Integrating information, financial, and material flows in a chemical supply chain

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Abstract
We address the flows involved in a real supply chain and discuss how they can be integrated for supply chain management. A scheduling model is proposed based on a State-Task Network representation to schedule order transactions and manufacturing operations in a make-to-order chemical plant. The proposed model is compared to scheduling models that focus on either the order transactions or the manufacturing operations. The advantage of the integrated approach is found in the accuracy of the solutions attained, whereas the siloed models produce suboptimal or infeasible solutions. Each model is compared in a stochastic discrete event simulation environment. An integrated scheduling model is also presented, which includes information, financial, and material flows along a three-echelon supply chain. This integrated model serves as a starting point for developing decision-support systems that take a more comprehensive view of the complex relationships amongst the different flows involved in real supply chains.

Keywords: Supply chain management, business processes, financial modeling, chemical process scheduling, logistics, inventory management.

1. Introduction

Management of real supply chains requires effective decision making across the different levels of time and space in the supply chain. Depending on the time scales of the decisions being made, these can be categorized as operational (short-term), tactical (mid-term), or strategic (long-term) (Shapiro, 1999). These decisions are made across and within the various geographically distributed actors in the supply chain, as well as the different business units and departments of the enterprises involved. Supply chain components include suppliers, manufacturing sites, distribution centers, and markets/customers, each of which are placed along the different tiers of the supply network. Supply chains also involve enterprise departments such as billing, accounting, sourcing, customer service, logistics, production, and maintenance. Each of these components and departments is managed by various agents that are constantly required to manage risk and respond to disruptions. The distributed nature of decision-making across the supply chain often results in a decentralized and siloed approach to supply chain management. Competing interests and priorities often lead to inefficiencies and hinder the ability of decision-makers to face and overcome the various challenges that can arise throughout the supply network.

Overcoming the challenges faced by real supply chains requires an integrated approach to supply chain modeling and management. Throughout the academic literature, most approaches to supply chain modeling fall into one of the following categories: bottom-up approaches or top-down approaches (Shapiro, 1999). Top-down methods focus on the operational decisions within supply chain management (e.g., design, planning, and scheduling) (Shah, 2005). On the other hand, bottom-up methods focus on the transactional processes in the supply chain, which are modeled in information management systems, such as Enterprise Resource Planning (ERP) systems (Shapiro, 1999). In the Process Systems Engineering (PSE) community, the need for a holistic approach to supply chain management has been emphasized, requiring a paradigm shift from operation-based decision support systems to integrated decision frameworks that account for the different areas (e.g., accounting, research and development, sustainability) and flows (material, financial, and information) that make up real supply chains (Laínez and Puigjaner, 2012). With the advent and widespread drive towards digitalization in the fourth industrial revolution, a clear opportunity has emerged for a more holistic approach to supply chain management. This endeavor requires viewing supply networks as systems that unite physical, information, and financial flows, with multiple interactions across the enterprise where material, data, humans, and intelligent agents interact in a coordinated fashion (Büyüközkan and Göçer, 2018).

Academic research in driving this transformation to supply chain management is still in its infant steps. However, important work has begun to move the PSE community in this direction. One such development in this space is that of Guillen *et al.* (2006), who present a planning/scheduling model for a chemical supply chain that integrates process operations and financial decisions. Their work is unique in that the objective of the supply chain planning and scheduling is to maximize shareholder equity, which is modeled via a cash flow model. This work highlights the value obtained when financial and material flows are integrated in supply chain operations. The authors contrast the integrated approach to a sequential and hierarchical approach where financial decisions are made in response to the optimization of the physical operation of the supply chain. The authors show that sequential decision making, as is typically done in real enterprises, results in reduced shareholder equity and less balanced financial and inventory loads. Another work that proposes integrating financial and physical flows in supply chains is that of Comelli *et al.* (2008), which implements activity-based costing and payment terms in supply chain tactical planning. Although these works and others are valuable in integrating physical and financial flows in supply chains, they do not consider the information flows in supply chain business processes, which are key drivers in real supply chains and an area that has received very little attention in PSE.

Information flows in a supply chain are managed by end-to-end business processes, which encompass the transactions that occur on various requests along a supply chain. These requests can be external customer orders, which are governed by the order-to-cash process, or inventory replenishment orders, which are governed by the source-to-pay process. Scheduling of events in business processes has been studied principally by the computer science and information systems communities (Xu *et al.*, 2010). The business process scheduling in these works targets purely transactional business processes, such as banking processes that are executed in the cloud (Hoenisch *et al.*, 2016). However, when business processes involve physical goods, such as in material procurement or physical goods sales, the associated business processes become tightly coupled with the material flows and processes in the system. Although scheduling business processes in this context has not received much attention, their close integration with physical and financial flows is critical in chemical supply chains, where business processes like the order-to-cash process depend on the availability of inventory and the manufacturing of goods.

The present work seeks to address this gap in the supply chain management literature and bridge the two approaches to supply chain modeling discussed by Shapiro (1999). As a first step in accomplishing this, a framework is presented to integrate the material flows in a chemical batch plant with the information flows in the order fulfillment process. Prior work by the authors includes the development of scheduling models to optimize the order transactions in the order-to-cash process (Perez *et al.*, 2021), which have then been integrated with discrete event simulation in a digital twin framework for supply chain business processes (Perez *et al.*, 2022). However, this prior work focuses primarily on the information flows in the supply chain and represents any physical processes as nodes in the transactional process network with a lumped process duration. In this work, we provide a more comprehensive and detailed approach, which integrates manufacturing scheduling models with the order-to-cash process model. This approach provides a more complete and accurate view of the supply chain by accounting for both material and information flows. The use of chemical production and material availability models enables an accurate representation of the processing times in the chemical manufacturing steps, which in turn allows the optimization models to find better solutions when scheduling customer orders. The present work also takes a step further by presenting an integrated model that brings together the various material flows across the supply chain, including raw material suppliers, manufacturing sites, distribution centers, and final customers. Coupled to this supply chain model are models for batch production scheduling at manufacturing sites, inventory management at storage locations, order-to-cash business transactions at demand facing nodes, source-to-pay transactions at supply facing nodes, and financial assets, liabilities, and shareholder equity. This integrated model is built using concepts from both the State-Task Network (Kondili *et al.*, 1993) and Resource-Task Network (Pantelides, 1994) paradigms. Furthermore, this work builds on the prior work by Guillen *et al.* (2006) and Perez *et al.* (2021, 2022) to take a step forward in the development of a holistic digital supply chain management system that couples all major supply chain flows: information flows in ERP systems, material flows in production and distribution processes, and financial flows in accounting processes.

The paper is structured as follows: the different components and flows in a supply chain are described and modeled via Task Network models in **Section 3**. These models include a graphical (network-based) abstraction to describe the material, information, and financial flows and processes in a supply chain. For each representation, a discrete-time Generalized Disjunctive Programming (GDP) optimization model is defined. An illustrative example is given in **Section 4** to integrate the detailed chemical plant scheduling models with the order-to-cash process in a dynamic (online) scheduling environment. The benefits of an integrated model over a transaction-focused or material-focused model are presented. **Section 5** describes a holistic Task Network representation that brings together all of the processes described in **Section 3** for the scheduling of supply chain material, financial, and transactional processes. **Section 6** presents concluding remarks and future directions to extend the work presented here.

2. Nomenclature

	Description
Sets	
$a \in A$	Agents
$a \in A_l$	Agents capable of executing transaction l
$i \in I$	Processes
$i \in I_k^{pred}$	Processes producing state k (predecessor processes)
$i \in I_k^{succ}$	Processes consuming state k (successor processes)
$i \in I^{super}$	Super-transaction tasks used in integrated model
$j \in J$	Processing equipment
$j \in J_i$	Processing equipment used for process i
$k \in K$	States
$k \in K^{arrived}$	Raw material arrival states
$k \in K^{feed}$	Feedstock material states
$k \in K^{inv}$	Inventory storage states

$k \in K^{fulfilled}$	Fulfilled (delivered) material states at external customers
$k \in K^{prod}$	Finished product material states
$k \in K^{shortfall}$	Inventory position shortfall states
$k \in K^{store}$	Downstream finished product storage states
$k \in K^{super}$	States connected to a super-transaction task
$k \in K^{AP}$	Accounts payable state
$k \in K^{AR}$	Accounts receivable state
$k \in K^{MTO}$	Make to order material states
$l \in L$	Transactions
$l \in L_s^{pred}$	Transaction producing information state s (predecessor transaction)
$l \in L_k^{pred}$	Interface transaction producing material state k
$l \in L_s^{succ}$	Transaction consuming information state s (successor transaction)
$l \in L_k^{succ}$	Interface transaction consuming material state k
$l \in L_o^{super}$	*Issue Goods & Receive Payment* super-transaction for order o
$s \in S$	Information states
$t \in T$	Timepoints
$(o, l, a) \in \Omega$	Active business process tasks (transaction l on order o by agent a)
Parameters	
$\alpha_{i,j}$, $\beta_{i,j}$	Fixed and variable operating cost factors for process i performed on equipment j
$\gamma_{l,a}$	Cost of preempting (interrupting) transaction l being performed by agent a
$\rho_{i,k}^{cons}$	Consumption ratio for state k involved in process i
$\rho_{i,k}^{prod}$	Production ratio for state k involved in process i
$\rho_{i,k,\theta}^{fixed}$	Fixed production/consumption ratio for state k in process i started θ periods ago
$\rho_{i,k,\theta}^{var}$	Variable prod. /cons. ratio for state k in process i started θ periods ago
$\tau_{i,j,k}$	Time to produce state k in process i in equipment j
$\overline{\tau}_{i,j}$	Total duration of process i in equipment j
$\tau_{o,l,a}$	Total duration of transaction l by agent a on order o
t_o^r, t_o^e, t_o^d, t_o^{ls}	Release, earliest fulfillment, due, and lost sales dates for order o
p_k	Price of material k
$q_{o,k}$	Amount of material k required to fulfill order o
$\overline{q}_o$	Amount of finished good requested in order o
w_k	Weighing coefficient for state k
z_o	Profit (or revenue) of order o. Continuous variable in Example 1.
ROP_k	Reorder point for material k
TIP_k	Target inventory position for material k
S_k^{min}, S_k^{max}	Lower and upper bounds on the level of state k
$V_{i,j}^{min}$, $V_{i,j}^{max}$	Lower and upper bounds on the batch size of process i in equipment j
V_i^{min}, V_i^{max}	Lower and upper bounds on the batch size of task i
Continuous Variables	
t_o^{exit}	Time that order o is fulfilled
$B_{i,t}$	Batch size for task i started at time t
$B_{i,j,t}$	Batch size for task i, j (process i in equipment j) started at time t
$N_{i,t}$	Task i started at t
$S_{k,t}$	State level for state k at time t
$S_{k,t}^{max}$	Upper bound on state k at time t

