

Combinatorial Framework for Effective Scheduling of Multipurpose Batch Plants

E. Sanmartí and L. Puigjaner

Chemical Engineering Dept., Universitat Politècnica de Catalunya, E.T.S.E.I.B., Diagonal 647,
E-08028 Barcelona, Spain

T. Holczinger and F. Friedler

Dept. of Computer Science, University of Veszprém, Veszprém, Egyetem u. 10, H-8200, Hungary

The production scheduling of multipurpose batch plants is considered. A novel graph representation that looks at the specific characteristics of production scheduling in chemical processes is proposed. In these graphs, the nodes represent the production tasks, the arcs of the precedence relationships among them. The representation is flexible enough to consider a wide variety of production structures, including complex recipes. Both nonintermediate storage (NIS) and unlimited intermediate storage (UIS) transfer policies can be considered simply by choosing the appropriate precedence relationships. This representation provides the opportunity of incorporating highly efficient graph algorithms together with an appropriate branch-and-bound algorithm for solving multipurpose scheduling problems. The efficiency of the proposed method is established by solving examples and a complex case study.

Introduction

Multipurpose batch plants are characterized by their flexibility and ability to produce a large number of different products in different qualities so as to satisfy the client's demand, and by the possibility of considering alternate production paths for the same product in order to reduce costs. This high degree of flexibility is one of the major sources of the complexity of scheduling problems. In practice, a large number of variables have to be introduced (e.g., for tasks to equipment assignments, products, and/or task sequencing and task timing) to describe the problem appropriately in a mathematical programming model that is difficult or frequently impossible to solve by available general-purpose solvers. Simplifying assumptions such as reducing the search space to permutation schedules (see, for example, Reklaitis, 1981), in which complete batches are sequenced instead of tasks, may result in valuable solutions; nevertheless, optimality cannot be guaranteed in most cases.

Short-term scheduling of chemical multipurpose batch plants has similarities with the general job-shop problem, which has been widely treated in operations research. The approach traditionally used is based on a graph representa-

tion of the scheduling problem combined with a branch-and-bound (B&B) algorithm (see, e.g., Adams et al., 1988; Carlier and Pinson, 1989). For the job-shop scheduling problem, B&B algorithms are usually coupled with specific heuristics that greatly accelerate the convergence with the optimal or near-optimal solutions. The scheduling of chemical batch plants, however, substantially differs from the job-shop scheduling problems. The former is usually more complex than the latter, since additional conditions have to be considered, for example, the storage of intermediate liquid materials that do not occur in the discrete mechanical manufacturing industry. Another key difference is the presence of unstable intermediate products that may require immediate transfer. These differences prevent the direct adoption of the graph representation and algorithms developed for job-shop scheduling to batch chemical processes. Thus, batch chemical systems are usually scheduled by using other techniques, mainly mathematical programming (see, for example, Voudouris and Grossmann (1994) and Sanmartí et al. (1996)), sequencing and scheduling via tailored heuristics or stochastic (simulated annealing, genetic algorithms) methods (see, for example, Kudva et al. (1994), Graells et al. (1996), Hasebe et al. (1996), and Murakami et al. (1997)).

Correspondence concerning this article should be addressed to L. Puigjaner.

The selection of the representation technique in solving any complex problem like scheduling has major importance for several reasons [see, for example, state-task network (STN) representation by Kondili et al., 1993; resource-task network (RTN) representation by Schilling and Pantelides, 1996; event operation network (EON) representation by Graells et al., 1998]. A convenient representation may provide the opportunity of exploiting the unique features of the problem, resulting in a procedure with a higher efficiency. Furthermore, if the representation explicitly expresses the crucial points, it may contribute to an understanding of the depth of the problem that may facilitate the development of new algorithms or the improvement of available ones. The generality of the chosen representation technique also determines the range of problems that can be treated.

Kondili et al. used a discrete representation of time and introduced the state-task network representation of the process. The major advantage here is the ability to consider very general-process recipes involving batch splitting and mixing, material recycles, storage policies, resource constraints, and so on. The formulation of Kondili et al. is based on the definition of binary variables that indicate whether tasks start in specific pieces of equipment at the start of each time period. However, the major problems with this approach are the large size of the resultant mixed-integer linear programming (MILP) model and mapping the discretization points with the actual points in time when the events take place. This forms the basis of several other pieces of research that are aimed at taking advantage of the representational capabilities of the formulation while improving its numerical performance. Sahinidis et al. (1991) disaggregated the model in a way that solution efficiency is improved despite the large nature of this model. Shah et al. (1993) modified the allocation constraints to generate the smallest possible integrality gap for this type of formulation. In addition, Elkamel (1993) proposed a heuristic decomposition method to solve separate scheduling problems for parts of the overall scheduling problem. In a later work, Yee and Shah (1997, 1998) considered the further use of heuristics embedded in the formulation. Pantelides et al. (1994) presented a critique of the STN and associated scheduling formulations. They then proposed an alternative representation, the resource-task network (RTN), based on a uniform description of all resources. Here tasks are assumed to only consume and produce resources instead of materials.

As for continuous representation of time, Zhang and Sargent (1994, 1996), presented a continuous-time formulation based on the RTN representation. They composed an MILNP representation that was solved using the liberalization procedure. Schilling and Pantelides (1996) proposed a hybrid B&B solution procedure that works well in reduced scenarios. Pinto and Grossmann (1995) used preordering constraints and a decomposition scheme for large systems that minimize earliness and eliminates unnecessary setups. Graells et al. (1998) presented the EON representation that simplifies the timing subproblem. Together with the process-material network (PMN) representation, the EON provides a realistic and robust framework for detailed process simulation at the scheduling level.

A large portion of the most recent research in scheduling relates to the development of mathematical models as the best way of representing the complex interactions between

resource allocation, task timing, materials flows, and equipment capacities (see, for example, recent reviews in this area by Shah, 1998; Pekny and Reklaitis, 1998; Pinto and Grossmann, 1998; Puigjaner, 1999). In the present work, a new graph representation appropriate for combinatorial algorithms is introduced. The article describes a general framework for solving different types of multipurpose batch scheduling problems. Therefore, it provides a good basis for effective algorithms to solve a large variety of scheduling problems.

Problem Definition

Three types of information define a multipurpose batch-scheduling problem; these are the recipes of each product, tasks to equipment assignments, and the amount to be produced from each product.

A recipe is an entity that contains the minimum set of information that uniquely defines the manufacturing requirements for a specific product. The ISA SP88 standard defines four levels for the types of recipes that are used in batch processes, depending on the user requirements. These levels are:

- General recipe identifies raw materials, their relative quantities, and the required processing. It is considered as enterprise-level information, and is therefore equipment independent. Besides it is not specific to a particular site.
- Site recipe is a combination of site-specific information and the general recipe (it is specific to a particular site).
- Master recipe includes information about required process cell equipment, raw materials with corresponding quantities, and the procedure for making the product. It can be derived from a general recipe or a site recipe.
- Control recipe includes additional information about the process units that are used in manufacturing a single batch of a single product. This recipe is created from the master recipe when a batch is scheduled for production.

Based on the four types of recipes, the master recipe is to be considered for the scheduling of batch processes. This master recipe can be conveniently represented as a directed graph, where the nodes represent the production tasks and the arcs the precedence relationships among them. Note that the production time (PT) and the set of plausible equipment (Eq.) of a task are given at the corresponding node. Figure 1 illustrates the conventional representations of the recipe of a product composed by three reaction stages. Natu-

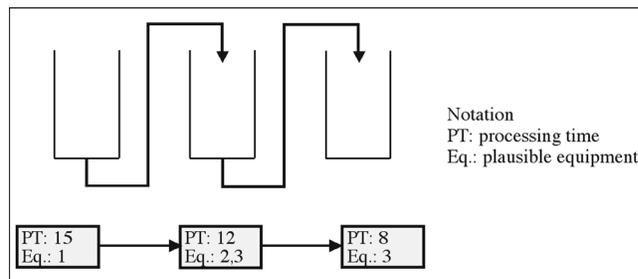


Figure 1. Conventional representations of a recipe composed of three consecutive reaction stages.

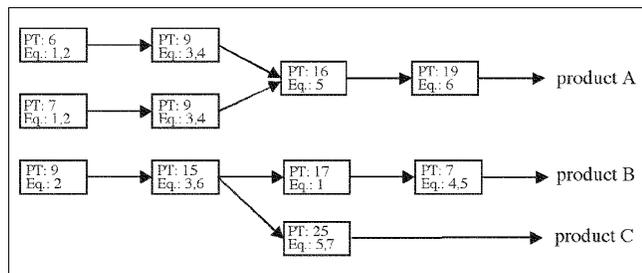


Figure 2. Conventional representation of two master recipes of three products.

rally, complex recipe structures can also be represented in this way, as illustrated in Figure 2, where, for example, two intermediates are produced, mixed, and further processed in the production of *A*.

