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Addressing the Scheduling of Chemical Supply Chains under Demand Uncertainty

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A multistage stochastic optimization model is presented to address the scheduling of supply chains with embedded multipurpose batch chemical plants under demand uncertainty. In order to overcome the numerical difficulties associated with the resulting large-scale stochastic mixed-integer-linear-programming (MILP) problem, an approximation strategy comprising two steps, and based on the resolution of a set of deterministic and two-stage stochastic models is presented. The performance of the proposed strategy regarding computation time and optimality gap is studied through comparison with other traditional approaches that address optimization under uncertainty. Results indicate that the proposed strategy provides better solutions than stand-alone two-stage stochastic programming and two-stage shrinking-horizon algorithms for similar computational efforts and incurs much lower computation times than the rigorous multistage stochastic model. © 2006 American Institute of Chemical Engineers *AIChE J,* 52: 3864-3881, 2006
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Introduction

The concept of Supply Chain Management (SCM), which appeared in the early 1990s, has recently raised a lot of interest since the opportunity of an integrated management of the supply chain (SC) can reduce the propagation of unexpected/undesirable events through the network, and can affect decisively the profitability of all the members. SCM looks for the integration of a plant with its suppliers and its customers to be managed as a whole, and the co-ordination of all the input/output flows (materials, information and finances) so that products are produced and distributed at the right quantities, to the right locations, and at the right time.[1] The main objective is to achieve suitable economic results together with the desired consumer satisfaction levels.

The design of a new SC, the retrofitting of an existing SC, or the planning of the operation of the chain to meet ever-changing market conditions can all be posed as a large-scale dynamic decision problems.[2] The computational challenges associated with these problem features are receiving increasing attention both in the operations research (OR) literature, and in the process systems engineering (PSE) community, and as a result of this effort, significant progress has been made in problem formulations and decomposition strategies.

This work focuses on the operational level of the SCM problem and addresses the multisite scheduling under uncertainty of a SC comprising several plants, warehouses and retailers, and including also the transport of materials between the various nodes embedded in the network. To tackle this problem, a rigorous scenario-based multistage stochastic mathematical model is derived, and several decomposition strategies are investigated aiming at the overcoming of the numerical difficulties associated with the computation of the underlying large-scale stochastic mixed-integer-linear-problem (MILP).

The article is organized as follows. First, a critical review of previous work on SC modeling and design is given. A formal definition of the problem is then presented and the underlying multistage stochastic model is derived. Various approaches that deal with optimization under uncertainty are next introduced, and the proposed decomposition strategy suggested to overcome the numerical difficulties of the aforementioned multistage stochastic model is described. Finally, some computa-

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tional results that highlight the advantages of our proposed approach are given together with the conclusions of the work.

Literature review

Numerous attempts have been made to model and optimize the SC behavior. Deterministic strategies[3,4] consider all model parameters, such as cost coefficients, production rates, demand, and so on, as being known. This assumption is usually not realistic due to the presence of numerous sources of technical and commercial uncertainty in the SC operation. Literature reveals that the most important and extensively studied source of uncertainty has been demand.[5,6] The emphasis on incorporating demand uncertainty into the planning decisions is appropriate given the fact that effectively meeting customer demand is what mainly drives most SC planning initiatives. Several approaches dealing with the uncertainty at different levels of the SC have been proposed.

Simulation-based approaches

A research stream in SCM under uncertainty has been oriented through simulation-based approaches. Dynamic process simulation has long been recognized as a useful tool for understanding and improving processes. Similarly, SC simulation is becoming a popular tool to formulate policies. In almost all the cases, the simulations are stochastic in that they repetitively sample the necessary parameters values from probability distributions of uncertain parameters to build-up distributions of performance measures, rather than point values.

Simulation approaches in the area of SCM under uncertainty usually work at a operational/tactical level. Part of the effort has been oriented through control theory in which the uncertainty is modeled as disturbances arriving to a dynamic model of the system.[7-9]

Multiagent-based approaches have also been applied for simulating distributed systems with somewhat decentralized decision-making (especially for short-term decisions).[10,11] In all the cases, the different players in the SC are represented by agents who are able to make autonomous decisions based on the information they have available and the messages they receive. The agents include warehouses, customers, plants and logistics functions.

Optimization-based approaches

Concerning the solution approaches available in the literature to deal with optimization under uncertainty, which addresses problems where a sequence of decisions must be computed under an uncertain environment, one can find two major methodologies from different research streams that formulate, and solve them by using a probabilistic representation of the uncertainty: stochastic optimal control and multi-stage stochastic programming. These two methodologies have been shown to be equivalent in that the decision prescribed by the optimal policy found by stochastic optimal control is the same as the corresponding optimal decision found by stochastic programming.[12]

Multistage stochastic programming with recourse

Multistage stochastic programming deals with problems that involve a sequence of decisions reacting to outcomes that evolve over time. At each stage, one makes decisions based on currently available information, that is, past observations and decisions, prior to the realizations of future events. The multistage stochastic programming has been extensively applied to solve tactical/strategic SCM problems.

Contributions belonging to this group differ primarily in the selection of the decision variables and the way in which the expected value term, which involves a multidimensional integral accounting for the probability distribution of the uncertain parameters, is computed. In view of this, two distinct methodologies for representing uncertainty can be identified within probabilistic methods. These are the scenario-based approach and the distribution-based approach.

In the former approach,[13–19] the uncertainty is described by a set of discrete scenarios capturing how the uncertainty might play out in the future. Each scenario is associated with a probability level representing the decision maker's expectation of the occurrence of a particular scenario. The scenario-based approach avoids the problem of multivariate integration when the random variables follow multidimensional continuous distributions. This is achieved by generating a finite set of scenarios, from sampling or a discrete approximation of the given distributions, to represent the probability space. With the scenarios or scenario tree specified, the stochastic program becomes a deterministic equivalent program.

In those cases where a natural set of discrete scenarios cannot be identified and only a continuous range of potential futures can be predicted, a distribution-based approach must be used.[5,6] By assigning a probability distribution to the continuous range of potential outcomes, the need to forecast exact scenarios is obviated.

Stochastic optimal control

Stochastic optimal control, or Markov decision process, characterizes a sequential decision problem in which the decision makers choose an action in the state occupied at any decision epoch according to a decision rule or policy. Dynamic programming provides a framework for studying such problems, as well as for devising algorithms to compute an optimal control policy. In the area of SCM, the stochastic optimal control has been mainly applied to solve operational/tactical problems.[20,21]

Finally, the most preferred nonprobabilistic method to cope with the uncertainty in SCM has been fuzzy programming.[22,23]

Operational approaches for SCM

A literature review with regard to operational approaches for SCM reveals that from an operational perspective, and due to the complexity associated with the interdependencies between the production/distribution tasks of the network, the detailed scheduling of the various processes of the SC has been left to be decided locally. Therefore, while the single-site production scheduling problem has been an active area of research in the chemical engineering community over the last decade,[24] the multisite case has so far received little attention.

Few works can be found in the literature dealing with the multisite scheduling problem. Almost all of them are deterministic approaches that consider all model parameters as being known.[25,3,26,27,28] On the other hand, research in the area of batch plants with demand uncertainty has focused more on the design aspect[29-31] than on operations scheduling. The scheduling of batch plants under demand uncertainty has emerged only recently as an area of active research.[32-34] The prevalent approach here is through the use of probabilistic models that describe the uncertain parameters in terms of probability distributions. Specifically, the two-stage stochastic programming approach has been the most preferred method over the last years.

Compared to these deterministic multisite scheduling approaches that have been presented in the literature to date, the methodology proposed in this article focuses on developing a model, and a solution strategy for a broader problem that deals with the scheduling of chemical SCs under demand uncertainty considering the possibility of modifying the original schedule as information arrives and uncertainty evolves over time. A multistage stochastic programming model is derived to tackle this problem. Such model exhibits binary variables not only in the first stage, but also in periods beyond the first one due to the possibility of further modifications to the original schedule once this is fixed at time zero. A decomposition strategy is also introduced aiming at the overcoming of the numerical difficulties associated with the aforementioned model.

Problem statement

Production-distribution networks that can be described through the state-task-network (STN) representation[35] are considered in this work. Materials are manufactured in multipurpose batch chemical plants, and stored in warehouses prior to being sent to final markets where they become available to customers. The following data is assumed to be known in advance:

- Set of raw materials, intermediate and final products to be manufactured, stored and transported through the nodes of the network.
- Set of production recipes and prices of final products.
- Structure of the embedded plants, that is, number of equipment units, their capacities and suitabilities for the labor tasks.
- Cost functions associated with raw materials, utilities consumption, holding inventory over the horizon and lost demand due to inadequate production.

It is assumed that sales of products are executed at the end of each of the periods of time in which the time horizon is divided. The demand associated with each of these periods cannot be perfectly forecast, and its uncertainty is represented by a set of scenarios with given probability of occurrence. Decisions regarding scheduling tasks are made in stages as information arrives and uncertainty unveils over time. Therefore, while the scheduling decisions regarding the whole SC (number of tasks to be performed, batch sizes, assignment and sequencing decisions) must be taken at the beginning of each period, that is, prior to the realization of the uncertainty, sales are computed once the random events take place at the end of the period, that is, beginning of the next one. Thus, the problem contemplated involves a sequence of decisions, that is, schedules, purchases of raw materials and sales of final products, that react to outcomes, that is, demand realization, that evolve over time. The model presented in this work assumes that all scheduling decisions are taken and completed within a period of time, that is, the tasks do not occur (spill) across successive

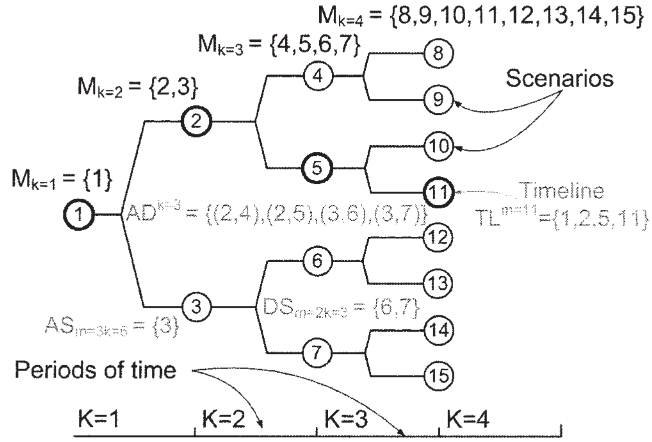

Figure 1. Scenario tree.

periods. Let us mention at this point that unlike other works in the literature, it is considered in this work that some of the demand can actually be left unsatisfied because of limited production capacity considerations.

Modeling assumptions

It is assumed that the time horizon is divided in $|K|$ periods, wherein the random variable (demand) takes a finite number of possible realizations. Each set of possible outcomes in each of the given periods is called a scenario.