$S_{o,t}^{exit}$	Removal (fulfillment) of order o at time t
$S_{k,t}^{demand}$	External demand (removal) of state k at time t
$S_{k,t}^{supply}$	External supply (addition) of state k at time t
Boolean Variables	
BL_o	Order o is fulfilled late (backlogged)
$D_{o,t}$	Order o delivered at time t
LS_o	Order o is a lost sale
OT_o	Order o is fulfilled on-time
$W_{i,t}$	Task i starts at t
$W_{i,j,t}$	Task i, j (process i in equipment j) starts at time t

3. Supply Chain Component Models

As introduced previously, real supply chains are complex networks that link various entities (geographically distributed physical assets, business units, organizations, and enterprises), which interact throughout the different levels of decision-making (operational, tactical, and strategic). The links between these entities can be divided into three general types of flows: information, material, and financial (Laínez and Puigjaner, 2012). **Figure 3.1.1** provides a diagram of the different components in a real supply chain as they interact with each of these flows. At the enterprise level, information flows are governed by business processes, in which information flows into and out of a network of transactional events. These business processes are managed via enterprise resource planning (ERP) systems. Material flows are found within and between physical supply chain nodes (suppliers, manufacturing sites, and distribution centers). Physical events control the flow of materials as they are transported, stored, and transformed from raw materials, to intermediates, and ultimately to finished goods and byproducts. Financial flows occur whenever a commercial transaction takes place, such as when raw materials are purchased, finished goods are sold, operational expenses are paid for, capital is invested, and dividends are disbursed. From an accounting perspective, at each financial transaction a balance is made between assets, liabilities, and shareholder equity. Each financial flow increases or decreases the amount in each of these financial categories.

Although each of the three types of flows are managed by different organizations within an enterprise, the next generation supply chain must account for the interwoven nature of these flows throughout the supply network. These types of flows are discussed and modeled in the next subsections.

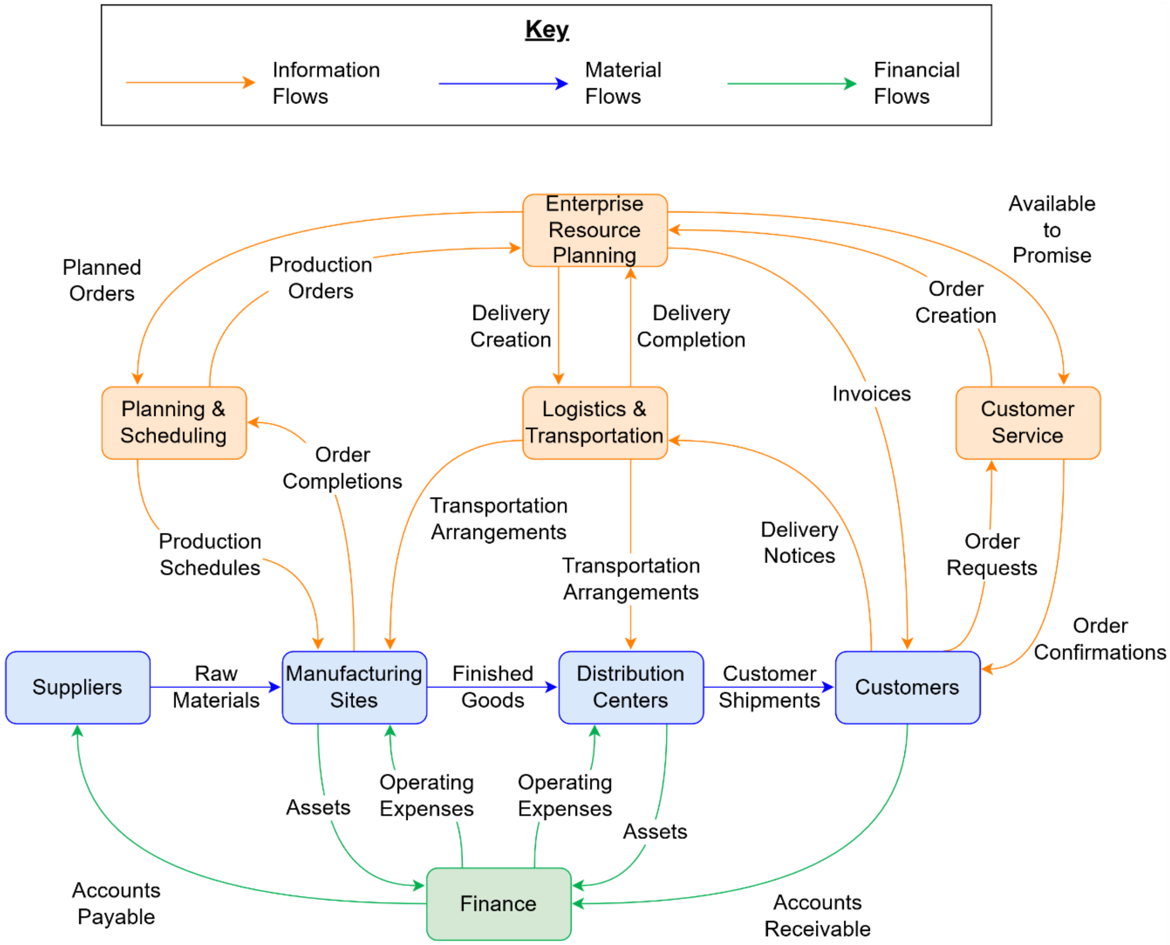

Figure 3.1.1. Components and flows in a real supply chain.

3.1 Material Transformation Processes

One of the main physical processes in a supply chain, and especially in a chemical supply chain, is that of processes that transform matter into different physical and chemical forms. The material transformation processes in a supply chain occur in manufacturing facilities (i.e., chemical plants), where production schedules are usually required to produce the desired finished goods subject to resource limitations and demand for the different products. Chemical process scheduling is a key area of PSE and has been studied for several decades. Many mathematical formulations have been proposed to obtain schedules that are optimal for some desired performance indicator, such as cost or makespan. The reader is referred to key reviews in the area of chemical batch scheduling for further detail on the various models available (Harjunkoski *et al.*, 2014; Maravelias, 2021; Méndez *et al.*, 2006).

In this work, we model material processes and flows in a supply chain using the State-Task Network (STN) model (Kondili *et al.*, 1993; Shah *et al.*, 1993), which is a discrete-time mixed-integer programming scheduling model that represents a process as bipartite graphs with *state* nodes (e.g., materials) and *task* nodes (e.g., unit operations). In this model, *tasks* consume or produce the *states* associated with each task. State balances are performed at each timepoint along the scheduling horizon. The STN model can be used to model continuous, batch, or semi-continuous processes (Maravelias, 2021). An example of a STN bipartite graph representation of a chemical plant is given in **Figure 3.1.2**, which models the chemical plant presented in Kondili *et al.* (1993). The plant shown is a batch plant with three raw materials (A, B, and C), four intermediate materials (HotA, AB, BC, and E), two final products (P1 and P2), two multipurpose reactors (50 and 80 kg capacity), one heater (100 kg capacity), and one distillation column (200 kg capacity). There are five unit operations in the batch plant: Heating, Reaction 1, Reaction 2, Reaction 3, and Separation. Processing times, intermediate storage capacities, and reaction stoichiometries (on a mass basis) are given in **Figure 3.1.2**, where task nodes are aggregated by unit operation (e.g., Reaction 1 in the 50 kg Reactor and Reaction 1 in the 80 kg Reactor are represented by a single blue rectangular node). Storage limits for raw materials and final products are not considered, but could be included if desired. The general plant topology given in **Figure 3.1.2** contains key features of material transformation processes, including processes with single and multiple inputs and outputs, material recycles, storage capacity limits, resource constraints, and intermediate material draws. With these features, the proposed mathematical scheduling model can be readily extended to more complex physical processing networks.

