Unit	Washing time (h)	Contaminant conc. (ppm)		Flow(kg)	
			Source	Sink	Source	Sink
Heating (H)	HR	0				
Reaction 1 (R1)	RR1	0.2	250 \pm 25	600	80 \pm 20	80
	RR2	0.2	250 \pm 25	600	80 \pm 20	80
Reaction 2 (R2)	RR1	0.2	500 \pm 50	800	100 \pm 20	100
	RR2	0.2	500 \pm 50	800	100 \pm 20	100
Reaction 3 (R3)	RR1	0.2	400 \pm 40	850	120 \pm 20	120
	RR2	0.2	400 \pm 40	850	120 \pm 20	120
Separation (S)	SR	0				

From RO 1, the calculated external resource requirement is 10.8% greater than the deterministic solution handling any realization for uncertain parameters (scenario (iii)) in the bounded region. Detailed results with different scenarios are tabulated in Table 5.

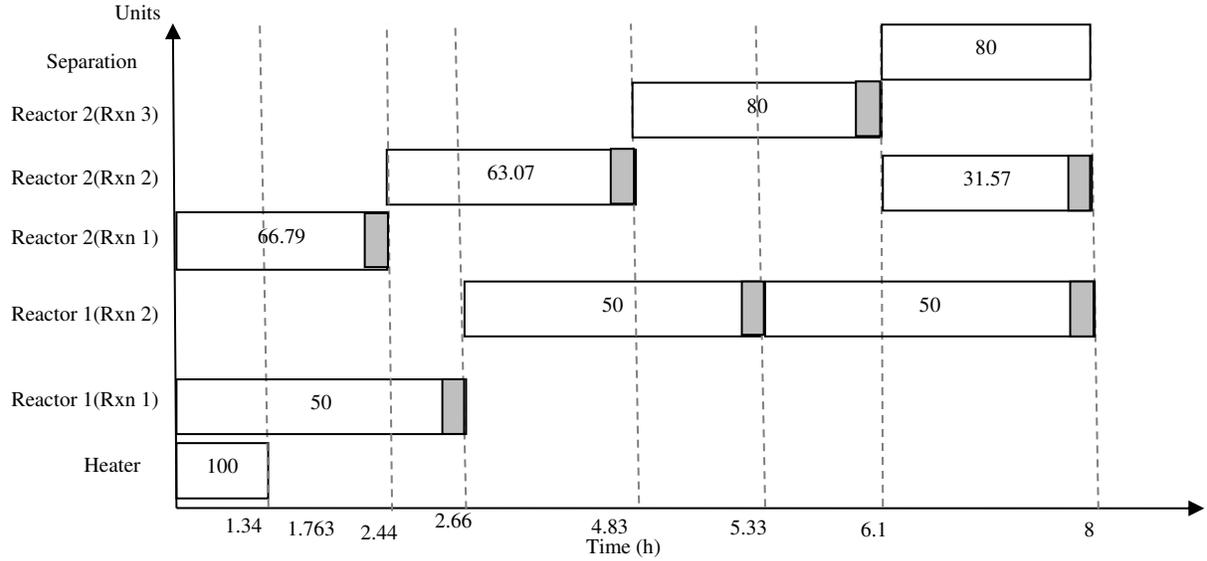


Fig. 3 Maximum production schedule for Example 2

Next, RO 2 results in linear formulation for the first scenario and nonlinear for the second and third scenario. The MINLP is solved with different reliability levels, with the maximum level of uncertainty in the bounded interval. The size of the problem is increased resulting in complications associated with nonlinear optimization. Executing the problem for the worst-case with a 100% probability of constraint violation results in the most conservative solution comparatively. For other reliability levels, the model becomes infeasible. In order to avoid this complexity related to nonlinear formulation and infeasible results, RO 3 formulation is explored.

Table 5. Example 2 results and solution statistics

<i>Flow Uncertainty</i>	Nominal	RO 1	RO 2	RO 3					
				Budget Parameter (Γ_f^b)					
				0	0.25	0.5	0.75	1	
Objective (kg)	280	290	293.4	300.6	280	282.5	285	287.5	290
Const. violation prob.			0.8	0.2	0.75	0.68	0.625	0.56	0.5
Single equations	6599	6599	6599	6599	6629	6629	6629	6629	6629
Single variables	4296	4296	4296	4296	4356	4356	4356	4356	4356