This conventional representation is similar to the flow-sheet representation of continuous plants (see Reklaitis (1991)), the only role of the arcs being to express the order of tasks; all other information is related to the nodes of the graph. For combinatorial algorithms of scheduling, however, it is beneficial to distribute information between nodes and arcs: processing times are assigned to the arcs instead of nodes. Figure 3 shows the graph-representation of recipes given on Figure 2, where S_i denotes the set of those equipment units that can perform the task represented by node i (such as $S_1 = \{1,2\}$); in addition, an additional node (the so-called product node) is introduced for each product. In this representation, the value assigned to an arc expresses the lower bound for the difference between the starting times of the two related tasks. The processing time of a task may be different for different equipment units. In this case, the weight of the arc is the minimum of the processing times of the plausible equipment units.

Formally, any recipe can be represented by an acyclic directed graph. Note that recycling in the process flow sheet does not result in a cycle in the graph of the recipe, since it is realized as a feedforward to the production of the next batch or some batch to be started later.

Graph Representations for Solving Scheduling Problems

Scheduling of batch chemical plants has been traditionally approached by tailored heuristics and mathematical programming, either MILP or mixed-integer nonlinear programming (MINLP). The graph-theoretic approach has also been used frequently in solving complex combinatorial problems, including scheduling. These applications in scheduling, however, have been limited to the general job-shop-scheduling problem of the mechanical industry where intermediates can be stored between operations, that is, for an unlimited intermediate storage (UIS) policy. In solving a chemical scheduling problem, however, the liquid, and sometimes the unstable nature of the intermediate products, has to be considered. Unlike solids, liquid intermediates have to be stored in specific vessels that have to be available at each specific equipment unit. Consequently, more sophisticated graph representation and algorithms are required in order to represent this

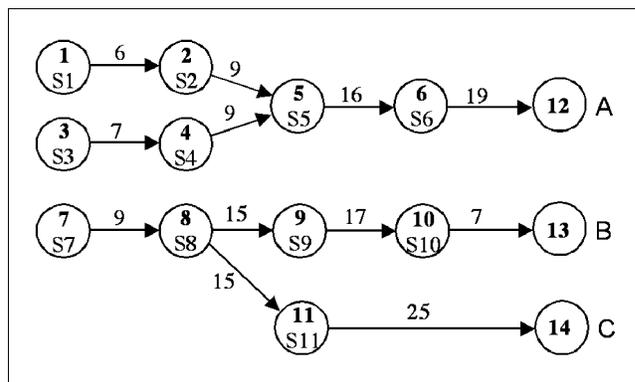


Figure 3. Graph representation of the two recipes in Figure 2.

situation. Furthermore, liquid intermediates are frequently unstable, and they have to be transferred immediately after processing.

Graph representation for the unlimited intermediate storage policy

Assume that the number of batches of each product to be produced is already known and definite assignments of equipment to tasks are given. Then, the sequence of the tasks to be processed can be represented in a graph (Adams et al., 1988) where the task sequence of all equipment units is defined by a set of conjunctive arcs that connect the tasks assigned to the same equipment unit. These arcs have the same weight as the processing time of the tasks that introduce a set of precedence constraints in addition to the constraints imposed by the recipe. For example, 1–6–7 is the task sequence of equipment unit E1 shown in Figure 4b for the scheduling problem specified by the recipe on Figure 4a. In this example, E1 is assigned to each of tasks 1, 6, and 7 where, $E1 \in S_1, S_6, S_7$. It can be observed in Figure 4b that task 6 is subject to two precedence constraints: it cannot start before task 5 is completed (because of the recipe) and before task 1 has finished (because of the sequence).

This type of graph representation is useful in solving the job-shop problems with the UIS policy; however, it may not be appropriate for nonintermediate storage (NIS) cases. For the former, it is assumed that an equipment unit is available immediately after it processes a task, that is, the intermediate product that has been generated in this task is removed from the equipment unit and stored until the next task in the recipe starts its processing. In most of the chemical batch processes, however, the NIS transfer policy is to be followed instead of the UIS policy.

S-graph for nonintermediate storage policy

In the NIS case, an equipment unit is not free after processing a task until the material stored in it has been transferred to the equipment unit assigned to the next task in the recipe. Arc or arcs express these additional constraints imposed by the NIS policy. Let τ_j denote the set of tasks that follow task j according to the recipe. If equipment unit E_i is assigned to task j after completion of task k , then a zero-

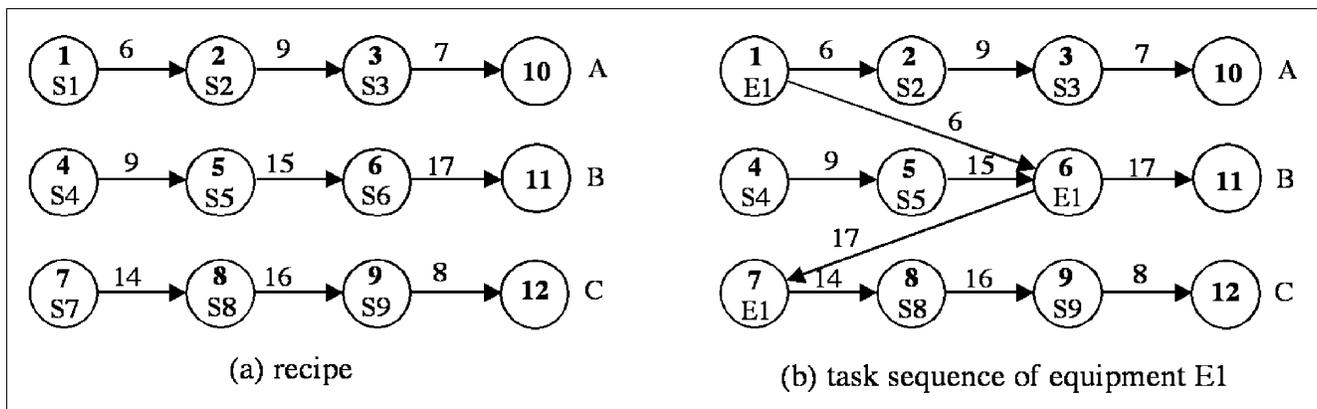


Figure 4. Task sequence for equipment unit E1 included in sets of equipment units S1, S6, and S7: appropriate only for UIS transfer rule.

weighted arc (or an arc whose weight is equal to the length of the changeover time if applicable) is established from each element of τ_j to k . This method of representation is called *S-graph*. The task sequence of equipment E1 given in Figure 4b is given via S-graph in Figure 5. Instead of connecting the node of tasks 1 to 6, and then that of 6 to 7 by arcs weighted by the length of the processing time, as shown in Figure 4b, zero weighted arcs are used to connect the node of tasks 2 to 6 and that of tasks 11 to 7, respectively.

A feasible schedule for the UIS transfer policy may not be feasible for the NIS case. This infeasibility can be detected in the S-graph representation by finding a directed cycle in the graph, while it cannot be recognized on the conventional representation. For example, Figure 6 shows the Gantt chart of an infeasible schedule of the scheduling problem specified by the recipe in Figure 4a for the NIS policy; nevertheless, it is an optimal schedule for the UIS policy. The Gantt chart given in Figure 6 shows the transfer of material from equipment unit E1 (task 1) to equipment unit E3 (task 2) simultaneously with the transfer from E3 (task 5) to E1 (task 6). This transfer of material can only be performed if an intermediate storage is available to store one of the products while the other is being transferred, which is the case of the UIS policy. An optimal solution for the NIS policy of the same example is given in Figure 7.

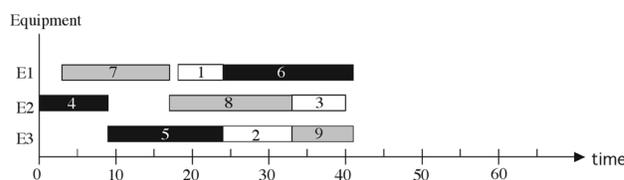


Figure 6. Gantt chart of the optimal schedule for UIS transfer policy for recipe given in Figure 4a; it is infeasible for NIS.

Although conventional representation is not convenient for NIS, an S-graph can represent both NIS and UIS scheduling problems correctly. For simplicity, in this article the mathematical formulation and the algorithms will be introduced for only the NIS case.