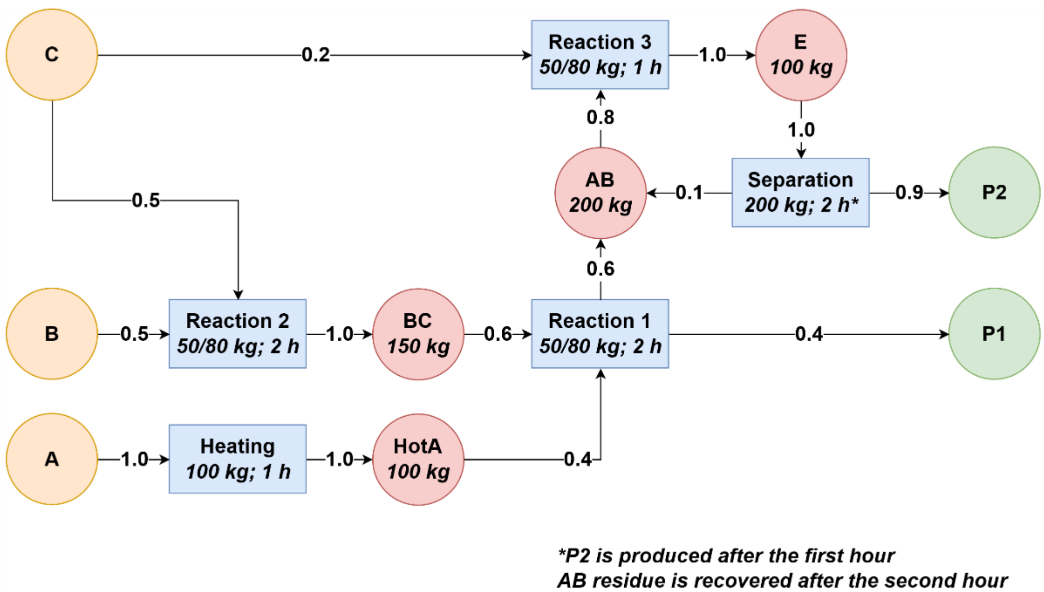

Figure 3.1.2. Compact STN diagram for the chemical batch plant in Kondili *et al.* (1993). States are indicated by circular nodes and tasks by rectangular nodes. Capacities and processing times are shown under each unit operation. Tank capacities are shown for the intermediate materials. Unit operation reaction stoichiometries (referred to as bill of materials in supply chain) are shown on a mass basis over each directed edge.

We now describe the STN model for the plant (Kondili *et al.*, 1993) in the form of a Generalized Disjunctive Programming (GDP) model (Castro *et al.*, 2018; Grossmann and Trespalacios, 2013). The principal model constraint is a state balance about each material state node as given in (3.1.1), where the amount of state k at timepoint t ($S_{k,t}$) is updated from its the value in the previous timepoint ($t-1$) by:

- Adding any amount produced from batches of material in tasks i, j (process i performed on equipment j) triggered $\tau_{i,j,k}$ periods ago ($B_{i,j,t-\tau_{i,j,k}}$),
- Subtracting any amount consumed in batches of material that have entered production in the current period ($B_{i,j,t}$),

- Adding any external supply of material ($S_{k,t}^{supply}$), and
- Subtracting any external demand for the material ($S_{k,t}^{demand}$).

$\rho_{i,k}^{prod}$ and $\rho_{i,k}^{cons}$ are the production and consumption ratios for material in state k in process i, sets I_k^{pred} and I_k^{succ} are the physical process predecessors and successors to node k, and set J_i is the set of equipment that can perform process i.

$$S_{k,t} = S_{k,t-1} + \sum_{i \in I_k^{pred}} \rho_{i,k}^{prod} \cdot \sum_{j \in J_i} B_{i,j,t-\tau_{i,j,k}} - \sum_{i \in I_k^{succ}} \rho_{i,k}^{cons} \cdot \sum_{j \in J_i} B_{i,j,t} + S_{k,t}^{supply} - S_{k,t}^{demand} \qquad \forall k \in K, t \in T \tag{3.1.1}$$

(3.1.2) is a disjunction constraint that allows the batch of material $B_{i,j,t}$ from task i, j, starting at timepoint t to have a nonzero value between a minimum batch size $V_{i,j}^{min}$ and a maximum batch size $V_{i,j}^{max}$ if the task is triggered at time t, meaning $W_{i,j,t} = True$. Otherwise, the bounds on the batch size reduce to zero.

$$\begin{bmatrix} W_{i,j,t} \\ V_{i,j}^{min} \leq B_{i,j,t} \leq V_{i,j}^{max} \end{bmatrix} \vee \begin{bmatrix} \neg W_{i,j,t} \\ B_{i,j,t} = 0 \end{bmatrix} \qquad \forall i \in I, j \in J_i, t \in T \tag{3.1.2}$$

The cardinality constraint in (3.1.3) allows *at most* 1 task triggering Boolean variable to be true from the set of processes that equipment j can execute within a window of $\bar{\tau}_{i,j} - 1$ periods, where $\Gamma(n,\cdot)$ is the *at most n* predicate (Perez and Grossmann, 2023) and $\bar{\tau}_{i,j}$ is the total duration of task i, j. This cardinality rule is the logical equivalent to the knapsack constraint on the reformulated binary variables ($\sum_{i \in I_j} \sum_{t'=t-\bar{\tau}_{i,j}+1}^{t} W_{i,j,t'} \leq 1$) proposed by Shah *et al.* (1993) for the STN model. The constraint ensures that processing equipment cannot begin another batch before the current batch has completed. Although cardinality rules are not used in the traditional GDP formulation, they have been recently introduced in an extended GDP formulation to allow higher-order logic constraints such as this resource assignment constraint (Perez and Grossmann, 2023).

$$\Gamma\left(1, W_{i,j,t'} \;\; \forall i \in I_j, t' \in \{t - \bar{\tau}_{i,j} + 1, \dots, t\}\right) \qquad \forall j \in J, t \in T \tag{3.1.3}$$

The variable domain and bounds for the GDP STN model are given in (3.1.4) – (3.1.6). The external supply and demand of material ($S_{k,t}^{supply}$ and $S_{k,t}^{demand}$) are usually parameters, but can in some cases be modeled as variables in the space of the non-negative reals. The lower and upper bounds on a material state are given by S_k^{min} and S_k^{max}, respectively, which can be used to enforce a minimum and maximum inventory level for material k.

$$B_{i,j,t} \in \mathbb{R}: 0 \leq B_{i,j,t} \leq V_{i,j}^{max} \qquad \forall i \in I, j \in J_i, t \in T \tag{3.1.4}$$

$$S_{k,t} \in \mathbb{R}: S_k^{min} \leq S_{k,t} \leq S_k^{max} \qquad \forall k \in K, t \in T \tag{3.1.5}$$

$$W_{i,j,t} \in \{True, False\} \qquad \forall i \in I, j \in J_i, t \in T \tag{3.1.6}$$

In discrete-time scheduling applications, the objective function defined by the feasible space given in (3.1.1) – (3.1.6) depends on the desired targets, but is usually a minimization of cost or a maximization of profit, where operating costs can be modeled as being proportional to the batch size of each task (with some fixed setup cost if desired), and sales are driven by the price of the materials demanded. Additional model features such as cleaning steps (e.g., changeovers) and non-equipment resource availability can also be included in the STN formulation (Méndez *et al.*, 2006). However, when such features are desired, it is often advantageous to switch over to a RTN model (Brunaud *et al.*, 2020).

3.2 Supply Chain Inventory Processes

We refer to inventory processes in a supply network as the processes that regulate the storage and distribution of inventory throughout the supply chain network. Some key terms in this space are:

- Safety stock: the inventory held to buffer against fluctuations (uncertainty) in demand and supply.
- Cycle stock: the inventory used to satisfy demand during a replenishment cycle.
- Inventory backlog: the inventory promised to customers (internal and external) that is overdue (e.g., due to a stockout).
- Inventory level: the difference between the on-hand inventory and inventory backlog.
- Inventory position: inventory "owned" at a location. Owned means that backlogs are deducted, and incoming inventory (in-transit) is included. This is equivalent to the sum of the inventory level and the replenishment orders that have already been placed.
- Reorder point: the parameter which triggers a replenishment order when the inventory position is less than or equal to its value.
- Replenishment policy: the decision rule used to determine 1) when to place a replenishment order and 2) the size of the order. Different types of policies exist, including order-up-to (s, S) and fixed-order-quantity (r, Q) (Brunaud, Laínez-Aguirre, *et al.*, 2019). Among these policies a key decision is how inventory is monitored, which can be periodic or continuous (Shenoy and Rosas, 2018).

We propose a STN formulation for inventory control in a supply chain. Using a STN formulation allows integrating inventory decisions with other supply chain decisions in Example 2 (see **Section 5**). This formulation monitors the target inventory position shortfall (PS) as an additional state node to trigger a replenishment order when the position shortfall is at least equal to the difference between the target inventory position of material m (TIP_m) and the reorder point (ROP_m). **Figure 3.2.1** illustrates the STN structure for the supply of material A in the Kondili plant from the previous section. The green node represents a new state node that measures the inventory required to reach the target inventory position for feedstock A. This state represents the complement of the inventory position and is bounded between 0 and TIP_A. A shortfall of 0 indicates that the inventory position of A is at its target. The reorder point ROP_A is the inventory position at which a replenishment order of A is triggered. This value is often calculated by summing the cycle and safety stocks to ensure that the demand over the supply lead time can be met up to a certain level of uncertainty (Eruguz *et al.*, 2016).

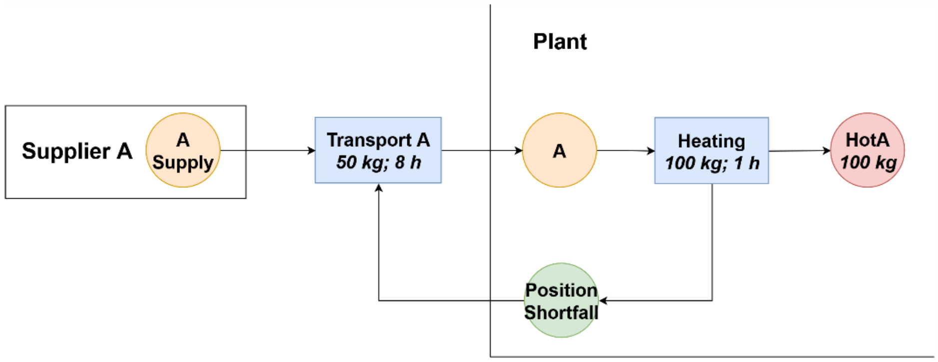

Figure 3.2.1. Example STN representation for the supply and monitoring of inventory.