Discrete variables	940	940	940	940	940	940	940	940	940
Concentration Uncertainty				Budget Parameter(Γ_c^b)					
				0	1.5	3	4.8	6	
Objective (kg)	280	324.44	298.82	Infeasible	280	290.37	295.76	299.3	300.76
Const. violation prob.			1		0.68	0.46	0.27	0.156	0.015
Single equations	6599	6599	8460		7499	7499	7499	7499	7499
Single variables	4296	4296	6457		5226	5226	5226	5226	5226
Discrete variables	940	940	940		940	940	940	940	940
Flow and Concentration Uncertainty				Budget Parameter (Γ_f^b, Γ_c^b)					
				0	.25,1.5	0.5,3	.75,4.8	1,6	
Objective (kg)	280	310.23		Infeasible	280	283.3	301.31	307.55	310.23
Single equations	6599	6599			7529	7529	7529	7529	7529
Single variables	4296	4296			5286	5286	5286	5286	5286
Discrete variables	940	940			940	940	940	940	940
Type	MILP	MILP		MINLP				MILP	
Solver	XPRESS	XPRESS		DICOPT				XPRESS	

For RO 3 formulation, Γ_f^b takes a value between [0, 1] and budget parameter Γ_c^b takes a value between [0, 6]. It may be noted that variation in the level of uncertainty does not affect the size of the problem. For scenario (iii), combinations of several different budget parameters are used to solve the problem, results are summarized in Table 5. For the level of uncertainty to be 80% in available internal source parameters, the objective value is calculated to be 307.55kg. A higher value of budget parameter consequently represents more contaminated internal sources with lower availability of internal sources. Increasing their respective budget parameter, the tendency of robust formulation to seek more use of external resource to satisfy the deterministic demand. The objective value calculated using RO 3 could save 2.68 kg of resource compared to RO 1 in 8 hours. However, the figure does not seem to be large but could approximately save more than 2500kg of water per year (assuming around 300 days of operation/year). A comparison of the models and solution statistics for the nominal and robust solutions is available in Table 6.

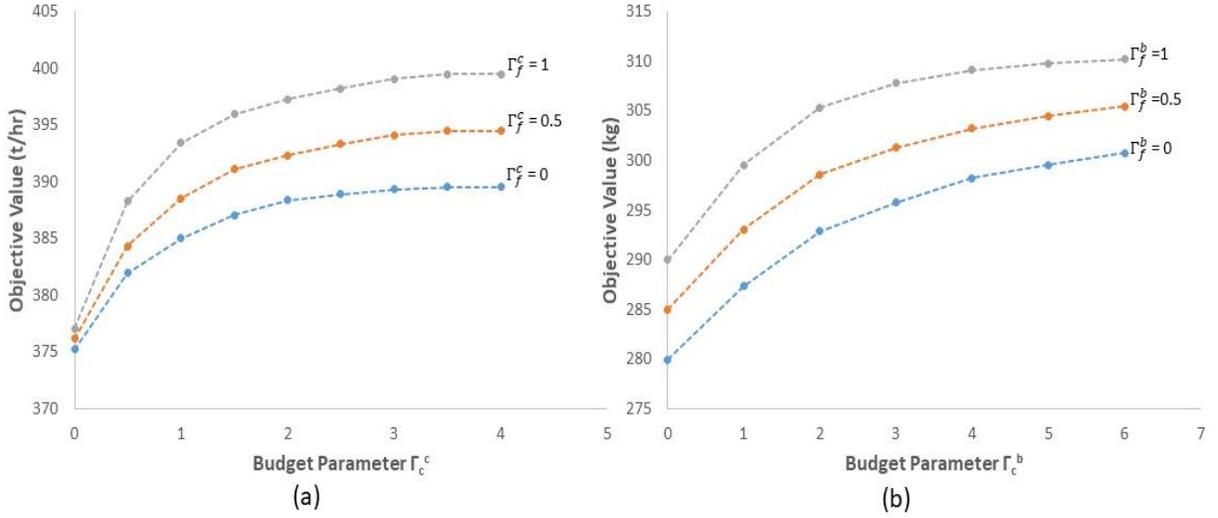


Fig. 4 Effect of uncertainty on objective value using RO 3 (a) continuous process (b) batch process

The effect of uncertainty on objective value is elaborated using Fig 4. For any realization of the budget parameter as uncertainty level in Γ_f^b , the nature of the curve for varying Γ_c^b is observed to be similar. Table 4 shows that six sources are available for two reactions in reactor three, being an L.H.S. uncertainty Γ_c^b can vary between (0,6). During this range, the objective value fluctuates stating that all certain parameters affect optimality unlike Example 1. In spite of six internal sources, Γ_f^b can take values between [0,1] because of R.H.S. uncertainty and worst-case solution can be obtained at $\Gamma_f^b = 1$.