Mathematical Formulation of the S-Graph

Formally, directed graph G can be given as a pair (N, A) , where N is a finite set, the set of nodes, and A is a set of pairs of nodes identifying the arcs of the graph (that is, $A \subseteq N \times N$). In an S-graph, two classes of arcs, the so-called recipe-arcs and schedule-arcs, are specified. Therefore, an S-graph is given in the form of $G(N, A_1, A_2)$, where N, A_1 , and A_2 denote the sets of nodes, recipe-arcs, and schedule-arcs, respectively. It is supposed that $A_1 \subseteq N \times N, A_2 \subseteq N \times N$, and $A_1 \cap A_2 = \emptyset$; furthermore, a nonnegative value, $c(i, j)$, which denotes the weight of arc (i, j) , is assigned to each arc. In practice, if the arc is established from node i to node j , that is, $(i, j) \in A_1 \cup A_2$, then it is supposed that the task corresponding to node j cannot start its activity earlier than $c(i, j)$ after the task corresponding to node i starts. Specific types of S-graphs are identified for a recipe (that is, recipe-graph) and for a schedule of all tasks (that is, schedule-graph).

Recipe-graph

A recipe defines the order and type of tasks, the material transfers among them, and the set of plausible equipment units of each task. This type of information should be represented by the graph of a recipe.

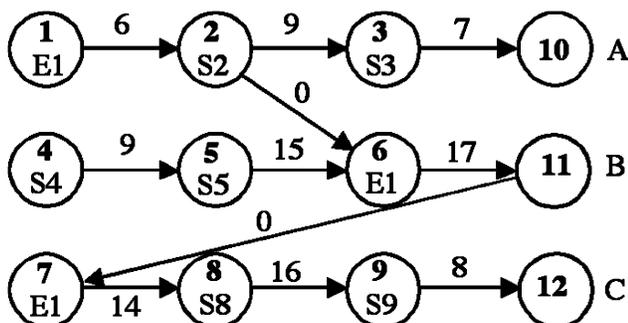


Figure 5. S-graph representation of task sequence 1-6-7 of Figure 4b for equipment unit E1 with NIS policy.

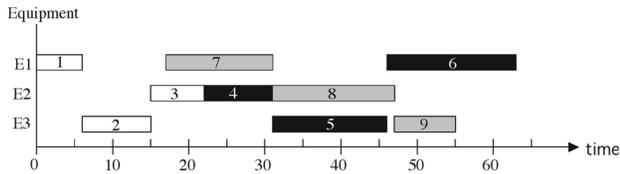


Figure 7. Gantt chart of the optimal schedule for NIS transfer policy for recipe given in Figure 4a.

Let one node be assigned to each task (task node) and one to each product (product node). An arc is established between the nodes of consecutive tasks determined by the recipe, and one is also established from each task node that generates the product to the corresponding product node. The weight of an arc is specified by the processing time of the task corresponding to the initial node of the arc if a single equipment unit is available for this task and the minimum of the processing times of all equipment unit if more than one equipment unit is available.

If multiple batches of a product are to be produced, the task nodes, the product nodes, and the arcs are multiplied appropriately. The resultant graph is called task network, where N_t and N_p denote the set of its task nodes and product nodes, respectively ($N_t \cap N_p = \emptyset$).

In practice, the inputs of a task may not need to be available at the same time; instead, further constraints may need to be applied on the timing of these inputs. Stated formally, the timing of the feeds is to be given as a partial order on their starting times. In the simplest case, all inputs must be available simultaneously. In Figure 8, according to this representation technique, task 4 has three different inputs that are produced in parallel by tasks 1, 2, and 3. Obviously, three pieces of equipment must be prepared simultaneously to feed task 4.

In general, the practical order of the inputs of a task is given by the so-called feed-precedence graph of the task. For example, suppose that input 1 precedes input 3, and input 1 is available simultaneously with input 2 in the part of a task network given in Figure 9a. Additional nodes and arcs express the order of precedence of the feeds of task 4 according to Figure 9b.

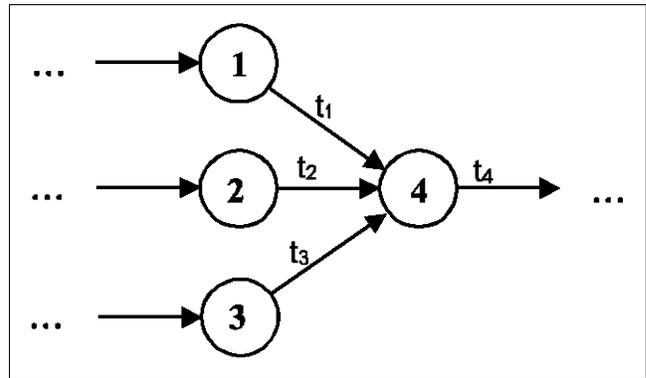


Figure 8. Part of a recipe-graph: simultaneous input streams to task 4.

The task network extended with a feed-precedence graph is called recipe-graph. It represents all structural information given in a recipe. If $G(N, A_1, A_2)$ is a recipe-graph, it is acyclic, $N = N_t \cup N_p$, and $A_2 = \emptyset$.

For simplicity, the partial ordering of the timing of the feeds of a task is not examined here (for more details of the feed-precedence graph, see Appendix A). Let $N_i (\subset N_t)$ be the set of nodes of those tasks that can be performed by equipment unit i . It is supposed that there is at least one equipment unit available that can be assigned to a task, that is, the set of task nodes can be given as $N_t = N_1 \cup N_2 \cup \dots \cup N_n$, where N_i and N_j ($i, j = 1, 2, \dots, n$) are not necessarily disjoint.

Example 1. Suppose that two batches of product A and one batch of product B are to be produced, where product A is produced in two consecutive steps. The first step can be performed by any equipment unit given in set S1, and step 2 can be performed by any equipment unit given in set S2. Product B is produced in three consecutive steps that can be performed by any of the elements of sets S3, S4, and S5, respectively. The resulting recipe-graph is given in Figure 10.

Schedule-Graph

A specific S-graph, termed schedule-graph, is introduced to describe a single solution of a scheduling problem; there

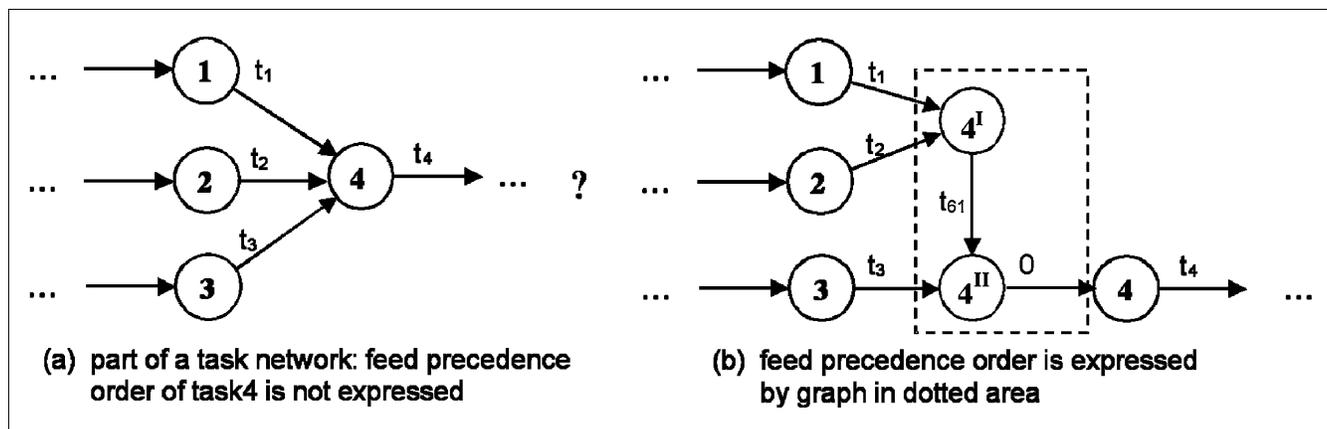


Figure 9. Part of a recipe-graph for illustrating feed-precedence graph.

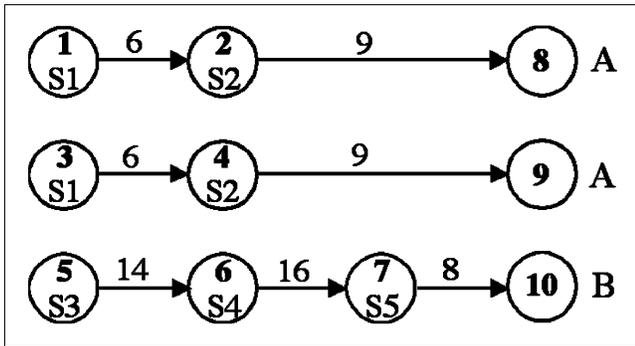


Figure 10. Recipe-graph: two batches for product A and one batch for product B.

exists one schedule-graph for each feasible schedule of the problem. S-graph $G'(N, A_1, A_2)$ is called a schedule-graph of recipe-graph $G(N, A_1, \emptyset)$, if all tasks represented in the recipe-graph have been scheduled by taking equipment-task assignments into account. The schedule-graph of the optimal schedule can be effectively generated by an appropriate search strategy, as will be shown later.