For the replenishment to occur, there is a transportation task that links the supply of raw material A at the external supplier with the amount of A available at the plant. This transportation task takes two inputs, the availability of material A at the supplier node, and the position shortfall (PS) of A at the plant. Each time the Heating unit operation is triggered, the PS level increases by the amount of A that was consumed ($\rho_{Heat,PS}^{prod} = 1$). Note that the PS level increases when the Heating step is triggered, rather than when it ends. This results in a minor change to the state balance from (3.1.1), which is shown in (3.2.1), where the $-\tau_{i,j,k}$ in the time index of the Batch variable in the second term is removed. The minimum "batch size" for the transportation event is set to $V_{Trans,j}^{min} = TIP_A - ROP_A$. This ensures that the replenishment can only be triggered when the inventory position drops to or below the reorder point ROP_A, at which point, the position shortfall is "consumed" to reach the target inventory position. See **Appendix A** for a numerical example of these inventory dynamics.

$$S_{k,t} = S_{k,t-1} + \sum_{i \in I_k^{pred}} \rho_{i,k}^{prod} \cdot \sum_{j \in J_i} B_{i,j,t} - \sum_{i \in I_k^{succ}} \rho_{i,k}^{cons} \cdot \sum_{j \in J_i} B_{i,j,t} \qquad \forall k \in K^{shortfall}, t \in T \qquad (3.2.1)$$

By defining a state for the inventory position shortfall in the STN model, classical inventory policies for supply networks such as the order-up-to or (s, S) policy can be integrated with material transformation processes. The example shown here represents an order-up-to policy with continuous review. Periodic review can also be represented by fixing the transportation trigger Boolean variable $W_{Trans,j,t}$ to 0 for all t not belonging to a review period. Fixed-order-quantity policies can also be modeled by fixing the lower and upper bounds on the transportation "batch size" $B_{Trans,j,t}$ to equal the fixed order size.

3.3 <u>Business Processes</u>

The principal end-to-end business processes in a supply chain are the source-to-pay (S2P), forecast-to-plan (F2P), plan-to-produce (P2P), plan-to-move (P2M), inquiry-to-order (I2O), and order-to-cash (O2C) processes. These processes map the necessary steps that need to be performed between each end in the process. For example, the order-to-cash process contains the transactions that occur on a customer order until the goods are delivered, and payment is received from the customer on the invoice sent. These processes are often described as being linear, as the one shown in **Figure 3.3.1A**. However, in practice, they can be much more complex, involving parallel paths, alternate paths, and recycles to address inconsistencies and respond to system disturbances. **Figure 3.3.1B** illustrates some of the complexities observed in real business processes.

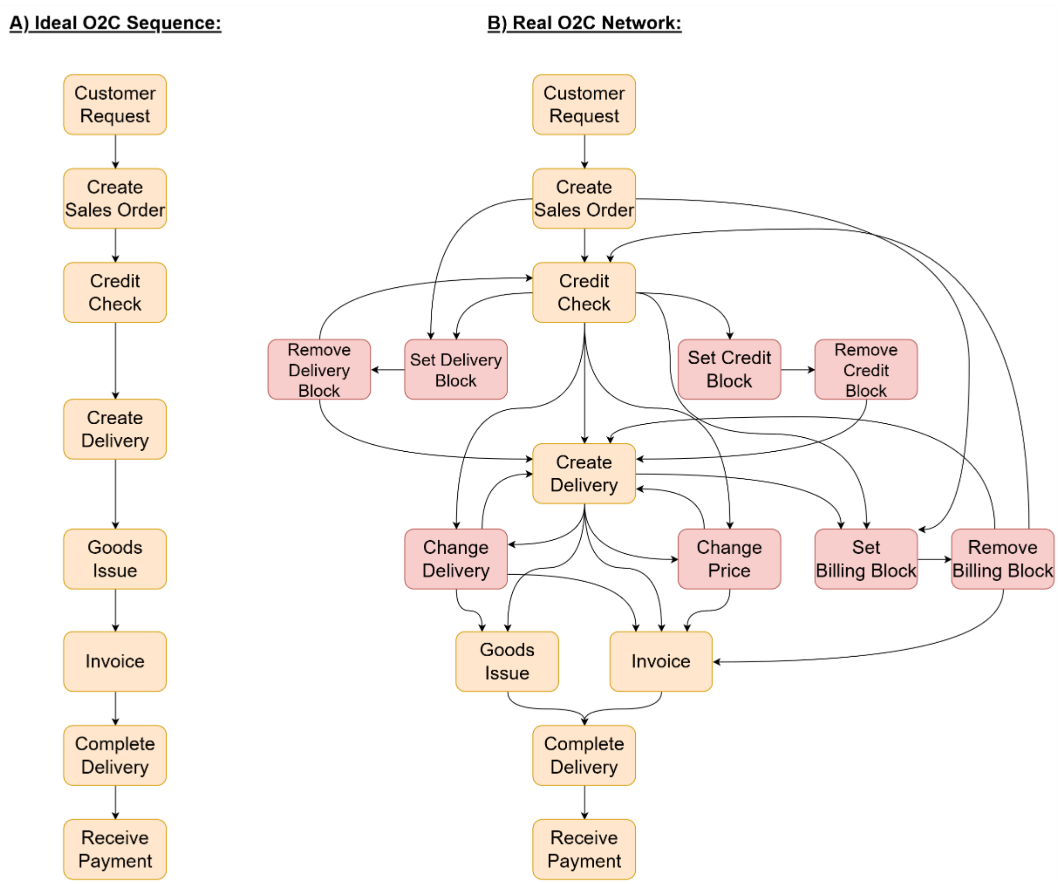

Figure 3.3.1. A) ideal linear order-to-cash process network (left), B) real order-to-cash process network with parallel events, alternate paths, recycles, and exceptions (right).

For the purposes of the work shown in this paper, we focus primarily on the order-to-cash (O2C) and source-to-pay (S2P) business processes because they link the enterprise supply chain to external customers and suppliers. However, the models presented here can be extended to the other relevant business processes. We note that although **Figure 3.3.1A** gives the main steps in the order-to-cash sequence, the actual event names and connections can vary among different enterprises. The same is true for other business processes. Prior work has shown that business processes can be modeled as flexible flowshop or jobshop networks where orders are processed by agents that execute the various transactions at each stage in the network (Perez *et al.*, 2021). With this flexible flowshop/jobshop modeling approach, business processes can be scheduled via heuristics or mathematical optimization. In our prior work, classical models from chemical batch scheduling were extended to applications in business processes. Among the different scheduling models compared, the discrete-time State-Task Network (STN) and Resource-Task Network (RTN) models proved to be advantageous for modeling business processes due to their model tightness and amenability to significant model reduction by commercial solvers during presolve (Perez *et al.*, 2021).

The general RTN representation of a business process model is given in **Figure 3.3.2**, which shows orders $1, \dots, |O|$ transitioning through states $1, \dots, |S|$ as they flow down the business process. The transition from one state to another occurs when a business transaction is performed (e.g., run credit check, create delivery, and record goods issue). Each of the transactions $1, \dots, |L|$ are executed by an agent, which can be a computer-based agent in the case of robotic process automation (RPA) (van der Aalst *et al.*, 2018) or a human agent (e.g., planner, scheduler, customer service representative). The double arrow on the agent nodes indicates that agents are consumed (locked) during a transaction and produced (released) when a transaction ends.

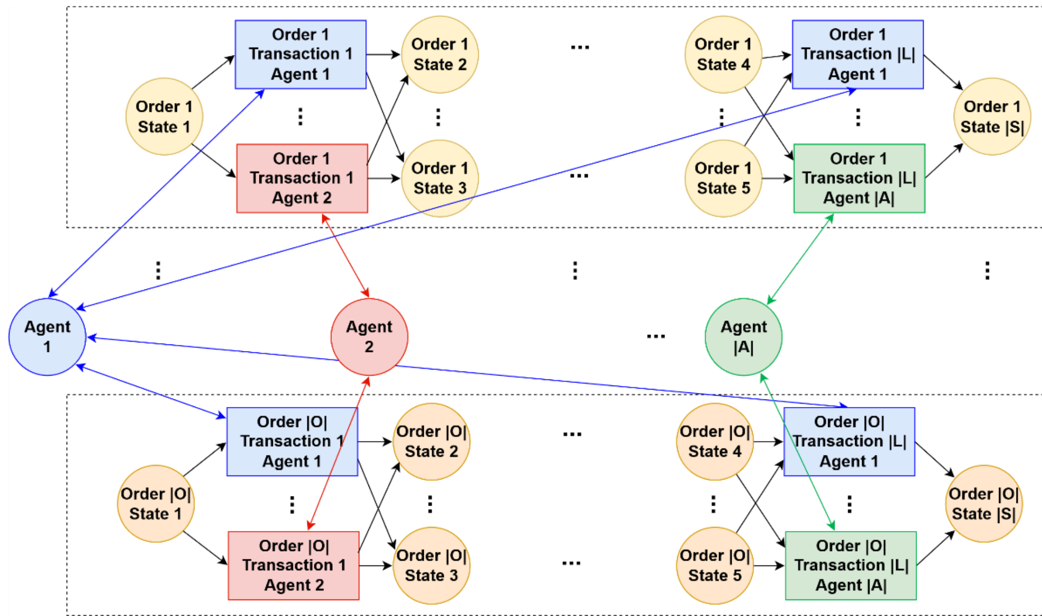

Figure 3.3.2. Detailed RTN representation of a business process network. Rectangular nodes represent task o, l, a for transactional event $l \in L$ that is executed on order $o \in O$ by agent $a \in A$. Circular nodes indicate the network resource o, s for order $o \in O$ in information state $s \in S$, or the individual $a \in A$ that is used in each transactional node.