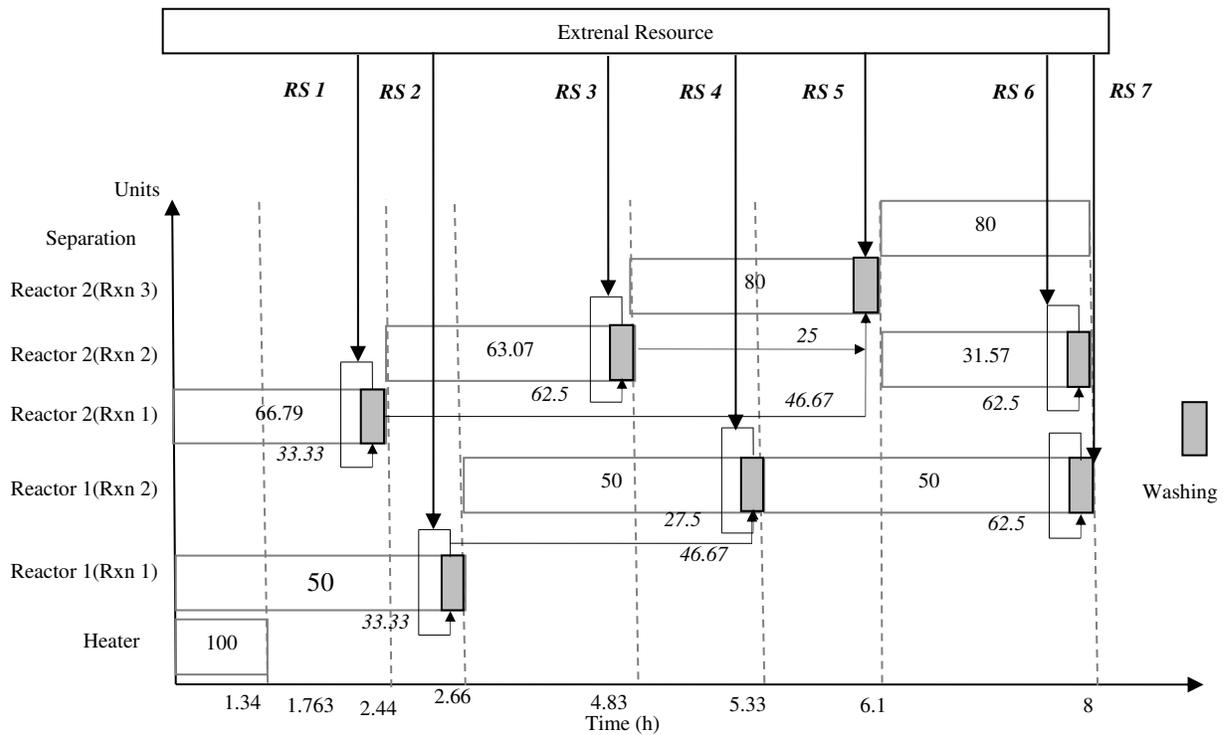


Fig. 5 Possible RAN for Example 2

Fig. 5 represents the schematic of a possible RAN, where the resource stream data obtained from different models for the third scenario is present in Table 6. Although the schedule for RAN is not affected in this example, the resource stream data obtained is affected. For a case in RO 3 and RO 1, it can be observed that RS 5- RS 7 are changed and no effect is being observed in RS 1-RS 4. Such type of examination would help the planner to design the flexible allocation network to entertain robust feasible results.

Table 6. Resource stream data for Fig. 5

Resource Stream (RS)	Nominal	RO 1	RO 3
RS 1	46.67	48	48
RS 2	46.67	48	48
RS 3	37.5	41.176	41.176

RS 4	25.83	41.176	41.176
RS 5	48.33	49.524	53.291
RS 6	37.5	41.176	35.345
RS 7	37.5	41.176	40.62
Net resource required	280	310.23	307.55

5. Conclusion

In this work, robust formulations are proposed to target the minimum resource requirement continuous and batch processes under uncertainty. The aim of the formulations is to produce robust solutions which are in sense to immune against any realizations of uncertainty in a known bounded interval. The approach is applied to address the defined problem with uncertain flow rate and contaminant concentration of internal resources. Robust counterpart formulations are generated using three popular methodologies and compared with the deterministic case. Implementation of the proposed formulations is elucidated with two illustrative examples, one each for continuous and batch process. Computational results demonstrate that RO 3 approach is comparatively effective way to address resource targeting problem under uncertainty. Whereas, RO 2 leads to infeasible solutions for certain scenarios in the batch process due to complexity related to nonlinearity. Also, RO 1 turns out to be a special case of RO 3 when the budget parameter is set to its maximum attainable value. RO 3 is advantageous because it maintains the linearity without substantially increasing the size of the problem, it also has the ability to control the degree of conservatism for any constraint and ensure the viability using a budget parameter for the robust optimization problem. In an illustrative example, it is also evaluated that with a certain level of risk, 2500kg of water could be saved. In future work, the model formulations would be readily expanded to multiperiod aspects. The ideology could be applied to other various aspects of process integration and other similar models of resource allocation networks; eg. hydrogen integration systems, carbon management networks.