Example 2. Three products are to be produced according to the recipe given in Figure 11. One equipment unit can be assigned to each task according to the following: $S1 = \{E1\}$, $S2 = \{E3\}$, $S3 = \{E2\}$, $S4 = \{E2\}$, $S5 = \{E3\}$, $S6 = \{E1\}$, $S7 = \{E1\}$, $S8 = \{E2\}$, and $S9 = \{E3\}$. There are eight different solutions represented by the eight schedule-graphs given in Figure 12.

For the formal definition of a schedule-graph, suppose that S-graph $G'(N, A_1, A_2)$ is given where $G(N, A_1, \emptyset)$ is a recipe-graph and $A_2 \subseteq N \times N$. Let M_i ($i = 1, 2, \dots, n$) denote the set of nodes of those tasks that are to be performed by equipment unit i according to S-graph $G'(N, A_1, A_2)$. It is assumed that exactly one equipment unit is assigned to each task, that is, $M_i \cap M_j = \emptyset$ ($i \neq j, i, j = 1, 2, \dots, n$). Therefore, M_1, M_2, \dots, M_n is such a partitioning of the set of task nodes $N_i = N_1 \cup N_2 \cup \dots \cup N_n$ that $M_i \subseteq N_i$ ($i = 1, 2, \dots, n$).

A specific graph, called component-graph, will be identified to show the activity of each equipment unit. Stated formally, S-graph $G'_i(N'_i, A_{1i}, A_{2i})$ ($\subseteq G'(N, A_1, A_2)$) is the component-graph of equipment unit i ($i = 1, 2, \dots, n$) if

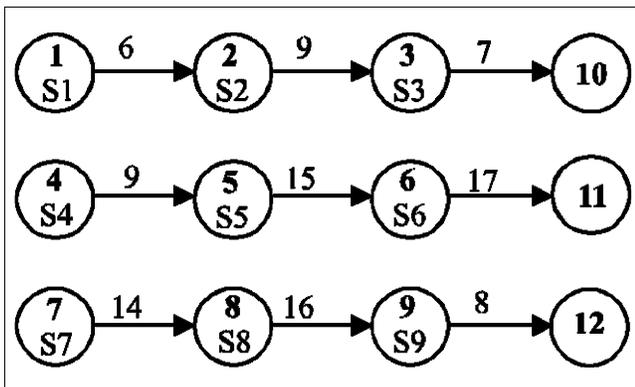


Figure 11. Recipe-graph of Example 2.

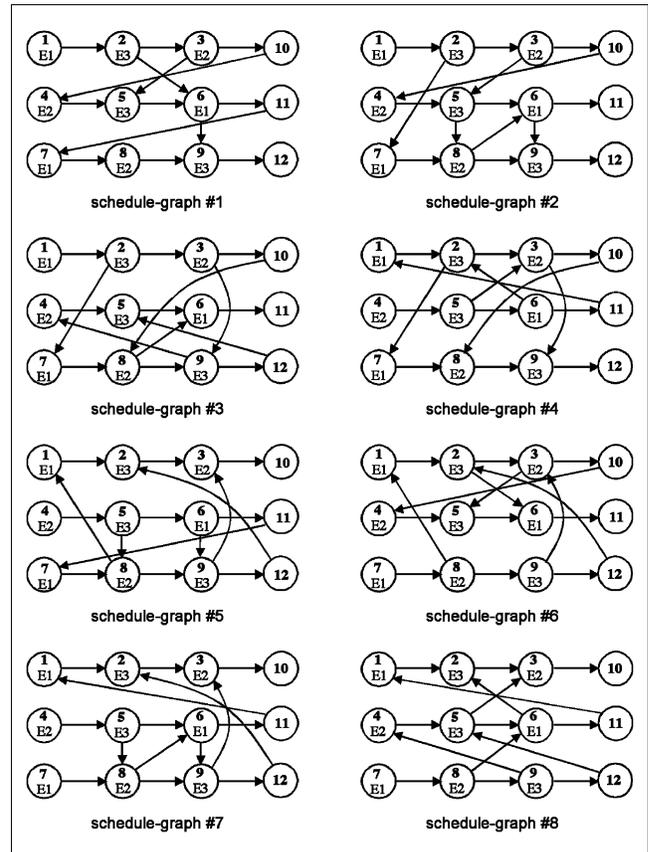


Figure 12. All schedule-graphs of Example 2.

- N'_i includes all nodes of M_i and the end nodes of all arcs in A_1 starting from any elements of M_i (i.e., $N'_i = M_i \cup \{k : (j, k) \in A_1, j \in M_i\}$);

- A_{1i} includes all recipe-arcs of G' , starting from any elements of M_i (i.e., $A_{1i} = \{(j, k) : (j, k) \in A_1, j \in M_i\}$);

- A_{2i} includes all schedule-arcs of G' , starting from the end node of an arc of A_{1i} and pointing to any elements of M_i (i.e., $A_{2i} = \{(j, k) : (j, k) \in A_2, k \in M_i, \text{ and } \exists l \in M_i \text{ such that } (l, j) \in A_{1i}\}$).

S-graph $G'(N, A_1, A_2)$ is defined to be a schedule-graph for recipe-graph $G(N, A_1, \emptyset)$ and equipment assignments M_i ($i = 1, 2, \dots, n$) if it satisfies the following four axioms.

(SG1)

G' is acyclic

(SG2)

G'_i defines total order on $M_i \cup \{j\}$ for all $j \in N'_i$ and $i = 1, 2, \dots, n$.

(SG3)

The out-degree of every node of N'_i ($i = 1, 2, \dots, n$) is at most 1 according to the arcs in A_{2i} .

(SG4)

Schedule-graph G' is the union of its component schedule-graphs, that is, $G' = \bigcup_{i=1}^n G'_i$.

It is important to examine the relation between a schedule-graph and the set of feasible schedules of a scheduling problem. Solving a practical problem, arc (i, j) of an S-

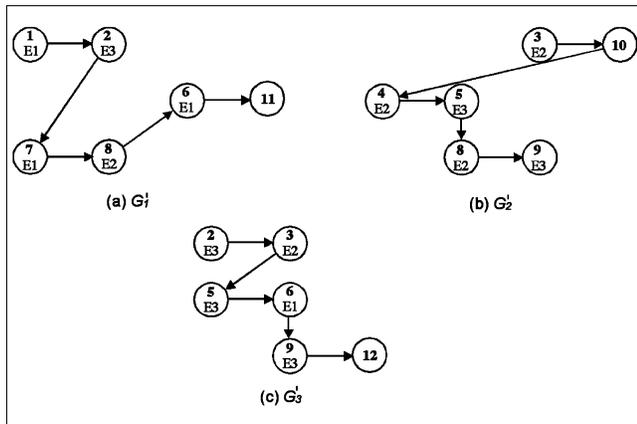


Figure 13. Component-graphs of schedule-graph No. 2 of Figure 12.

graph expresses that the processing time of the task represented by node j must start at least $c(i, j)$ time later than the task of node i started. Therefore, the violation of axiom (SG1) cannot result in a feasible schedule; that is, either the time precedence or the NIS policy is violated. If (SG1) is satisfied, the violation of axiom (SG2) implies that the scheduling is incomplete, since the order of certain tasks is not determined. Although axioms (SG3) or (SG4) are not necessarily satisfied by a feasible schedule, the optimal solution can always be generated by reducing the search to those S-graphs that satisfy (SG3) and (SG4). Consequently, the optimal solution can always be generated from the set of all schedule-graph.

Example 2 Revisited. Component-graphs G'_i ($i = 1, 2, 3$) of schedule-graph #2 shown in Figure 12 with equipment-task assignments $M_1 = \{1, 7, 6\}$, $M_2 = \{3, 4, 8\}$, $M_3 = \{2, 5, 9\}$ are given in Figure 13. Obviously, the schedule-graph with these equipment-task assignments satisfies axioms (SG1) through (SG4).

Basic Algorithm for Optimal Scheduling

The recipe-graph of a scheduling problem is always a sub-graph of any of its schedule-graphs with identical sets of nodes. Each arc of a schedule-graph that does not belong to its recipe-graph is a schedule-arc. Extending the recipe-graph

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procedure main
notation:  $n$ : number of equipment units
 $N_i$  ( $i = 1, 2, \dots, n$ ): set of tasks that can be performed by equipment unit  $i$ 
 $last\_node$ : set of pairs  $(i, j)$ , where  $i$  is an equipment unit and  $j$  is a task (node)
 $PP = (G(N, A_1, A_2), bound, last\_node, SOUN)$ 
input: recipe-graph  $G(N, A_1, \emptyset)$  and  $N_i$  ( $i = 1, 2, \dots, n$ )
begin
 $SET = \emptyset$ ;  $bound = 0$ ;  $SOUN = N_1 \cup N_2 \cup \dots \cup N_n$ ;  $last\_node = \emptyset$ ;  $current\_best = \infty$ ;
put  $(G(N, A_1, \emptyset), bound, last\_node, SOUN)$  into  $SET$ ;
while  $SET \neq \emptyset$  do
begin
select and remove one element from  $SET$ , it is denoted by  $PP$ ;
branching( $PP$ );
end;
if  $current\_best < \infty$  then print solution;
end

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Figure 14. Main procedure of the scheduling algorithm.