The description of scenarios when talking about multistage stochastic programming is often made on a tree, such as that in Figure 1. Here, it is considered that there are $|M_K|$ scenarios that are evident in the last stage K with a probability equal to $Prob_{mK}$. In previous stages, we have a more limited number of possible realizations, which we call the stage k *scenarios* and represent by m_k. M_k denotes the set of scenarios till the end of period (k-1). E.g., M_1 consists only of the root node (1), M_2 consists of nodes at the end of period 1, that is, 2-3, and so on. Each of these period k scenarios is said to have a single *ancestor* scenario in stage k-1, and one or several *descendant* scenarios in stage k+1. We define AD^k to be the set of binary tuples representing all possible ancestor-descendant combinations at stage k of the scenario tree. For the example presented in Figure 1, $AD^3 = \{(2,4),(2,5),(3,6),(3,7)\}$, as it is depicted in the same figure. DS_{mk} represents the set of descendant scenarios of scenario m_k. For example, for m = 2 and k = 3, $DS_{mk} = \{6,7\}$, as it is depicted in the same figure. Finally, AS_{mk} represents the ancestor scenario of scenario m_k. For instance, for m = 3 and k = 6, $AS_{mk} = \{3\}$, as it is also shown in the figure.

Different scenarios at stage k may correspond to the same m_k realizations, and are only distinguished by differences in their ancestors.[36] Moreover, the root node of the scenario tree represents the initial state of the system, while the leaves of the tree are the end of the time horizon. Furthermore, every unique path from the root node to a leaf node represents one unique time-line (a unique future) along which the scheduling decisions executed could live through. Therefore, TL^{mK} represents the set of stage k *scenarios* belonging to the time-line that ends in scenario m_K at final stage K. For the example presented before, we have $TL^{11} = \{1,2,5,11\}$. The problem then is to obtain a schedule that maximizes the expected profit. This can be achieved by matching demand as closely as possible, thus, reducing inventories and minimizing the labor costs, and the costs for underproduction.

Multistage stochastic programming approach

In a multistage stochastic optimization approach the uncertain model parameters are considered random variables with an associated probability distribution, and the decision variables are classified into several stages. The first-stage variables correspond to those decisions which need to be made here-and-now, prior to the realization of the uncertainty. The k-stage variables (k>1) correspond to those decisions made after the uncertainty associated with the stages up to k-1 is unveiled. After the decisions up to k-1 are taken, and the random events up to k-1 are realized, the k-stage decisions are made subject to the restrictions imposed by the k-stage problem. Due to the stochastic nature of the performance associated with the *k*-stage decisions (k>1), the objective function consists of the sum of the first-stage performance measure, and the expected performance corresponding to the variables beyond the first period of time.

Therefore, having in mind the concepts previously presented, it is possible to formulate the scheduling problem as a ($|K| + 1$)-stage stochastic MILP whose solution involves the computation of the scheduling decisions to be implemented at each node in the scenario tree. Three types of constraints are considered within this formulation, the assignment, the mass balance and the capacity constraints. The mathematical formulation next derived is based on the STN representation,[35] which implies the discretization of each time period k into $|T|$ scheduling intervals of lower length. The mass balance equations have been modified to properly model the transport of materials between the nodes of the SC. To decouple units from tasks, we use the following rule: If a task *i* can be performed in two units *j* and *j′*, then two tasks i (performed in unit *j*), and *i′* (performed in unit j′) are defined.[37,38] The involved sets of equations are described in detail next.

Assignment Constraints. The basic assignment constraint 1 has been taken from the work of Shah et al.[39] in which the authors reformulated the original assignment constraint used by Kondili et al.[35]

$$\sum_{i \in I_j \cap NTR} \sum_{t'=t-pt_i+1}^{t} W_{it'km_k} \leq 1 \qquad \forall j \in J, \quad \forall t \in T, \quad \forall k < |K|, \quad \forall m_k \in M_k \quad (1)$$

This constraint implies that unit j cannot be assigned to tasks other than i during the interval [t-p_i+1,t] in every period k and scenario m_k, and, thus, ensures that at most one of these suitable tasks *i* is assigned to unit *j* during the defined interval in every period and scenario. It is only applied for production equipments ($i \in I_j \cap NTR$), and not for transport ones ($i \in I_j \cap TR$), that is, trucks. For transport equipments, it is necessary to consider both, the time required to transport materials from one node to another, and the time spent in coming back to the origin once the transport task has been accomplished as stated by Eq. 2

$$\sum_{i \in I_j \cap TR} \sum_{t'=t-2pt_i+1}^{t} W_{it'km_k} \leq 1 \qquad \forall j \in J, \quad \forall t \in T, \quad \forall k < |K|, \quad \forall m_k \in M_k \quad (2)$$

When transport tasks are carried out by external suppliers, which turns out to be a common situation, it seems reasonable to model them as an external utility consumed by the network. In this case the assignment constraints corresponding to the transport tasks can be omitted.

Mass balance Constraints. Here it is considered that scheduling decisions are taken within each period of time and are linked to adjacent periods of the scenario tree through the initial amounts of materials. Hence, the mass balances are enforced via the following constraints

$$S_{st0km_k} + Purch_{skm_k} = \sum_{i \in SI_s} B^I_{istkm_k} + Sales_{skm_k} \qquad \forall s \in S, \quad \forall k < |K|, \quad t = 1, \quad \forall m_k \in M_k \quad (3)$$

$$S_{st-1km_k} + \sum_{i \in SO_s} B^O_{ist-pt_ikm_k} = S_{stkm_k} + \sum_{i \in SI_s} B^I_{istkm_k} \qquad \forall s \in S, \quad \forall k < |K|, \quad \forall t > 1, \quad \forall m_k \in M_k \quad (4)$$

$$S_{st0km_k} = S_{stkm_k} + Sales_{skm_k} \qquad \forall s \in S, \quad k = |K|, \quad t = 1, \quad \forall m_k \in M_k \quad (5)$$

$$S_{st-1km_{k-1}} = S_{st0km'} \qquad \forall s \in S, \quad \forall k > 1, \quad t = |T|, \quad \forall m_{k-1}, \quad m'_k \in AD^k \quad (6)$$

$$S_{0_s} = S_{st0km_k} \qquad \forall s \in S, \quad k = 1, \quad \forall m_k \in M_k \quad (7)$$

That is, in Eq. 3 it is stated that the initial amount of state *s* plus the amount purchased must equal the holdup plus the amount consumed, and the sales. In this equation it is assumed that purchases and sales of products take place in the first time interval of each period of time in which the time horizon is divided. For final products (sFP) $Purchases_{st}$ should be removed if the possibility of outsourcing is not contemplated. Moreover, for raw materials (sRM) $Sales_{st}$ should be removed, and for intermediate products (sIP), both should be removed. Equation 4 represents the mass balance for time intervals beyond the first one. In this equation, we only consider the amount of materials in state s produced in time interval *t*, thus, omitting the purchases and sales terms. Constraint 5 is suitable for the first time interval of the last period of time, for which only sales decisions are computed. Finally, Eqs. 6 and 7 are applied to connect each scenario in stage k+1 with its *ascendant* scenario in stage *k* through the initial amounts of materials in state *s*

$$Sales_{skm_k} = Dem_{skm_k} \qquad \forall s \in S, \quad \forall k \in K, \quad \forall m_k \in M_k \quad (8)$$

In Eq. 8 it is stated that the sales can be lower or equal than the demand as it is assumed that some of the demand can be left unsatisfied because of limited production capacity or due to risk management considerations.

$$B^{I}_{istkm_k} = B_{itkm_k} \cdot (-\rho^{I}_{is}) \qquad \forall\, i \in NTR, \quad \forall\, s \in SI'_i, \quad \forall\, t \in T, \quad \forall\, k < |K|, \quad \forall\, m_k \in M_k \quad (9)$$

$$B^{O}_{istkm_k} = B_{itkm_k} \cdot \rho^{O}_{is} \qquad \forall\, i \in NTR, \quad \forall\, s \in SO'_i, \quad \forall\, t \in T, \quad \forall\, k < |K|, \quad \forall\, m_k \in M_k \quad (10)$$

Equations 9 and 10 compute the amounts of materials produced (continuous variable B^{O}_{istkmk}) and consumed (B^{I}_{istkmk}) from the batch size of task i started in time interval t (B_{itkmk}) and scenario m_k of period k. These equations are valid for nontransport tasks (iNTR) with constant values of mass fractions for consumption and production of states ($\rho^{\mathrm{I}}_{\mathrm{is}}$ and $\rho^{\mathrm{O}}_{\mathrm{is},}$ respectively)

$$\sum_{s \in SI'} B^{I}_{istkm_k} = B_{itkm_k} \qquad \forall\, i \in TR, \quad \forall\, t \in T, \quad \forall\, k < |K|, \quad \forall\, m_k \in M_k \quad (11)$$

$$B^{I}_{istkm_k} = \sum_{s' \in SO'_i \cap TSO_s} B^{O}_{is'tkm_k} \qquad \forall\, i \in TR, \quad \forall\, s \in SI'_i, \quad \forall\, t \in T, \quad \forall\, k < |K|, \quad \forall\, m_k \in M_k \quad (12)$$

On the other hand, constraints 11 and 12 are applied to model the transport tasks (iTR), which can operate over a range of mass fractions rather than for a given fixed value as occurred with the production ones. Therefore, Eq. 11 forces the summation over s of the continuous variable B^{I}_{istkmk} to be equal to the batch size of the transport task i (B_{itkmk}) started in time interval t in scenario m_k of period k. Equation 12 links the input and output states of a transport task i by forcing the total amount of output states s' coming from state s ($s' \in TSO_s$) to equal the input flow of s.

Capacity Constraints. The capacity limits for equipment and storage tanks can be expressed as follows

$$B^{MIN}_i \cdot W_{itkm_k} \le B_{itkm_k} \le B^{MAX}_i \cdot W_{itkm_k} \qquad \forall\, i \in I, \quad \forall\, t \in T, \quad \forall\, k < |K|, \quad \forall\, m_k \in M_k \quad (13)$$

$$0 \le S_{stkm_k} \le C_s \qquad \forall\, s \in S, \quad \forall\, t \in T, \quad \forall\, k < |K|, \quad \forall\, m_k \in M_k \quad (14)$$

Equation 13 bounds the batch size of each task i, while constraint 14 enforces the condition for which the amount of material in state s must be lower than the capacity of its storage tank in any time interval t within period k in scenario m_k

$$U_{utkm_k} = \sum_{i \in I_j} \sum_{t'=1}^{pt_i - 1} \alpha_{ui} \cdot W_{it-t'km_k} + \beta_{ui} \cdot B_{it-t'km_k} \qquad \forall\, u \in U, \quad \forall\, j \in J, \quad \forall\, t \in T, \quad \forall\, k < |K|, \quad \forall\, m_k \in M_k \quad (15)$$

$$0 \le U_{utkm_k} \le U^{\max}_{uk} \qquad \forall\, u \in U, \quad \forall\, t \in T, \quad \forall\, k < |K|, \quad \forall\, m_k \in M_k \quad (16)$$

Finally, for the utility requirements, we assume that the total consumption of utility u in time interval t within period k in scenario m_k can be expressed by Eq. 15, where fixed and variable coefficients for consumption of utility u by task i are introduced (α_{ui} and β_{ui}). The amount of utility consumed in a given period is also constrained to be lower than the maximum available one $U^{\mathrm{max}}_{\mathrm{uk}}$, as stated in Eq. 16.