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Conflict of interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

References

- Al-redhwan SA, Crittenden BD, Lababidi HMS (2005) Wastewater minimization under uncertain operational conditions. *Computers and Chemical Engineering* 29:1009–1021. <https://doi.org/10.1016/j.compchemeng.2004.11.002>
- Arya D, Shah K, Gupta A, Bandyopadhyay S (2018) Stochastic Pinch Analysis to Optimize Resource Allocation Networks. *Industrial and Engineering Chemistry Research* 57(48): 16423–16432 <https://doi.org/10.1021/acs.iecr.8b03935>
- Bandyopadhyay S (2020) Interval Pinch Analysis for Resource Conservation Networks with Epistemic Uncertainties. *Industrial and Engineering Chemistry Research* 59:13669–13681. <https://doi.org/10.1021/acs.iecr.0c02811>
- Ben-tal A, Nemirovski A (2000) Robust solutions of Linear Programming problems contaminated with uncertain data. *Mathematical Programming* volume 88:411–424 <https://doi.org/10.1007/PL00011380>
- Bertsimas D, Sim M (2004) The price of robustness. *Operations Research* 52:35–53. <https://doi.org/10.1287/opre.1030.0065>
- Chaturvedi ND, Bandyopadhyay S (2014) Simultaneously targeting for the minimum water requirement and the maximum production in a batch process. *Journal of Cleaner Production* 77:105–115. <https://doi.org/10.1016/j.jclepro.2013.11.079>
- Chwan D, Foo Y (2009) State-of-the-Art Review of Pinch Analysis Techniques for Water Network Synthesis. *Industrial and Engineering Chemistry Research* 48:5125–5159. <https://doi.org/10.1021/ie801264c>
- FICCI (2011) Water Use in Indian Industry Survey. FICCI Water Mission, New Delhi http://ficci.in/Sedocument/20188/Water-Use-Indian-Industry-survey_results.pdf
- Foo D (2012) Process Integration for Resource Conservation (1st ed.). CRC Press.

<https://doi.org/10.1201/b12079>

Gleeson T, Wada Y, Bierkens MFP, Van Beek LPH (2012) Water balance of global aquifers revealed by groundwater footprint. *Nature* 488:197–200.

<https://doi.org/10.1038/nature11295>

Gomes JFS, Queiroz EM, Pessoa FLP (2007) Design procedure for water/wastewater minimization : single contaminant. *Journal of Cleaner Production* 15:474–485.

<https://doi.org/10.1016/j.jclepro.2005.11.018>

Gouws JF, Majozi T, Chwan D, et al (2010) Water Minimization Techniques for Batch Processes. *Industrial and Engineering Chemistry Research* 49:8877–8893

<https://doi.org/10.1021/ie100130a>

Grossmann IE, Apap RM, Calfa BA, et al (2017) Mathematical Programming Techniques for Optimization under Uncertainty and Their Application in Process Systems Engineering. *Theoretical Foundations of Chemical Engineering* 51:893–909.

<https://doi.org/10.1134/S0040579517060057>

Hanjra MA, Qureshi ME (2010) Global water crisis and future food security in an era of climate change. *Food Policy* 35:365–377. <https://doi.org/10.1016/j.foodpol.2010.05.006>

Klemeš JJ (2013) Handbook of Process Integration (PI): Minimisation of Energy and Water Use, Waste and Emissions Woodhead Publishing 353-382.

<https://doi.org/10.1533/9780857097255.3.353>

Kumawat PK, Chaturvedi ND (2020) Robust targeting of resource requirement in a continuous water network. *Chemical Engineering Transactions* 81:1003–1008.

<https://doi.org/10.3303/CET2081168>

Lee JY, Foo DCY (2017) Simultaneous Targeting and Scheduling for Batch Water Networks. *Industrial and Engineering Chemistry Research* 56:1559–1569.

<https://doi.org/10.1021/acs.iecr.6b03714>

Li Z, Ierapetritou MG (2008) Robust optimization for process scheduling under uncertainty. *Industrial and Engineering Chemistry Research* 47:4148–4157.

<https://doi.org/10.1021/ie071431u>

Lin X, Janak SL, Floudas CA (2004) A new robust optimization approach for scheduling under uncertainty: I. Bounded uncertainty. *Computers and Chemical Engineering* 28:1069–1085.

<https://doi.org/10.1016/j.compchemeng.2003.09.020>

Majozi T. (2010) Introduction to Batch Chemical Processes. In: *Batch Chemical Process Integration*. Springer, Dordrecht 1-11. https://doi.org/10.1007/978-90-481-2588-3_1

Mei I, Chew L, Tan RR, et al (2009) Game theory approach to the analysis of inter-plant water integration in an eco-industrial park. *Journal of Cleaner Production* 17:1611–1619.

<https://doi.org/10.1016/j.jclepro.2009.08.005>

Poplewski G, Foo DCY (2021) An extended corner point method for the synthesis of flexible water network. *Process Safety and Environmental Protection* 148:210–224.