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procedure branching(PP)
comment: generates all child partial problem of partial problem  $PP$ 
notation:  $graph(PP) = G(N, A_1, A_2)$ 
 $bound(PP) = bound$ 
 $last\_node(PP) = last\_node$ 
 $SOUN(PP) = SOUN$ 
begin
let  $EQ$  be an equipment unit that can be assigned to an unscheduled task (node);
let  $SO = N_{EQ} \cap SOUN(PP)$ ;
for all  $k \in SO$  do
begin
if there is no pair  $(i, j) \in last\_node$  such that  $i = EQ$  then
begin
put  $(graph(PP), bound(PP), last\_node(PP) \cup \{(EQ, k)\}, SOUN(PP) \setminus \{k\})$ 
into  $SET$ ;
end;
else
begin
let  $G_0(N, A_1, A_2) = graph(PP)$ ;
for all  $(j, l) \in A_1$  do
begin
update  $c(j, l)$ ;
 $G_0(N, A_1, A_2) = G_0(N, A_1, A_2) \cup \{(l, k)\}$ ;
end;
 $bounding(G_0(N, A_1, A_2), bound)$ ;
if  $bound < current\_best$  then
begin
if  $SOUN(PP) \setminus k = \emptyset$  then
update  $current\_best$ ,  $SET$ , and  $solution$ ;
else
put  $(G_0(N, A_1, A_2), bound, last\_node(PP) \cup \{(EQ, k)\} \setminus \{(EQ, j)\}, SOUN(PP) \setminus \{k\})$  into  $SET$ ;
end;
end;
end;
end;
return;
end;

```

Figure 15. Branching procedure of the scheduling algorithm.

with arcs in all possible directions by taking axioms (SG1) through (SG4) into account, constraints on the assignments can result in all schedule-graphs. Consequently, all schedule-graphs and the related assignments can be generated in a finite number of steps. This graph generation can be performed conveniently by a B&B algorithm, where an equipment unit is assigned to a task and the order of this task is determined in each branching step.

Branching algorithm

In the proposed B&B procedure for generating all schedule-graphs, one S-graph and a partial assignment belong to a partial problem and also to a node of the enumeration tree. The recipe-graph with no assignment serves as the root of the tree. At any partial problem, one equipment unit is selected and then all child partial problems are generated to unscheduled tasks through the possible assignments of this equipment unit. The processing time of a task may depend on the assigned equipment unit; therefore, assigning an equipment unit to a task may modify the weight of the recipe-arcs, starting from the node representing the task. This procedure is given in Figures 14 and 15. For simplicity, it is assumed that there is exactly one equipment unit to perform a task. The main procedure initializes the values of the variables (Figure 14) prior to calling the branching algorithm (Figure 15).

There is a high degree of freedom in realizing the branching algorithm to select the appropriate or the most effective search strategy. For instance, the order of the selection of equipment units can greatly affect the efficacy of the algo-