Although **Figure 3.3.2** provides the most general and flexible graphical representation of a business process using RTN, the scheduling model used for these processes in this work is a STN, which can be viewed as a specialized version of the RTN. As a more general formulation, RTN is particularly effective when: 1) identical resources are used, 2) resources are consumed or produced in discrete or continuous quantities, or 3) changeover (e.g., cleaning) steps are required between tasks (Brunaud *et al.*, 2020; Méndez *et al.*, 2006). For business processes, most agents are unique, consumption and production of order states occur only at the beginning and end of a transaction, and changeover events are not required since these are not material processing tasks. In addition to being well suited for business process scheduling, prior work has shown that using STN for business processes results in models with fewer variables and constraints, which speeds up the scheduling optimization (Perez *et al.*, 2021). The STN model representation is equivalent to that of **Figure 3.3.2** without the agent nodes. Instead, each order subnetwork is linked implicitly with agent assignment constraints (analogous to (3.1.3)). The detailed STN model is presented in Perez *et al.* (2022), and is reproduced in **Appendix B** in GDP form.

3.4 Financial Processes

Financial processes govern the cash flow throughout the supply chain. Previous research in this area in PSE includes that of Yi and Reklaitis (2004), who model cash as a storage unit in a batch storage network. Their work shows that integrating material and financial flows allows obtaining a more accurate network design that ensures that cash inventory is not depleted. As mentioned in the Introduction (**Section 1**), Guillén *et al.* (2006) integrate material planning and scheduling decisions with financial ones, accounting for the various financial entities in a supply chain, and proposing an objective function that targets maximizing shareholder equity. Other works in the literature discuss applications of financial models in supply chain, with some addressing their integration with physical flows (Abdollahzadeh *et al.*, 2018; Comelli *et al.*, 2008; Kees *et al.*, 2019; Pfohl and Gomm, 2009). Integrating financial flows with inventory modeling allows modeling working capital, which is the sum of inventory assets and accounts receivable, minus accounts payable.

We propose modeling the financial balance sheet of an enterprise as a RTN. This allows us to model supply chain financial processes in a way that can be linked with the other supply chain process models discussed in this paper. The balance sheet of a company is a financial statement that balances the assets in a company with the sum of its liabilities and shareholder equity, which enables the company to finance its assets and operations. Some examples of how financial transactions are logged in the balance sheet at a high level are given below:

- Purchase of raw materials: The increase in inventory assets is equal to the increase in accounts payable (liability) owed to the supplier and shipper.
- Production of finished goods: The assets decrease by the value of the raw materials consumed and increase by the value of the finished goods produced at that location. The net change in asset value is balanced with the accounts payable for production (e.g., operating expenses).
- Shipping a finished product from one location to another: The value of the supply chain assets changes by the difference in the value of the assets at the receiving node and the value of the assets at the supplying node. This change is balanced by the accounts payable for shipping.
- Sale of finished goods: The assets increase by the accounts receivable associated with the sale, and decrease by the value of finished goods sold. This change in assets is balanced by the accounts payable for delivery (liability) and the increase in profit, which is initially recorded as a sale in the income statement and eventually as retained earnings (shareholder equity) in the balance sheet. For the proposed dynamic financial modeling in this section, profit from sales is recorded as shareholder equity.
- Paying expenses: When the liability for accounts payable is decreased by fulfilling the respective payments, the cash (asset) decreases by an equal amount.
- Receiving payments: When customers pay for the goods received, the net change in assets is zero. The assets decrease by the amount received for accounts receivable, which increases the cash (asset) by that same amount.
- Paying dividends: When dividends are paid out to shareholders, the cash (asset) decreases by the same amount that the earnings (shareholder equity) decrease.

In aligning with the Task Network approach used in the previous sections to model material and information processes, we propose a new application of RTN to represent financial processes. RTN was chosen to model financial processes instead of STN because invoices are produced and consumed in discrete quantities, while assets and liabilities are produced and consumed in variable (continuous) quantities, which can be explicitly modeled with RTN. Furthermore, the concept of financial entities such as assets, liabilities, and shareholder equity can intuitively be referred to as financial resources. **Figure 3.4** shows the RTN graph where assets, accounts payable, accounts receivable, earnings, cash, dividends, and invoices are modeled as resources. On the left side of the graph, receiving inventory (asset value) is a financial transaction that produces the inventory asset and an invoice that must be paid. This transaction also increases the level of the accounts payable resource. The payment delay task represents the time allowed by contract for paying an invoice (payment terms). When the invoice payment transaction is performed at the end of the payment terms, the accounts payable resource is consumed, along with the invoice and the cash required for the payment. On the right side of the graph, selling inventory (asset value) is a financial transaction that produces an invoice sent to the customer, accounts receivable, and earnings (shareholder equity). Depending on the nature of the sale, it can also add to the level of the accounts payable for any shipping costs. Once the payment terms on the customer invoice expired, the customer is expected to pay the invoice, which consumes the accounts receivable and produces cash (asset). The cash can then be used to pay dividends, during which the shareholder equity decreases by the amount paid out to shareholders.

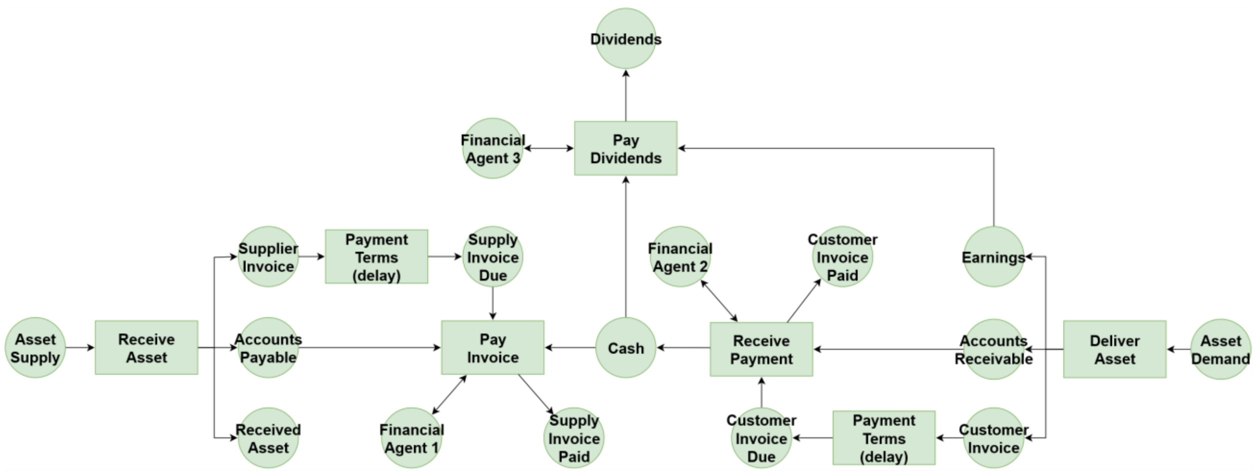

Figure 3.4. RTN representation of assets, liabilities, shareholder equity, and invoice states being transformed by supply chain financial processes.

It has now been shown that task network models (STN and RTN) can be applied not just to physical entities and processes, but also to information states and transactions, as well as financial entities and transactions. Thus, the STN and RTN models have been extended from their original use case in chemical batch scheduling to novel applications in inventory control, business processes, and dynamic accounting modeling, which are all key components in a real supply chain. Taking this modeling approach can then be used to optimize integrated flows in a supply chain, as is shown in the next sections.

4. Example 1: Integrating business processes scheduling with batch chemical process scheduling

This section illustrates how business processes can be modeled alongside material transformation processes using mathematical optimization, discrete event simulation, and the integration of these two for online scheduling in a simulation environment. The example given highlights the benefits of an integrated model for a make-to-order specialty chemicals plant, which allows finding the optimal sequencing of customer order transactions and production batches to maximize the profit generated from order fulfillment.

Consider the STN of a simplified order fulfillment business process given in **Figure 4.1**, which includes a create sales order step, followed by a credit check, which then enables two parallel transactions (create & send invoice and create shipment documents), followed by a goods issue step, meaning that the goods are sent to the customer. The system has two agents, one performs the order creation, credit check, and invoicing steps, and the other performs the document creation and goods issue steps. All transactions have a duration of 1 h on average. Note that since there are two parallel paths in the network, the credit check step produces two identical order states (*Order Checked A* and *Order Checked B*) to enable both paths, while maintaining all order states bounded by 0 and 1.

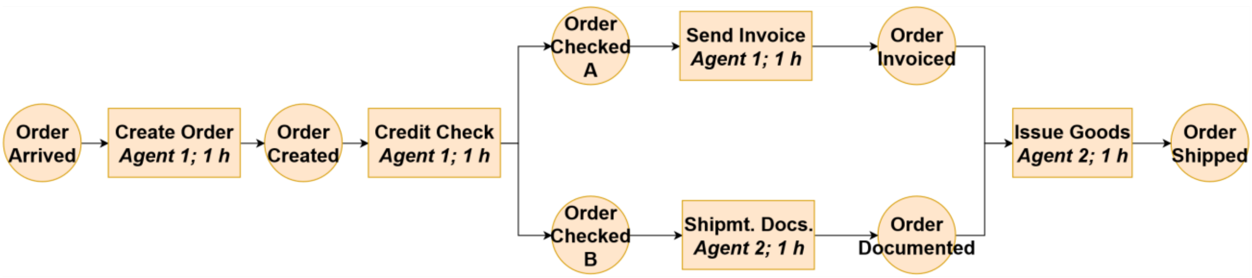

Figure 4.1. STN for a simplified order fulfillment process with agents assigned and processing durations indicated in each task node.