Objective Function. The presented model accounts for the maximization of the total expected profit (Eq. 18). Revenues are obtained through sales of final products, while costs are due to the underproduction, that is, leaving part of the demand unsatisfied, purchases of raw materials, consumption of utilities and inventories as stated by Eq. 17

$$\begin{aligned} Profit_{m_K} = {} & \sum_{s \in S} \sum_{k \in K} \sum_{m'_k \in TL^{mK}} Sales_{skm'_k} \cdot Prices_s \\ & - \sum_{s \in S} \sum_{k \in K} \sum_{m'_k \in TL^{mK}} (Dem_{skm'_k} - Sales_{skm'_k}) \cdot UDCost_s \\ & - \sum_{s \in S} \sum_{k \in K} \sum_{m'_k \in TL^{mK}} Purch_{skm'_k} \cdot RMCost_s \\ & - \sum_{s \in S} \sum_{t \in T} \sum_{k \in K} \sum_{m'_k \in TL^{mK}} S_{stkm'_k} \cdot ICost_s \\ & - \sum_{u \in U} \sum_{t \in T} \sum_{k \in K} \sum_{m'_k \in TL^{mK}} U_{utkm'_k} \cdot UCost_u \end{aligned} \quad (17)$$

$$E[Profit] = \sum_{m_K} Prob_{m_K} \cdot Profit_{m_K} \quad (18)$$

Finally, the overall problem (model SCHEDMS) can be expressed as follows

$$maximize\ E[Profit]$$

subject to

$$constraints\ 1\text{–}18$$

This multistage stochastic formulation leads to a large-scale MILP that presents a high number of integer variables, which grows exponentially with the number of scenarios under study.

Two-stage stochastic programming approach

The solution of the K+1-stage stochastic program described before could be in principle addressed by means of mathematical programming tools. However, this would lead to high-computational requirements owing to its scale and complexity, which would make its implementation in a real scenario at present rather difficult. Therefore, in order to overcome the numerical difficulties associated with the resolution of the multistage formulation when a high number of scenarios and/or time periods are considered, it seems convenient to formulate the problem as a two-stage stochastic program regardless of the number of periods in which the demand resolves, thus, decreasing the total number of integer variables. The resulting two-stage model involves integer first-stage variables (scheduling decisions), and continuous second-stage ones (sales and inventory profiles). The two-stage formulation provides the same solution as the multistage formulation if the uncertainty in the demand resolves itself in only one stage, that is, it is only considered one period of time ($|K| = 1$). If this is not the case ($|K| > 1$), the solution computed by the two-stage model will be lower or equal to that provided by the *k*-stage formulation, since it will not consider the possibility of further modifications to the original schedule once this is fixed at time zero. Furthermore, the decomposable structure of the resulting two-stage program, that presents a convex and closed second-stage feasible region, could be exploited to reduce the computational requirements of the model.[40]

In our problem, decision variables related to the production schedule should be considered as first-stage decisions since they have to be taken at the beginning of the time horizon, that is, before the uncertainty is unveiled. On the other hand, the sales and, thus, the inventory profiles are second-stage variables. Therefore, at the end of the scheduling horizon, a different profit value is obtained for each particular realization of demand uncertainty, and the proposed model accounts for the maximization of the expected value of this profit distribution. Having in mind that there are $|K|$ periods in which decisions can be adapted to face the realization of uncertainty, it follows that for problems with $|K| > 1$ periods the two-stage stochastic formulation may lead to suboptimal solutions, as it is not considering the possibility of further modifications to the original schedule once this has been fixed at time zero.

Solution of two-stage stochastic models within a shrinking-horizon framework

Recently, Balasubramanian and Grossmann[41] applied an approximation strategy to solve large-scale stochastic multistage MILP, based on the solution of a series of two-stage models within a shrinking-horizon approach, thus, overcoming the computational difficulties associated with the problem sizes resulting from the former formulation.

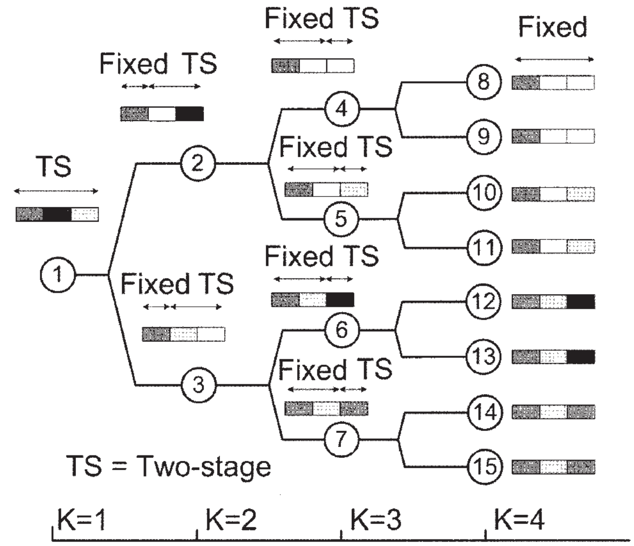

Figure 2. Two-stage models solved within a shrinking-horizon strategy.

Within this framework, two-stage stochastic models (SCHEDTS), which are used as simplifications of the original multistage problem, are formulated for the entire horizon of $|K|$ time periods. Although the solution of the model provides decisions for the entire horizon, only the decisions for the first time period are implemented. The state of the system is updated at the end of the first time period, and an approximate model is solved for the remaining $|K| - 1$ time periods (with decisions for the elapsed first time period already fixed). The algorithm (see algorithm 1) proceeds in this manner until decisions have been fixed for the entire horizon (see Figure 2).

The generic two-stage models (SCHEDTS) that are solved at the different nodes of the tree can be easily derived from the multistage stochastic model previously presented by defining the variables representing the scheduling decisions as not scenario-dependent, that is, the scheduling decisions are fixed at time zero and are not modified over time

Algorithm 1 Algorithm shrinking-horizon two-stage (SHT)
for k=1 to $|K|$ - 1 **do**

  for m_k = 1 to $|K|$ - 1 **do**

    Determine the set of all the descendant scenarios of m_k

    Solve SCHEDTS fixing S_{st0kmk} and with all the descendant scenarios of m_k

    Store W_{itk}, B_{itk}, B^{I}_{istk}, B^{O}_{istk}, $Purch_{skmk}$, $S_{st=|T|kmk}$ and $Sales_{skmk}$

  end for

end for

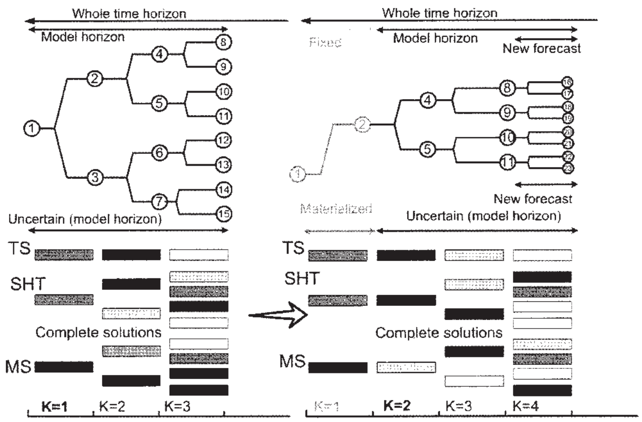

Figure 3. Rolling horizon strategy.

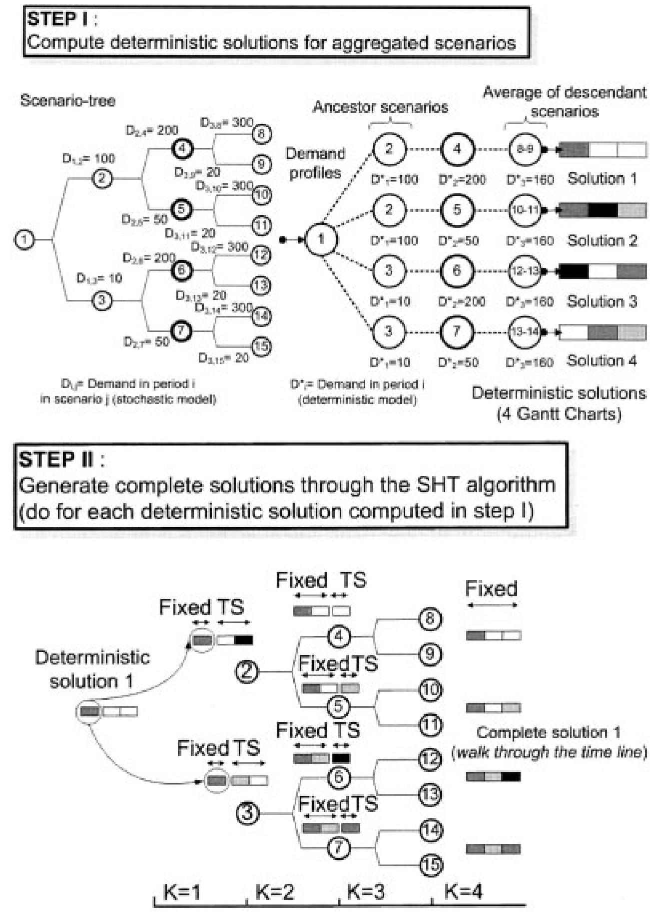

Figure 4. (a) Proposed approach (I). (b) Proposed approach (II).

The authors showed that the proposed approximation strategy provides an expected profit within a few percent of the multistage stochastic MILP result in a fraction of the computation time, and provides significant improvement in the expected profit over two-stage stochastic programming and similar shrinking-horizon deterministic approaches. This improvement is due to the consideration of further modifications to the original schedule in order to react to the realization of the uncertainty. However, the solution provided by this strategy may still be suboptimal compared to the multistage stochastic model.

Approximation approach

The multistage and two-stage stochastic programming approaches consider that in all the periods of time only demand forecasts within the initial time horizon are available. However, in practice, this is not the case, since these forecasts are usually recomputed within each period of time once the demand that finally materializes in the previous period is unveiled. This provides additionally forecasts for periods beyond the horizon considered at time zero. For this reason, in practice, demand and other uncertainties are accommodated in part by strategies that address optimization under uncertainty, that is, multistage and two-stage stochastic programming approaches and shrinking horizon algorithms, in the so-called rolling horizon mode.[42] That is, the operating horizon is divided into a certain number of periods, and the model with suitable demand forecasts is solved to yield scheduling decisions for each period, and only those belonging to the first period are implemented. At the end of the first period, the state of the system, including inventory levels, is updated and the cycle is repeated with the horizon advanced by one period considering the demand forecast for the new period, which is now available, as it is depicted in Figure 3. This means that if we were to implement the two-stage programming approach and the two-stage shrinking-horizon strategy in real time, both would lead to the same scheduling decisions, since the latter applies two-stage model to compute the scheduling decisions of the first node of the scenario tree, which are those to be executed in real time.