```

procedure bounding ( $G(N,A)$ , bound)
begin
  for all  $s \in N_p$  do cycle_search ( $s, \{s\}$ );
  if no cycle then
    bound = longest_path ( $G(N,A)$ );
  else
    bound =  $\infty$ ;
end;

```

Figure 16. Bounding procedure of the scheduling algorithm.

rithm. To schedule the “busiest” unscheduled equipment unit results in an effective search in most cases.

Bounding

The bounding procedure given in Figure 16 first tests the feasibility of a partial problem. If this test is proved positive, it determines a lower bound for the makespan of all solutions that can be derived from this partial problem. If no waiting time is limited, a schedule-graph is feasible if and only if it is acyclic. Thus, the feasibility of a partial problem is tested by a cycle search algorithm. Note that it can be realized by an efficient (polynomial) algorithm (see Appendix B for the algorithm). If the waiting time is limited for some intermediate products, further examination is required, for example, by solving an LP problem.

Obviously, the S-graph of a partial problem is a subgraph of the S-graph of any of its child partial problems. Since an additional arc does not decrease the length of the longest path of a graph, the length of the longest path of any subgraph of a schedule-graph is a lower bound of the longest path of the schedule-graph. Moreover, the length of the longest path of a schedule-graph is also a lower bound of the makespan of the corresponding solution. Consequently, the following proposition is true.

Proposition 1. The longest path of any subgraph of a schedule-graph provides a lower bound of the makespan of the solution related to the schedule-graph.

The longest path of a graph can be generated efficiently by a polynomial time algorithm; thus, it can be applied effectively in solving scheduling problems (see Appendix B for the algorithm).

At certain partial problems of the B&B algorithm, especially at the highest levels of the enumeration tree, the longest path may not give a sharp lower bound simply because no or

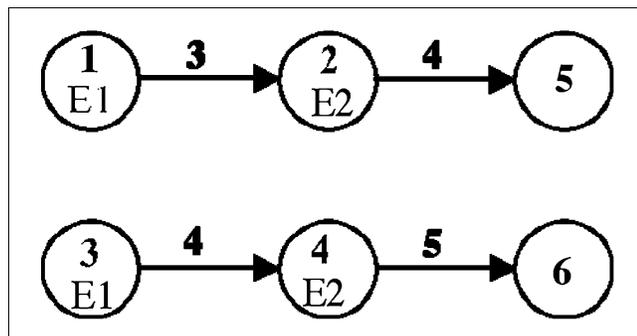


Figure 17. Recipe-graph for the illustrative example.

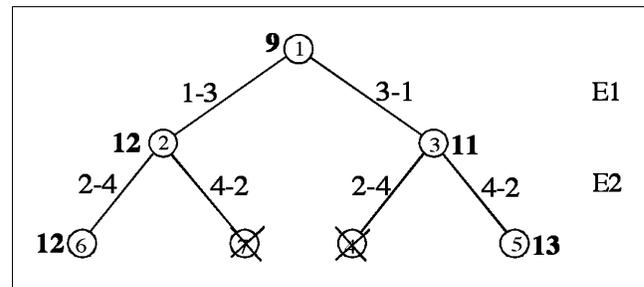


Figure 18. Search tree for the illustrative example: nodes represent partial problems, arcs labeled by the sequence of equipment units, and bold numbers show the lower bounds.

only few schedule arcs are considered. In general, this bound can be sharpened by solving a specific LP problem based on the result of the longest-path algorithm (see Appendix C for the details) in return of an additional computational effort.

If the waiting times of some intermediate products are limited, LP relaxation is to be used to test the feasibility and generate a lower bound. Each time that the lower bound of the partial schedule of a node (partial problem) is greater than the current upper bound or the partial schedule is cyclic (i.e., it is structurally infeasible), this partial schedule and the corresponding node on the enumeration tree are pruned.

Illustrative example

The recipe-graph is shown in Figure 17, where one batch of each of the two products is to be generated. The search tree is depicted in Figure 18. The nodes of the tree represent the partial problems, and they are numbered in the order in which the proposed base algorithm generates them. The branches are identified by the task sequence they introduce. The lower bound associated with each of the feasible partial problems is shown in boldface. The node of an infeasible partial problem is crossed (such as No. 4 and No. 7). The S-graphs that correspond to these partial problems are shown in Figure 19.

The root of the search tree (partial problem No. 1) corresponds to the recipe-graph, the longest path, that is, the lower bound of its makespan is 9. From this partial problem, two branches, partial problems No. 2 and No. 3, are generated for the sequence of equipment unit E1: 1–3 and 3–1, with a lower bound of 12 and 11, respectively. The branch with the best lower bound is partial problem No. 3, and it is selected to continue expanding the tree. From this partial problem, two branches (partial problems No. 4 and No. 5) are generated: sequences 2–4 and 4–2 for equipment unit E2. Both partial problems are complete schedules, that is, they can lead to a new upper bound for the minimum makespan. Partial problem No. 4 contains a cycle; it must be discarded. Partial problem No. 5 represents a complete schedule with a makespan of 13, that is, it is an upper bound for the optimal makespan. Partial problem No. 2 is the next branch to be expanded, from which sequences 2–4 and 4–2 for equipment unit E2 are generated (partial problems No. 6 and No. 7); both are complete schedules. Partial problem No. 6 corre-

sponds to a schedule with a makespan of 12; it is better than the current upper bound, and accordingly is set as the new upper bound of the minimum makespan. Partial problem No. 7 is not explored, since the lower bound of its ancestor (partial problem No. 2) is no better than the current upper bound.

Program Realizations and Applications

The algorithms outlined in the subsections on the branching algorithm and bounding are considered as a framework for developing efficient algorithms for solving complex scheduling problems. Although this framework is itself useful in solving scheduling problems, it is considered as a base in developing an efficient solver for complex scheduling problems by embedding additional acceleration tools. These tools

can be either general-purpose, that is, valid for any problem, or specific to a class of problems. The former type of tool exploits the properties of all scheduling problems. For example, a partial problem of the B&B procedure can be pruned if all leaves that can be derived from it are cyclic. Another type of acceleration tools exploits the properties of a special class of problems. While, the problem type of independent tools is to be realized in any scheduling program based on the framework, the specific tools are to be developed for extremely complex problems whenever the general-purpose algorithm is incapable of generating the optimal solution in a realistic time period. Both types of tools may guarantee the optimality of the solution. The present article examines the program realizations of the pure framework and its acceleration with a general type of tool.

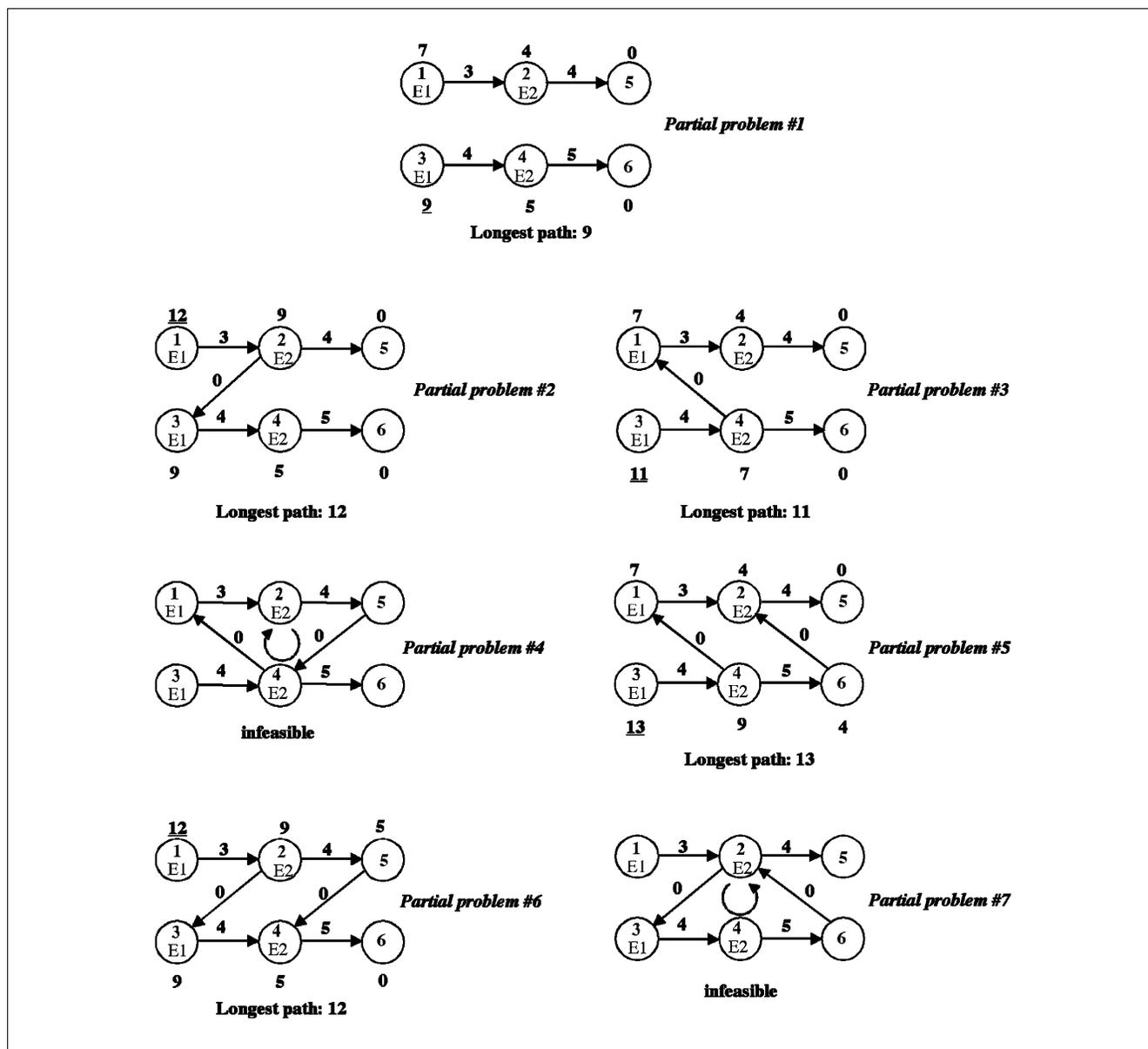


Figure 19. S-graphs of the partial schedules generated according to the search tree given in Figure 18; longest path algorithm determines the lower bound.

Table 1. Recipes of Example 3

Task	Product A		Product B		Product C		Product D	
	Eq.	Time (h)						