Executing this order fulfillment process without considering the material transformation processes, assumes that the supply of products is unlimited or available immediately upon request. This is usually not the case in real systems, especially those that are make-to-order such as specialty chemicals. We now describe a model that integrates the order fulfillment process with the processes in the chemical batch plant used to manufacture the specialty chemicals. For the chemical batch plant, we use the Kondili *et al.* (1993) plant from **Section 3.1**. **Figure 4.2** shows the integrated STN model for this system.

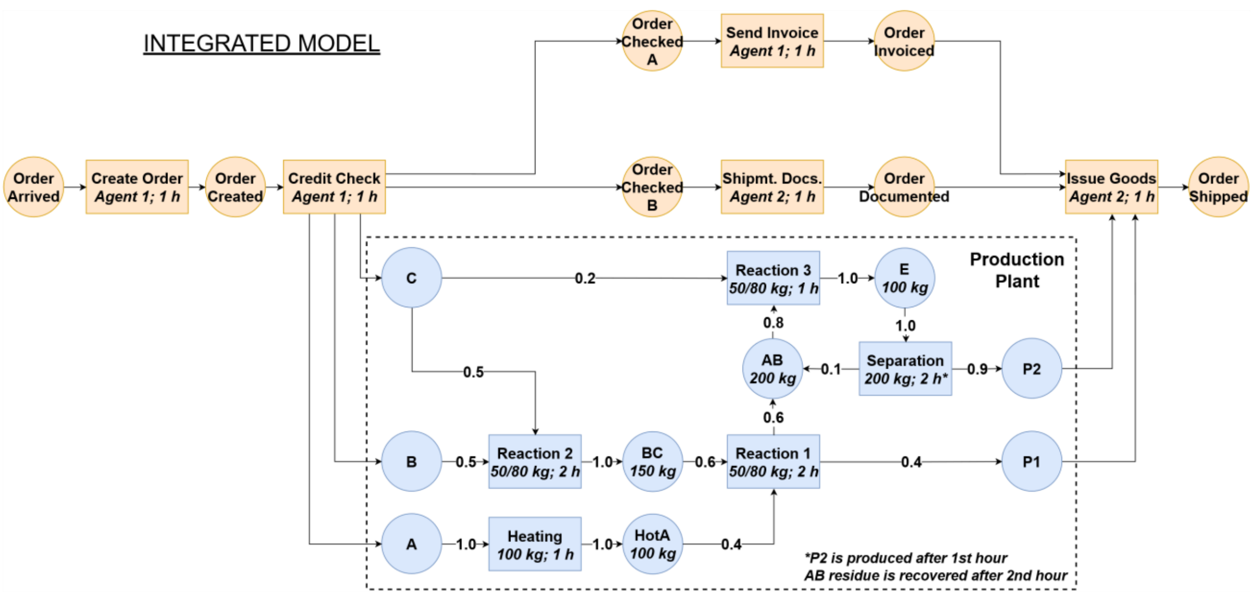

Figure 4.2. Integrated STN for order fulfillment and chemical batch processing. Assigned agents and mean processing times are indicated in the transactional task nodes. Equipment capacities and processing times are indicated in the physical task nodes. Material capacity limits, if any, are indicated in the material state nodes.

The link between the business process and the manufacturing process occurs at the material input and output interfaces. Once a make-to-order request enters the system and is approved (i.e., passes the credit check step), the raw material inventory for that order is released to manufacturing (becomes available). This is seen in the STN graph where the *Credit Check* transaction "produces" material in the A, B, and C material states. The second linkage between the two models occurs at the goods issue step, which cannot be executed until the material requested by the customer is available. The goods issue transaction consumes not just the order invoiced and order documented states, but also consumes the amount of P1 or P2 material requested by the customer.

Since the touch points between the models occur at the material boundaries, the models can be integrated with linking constraints that involve the triggering of the transactional events at the interface (*Credit Check* and *Issue Goods* transactions), and the external supply and demand on the physical model ($S_{k,t}^{supply}$ and $S_{k,t}^{demand}$ continuous variables for $k \in \{A, B, C, P1, P2\}$ from **Section 3.1**, respectively). The linking constraints are given in (4.1) – (4.2), where the supply and demand of material states are linked to the "batch sizes" of the transactions upstream (L_k^{pred}) and downstream (L_k^{succ}) of the feedstock (K^{feed}) and product (K^{prod}) material states. $q_{o,k}$ is the amount of material k required to fulfill order o. For product nodes, this amount is the order quantity, and for feedstock nodes, this amount can be obtained by propagating the reaction stoichiometries up the network.

$$S_{k,t}^{supply} = \sum_{o \in O} q_{o,k} \cdot \sum_{a \in A_l} B_{o,l,a,t-\tau_{o,l,a}} \qquad \forall k \in K^{feed}, l \in L_k^{pred}, t \in T \quad (4.1)$$

$$S_{k,t}^{demand} = \sum_{o \in O} q_{o,k} \cdot \sum_{a \in A_l} B_{o,l,a,t} \qquad \forall k \in K^{prod}, l \in L_k^{succ}, t \in T \quad (4.2)$$

The domains and bounds for the material supply and demand variables are given in (4.3) – (4.4).

$$S_{k,t}^{supply} \in \mathbb{R}: 0 \leq S_{k,t}^{supply} \leq \sum_{o \in O} q_{o,k} \qquad \forall k \in K^{feed}, t \in T \quad (4.3)$$

$$S_{k,t}^{demand} \in \mathbb{R}: 0 \leq S_{k,t}^{demand} \leq \sum_{o \in O} q_{o,k} \qquad \forall k \in K^{prod}, t \in T \quad (4.4)$$

While various objective functions can be used, the simplest one is to maximize the system profit, which is the difference between the sum of the order revenues z_o and the operating costs for each scheduled material transformation process as given in (4.5), where $\alpha_{i,j}$ is the fixed setup cost, and $\beta_{i,j}$ is the variable operating cost ratio for task i,j (process i in equipment j). The integrated model, referred to as IM hereafter, is given by the plant scheduling model in (3.1.1) – (3.1.6), the transactional model in (B.1) – (B.11) and (B.13) – (B.20) (see **Appendix B**), and linking constraints and objective function in (4.1) – (4.5).

$$\max \sum_{o \in O} z_o - \sum_{t \in T} \sum_{i \in I} \sum_{j \in J_i} \left(\alpha_{i,j} \cdot W_{i,j,t} + \beta_{i,j} \cdot B_{i,j,t}\right) \quad (4.5)$$

This integrated model is based on the following assumptions:

- The plant is make-to-order and raw materials are readily available. However, note that make-to-stock and material supply considerations can also be included, as shown in Example 2 in **Section 5**.
- Utilities and labor at the plant are not considered. These could be accounted for by explicitly modeling these resources, in which case a Resource-Task Network (RTN) (Pantelides, 1994) representation is recommended.
- Task processing times include any setup and material transfer times. Changeovers are not considered, but could be introduced with additional constraints (Méndez *et al.*, 2006).
- Working shifts for agents are not included. These could be included by introducing additional constraints on when agents can perform transactions.
- Customer orders are only fulfilled in their entirety. In other words, order splitting or partial fulfillments is not allowed.
- Order revenue can be modeled as a piecewise linear function as described in **Appendix B**.

For Example 1, we also show how the information and material processes can be simulated via discrete event simulation (DES). DES is used to validate the integrated model in a stochastic environment via a rolling horizon approach. The reader is referred to our prior work on the integration between DES and deterministic mathematical optimization for online scheduling of business processes in supply chains (Perez *et al.*, 2022). We have extended the digital twin framework presented in Perez *et al.* (2022) to allow for online scheduling of both customer order transactions and chemical batch production.

Figure 4.3 shows the queueing network representation for DES that corresponds to the integrated STN representation in **Figure 4.2**. The DES model proposed has 6 queues, one for each type of resource in the system (Agent 1, Agent 2, 50 kg Reactor, 80 kg Reactor, Heater, and Distillation Column). Note that because the two reactors have different capacities, they are modeled as separate queue-server entities. For identical reactors, a single queue can be used with two servers, which is analogous to what is done in the RTN models when identical processing units are available. There are also 9 buffer tanks that represent the material storage units in the system. The contents in the feedstock and intermediate material tanks are routed to one of the reactor queues where the reaction to be performed is assigned based on the process schedule, reaction recipes, and resource availability. Produced materials are then routed to the correct storage tanks based on the recipes for the executed reactions. The heater and distillation column do not require routing nodes as they are single-task operating units used at the beginning and end of the physical process network.

On the transactional side, an order routing step is used to send order information to the assigned agent queue for processing. For transactions in series, such as the order creation and credit check transactions, the order routing routine is single-input-single-output. For parallel transaction pathways and interface points, the routing is single-input-multiple-output, multiple-input-single-output, or multiple-input-multiple-output. For example, when the *Credit Check* is performed on an order by Agent 1, the order routing routine, unlocks material in raw material storage tanks A, B, and C, and sends an order invoicing job to the queue of Agent 1 and an order shipment documentation job to the queue of Agent 2. Routing decisions are governed by the STN model of the system.