To improve these decisions implemented in real time, it is proposed in this work to consider the effect that the first-stage variables have on time periods beyond the first one when computing such variables. This is accomplished by combining the two-stage stochastic shrinking-horizon algorithm developed by Balasubramanian and Grossmann[41], with a deterministic scheduling formulation. A deterministic scheduling model is used to find potential candidate solutions for the first period of time in which the time horizon is divided. For each of these candidates, an adequate algorithm can be applied (for example, the shrinking-horizon algorithm) to assess them in terms of expected profit and produce complete solutions, that is, a *walk through the time-line*, considering all the nodes of the scenario tree

Algorithm 2 Algorithm deterministic shrinking-horizon two-stage (DSHT)

fix k

for $m_k = 1$ to $|M_k|$**do**

Compute the demand associated with each average scenario m^*_k as follows:

Solve SCHEDTS for average m_k

Store W_{itk}, B_{itk}, $B^I{}_{istk}$, $B^O{}_{istk}$, $Purch_{sk}$, S_{st+Tk} and $Sales_{sk}$ belonging to k=1

for k' = 2 to |K| - 1 **do**

for $m_{k'}=1$ to $|M_{k'}|$**do**

Determine the set of all the descendant scenarios of $m_{k'}$

Solve SCHEDTS fixing $S_{st0kmk'}$ and with all the descendant scenarios of m_k

Store $W_{itk'}$, $B_{itk'}$, $B^I_{istk'}$, $B^O{}_{istk'}$, $Purch_{sk'mk'}$, $S_{st=|T|k'mk'}$ and $Sales_{sk'mk'}$

end for

end for

Let X^{mk} be the approximated solution to SCHEDMS

end for

Use $x^*=\text{argmax}\{Obj(x^{mk})|m_k=1, 2, _k|\}$ as the estimate of the optimal solution of SCHEDMS

Therefore, the proposed approximation method (algorithm 2) comprises two steps. In first place, the deterministic formulation is applied to a set of aggregated scenarios computed from the scenario tree, thus, providing scheduling decisions for the first period of time. To generate these aggregated scenarios, it is proposed to fix a period of time *k* of the scenario tree, and then compute a set of $|M_k|$ aggregated scenarios. Each of these aggregated scenarios is associated with a scenario m_k of *k* and comprises a set of possible outcomes of the demand in each time period (that is, a demand profile for the entire time horizon). For periods from one to *k*, the demands are given by the ancestor scenarios of m_k. For periods beyond *k*, the demands are computed as the average of the descendant scenarios of m_k. These aggregated scenarios associated with *k* are labeled as m^*_k. Second, a set of two-stage models solved within a shrinking-horizon approach are used to compute the decision variables of those nodes of the scenario tree beyond the first period of time, and also to assess the deterministic solutions in terms of the expected profit achieved at the end of the time horizon.

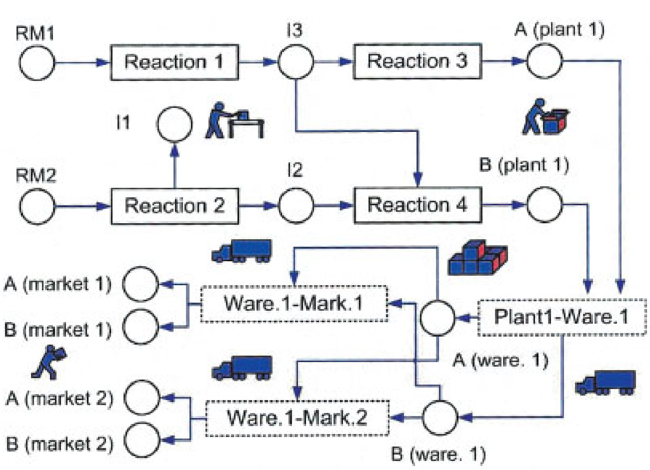

Figure 5. STN representation of case study 1.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Thus, our approach aims to improve the decisions of the first period of time which are implemented when such algorithm is applied in real time within a rolling-horizon strategy. As it will be shown through the case study, this improvement is achieved using similar computational efforts as the SHT, but with much lower computational effort than the multistage stochastic model.

Figure 4a and b illustrates the way in which the proposed strategy is applied to a simple case study comprising three periods of time, and two possible outcomes for the demand with equal probability of occurrence per period. In this case, four aggregated scenarios (that is, four demand profiles) are considered. These aggregated scenarios are generated taking as reference the scenarios in time period 2 and following the procedure described earlier. Thus, the demands of periods earlier than 2 are taken from the ancestor scenarios of the

Table 1. Processing Times of Tasks *i* (pt_i (h))

Task	pt_i	Task	pt_i
R1-RI1	4	R4-RII	6
R1-RI2	4	P1-W1	0
R2-RI1	4	W1-M1	0
R2-RI2	4	W1-M2	4
R3-RII	6		

Table 2. Maximum Batch Size of Task i (B_i^{MAX} (kg))

Task	B_i^{MAX}	Task	B_i^{MAX}
R1-RI1	100	R4-RII	250
R1-RI2	100	P1-W1	unlim.
R2-RI1	100	W1-M1	unlim.
R2-RI2	100	W1-M2	unlim.
R3-RII	250		

scenarios in period 2, while the demand in period 2 must equal the demand of the scenario used as reference. Finally, the demand for periods beyond the second one are computed by calculating the average of the descendant scenarios of the scenario taken as reference. For the first demand profile of the example depicted in Figure 4, which takes the scenario 4 as reference, we have that the demand of the first period is equal to 100, which is the demand in the ancestor scenario of scenario 4 (that is, scenario 2). The demand in period 2 is equal to the demand in scenario 4 (that is, 200). Finally, the demand in period 3 is determined by computing the average of the demand in the descendant scenarios of scenario 4 (that is, scenarios 8 and 9). In this case, assuming that each value of the demand has a 0.5 probability of occurrence, we have an average demand equal to 160 for period 3.

The deterministic formulation is then applied to each of the 4 demand profiles previously generated. This provides 4 deterministic solutions (that is, 4 Gantt Charts for the whole SC). Each of these deterministic solutions comprises a set of planning decisions that cover the entire time horizon. Our strategy proposes to keep those decisions belonging to the first period of time and discard the others. These decisions are then evaluated through the two-stage shrinking horizon strategy, which provides solutions for the remaining nodes of the scenario tree, and assess the first-stage solutions in terms of the expected profit achieved at the end of the time horizon. Figure 4b illustrates this part of the algorithm for the first deterministic solution. The decision variables of period 1 are fixed and the rest of variables are computed at each node in period 2 through a two-stage stochastic formulation that covers the whole time horizon. The decisions of period 2 are then frozen and those for periods beyond the second one are discarded. The procedure is then repeated until all the decisions in the scenario tree are computed thus generating a complete solution for the stochastic problem (that is, *a walk through the time-line*). With the scenario tree solved, one can compute the expected profit achieved at the end of the time horizon. After repeating this process for each deterministic candidate solution, the algorithm chooses the best one in terms of its expected profit.

Table 3. Mass Fractions for Consumption and Production of States by Task i (ρ_{is}^{I} and ρ_{is}^{O} (adim.))

	State						
Task	RM1	RM2	I1	I2	I3	A	B
R1-RI1	−1				1		
R1-RI2	−1				1		
R2-RI1		−1	0.1	0.9			
R2-RI2		−1	0.1	0.9			
R3-RII					−1	1	
R4-RII				−0.9	−0.1		1

Table 4. Price of State s ($Price_s$ (m.u.))

State	$Price_s$	State	$Price_s$	State	$Price_s$
RM1	300	A(M1)	3,000	B(M1)	16,650
RM2	10,500	A(M2)	3,000	B(M2)	16,350

Table 5. Inventory Cost of State s ($ICost_s$ (m.u./h))

State	$ICost_s$	State	$ICost_s$	State	$ICost_s$
RM1	1	A(P1)	10	B(M1)	55
RM2	35	B(P1)	55	A(M2)	10
I1	35	A(W1)	10	B(M2)	55
I2	35	B(W1)	55		
I3	1	A(M1)	10		

Table 6. Penalization for Demand of State s Unsatisfied ($UDCost_s$ (m.u./kg))

State	$UDCost_s$	State	$UDCost_s$
A(M1)	20	B(M1)	110
A(M2)	20	B(M2)	110

Computational effort

If it is assumed that B binary variables are needed for describing the scheduling of a time period k, it follows that a deterministic model with K periods will require B•K binary variables. The same number of binaries are necessary for a two-stage stochastic formulation. In the case of a multistage stochastic model, considering that there are M possible scenarios per time period, the number of binaries required would be $B[(M^K - 1)/(M - 1)]$. In the shrinking-horizon algorithm, the multistage stochastic model is approximated by a series of MILPs smaller in size than the former. Specifically, we would solve the first two-stage stochastic model with B•K binaries at the root node of the scenario tree, M two-stage MILPs with B•(K-1) at level two of the scenario tree, and so on. Finally, at the leaf nodes M^{K-1} MILPs with B binary variables should be

Table 7. Demand of State s ($Demand_{skmk}$ (kg))

State	
$k = 1$	
A(M1)	316
A(M2)	0
B(M1)	0
B(M2)	155
$k = 2$	
A(M1)	(400, 731, 367, 705, 356, 703, 413, 709, 407, 669, 382, 678, 329, 688, 355)
A(M2)	0
B(M1)	0
B(M2)	(176, 318, 183, 405, 203, 386, 211, 353, 201, 413, 222, 353, 173, 347, 175)
$k = 3$	
A(M1)	(318, 318, 330, 324, 320, 318, 317, 469, 334, 502, 289, 380, 331, 336, 326)
A(M2)	0
B(M1)	0
B(M2)	(143, 183, 164, 156, 145, 169, 148, 225, 157, 202, 167, 222, 159, 211, 160)

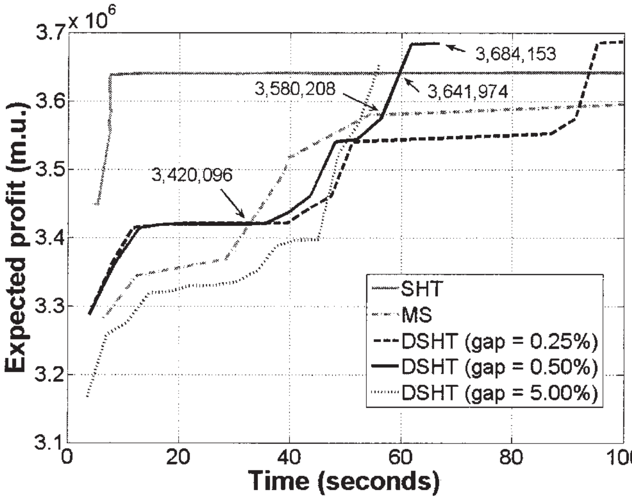

Figure 6. Case study 1a: computational results.