1	E1	6	E2	9	E4	8	E2	7
2	E3	9	E3	15	E1	14	E3	11
3	E4	7	E4	17	E2	16	E1	4

Table 2. CPU Time Usage (s)

No. of Batches	Proposed Basic Algorithm*	MILP* Sanmartí et al. (1996)	Makespan
4	0.13	3.86	47
5	1.01	51.9	62
6	4.48	—	73
7	62.24	—	87
8	297.5	—	92

*Solved by AMD K-7 Athlon 1 GHz.

Realization of the basic algorithm

The framework has been developed in C++ (it can be downloaded from <http://www.dcs.vein.hu/demo/sch/>). In order to illustrate this framework, we solve Examples 3 and 4.

Example 3. Four equipment units, E1, E2, E3, and E4, are available to generate four products, A, B, C, and D. The recipes of the products are given in Table 1.

The proposed basic algorithm and the solution of the MILP model presented in Sanmartí et al. (1996) have been compared by solving this example in generating a different number of batches of the products. The base problem considers the production of one batch of each product, that is, four batches altogether. Then, in order to generate up to eight batches, the batches of each product were repeated once more. The results are shown in Table 2 where the MILP model has been solved with a generic solver (GAMS/OSL). For six, seven, and eight batches, the MILP did not arrive at the optimal solution in reasonable time (in several hours), or the solver crashed.

Example 4. This example was introduced by Voudouris and Grossmann (1994). Five equipment units (stages), E1, E2, E3, E4, and E5, are available to generate four products, A, B, C, and D. The recipes and the number of batches of the products are given in Table 3 and Table 4, respectively.

The makespan of the resultant solution is the same as that given by Voudouris and Grossmann (1994). The running time in solving the basic algorithm using AMD K-7 Athlon 1 GHz was 20.07 s compared to 293 s using GAMS 2.25/Sciconic

Table 3. Recipes of Example 4

Task	Product A		Product B		Product C		Product D	
	Eq.	Time (h)						
1	E1	8	E1	7	E2	6	E2	4
2	E4	5	E3	3	E4	9	E3	6
3	E5	3	E5	4	E5	3	E5	4

Table 4. Number of Batches for Example 4

Product	A	B	C	D
Number of batches	3	3	2	2

2.11 in an IBM/R6000/Power 530 workstation for the model published by Voudouris and Grossmann. It can be seen that, without using any embedded acceleration tool, the basic algorithm obtains the optimal solution of the problem in a comparable or considerably lower CPU time than a general-purpose sophisticated MILP solver.

Acceleration of the basic algorithm

Even though the basic algorithm may solve scheduling problems up to a certain size, it may not be sufficiently effective for practical applications. The basic algorithm, however, can easily be accelerated by built-in combinatorial algorithms. A simple acceleration tool, the so-called loop prediction, is illustrated here. This tool tests whether an acyclic leaf can be derived from a partial problem. If the test is negative, the partial problem is to be pruned, since no feasible solution can be generated from this partial problem. This acceleration tool is realized by the loop search algorithm given in Appendix B. The program that has been developed in C++ can be downloaded from <http://www.dcs.vein.hu/demo/sch/>. A complex case study illustrates the behavior of the accelerated algorithm.

Case Study. Nineteen equipment units, E1 through E19, are available to generate ten products, A, B, C, ..., J. The recipes of the products are given in Tables 5 and 6. The changeover time is 60 min for equipment units E1, E2, E3, and E4, and 90 min for E5, E6, E7, E8, E9, E10, E11, E12, E13, E14, and E15; all other changeover times are zero.

The number of batches to be produced is given in Table 7 for each product; the sum of the number of batches is 33. The problem has been solved by the accelerated algorithm that required 25.27-s CPU time on a PC-Pentium 533 MHz. The resultant makespan is 7,740 min; Figure 20 shows the corresponding schedule-graph.

Table 5. Recipe for Products A, B, C, D, and E

Task	Product A		Product B		Product C		Product D		Product E			
	Eq.	Time (min)										
1	E1	300	E2	240	E2	240	E1	300	E2	240		
			E3	120	E3	120	E3	120	E4	240		
			E4	240								
2	E5	60	E6	120	E6	120	E6	120	E5	60		
			E7	90	E8	60	E7	90	E6	120		
			E8	60	E8	60	E10	120	E8	60		
			E10	120			E12	60	E9	90	E9	90
			E12	60			E14	120	E11	90	E10	120
			E14	120			E15	60			E12	60
			E15	60							E13	90
								E14	120			
								E15	60			
3	E16	720	E19	840	E17	540	E16	720	E17	540		
					E18	720	E17	540	E18	720		

Table 6. Recipes for Products F, G, H, I, and J

Task	Product F		Product G		Product H		Product I		Product J	
	Eq.	Time (min)								
1	E1	300	E2	240	E4	240	E1	300	E4	240
	E3	120	E3	120			E3	120		
2	E5	60	E5	60	E5	60	E10	120	E7	90
	E7	90	E10	120	E7	90	E11	90	E9	90
	E9	90	E11	90	E9	90	E12	60		
	E11	90	E12	60	E11	90	E13	90		
	E13	90	E13	90	E13	90	E14	120		
	E15	60	E14	120	E15	60				
3	E16	720	E16	720	E19	840	E19	840	E17	540
	E17	540	E17	540						
			E18	720						
			E19	840						

Table 7. Number of Batches of the Products

Product	A	B	C	D	E	F	G	H	I	J
Number of batches	2	3	5	2	5	4	5	5	1	1

Concluding Remarks

A new framework has been proposed for job-shop scheduling based on an S-graph representation. Instead of solving an MILP model of the scheduling problem, the procedure given in the article solves the problem by specific algorithms, including a sequence of efficient graph algorithms (e.g., longest path and cycle search algorithms) that exploit the unique feature of the scheduling problem. The solution of the complex examples illustrates the efficacy of the proposed framework.

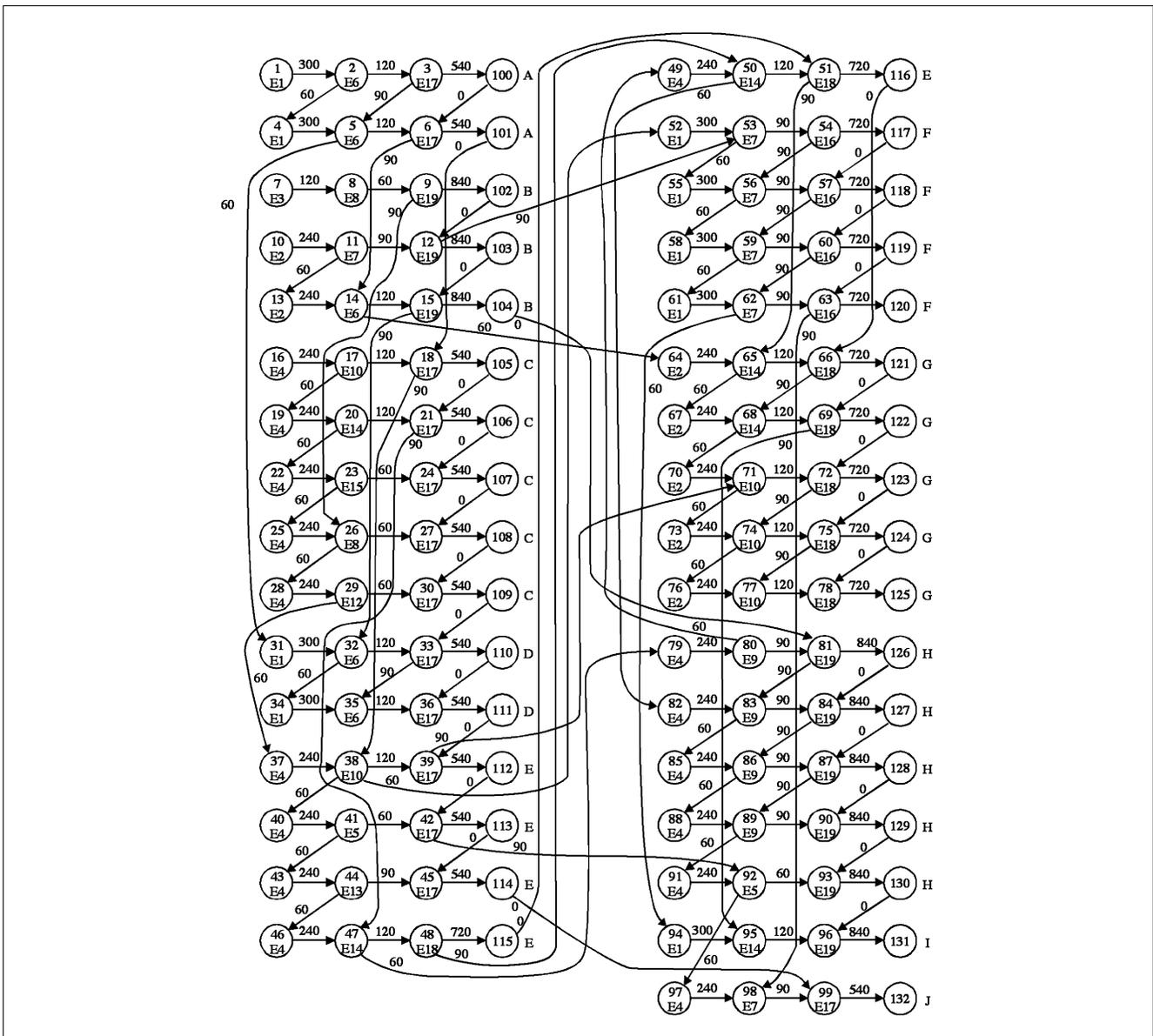


Figure 20. Schedule-graph of the optimal solution of the case study.

This framework provides the basis for further developments in solving special classes of scheduling problems, for instance, scheduling related to flexible recipes, complex recipes, and finite intermediate storage policy, which are the scope of our current work.

Acknowledgment

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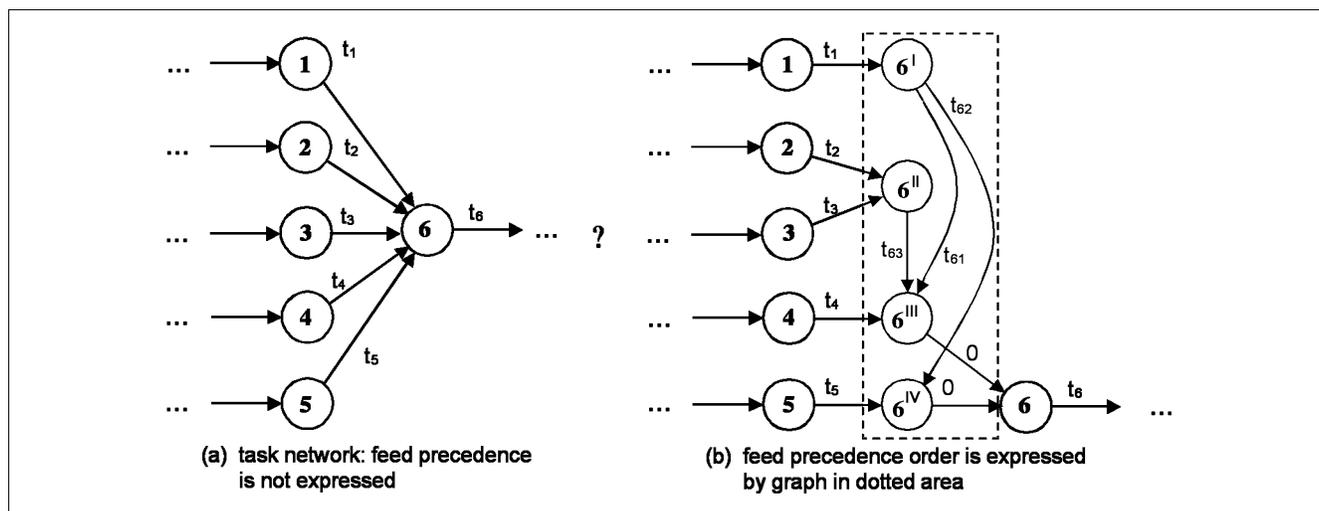


Figure A1. Part of a recipe-graph: complex procedure constraints are given on the inputs of task 6.

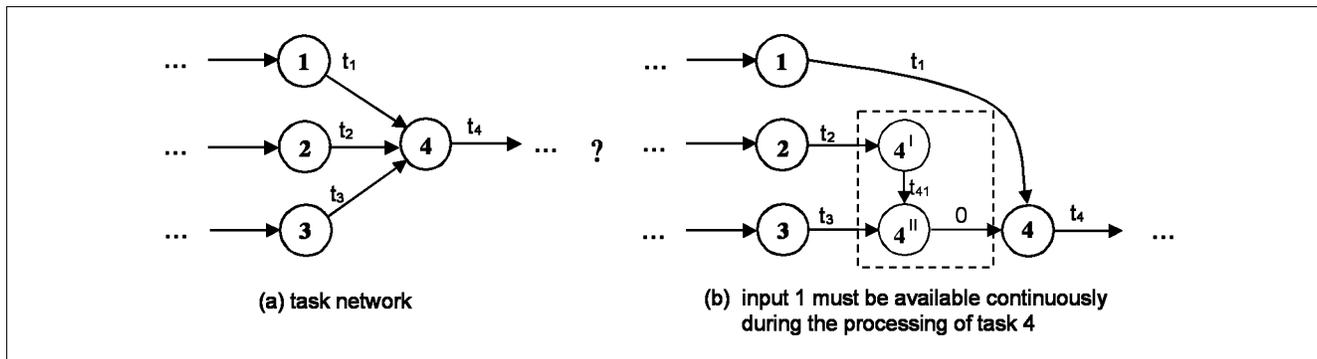


Figure A2. Fed-batch operation.

Appendix A: Feed-Precedence Graph

Suppose that a task has multiple inputs in the recipe. In the general case, certain inputs must be fed in parallel to the equipment, others in certain orders, and some have no relation given between them. The relationship between the feeds establishes a partial order among them. This partial order can be represented by an acyclic directed graph embedded in the task network. For example, suppose that input 1 must precede input 4 and 5, and input 2 must precede input 4 in