<https://doi.org/10.1016/j.psep.2020.09.050>

- Rodriguez-perez BE, Flores-tlacuahuac A, Sandoval LR, Lozano FJ (2018) Optimal Water Quality Control of Sequencing Batch Reactors Under Uncertainty. *Industrial and Engineering Chemistry Research* 57 (29): 9571-9590
<https://doi.org/10.1021/acs.iecr.8b01076>
- Sabouni MS, Mardani M (2013) Application of Robust Optimization Approach for Agricultural Water Resource Management under Uncertainty. *Journal of Irrigation and Drainage Engineering* 139:571–581. [https://doi.org/10.1061/\(asce\)ir.1943-4774.0000578](https://doi.org/10.1061/(asce)ir.1943-4774.0000578)
- Soyster AL (1973) Technical Note — Convex Programming with Set- Inclusive Constraints and Applications to Inexact Linear Programming. *Operations Research* 21(5):1019-1175
<https://doi.org/10.1287/opre.21.5.1154>
- Statyukha G, Kvitka O, Dzhygyrey I (2008) A simple sequential approach for designing industrial wastewater treatment networks. *Journal of Cleaner Production* 16:215-224.
<https://doi.org/10.1016/j.jclepro.2006.09.002>
- Tan RR (2011) Fuzzy Optimization Model for Source-Sink Water Network Synthesis with Parametric Uncertainties. *Industrial and Engineering Chemistry Research* 50: 3686–3694
3686 <https://doi.org/10.1021/ie101025p>
- Thiele DB (2007) INFORMS Tutorials in Operations Research Robust and Data-Driven Optimization : Modern Decision Making Under Uncertainty Robust and Data-Driven Optimization. *Tutorials in Operation Research*. <https://doi.org/10.1287/educ.1063.0022>
- Wang Y Smith R (1994) Wastewater Minimisation. *Chemical Engineering Science* 49:981–1006. [https://doi.org/10.1016/0009-2509\(94\)80006-5](https://doi.org/10.1016/0009-2509(94)80006-5).
- Weerasooriya RR, Liyanage LPK, Rathnappriya RHK, et al (2021) Industrial water conservation by water footprint and sustainable development goals: a review. *Environment, Development and Sustainability*. <https://doi.org/10.1007/s10668-020-01184-0>
- Zhang Z, Feng X, Qian F (2009) Studies on resilience of water networks. *Chemical Engineering Journal* 147:117–121. <https://doi.org/10.1016/j.cej.2008.06.026>