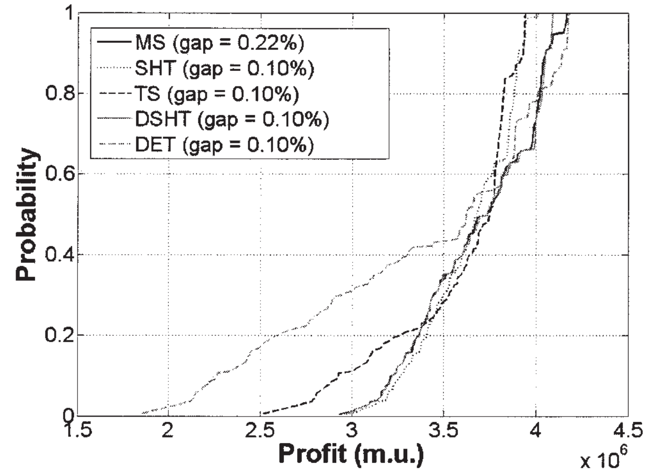

Figure 7. Case study 1a: probability curves.

computed. Eq. 19 shows the number of MILPs to be solved in this strategy

$$1 + M + M^2 + \cdots + M^{K-1} \tag{19}$$

The proposed algorithm implies the computation of a series of shrinking-horizon algorithms in which the first two-stage model is replaced by a deterministic formulation. Assuming that N deterministic candidates are evaluated, the overall algorithm would lead to the following number of MILPs

$$N \cdot (1 + M + M^2 + \cdots + M^{K-1}) \tag{20}$$

As it has been previously mentioned, the expressions given above provide the number of MILPs problems that are solved when a specific decomposition technique is applied and the number of binary variables required by each of these MILPs. This information provides an estimate of the computational effort associated with each algorithm.

The performance of the proposed algorithm can be enhanced in several ways. First, the number of iterations to be executed can be fixed, that is, decide beforehand the number of deterministic solutions that will be evaluated through the shrinking-horizon two-stage algorithm. A low-number of iterations will reduce the computational effort required but on the other hand may lead to solutions with higher-optimality gaps. Furthermore, the parameters of the MILP solver can be tuned according to the needs of our algorithm. Specifically, it is possible to change the relative optimality tolerance for the MILP models computed by the MILP solver, in this case CPLEX. Therefore, by increasing the optimality tolerance with which the models are solved, it is possible to decrease the computational effort of the overall algorithm, which on the other hand will also affect to the quality of the final solution.

Concerning the performance of the algorithm, two parameters will be analyzed, the optimality gap of the final solution and the computational time consumed. The optimality gap is determined considering the exact solution of the multistage stochastic model, or the solution of its LP relaxation if the model can not be solved to optimality. For the two-stage, shrinking-horizon two-stage and multistage approaches, it has been observed that the time consumed varies only with the optimality tolerance fixed to the solver. On the other hand, the time consumed by the proposed algorithm depends not only on the optimality tolerance fixed to the solver but also on the number of iterations. As it will be shown in the case study, the presented strategy provides solutions which are better than those given by the two-stage and shrinking-horizon two-stage approaches incurring similar CPU times. Moreover, these solutions exhibit low-optimality gaps, and the CPU times involved in their computation are much lower than those reported by the multistage stochastic formulation.

Computational results

Several examples to illustrate the performances of our algorithm are presented next. All the models were solved on a AMD Athlon 3000 computer using the MIP solver of CPLEX (7.0). All the examples have been adapted from other single-site scheduling case studies presented in the literature,[35, 43] which have been widely applied in the PSE community.

In this work, we have compared the computational results obtained with the various approaches over a range of values of the optimality gap fixed to the MIP solver, and therefore over

Table 8. Case Study 1a: Computational Results

	E[*profit*] (m.u.)	Gap (%)	Min. (m.u.)	Max. (m.u.)	CPU Time (s)
DET	3,384,691	8.42	1,843,056	4,177,601	0.89
TS	3,579,687	3.15	2,504,089	3,941,538	8.91
SHT	3,640,126	1.51	2,971,916	4,012,967	12.85
DSHT	3,687,421	0.23	2,940,654	4,091,780	401.70
MS	3,688,042	0.22	2,933,316	4,166,065	50,000.00

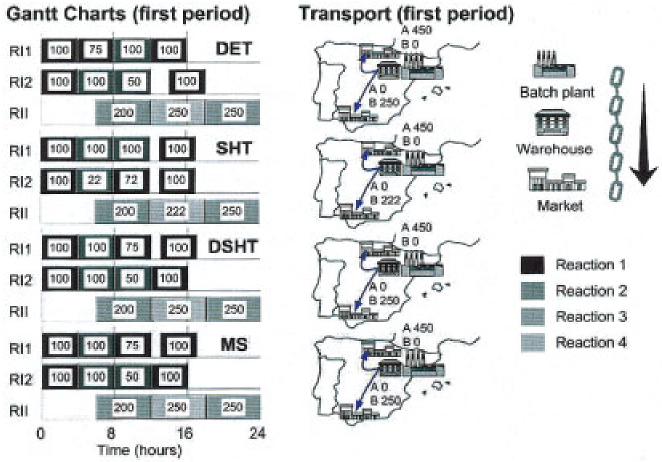

Figure 8. Case study 1a: schedules and transport decisions.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

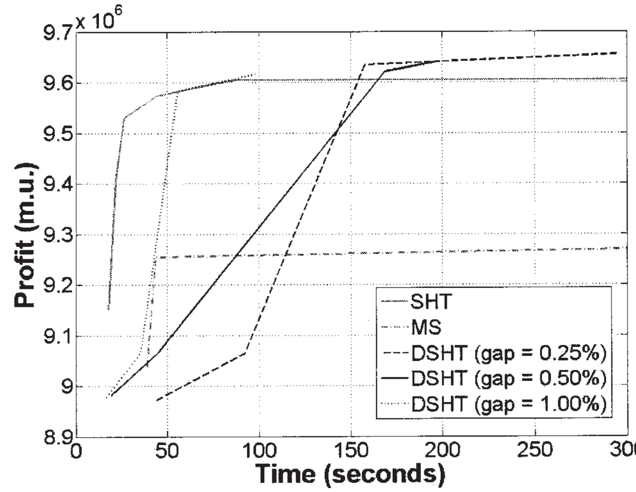

Figure 9. Case study 1b: computational results.

a range of computation times, rather than for a single value. This makes the difference with respect to other works in the literature in which the solutions are only compared for a given value of the optimality gap.[41] It is believed that our comparison provides a more accurate information regarding the performance of the different approaches, since the CPU time required in each case depends on the specific value of the optimality gap being analyzed. As it will be discussed later, each stochastic approach will perform better for a specific range of values of optimality gap depending on the example under study.

Let us notice at this point, that the optimality gap fixed to the multistage model represents indeed the "real" optimality gap of the problem, that is, it measures how far a solution is from the optimal solution of the overall problem. On the other hand, the optimality gap fixed to the subproblems to be solved within a decomposition strategy, for instance, to the two-stage shrinking horizon algorithm, measures for each two-stage stochastic subproblem in which the overall problem is decomposed, the difference between a solution and its optimal solution. In other words, both optimality gaps are not the same. In fact, the optimal solution of the multistage problem may not be reached even if we solve all the two-stage stochastic models computed within the shrinking-horizon strategy up to optimality.

Table 9. Demand of State *s* ($Demand_{skmk}$ (kg))

State	$Demand_{skmk}$
A(M1)	630
A(M2)	0
B(M1)	0
B(M2)	269
A(M1)	(653, 1461, 664, 1409)
A(M2)	0
B(M1)	0
B(M2)	(336, 509, 279, 647)
A(M1)	(612, 876, 627, 856)
A(M2)	0
B(M1)	0
B(M2)	(243, 361, 250, 334)
A(M1)	(676, 1406, 800, 1418)
A(M2)	0
B(M1)	0
B(M2)	(273, 618, 282, 564)

Example 1

Here, we investigate the scheduling under demand uncertainty of a SC comprising one plant, one warehouse and two final markets. The plant embedded in the SC (P1) manufactures two different products (A and B) which are stored in a warehouse (W1) prior to being sent to the final markets (M1 and M2) where they become available to customers. The STN representation of this example is given in Figure 5, while the data can be found in Tables 1 to 7. The structure of the plant has been adapted from the case study presented by Maravelias and Grossmann.[43] There are two types of reactors available for the process (type I and II) with different numbers of corresponding units available: two reactors (RI1 and RI2) of type I, but only one reactor (RII) of type II. Reactions R1 and R2 require a type I reactor, whereas reactions R3 and R4 require a type II reactor. The plant operates under a UIS policy (unlimited intermediate storage) for all the states. Two examples are presented that differ in the number of time periods, scenarios and the length of the time horizon. The initial inventories are assumed to be equal to zero for all the states. Two different types of utilities are considered, the first one, which is associated with the labor tasks, has a unitary cost of 0.25 m.u. while the second one, which corresponds to the transport services, costs 0.1 m.u. per unit. The fixed and variable coefficients for consumption of utility by tasks (α_{ui} and β_{ui}) are equal to 2,000 units of utility/h and 20 units of utility/kg•h, respectively for all the labor tasks and 50 units of utility/h and 5,000 units of utility/kg•h for transport ones. The availability of both utilities is assumed to be unlimited.

Example 1a

In this example, it is assumed a time horizon of 48 h, divided into two equally long time periods. Such periods are also divided into 24 scheduling intervals of 1 h each. 15 possible events in each period of time, that is, 15 possible values for the demand, are considered. This leads to 225 scenarios for the entire time horizon.

Table 10. Case Study 1b: Computational Results

	$E[profit]$ (m.u.)	Gap (%)	Min. (m.u.)	Max. (m.u.)	CPU Time (s)
DET	8,190,296	15.97	1,336,513	11,685,814	8.98
TS	9,306,710	4.51	5,465,061	11,272,959	35.05
DSHT	9,654,860	0.94	6,326,741	12,486,544	137.40
SHT	9,553,712	1.98	6,953,319	11,759,319	62.36
MS	9,638,721	1.12	6,133,053	12,650,022	50,000.00

Figure 6 shows the computational results obtained by applying the various approaches, that is, the two stage stochastic formulation (TS), the two-stage shrinking-horizon strategy (SHT), the proposed approximation method (DSHT), and the multistage stochastic formulation (MS). The curves shown in the figure have been obtained for each of these approaches by gradually changing the value of the optimality gap fixed to the solver. With regard to the presented approximation strategy, let us mention that such algorithm provides for each value of the optimality tolerance fixed to the solver as many solutions as aggregated scenarios are explored. In this work, the whole set of solutions provided by the DSHT, and not only the best one, have been plotted. Therefore, for a given number of aggregated scenarios explored, and for each value of the optimality gap for which the DSHT has been solved, one curve corresponding to the worst case of the algorithm has been plotted. This curve represents the evolution of the proposed algorithm in each iteration assuming that all the solutions are sorted in an ascendant way in terms of objective function value. It would be also possible to obtain another curve, the best case curve, which would represent the case in which the best solution is achieved in the first iteration of the algorithm. This curve would be an horizontal line intersecting the former in its highest point. In this case study, 15 aggregated scenarios have been explored in the DSHT strategy.