```

procedure cycle_search(i, LIST)
begin
  if pred(i) = ∅ then return no_cycle;
  for all j ∈ pred(i) do
    begin
      if j ∈ LIST then return cycle;
      LIST = LIST ∪ {j};
      cycle_search(j, LIST);
      if (cycle) then return cycle;
      LIST := LIST \ {j};
    end;
  return no_cycle;
end;

procedure pred(i)
begin
  pred(i) = set of nodes that have an arc to i;
end;

```

Figure B1. Cycle detection algorithm.

```

procedure longest_path (G(N,A))
begin
  for all j ∈ N do d(j) := 0;
  for all i ∈ N do
    begin
      LIST = {i}; longest = 0;
      while LIST ≠ ∅ do
        begin
          LIST = LIST \ {i};
          for each arc (i, j) ∈ A do
            begin
              if d(j) < d(i) + c(i, j) then
                begin
                  d(j) = d(i) + c(i, j);
                  longest = max(longest, d(j));
                  if j ∉ LIST then add node j to LIST;
                end;
            end;
          i = node in LIST with max d(i);
        end;
      end;
    end;
  end;

```

Figure B2. Longest path algorithm.

Figure A1a. Moreover, input 2 must be available simultaneously with input 3 in the task sequence. The additional nodes and arcs given in Figure A1b can express this order of precedence. These additional nodes are called feed-precedence nodes.

Note that for the so-called fed-batch operation, when a task has an input that must be fed continuously during the procedure of the task, the recipe-arc goes directly to the task node, bypassing the feed-precedence graph of the task if applicable (see Figure A2). The scheduling algorithm can simply take into account the feed-precedence graphs and the fed-batch operations.

Appendix B: Combinatorial Algorithms

The cycle-detection algorithm (Figure B1) is considered to be a feasible test of a partial problem of the proposed B&B algorithm, and the longest-path algorithm (Figure B2) is used in generating a lower bound of the makespan of a partial problem. More details of these algorithms can be found, for example, in Cormen et al. (1997).

Appendix C: LP Model for Determining a Lower Bound of a Partial Problem

Suppose that length L_j of the longest path to node j in the S-graph of a partial problem has been determined for all $j \in N$. Let \bar{M}_i denote the set of nodes given by formula $\bar{M}_i = \{j: j \in N_i \setminus M_i \& j \notin N_k \text{ for all } k \in \{1, 2, \dots, n\} \setminus \{i\}\}$ ($i = 1, 2, \dots, n$). Let c_i ($i = 1, 2, \dots, n$) be defined as

$$c_i = \max \left(\max_{j \in M_i} (L_j + t_{ij}), \min_{j \in N_i \setminus M_i} (L_j) \right) + \sum_{j \in \bar{M}_i} t_{ij},$$

where t_{ij} is the processing time of task j by equipment unit i .

The solution of LP problem

$$\begin{aligned}
 & \min X \\
 & \text{s.t.} \\
 & c_i + \sum_{j=1}^{m_i} x_{ij} \leq X \quad (i = 1, 2, \dots, n) \\
 & \sum_{i \in S_j} \frac{x_{ij}}{t_{ij}} \geq 1 \quad (\{j: j \in \{1, 2, \dots, |N_i|\} \& |S_j| > 1\}) \\
 & x_{ij} \geq 0 \quad (i = 1, 2, \dots, n, j = 1, 2, \dots, m_i)
 \end{aligned}$$

Table C1. Recipes of Example 5

Task	Product A		Product B		Product C	
	Eq.	Time (h)	Eq.	Time (h)	Eq.	Time (h)
1	E1	8	E1	9	E1	7
			E2	11	E2	7
2	E2	15	E3	5	E3	4
	E3	5				

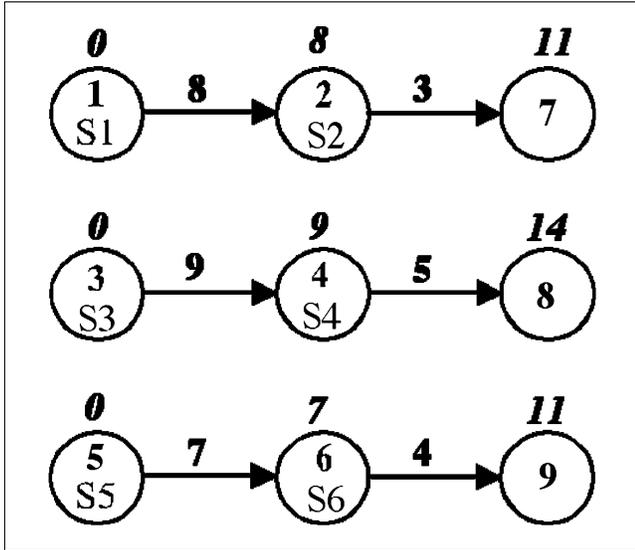


Figure C1. Recipe-graph of Example 5.

gives a lower bound for the partial problem, where
 n = number of equipment units;
 m_i = the cardinality of set $N_i \setminus (M_i \cup \bar{M}_i)$, that is, $m_i = |N_i \setminus (M_i \cup \bar{M}_i)|$ ($i = 1, 2, \dots, n$);
 N_i = the set of task nodes;
 S_j = set of equipment units that can perform task (node) j ($j = 1, 2, \dots, |N_i|$);

x_{ij} = (variable) processing time of equipment unit i in task (node) j ($i = 1, 2, \dots, n, j = 1, 2, \dots, m_i$); and
 X = (variable) lower bound for the partial problem.

Example C1. Three equipment units, E1, E2, and E3, are available to generate three products, A, B, and C. The recipes of the products are given in Table C1.

The recipe-graph of the example is given in Figure C1, where the value of the longest path to each node is given above the node.

The LP model will be given for the root of the enumeration tree of the B&B algorithm, that is, for the recipe-graph. Since $\bar{M}_1 = \{1\}$, $\bar{M}_2 = \emptyset$, $\bar{M}_3 = \{4,6\}$, $c_1 = 8$, $c_2 = 0$, and $c_3 = 16$, the LP problem to be solved is

min X

s.t.

$$\begin{aligned}
 8 + x_{13} + x_{15} &\leq X \\
 x_{22} + x_{23} + x_{25} &\leq X \\
 16 + x_{32} &\leq X \\
 \frac{x_{13}}{9} + \frac{x_{23}}{11} &\geq 1 \\
 \frac{x_{15}}{7} + \frac{x_{25}}{7} &\geq 1 \\
 \frac{x_{22}}{15} + \frac{x_{32}}{5} &\geq 1 \\
 x_{13}, x_{15}, x_{22}, x_{23}, x_{25}, x_{32} &\geq 0.
 \end{aligned}$$

The resulting lower bound is $X = 17.4$; it is a sharper bound than that given by the longest-path algorithm, or, 14.

Case Study Revisited. For the root of the enumeration tree, the lower bound given by the longest-path algorithm is 387 min, while it is 1,261 min when using the LP model.

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