Figures

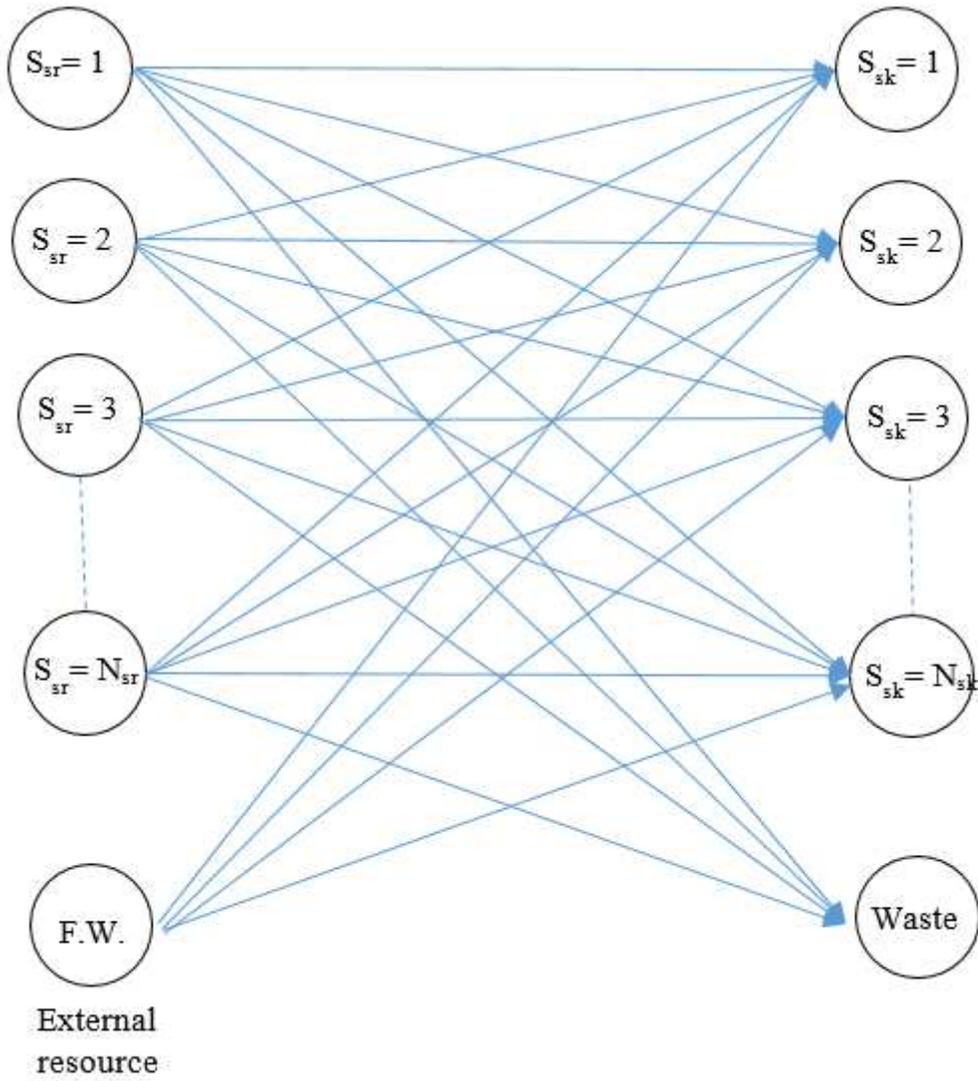


Figure 1

Schematic representation of continuous water network

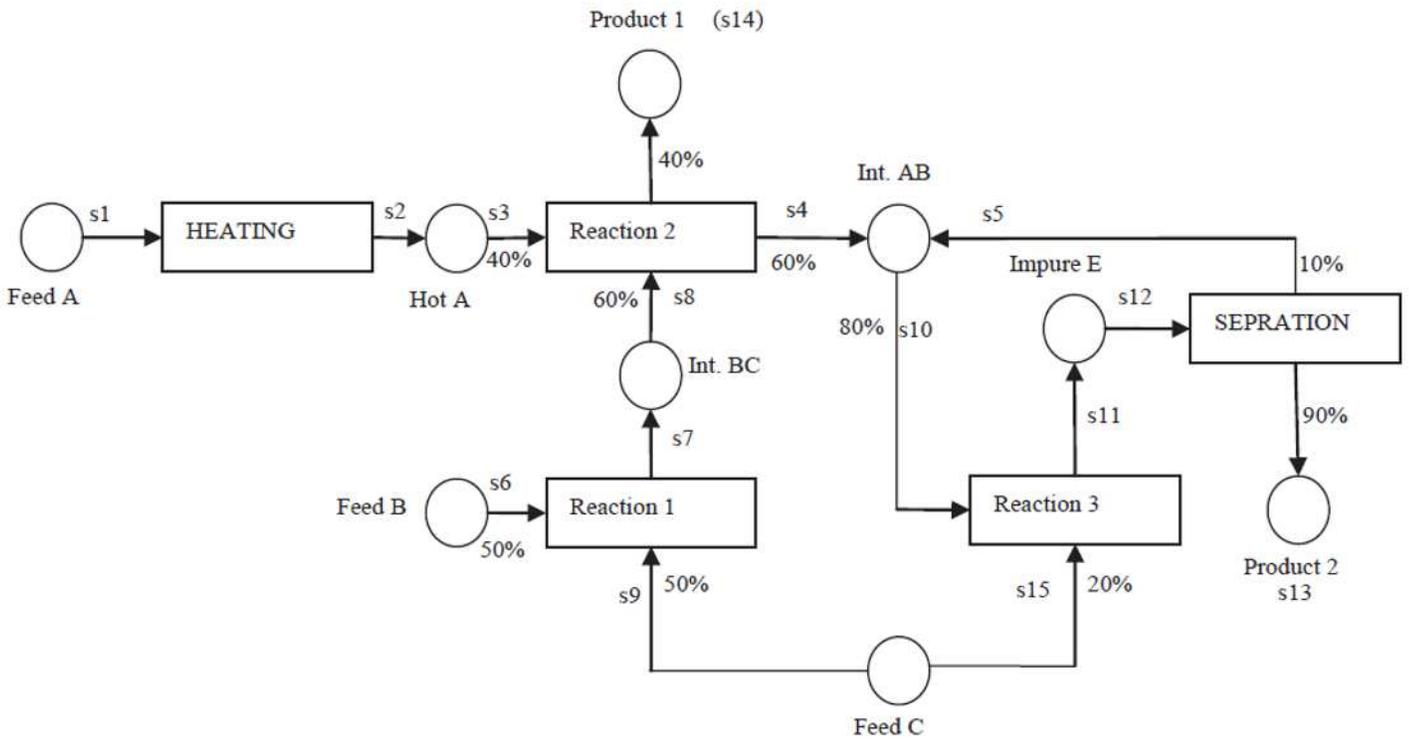


Figure 2

State Task Network (STN) representation of the two product batch process