After 50,000 s of computation time, the best solution obtained by the MS is equal to 3,688,042 m.u., still within 0.22% of the best relaxed solution (in our case 3,696,058 m.u.) obtained during the branch and bound procedure when the time limit of 50,000 s was exceeded. By increasing gradually the optimality tolerance of the solver up to 20%, different solutions were obtained, and the associated curve was plotted. This procedure was also followed with the SHT in order to obtain the points of its curve. In this case, the best solution computed in 50,000 CPU s by solving all the TS models of the SHT with an optimality gap of 0.05% is equal to 3,641,974 m.u., which is within 1.46% of the best solution. With regard to the approximation strategy, for the sake of simplicity, only three curves corresponding to the algorithm computed by solving all the deterministic, and TS subproblems with values of optimality gap equal to 0.25%, 0.50% and 5.00% have been plotted. As it can be observed, when the gap is decreased the worst case curve of the DSHT goes up and to the right, that is, the approximation strategy yields better solutions, but on the other hand leads also to higher computation times.

In the figure, one can see how the curve representing the MS intersects each of the worst case curves of the DSHT at least in one point. In the case of the curve computed with an optimality gap equal to 0.50%, it intersects in two points. The first intersection point yields an expected profit of 3,420,096 m.u., while the second one, leads to 3,580,208 m.u. Therefore, for objective function values below 3,420,096 m.u., the propose approach performs better than the MS since the curve associated with the latter lies entirely on the right side of that corresponding to the former, that is, the proposed approach leads to lower computation times than the MS formulation. The best solution computed by the DSHT with a gap of 0.50% is equal to 3,684,153 m.u. (within 0.32% of the best possible solution). As it can be observed in the figure, although the MS stochastic formulation can find better solutions than those provided by the DSHT algorithm it leads to a dramatic increase in CPU time. With regard to the SHT, its curve intersects the worst case curve of the proposed approach solved with a gap of 0.50% in an expected profit equal to 3,641,974 m.u. This value represents also the best solution that can be computed by the

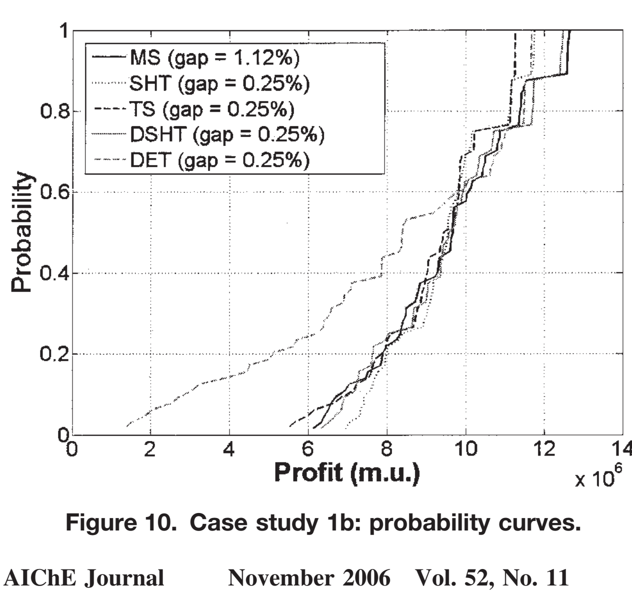

Figure 10. Case study 1b: probability curves.

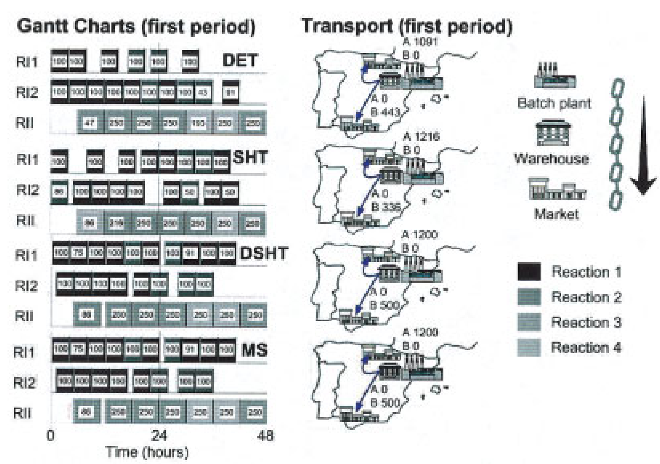

Figure 11. Schedules and transport decisions.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

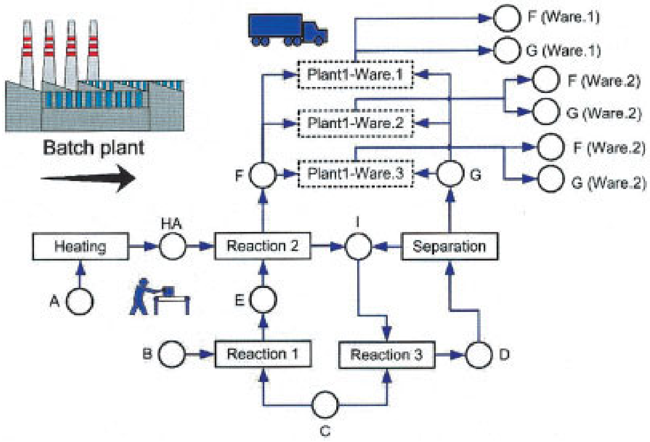

Figure 12. STN representation of case study 2 (I).

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

SHT algorithm. This means that for solutions below 3,641,974 m.u., the SHT strategy has a certain probability of yielding lower computation times than our algorithm. On the other hand, the SHT can not find solutions above 3,641,974 m.u., even if we solve all the TS subproblems up to optimality.

In Table 8, the expected profit and the minimum and maximum scenarios of the results computed by means of the SHT algorithm, the TS and the proposed strategy are given together, with the deterministic solution evaluated through the two-stage stochastic formulation (DET), and the best solution provided by the MS approach. All the models have been computed by fixing to the solver a tolerance, that is, an optimality gap, of 0.10%. The optimality gap of each solution, that is, the difference between the final solution provided by each approach, and the best relaxed solution (in our case 3,696,058 m.u.) obtained during the branch and bound procedure when the time limit of 50,000 s was exceeded, is also given in the table. Let us notice that although the optimality tolerance fixed to the solver is equal to 0.10% in all the cases, the overall solutions computed by the various approaches exhibit different optimality gaps, that is, the distances between the solutions provided by each specific algorithm and the optimal solution of the overall problem are not equal to 0.10%.

As it can be observed, the MS approach leads to the best solution although it is not capable of reaching the optimality gap of 0.10% after 50,000 CPU s. The proposed algorithm yields an expected profit which is very close to the one provided by the MS approach, and also incurs much less CPU time than the former. With regard to the TS and the SHT, let us note that both approaches yield lower computation times than the proposed algorithm, but they provide poorer solutions in terms of expected profit, that is, solutions with higher optimality gaps. Finally, the DET approach leads to the lowest CPU time, but also provides the poorest solution. One important thing to notice is that the deterministic formulation (nominal demands) predicts a solution that performs poorly under the uncertain environment, that is, the schedule obtained with the nominal parameters can be critically inefficient when another demand is ordered although it is the best one for the mean scenario. Indeed, although the profit of the deterministically generated schedule is higher than those of their stochastic counterparts in the nominal scenario, when the former is used in the presence of uncertainty, the expected profit value drops by nearly 24% (4,192,304 m.u. for the mean scenario and 3,384,691 m.u. under the uncertain environment).

Figure 7 shows the probability curves corresponding to the aforementioned solutions. As it can be observed, the solutions behave in different ways under the uncertain environment using as reference the MS solution. Specifically, the SHT provides a slightly conservative solution which exhibits low-probabilities of small profits, and also small probabilities of high-profits. On the other hand, the DSHT behave very similar to MS as it also involves high-probabilities of small profits, and also big benefits, thus, showing the trade-off between policies of risk-taker and risk-averse decision makers. For instance, the SHT provides a solution that yields a 9.3% probability of profits bellow 3,250,000 m.u., while the MS solution and the solution computed by the proposed algorithm lead to a 12.5%. On the other hand, the SHT provides a 1% probability of profits higher than 4,000,000 m.u., while the MS yields a 26.7% probability and the approximation algorithm a 27.6%.

Let us note also that the DET and the TS approaches provide the poorest solutions in terms of risk, since they lead to the highest probabilities of small profits. For instance, the DET curve yield a 38.2% probability of profits under 3,250,000 m.u., while the TS formulation provides a 19.6%. Moreover, this increase in risk is not compensated by an increase in opportunity, as occurred with the MS solution, and the solution computed with the proposed algorithm. Therefore, while the DET solution provides a 22.2% chance of benefits above 4,000,000 m.u., the TS one do not even show profits higher than 4,000,000 m.u. Similar conclusions can be derived from Table 8, in which the maximum and minimum scenarios associated with each solution are given. The SHT, which provides the more conservative solution, shows the highest minimum scenario, and also the lowest maximum. On the other hand, the MS formulation and the proposed approach, which involve riskier policies, yield lower minimum scenarios, but also provide the highest maximum scenarios. Let us notice at this point that the SHT applies a two-stage stochastic model to compute

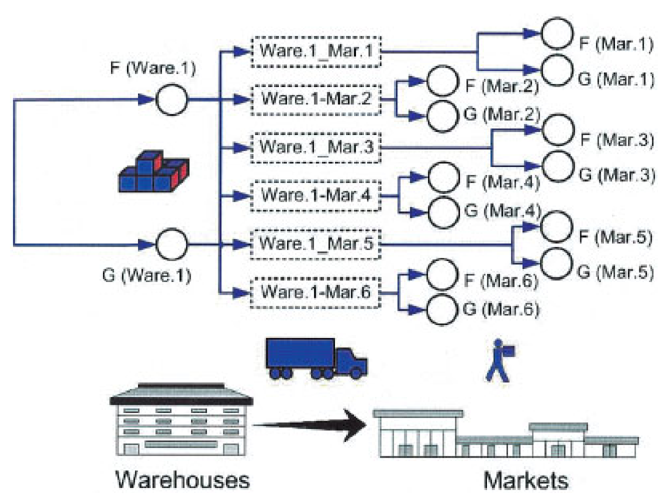

Figure 13. STN representation of case study 2 (II).