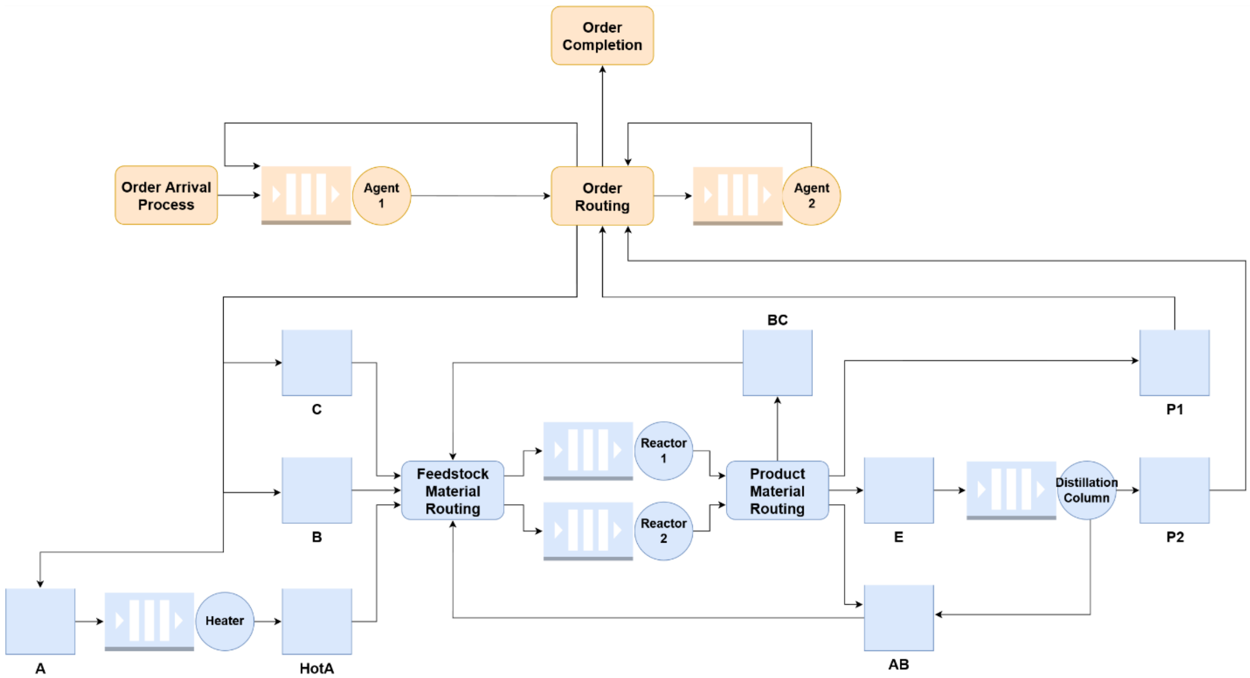

Figure 4.3. Queueing network for discrete event simulation of integrated information and material flows

The STN representation of the transaction-focused model is given in **Figure 4.4,** where the plant model is reduced to a single task for each product type (P1 and P2). The raw materials are lumped into a single state and the processing times along each product pathway are aggregated to obtain a total campaign duration. The *P2 Production* pathway includes all the processing steps involved in transforming raw materials A, B, and C into P2, with P1 and AB as byproducts. The operating capacities and stoichiometries shown in the graph are determined from the equipment and tank capacities at the plant. When running this transaction-focused model within the digital twin simulation environment, the DES also uses a lumped representation of the plant that operates on production campaign schedules for products P1 or P2.

The STN representation of the material-focused model is given in **Figure 4.5**, where the order creation and credit check steps are lumped into a single task (*Prepare Order*), and the transactions occurring in parallel to the manufacturing process are ignored. When running this model within the digital twin simulation environment, the transactional network is treated as a first-in-first-out (FIFO) system where the order priorities for the *Prepare Order* and *Issue Goods* transactions can be updated by the STN model.

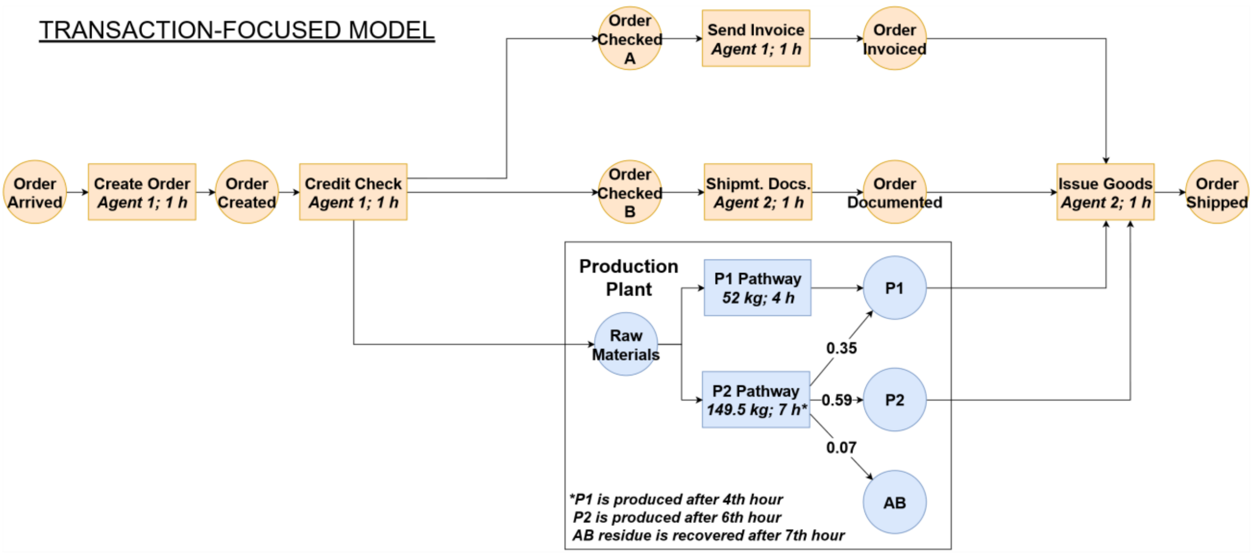

Figure 4.4. STN representation for the transaction-focused model.

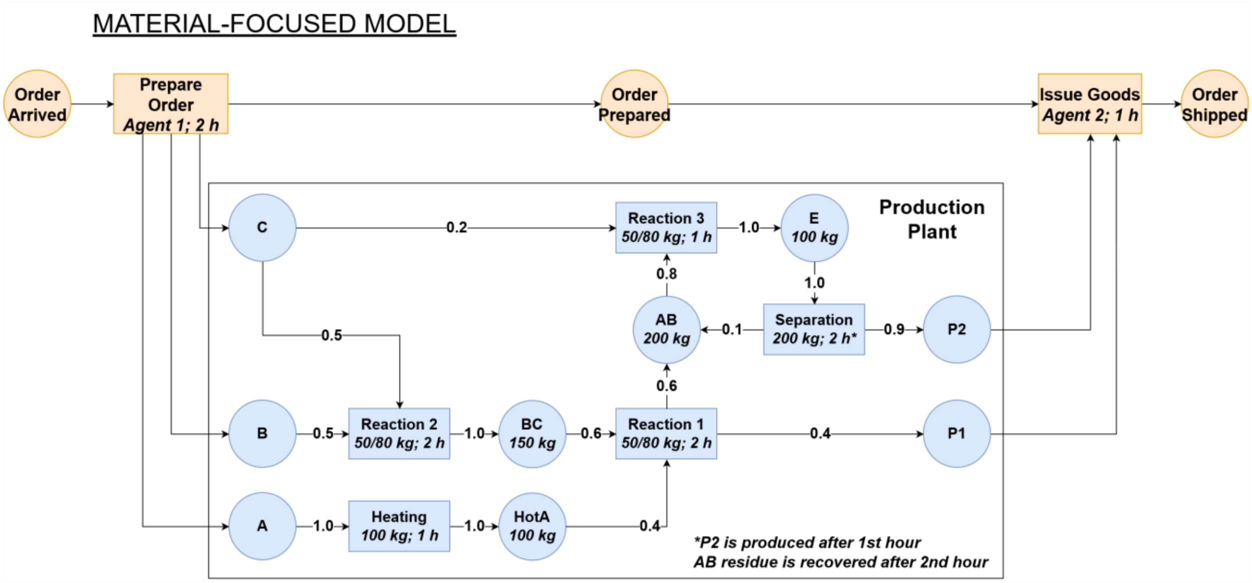

Figure 4.5. STN representation for the material-focused model.

For Example 1, the benefits of the integrated model are shown by comparing the solutions obtained when using the integrated model with those obtained from using a transaction-focused model that lumps the physical processes into single transaction nodes, and those obtained from a material-focused model that lumps the business transactions upstream and downstream of the manufacturing site into single processing nodes. For this comparison, we model a system where customer orders arrive continuously at random with interarrival times sampled from the $Poisson(\lambda = 1\ h)$ distribution. Material demand for P1 or P2 in each order is sampled from the positive side of the $Normal(\mu = 25\ kg, \sigma = 5\ kg)$ distribution with due dates sampled at random between 7 h and 20 h after each order arrives. The order profit at the due date is sampled uniformly between \$500 and \$1,000 with an early delivery incentive of 20% (decreasing linearly within the on-time delivery window), a late penalty of 10%, and a 10% depreciation up to the lost sales date, the latter of which is set at random and represents different customer patience levels after the due date. **Figure 4.6** shows the temporal evolution of the order profit throughout the 24 h horizon for the first 10 orders in the system. It can be seen that some orders have a higher profit than others throughout their lifetime, while the profit functions of others cross during the scheduling horizon (e.g., order 1 and 6 cross at t = 7 h). Overall, 26 orders enter the system during the simulation. The congestion in the system is shown in **Figure 4.7**, where the number of orders at each hour are shown throughout the 24 h horizon. The congestion in the system increases until t = 17 h, where the number of orders oscillates around 20.