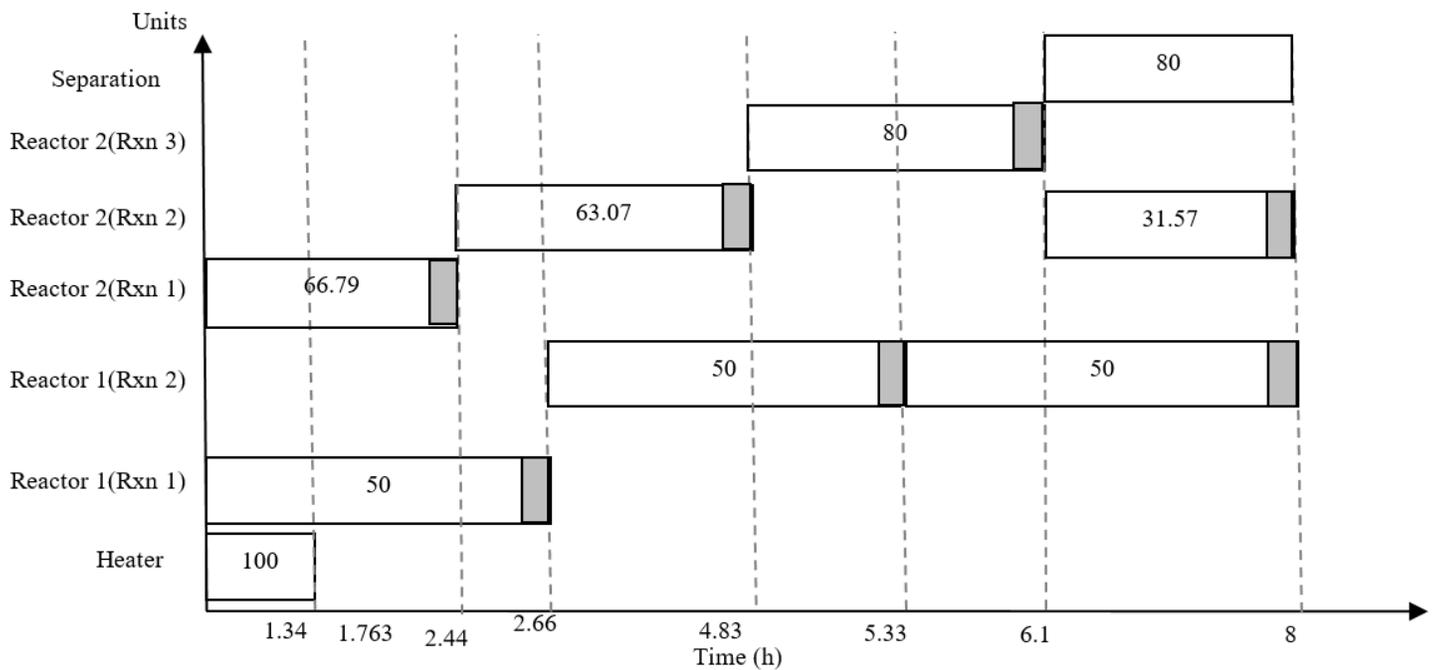


Figure 3

Maximum production schedule for Example 2

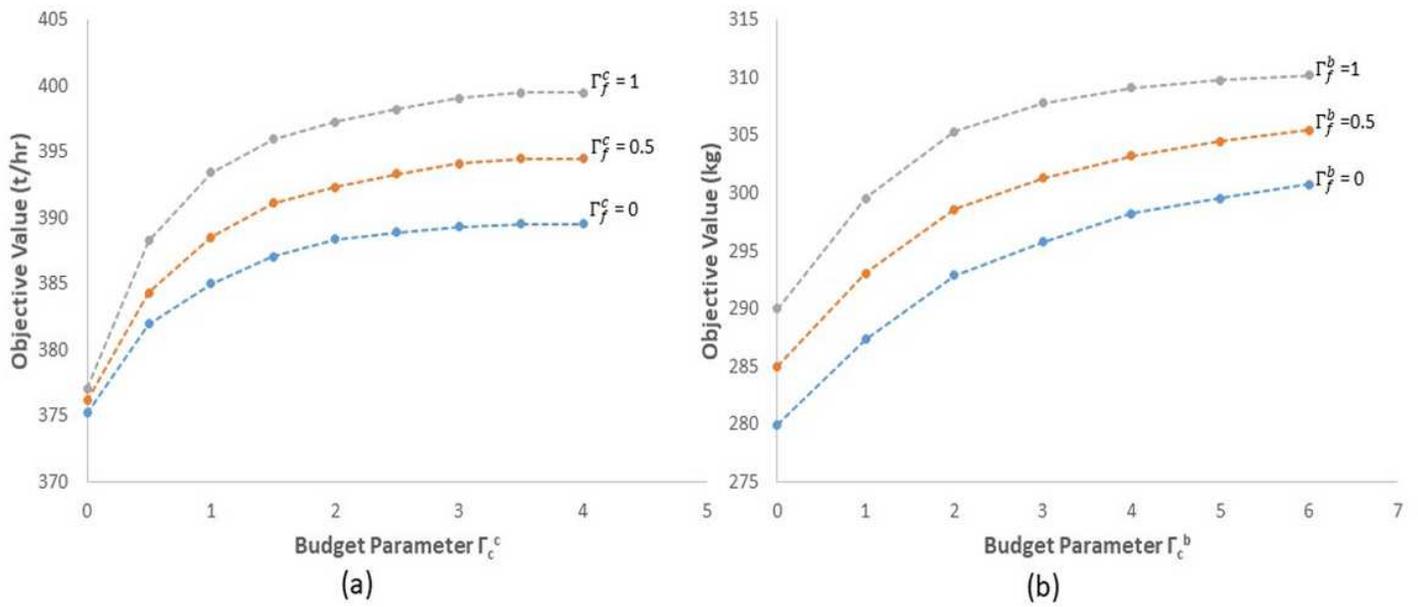


Figure 4

Effect of uncertainty on objective