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Table 11. Processing Times of Tasks i (pt_i (h))

Task	pt_i	Task	pt_i	Task	pt_i	Task	pt_i
Heating-H(P1)	8	Reaction1-RII(P2)	12	P2-W2	0	W2-M3	4
Reaction1-RI(P1)	12	Reaction2-RI(P2)	12	P2-W3	4	W2-M4	6
Reaction1-RII(P1)	12	Reaction2-RII(P2)	12	W1-M1	0	W2-M5	4
Reaction2-RI(P1)	12	Reaction3-RI(P2)	12	W1-M2	8	W2-M6	8
Reaction2-RII(P1)	12	Reaction3-RII(P2)	12	W1-M3	4	W3-M1	4
Reaction3-RI(P1)	12	Separation-S(P2)	8	W1-M4	8	W3-M2	4
Reaction3-RII(P1)	12	P1-W1	0	W1-M5	8	W3-M3	0
Separation-S(P1)	8	P1-W2	8	W1-M6	12	W3-M4	2
Heating-H(P2)	8	P1-W3	4	W2-M1	8	W3-M5	2
Reaction1-RI(P2)	12	P2-W1	8	W2-M2	0	W3-M6	4

Table 12. Maximum Batch Size of Task i (B_i^{MAX} (kg))

Task	B_i^{MAX}	Task	B_i^{MAX}	Task	B_i^{MAX}	Task	B_i^{MAX}
Heat.-H(P1)	500	Rea.1-RII(P2)	250	P2-W2	80,000	W2-M3	80,000
Rea.1-RI(P1)	250	Rea.2-RI(P2)	300	P2-W3	80,000	W2-M4	80,000
Rea.1-RII(P1)	200	Rea.2-RII(P2)	250	W1-M1	80,000	W2-M5	80,000
Rea.2-RI(P1)	250	Rea.3-RI(P2)	300	W1-M2	80,000	W2-M6	80,000
Rea.2-RII(P1)	200	Rea.3-RII(P2)	250	W1-M3	80,000	W3-M1	80,000
Rea.3-RI(P1)	250	Sep.-S(P2)	600	W1-M4	80,000	W3-M3	80,000
Sep.-S(P1)	500	P1-W2	80,000	W1-M6	80,000	W3-M4	80,000
Heat.-H(P2)	500	P1-W3	80,000	W2-M1	80,000	W3-M5	80,000
Rea.1-RI(P2)	300	P2-W1	80,000	W2-M2	80,000	W3-M6	80,000

the decisions of the first period of time. The conservative nature of the solution computed by the SHT may be, therefore, given by the assumption made in the TS formulation in which no modifications to the original schedule are permitted once this is fixed at time zero.

In Figure 8, for each approach, the schedules and the transport decisions associated with the first node of the scenario tree are given. The batch sizes and flows of materials given in the figure are expressed in Kg. Let us mention that all the schedules involve the execution of the same number of tasks, although the batch sizes are different in each case. Specifically, the solutions provided by the DET, the DSHT and the MS approaches exhibit the same batch sizes, which are higher than those computed by the SHT. The former represents a risky policy, while the latter can be seen as a conservative policy. Both policies are indeed reflected in the probability curves associated with the solutions, which were previously described.

Example 1b

In this example, it is assumed a time horizon of 144 h, divided into three equally long time periods. Each of these periods is also divided in 48 scheduling intervals of 1 h each. The scenario tree comprises 4 possible events in each period of time which leads to 64 scenarios for the entire time horizon. In this case, 4 aggregated scenarios haven been explored. Table 9 shows the demand data of this example.

Figure 9 shows the computational results obtained by applying the various approaches. After 50,000 s of computation time, the best solution obtained by the MS stochastic formulation is equal to 9,638,721 m.u., still within 1.12% of the best relaxed solution. The best solution computed in 50,000 CPU s by the SHT algorithm by solving all the two-stage stochastic models of the SHT with an optimality gap equal to 0.05% is equal to 9,603,712 m.u., which is within 1.47% of the best relaxed solution. With regard to the DSHT, three curves corresponding to the algorithm computed with gaps of 0.25%, 0.50% and 1.00% have been plotted.

The obtained figure is very similar to that of the previous case, and, therefore, similar conclusions can be derived. The MS formulation intersects the worst case curves of the DSHT computed with gaps of 0.25% and 0.50%, but lies completely on the right-side of the curve corresponding to a gap of 1.00%. This means that for expected profits bellow 9,615,490 m.u., which is the best solution achieved by the DSHT with a gap of 1.00%, the proposed algorithm performs better than the MS formulation. With regard to the SHT strategy, its curve intersects all the curves computed with the proposed approach in an expected profit equal to

Table 13. Mass Fractions for Consumption and Production of States by Task i (ρ_{is}^I and ρ_{is}^O (adim.))

	State								
Task	A	B	C	D	E	F	G	HA	I
Heating-H	−1							1	
Reaction1-RI		−0.9	−0.1		1				
Reaction1-RII		−0.9	−0.1		1				
Reaction2-RI					−0.6	0.9		−0.4	0.1
Reaction2-RII					−0.6	0.9		−0.4	0.1
Reaction3-RI			−0.9	1					−0.1
Reaction3-RII			−0.9	1					−0.1
Separation-S				−1			0.9		0.1

Table 14. Price of State s ($Price_s$ (m.u.))

State	$Price_s$	State	$Price_s$	State	$Price_s$	State	$Price_s$
F(M1)	6,600	F(M6)	7,500	G(M5)	27,000	A(P2)	300
F(M2)	6,600	G(M1)	24,000	G(M6)	25,500	B(P2)	600
F(M3)	6,000	G(M2)	24,000	A(P1)	360	C(P2)	1,200
F(M4)	5,700	G(M3)	25,500	B(P1)	660		
F(M5)	6,900	G(M4)	26,250	C(P1)	12,150		

Table 15. Inventory Cost of State s ($ICost_s$ (m.u./h))

State	$ICost_s$	State	$ICost_s$	State	$ICost_s$	State	$ICost_s$
A(P1)	0.6	A(P2)	0.5	F(W1)	10.0	F(M4)	9.5
B(P1)	1.1	B(P2)	1.0	F(W2)	10.0	F(M5)	11.5
C(P1)	20.3	C(P2)	20.0	F(W3)	10.0	F(M6)	12.5
D(P1)	20.3	D(P2)	20.0	G(W1)	40.0	G(M1)	40.0
E(P1)	10.8	E(P2)	10.5	G(W2)	40.0	G(M2)	40.0
F(P1)	10.5	F(P2)	10.0	G(W3)	40.0	G(M3)	42.8
G(P1)	40.3	G(P2)	40.0	F(M1)	11.0	G(M4)	43.8
HA(P1)	0.6	HA(P2)	0.5	F(M2)	11.0	G(M5)	45.0
I(P1)	0.8	I(P2)	20.0	F(M3)	10.0	G(M6)	42.5

Table 16. Penalization for Demand of State s Unsatisfied $UDCost_s$ ($UDCost_s$ (m.u./kg))

State	$UDCost_s$	State	$UDCost_s$	State	$UDCost_s$	State	$UDCost_s$
F(M1)	44	F(M4)	38	G(M1)	130	G(M4)	175
F(M2)	44	F(M5)	46	G(M2)	170	G(M5)	180
F(M3)	40	F(M6)	50	G(M3)	170	G(M6)	170

9,603,712 m.u. This represents also the best solution that the SHT can provide.

In Table 10 the expected profit and the minimum and maximum scenarios provided by the various approaches, with an optimality gap equal to 0.25% are given. As it can be observed, the proposed algorithm yields the highest expected profit also incurring much less CPU time than the MS approach, which provides the second highest expected profit. As occurred before, the SHT and TS approaches incur in less time than the proposed algorithm, but also lead to lower expected profits. Finally, although the DET approach incurs low CPU time it leads to the poorest profit, and when its solution is evaluated in the presence of uncertainty, the expected profit value drops by nearly 43% (11,728,621 m.u. for the mean scenario and 8,190,296 m.u. under the uncertain environment).

Figure 10 shows the probability curves corresponding to the aforementioned solutions. Again, the solution computed by the SHT turns out to be the most conservative, as it yields the lowest probabilities for small profits. On the other hand, it also leads to poor probabilities of high-profits. The MS formulation and the proposed algorithm lead to an increase in risk when compared to the solution provided by the SHT. However, such increase is compensated by and increase in opportunity. The TS approach and the DET solution lead to the riskiest solutions which do not even show high chances of big profits. Similar conclusions can be derived by looking at the values of the maximum and minimum scenarios corresponding to the approaches, which are shown in Table 10. The SHT provides the highest minimum scenario, while the DSHT and the MS approach lead to the highest maximum scenarios. On the other hand, the DET and the TS solutions lead to low-minimum scenarios, and also to small maximum scenarios.

In Figure 11, the schedules and the transport decisions associated with the first node of the scenario tree are given. In this case, the solutions provided by the MS, the DSHT and the DET approaches involve the execution of one more task (reaction 2) than the one computed by the SHT. The production rates computed by the DSHT and the MS are the same, and are higher than those given by the DET and SHT. Again, the former represents a risky policy, while the latter leads to a conservative, as it was previously mentioned when describing the probability curves associated with the solutions.

Example 2

Here we solve the scheduling under uncertainty of a SC comprising several plants, warehouses and retailers distributed in different locations. The plants embedded in the SC (P1 and P2) manufacture two different products (F and G) which are stored in three warehouses (W1 to W3) prior to being sent to six final markets (M1 to M6), where they become available to customers. The STN representation of the network under study is given in Figures 12 and 13, while the associated data are listed in Tables 11 to 17. The plants of the network are assumed to be multipurpose batch-chemical plants, with a structure adapted from the case study proposed by Kondili et al.[35] There is unlimited storage for all the states. The initial inventories are

Table 17. Demand of State s ($Demand_{skmk}$ (kg))

State	$Demand_{skmk}$
$k = 1$	
F(M1)	32
G(M1)	31
F(M2)	29
G(M2)	31
F(M3)	31
G(M3)	122
F(M4)	14
G(M4)	13
F(M5)	12
G(M5)	13
F(M6)	13
G(M6)	13
$k = 2$	
F(M1)	(39, 74, 38, 71, 37, 69, 37, 72)
G(M1)	(44, 78, 38, 72, 41, 76, 34, 69)
F(M2)	(43, 78, 31, 87, 36, 69, 33, 88)
G(M2)	(45, 64, 38, 71, 39, 70, 32, 81)
F(M3)	(33, 71, 37, 67, 36, 80, 35, 82)
G(M3)	(127, 276, 146, 266, 152, 340, 142, 282)
F(M4)	(14, 30, 14, 31, 12, 36, 14, 32)
G(M4)	(14, 33, 14, 33, 16, 29, 15, 34)
F(M5)	(15, 29, 15, 28, 16, 30, 14, 33)
G(M5)	(17, 31, 16, 32, 14, 28, 15, 27)
F(M6)	(15, 28, 15, 33, 14, 30, 15, 36)
G(M6)	(14, 31, 17, 29, 13, 30, 14, 32)
$k = 3$	
F(M1)	(31, 40, 33, 41, 30, 26, 31, 34)
G(M1)	(32, 37, 34, 37, 29, 38, 34, 38)
F(M2)	(32, 42, 31, 43, 30, 39, 32, 36)
G(M2)	(35, 29, 30, 26, 32, 48, 30, 39)
F(M3)	(33, 41, 32, 40, 33, 47, 31, 34)
G(M3)	(130, 125, 119, 121, 118, 171, 123, 136)
F(M4)	(13, 13, 13, 19, 13, 18, 13, 18)
G(M4)	(13, 10, 13, 12, 13, 16, 12, 18)
F(M5)	(14, 19, 13, 20, 13, 18, 13, 17)
G(M5)	(14, 16, 12, 18, 13, 18, 13, 17)
F(M6)	(12, 10, 13, 17, 13, 19, 14, 17)
G(M6)	(13, 18, 13, 16, 12, 17, 12, 15)

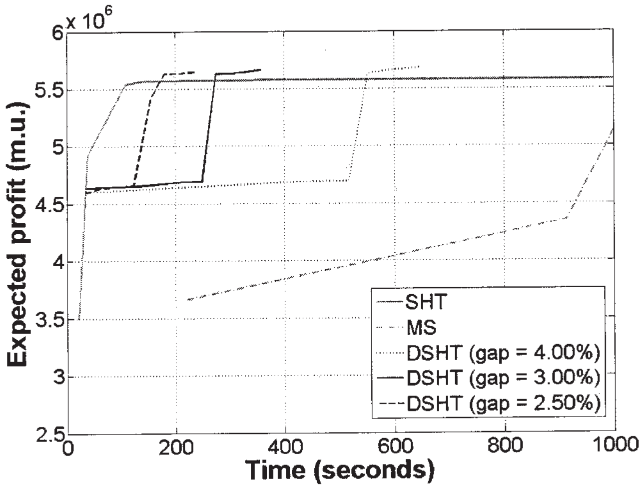

Figure 14. Case study 2: computational results.

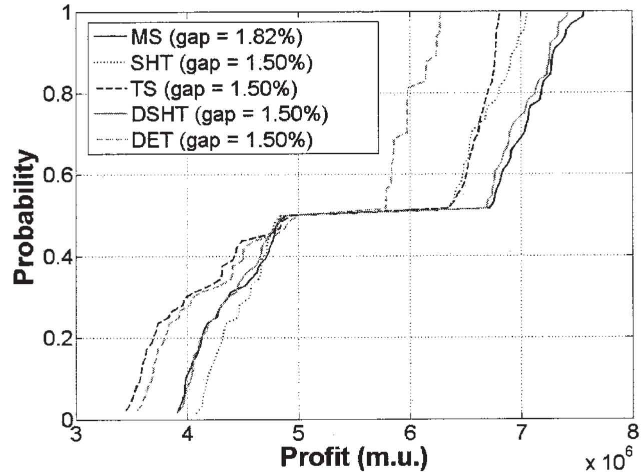

Figure 15. Case study 2: probability curves.

supposed to be equal to zero for all the states. Two different types of utilities are considered, the first one, which is associated with the labor tasks, has a cost of 0.25 m.u. per unit of utility consumed, while the second one, which corresponds to the transport services, costs 0.1 m.u. per unit. The fixed and variable coefficients for consumption of utility by tasks (α_{ui} and β_{ui}) are equal to 2,000 units of utility/h and 20 units of utility/Kg•h, respectively, for all the labor tasks, and 50 units of utility/h and 5,000 units of utility/Kg•h for transport ones. The availability of both utilities, as well as the capacities of the storages of raw materials, intermediate and final products are assumed to be unlimited.

In this example, it is assumed a time horizon of 144 h, divided into two equally long time periods. Such periods are also divided into 24 scheduling intervals of 2 h each. The scenario tree comprises 8 possible events in each period of time, which leads to 64 scenarios for the entire time horizon. In this case, 4 aggregated scenarios haven been explored.

Figure 14 shows the computational results obtained by applying the various approaches. After 50,000 s of computation time, the best solution obtained by the MS stochastic formulation is equal to 5,719,997 m.u., still within 1.82% of the best possible solution. The best solution computed by the SHT algorithm by solving all the two-stage stochastic models of the SHT with an optimality gap of 1% is 5,584,980 m.u., which is within 4.10% of the best solution. With regard to the DSHT, three curves corresponding to the algorithm computed with optimality gaps of 4.0%, 3.0% and 2.5% have been plotted.

The figure is very similar to that of the previous case, and, therefore, similar conclusions can be derived. In this case, the MS formulation lies completely on the right side of the three curves corresponding to the proposed algorithm.

In Table 18 the expected profit and the worst and best case scenarios of the results computed for a gap equal to 1.5% by means of the various approaches are given. As it can be seen, the MS formulation yields the highest expected profit, but incurs much more CPU time than the proposed algorithm, which provides the second highest expected profit. As occurred before, the SHT and TS approaches incur in lower times than those given by the proposed algorithm but also lead to lower expected profits. Finally, the DET approach leads to the poorest profit and when its solution is evaluated in the presence of uncertainty, the expected profit value drops by nearly 25% (6,311,588 m.u. for the mean scenario and 5,049,562 m.u. under the uncertain environment).

Figure 15 shows the probability curves corresponding to the aforementioned solutions. Again, the solution computed by the SHT turns out to be the most conservative, while the MS model and the proposed algorithm lead to an increase in risk which is compensated by and increase in opportunity. The TS approach and the DET solution lead to the riskiest solutions and do not even provide high chances of big profits. Similar conclusions can be derived by looking at the values of the maximum and minimum scenarios corresponding to the approaches, which are shown in Table 18. The SHT provides the highest minimum scenario while the DSHT and the MS approach lead to the highest maximum scenarios. On the other hand, the DET and the TS solutions lead to low-minimum scenarios, and also to small maximum scenarios.

Regarding the decision variables belonging to the fist period of time, which are not shown here due to space limitations, let us note that, again, the MS and the DSHT approaches lead to slightly higher production rates than the TS and the DET solutions.

Table 18. Case Study 2: Computational Results

	E[*profit*] (m.u.)	Gap (%)	Min. (m.u.)	Max. (m.u.)	CPU Time (s)
DET	5,049,562	13.30	3,533,201	6,278,033	130.27
TS	5,318,693	8.68	3,430,283	6,813,953	401.67
SHT	5,578,904	4.21	4,082,792	7,061,562	413.37
DSHT	5,679,799	2.48	3,908,463	7,424,297	7,237.14
MS	5,719,997	1.82	3,907,249	7,568,811	50,000.00

Conclusions

This article has addressed the scheduling of chemical supply chains under demand uncertainty. A multistage stochastic optimization formulation has been presented and an approximation strategy comprising two steps, and based on the resolution of a set of deterministic and two-stage models has been introduced aiming at the overcoming of the numerical difficulties associated with the resulting large-scale stochastic MILP.

The performance of the proposed strategy regarding computation time and optimality gap has been studied through comparison with other traditional approaches addressing optimization under uncertainty. The proposed strategy has been shown from numerical examples to provide better solutions than the standard TS formulation, and stand-alone two-stage shrinking-horizon algorithms also incurring lower computation times than the multi-stage stochastic formulation. Moreover, the decision variables belonging to the first period of time computed by the proposed algorithm are very similar to those provided by the multistage stochastic model, and the expected profit of the resulting solution is within few percent of the optimal one. The proposed approach seems to offer larger potential for results improvement as the number of periods and scenarios grows, because the underlying multistage stochastic formulation of the problem is likely to lead to intractable MILPs from the computational point of view.

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Notation

Indices

I = tasks
j = equipments
k = periods of time
m_k = scenarios in period k
m_k^* = average scenarios in period k
s = states
t = scheduling intervals
u = utilities

Sets

AD^k = binary tuples representing all possible ancestor-descendant combinations at stage k of the scenario tree
AS_{mk} = set of ancestor scenarios of m_k
DS_{mk} = set of descendant scenarios of m_k
FP = set of states corresponding to final products
I_j = set of tasks that can be performed in equipment j
IP = set of states corresponding to intermediate products
NTR = set of non transport tasks (production tasks)
RM = set of states corresponding to raw materials
S = set of states
SI_s = set of tasks receiving material from state s
SI'_i = set of states consumed by task i
SO_s = set of tasks producing material for state s
SO'_i = set of states produced by task i
TL^{mK} = set of stage k scenarios belonging to the time-line which ends in scenario m_K = at final stage $|K|$
TR = set of transport tasks
TSO_s = set of states s' coming from state s

Parameters

B_i^{MAX} = maximum batch size of task i
B_i^{MIN} = minimum batch size of task i
C_s = maximum storage for material in state s
Dem_{skmk} = demand of material in state s in period k in scenario m_k
Dem_{skm^*k} = average demand of material in state s in period k in average scenario m_k^*
$ICost_s$ = inventory cost of material in state s
$Price_s$ = price of material in state s
pt_i = processing time of task i
$RMCost_s$ = cost of raw material in state s
S_{0s} = initial amount of material in state s
U_{uk}^{max} = maximum consumption of utility u in period k
$UCost_u$ = utility cost of u
$UDCost_s$ = cost due to unsatisfied demand of material in state s

Variables

B_{itkmk} = batch size of task i started in time interval t at period k in scenario m_k
B_{istkmk}^I = amount of material in state s consumed by task i started in time interval t at period k in scenario m_k
B_{istkmk}^O = amount of material in state s produced by task i started in time interval t at period k in scenario m_k
E[Profit] = expected profit
$Profit_{mK}$ = profit of scenario m_K
$Purch_{skmk}$ = amount of material in state s purchased at period k in scenario m_k
S_{st0kmk} = initial amount of material in state s at the beginning of period k in scenario m_k
S_{stkmk} = amount of material in state s at the end of time interval t at period k in scenario m_k
$Sales_{skmk}$ = amount of material in state s sold at period k in scenario m_k
U_{utkmk} = consumption of utility u in scheduling interval t at period k in scenario m_k
W_{itkmk} = binary variable (1 if task i is started in interval t at period k in scenario m_k, 0 otherwise)

Greek symbols

α_{ui} = fixed coefficient for consumption of utility u by task i
β_{ui} = variable coefficient for consumption of utility u by task i
ρ_{is}^I = mass fraction for consumption of state s by task i
ρ_{is}^O = mass fraction for production of state s by task i
$Prob_{mK}$ = probability of scenario m_K

Scheduling models

SCHEDDET = deterministic scheduling formulation
SCHEDMS = multistage stochastic scheduling formulation
SCHEDTS = two-stage stochastic scheduling formulation

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