value using RO 3 (a) continuous process (b) batch process

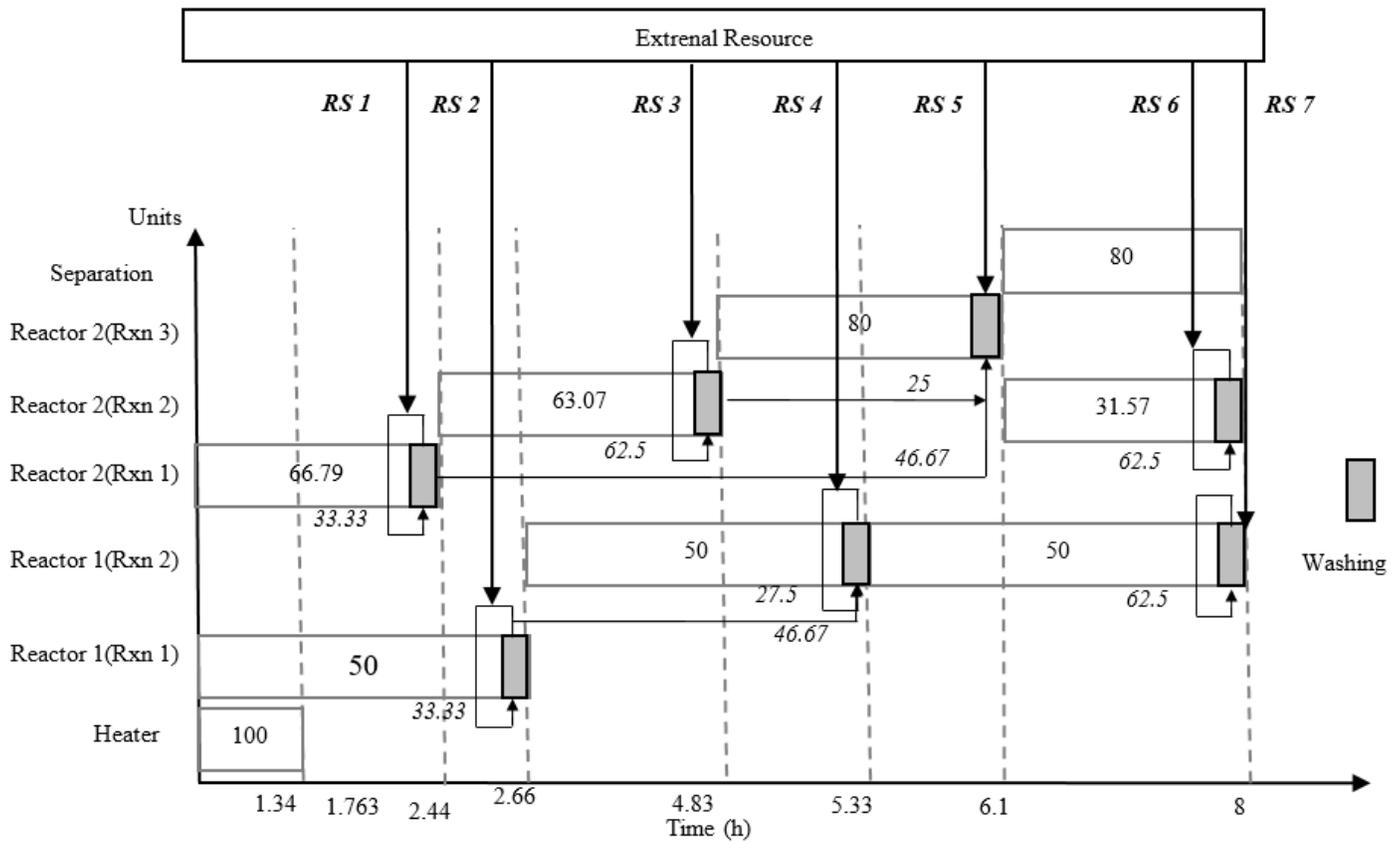


Figure 5

Possible RAN for Example 2

Supplementary Files

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