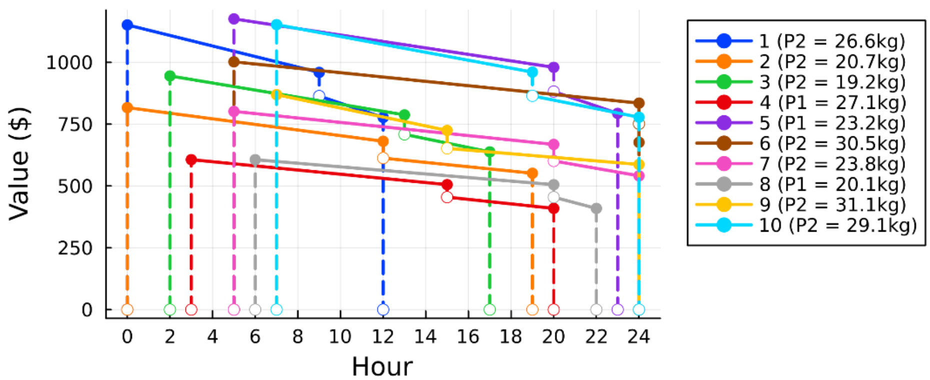

Figure 4.6. Order profit profiles used in Example 1 for the first 10 randomly generated orders (one piecewise linear function for each order).

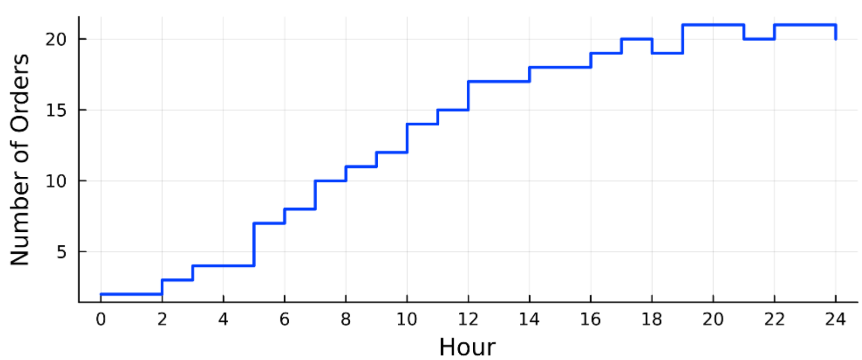

Figure 4.7. System congestion throughout the 24 h horizon.

Besides the uncertainty in the order arrivals, another area of uncertainty is that of the processing times of the human agents performing the business process transactions. This uncertainty is included by modeling the processing times for the transactional steps with the positive side of the $Normal(\mu = 1\ h, \sigma = 0.1\ h)$ distribution. This distribution is encoded in the discrete event simulation of the process. Since the scheduling models are deterministic, the average value is used during online optimization. However, if the time in service is nonzero when a scheduling event is triggered, the expected remaining processing time is used (i.e., $\mathbb{E}[\tau|\tau > \delta] - \delta$ where τ is the continuous random processing time and δ is the time in service).

For each of the models described in this section (integrated, transaction-focused, and material-focused), a stochastic discrete event simulation (DES) of the system is run, where the scheduling optimization model is triggered during the simulation whenever a new order arrives, for a total of 19 optimization (rescheduling) events. For greater detail on the algorithm behind the discrete event simulation model, the reader is referred to our work on a digital twin framework for supply chain business processes (Perez *et al.*, 2022). When a rescheduling is triggered, the system state (tank levels, active orders, queue states, and server states) are used to initialize and run the scheduling model. The duration of these scheduling events is the time required to build and solve the optimization problem. The schedules resulting from the optimization events are then used to actively update the plant schedule and order priorities in the queueing network as shown in **Figure 4.8**. The DES model was developed in the Julia programming language v1.8.3 (Bezanson *et al.*, 2017) by extending the simulation software described in Perez *et al.* (2022), which was used for business processes simulation. The extension allows integrating the business process queueing networks with the physical process queueing networks as shown in the above **Figure 4.3**. The integrated model (IM) presented is reformulated into a MILP via the Hull reformulation (Balas, 1998), and solved with Gurobi 9.5.2 using the JuMP modeling language v1.8.1 (Dunning *et al.*, 2017). An adaptive rolling horizon approach is used (Perez *et al.* 2022) with a time discretization of 6 min and an optimization time limit of 6 min. The 6 min value was selected based on the coefficient of variation of the transactional processing time distributions. The optimization-embedded DES is run on a Windows PC with 16 GB of RAM and an Intel-i7 3.60 GHz processor.

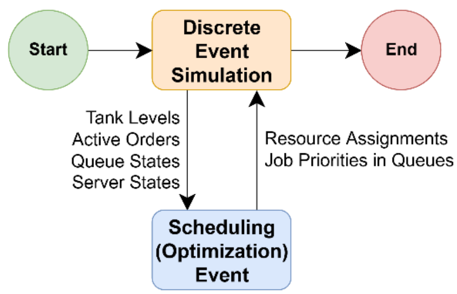

Figure 4.8. Block schematic for the optimization-embedded DES, where optimization events are triggered periodically and dynamically update production schedules and order transaction priorities.

Since the optimization model is being executed online during the simulation, an additional penalty is added to the objective function to discourage preempting transactional events. This is done by replacing the objective function in (4.5) with (4.6), where $\gamma_{l,a}$ is the cost of preempting transaction l being performed by agent a, and Ω is the set of all business process transactions that are active when the scheduling event is triggered ($t = 1$ in the scheduling model). For the current problem, the following parameter values are used: $\gamma_{l,a} = \$0.01$, $\alpha_{i,j} = \$0.001$ (small fixed-setup cost for physical processes), and $\beta_{i,j} = \$0$.

$$\max \sum_{o \in O} z_o - \sum_{t \in T} \sum_{i \in I} \sum_{j \in J_i} \left(\alpha_{i,j} \cdot W_{i,j,t} + \beta_{i,j} \cdot B_{i,j,t}\right) - \sum_{t \in T} \sum_{(o,l,a) \in \Omega} \gamma_{l,a} \cdot W_{o,l,a,1} \tag{4.6}$$

The results obtained from three modeling approaches (integrated, transaction-focused, and material-focused) on this problem set are given in **Table 4.1**. The largest optimization model sizes for each approach are given in **Table 4.2**, which correspond to the models optimized at t = 23 h, which is when the last order enters the system. See **Appendix C** for the CPU times and objective function value results of each optimization event in the simulation. The operating schedules obtained with the integrated and transaction-focused models are given in **Figure 4.9**. The results show that the integrated model provides a solution that is superior to that of the transaction-focused model by 8% in terms of profit, and fulfills 4 more orders on-time. The inferior performance of the transaction-focused model is a result of ignoring the availability of individual processing units at the plant and instead viewing the plant as a single resource. This is observed in the bottom Gantt chart in **Figure 4.9**, which shows a production schedule with three consecutive campaigns of product P2 (see **Figure 4.4**). Each time a P2 production campaign is run, the plant resource is locked for 7 h. As a result of ignoring the individual equipment availability, earlier processing steps cannot be used for additional production batches until the 7 h campaign ends, even though the equipment required for these processes is idle at the plant. For example, a second heating step could be performed simultaneous to one of the reactions or the separation step in the production campaign. Instead, the heater remains idle for 6 of the 7 h in the campaign. Another limitation of this lumped model is that intermediate storage and interactions between the P1 pathway and the P2 pathway are ignored. Thus, if the optimizer schedules a campaign to produce P1, the model does not consider that intermediate AB is produced, which could then be used to produce P2 in only 2 h, rather than having to run another P2 campaign (7 h). Thus, ignoring the details on the physical process side results in suboptimal schedules, which can increase the number of orders that are fulfilled late or become lost sales.

Table 4.1. Results from the online scheduling for each model.

Model	**System Profit**	**Orders On-time**	**Orders Fulfilled**
Integrated	$5,958	7	7
Transaction-focused	$5,499	3	7
Material-focused	$0	0	0

Table 4.2. Largest model size by model.

Model	**Binary Variables**	**Continuous Variables**	**Constraints**	**Model Generation Time* (s)**	**Model Solution Time (s)**
Integrated	68,182	46,781	298,430	4.3	89.1
Transaction-focused	66,496	12,775	222,951	3.8	22.1
Material-focused	44,548	62,566	259,414	2.0	8.9

*Time to construct and send model to solver.

On the other hand, the material-focused model does not fulfill any orders within the 24 h horizon, resulting in $0 profit. Since the scheduling model does not consider the parallel transactional network and the availability of agent resources assigned to parallel transactions, the model produces schedules that are infeasible in practice. This is observed in **Figure 4.10**, which shows the actual simulation results compared against two instances of the scheduling model (at t = 8 h and t = 14 h). Each of the *Goods Issue* events in the middle and bottom Gantt charts in **Figure 4.10** incurs in a resource violation because an order can only issue goods after the *Send Invoice* and *Create Shipment Documents* step, the former of which is done by Agent 1 who is fully booked on creating orders and running credit checks since the start of the simulation. The optimization assigns a higher priority to the *Prepare Order* transactions such that the *Send Invoice* transactions are always moved to the end of the FIFO queue for Agent 1. Thus, ignoring the business process network and agent resource availability results in infeasible schedules that introduce significant delays in fulfilling customer orders. These delays often result in inventory buildup (see **Figure 4.11**), and late order fulfillments or cancellations. Such a disconnect between plant scheduling and the timing of transactional processes is what generally occurs in practice.

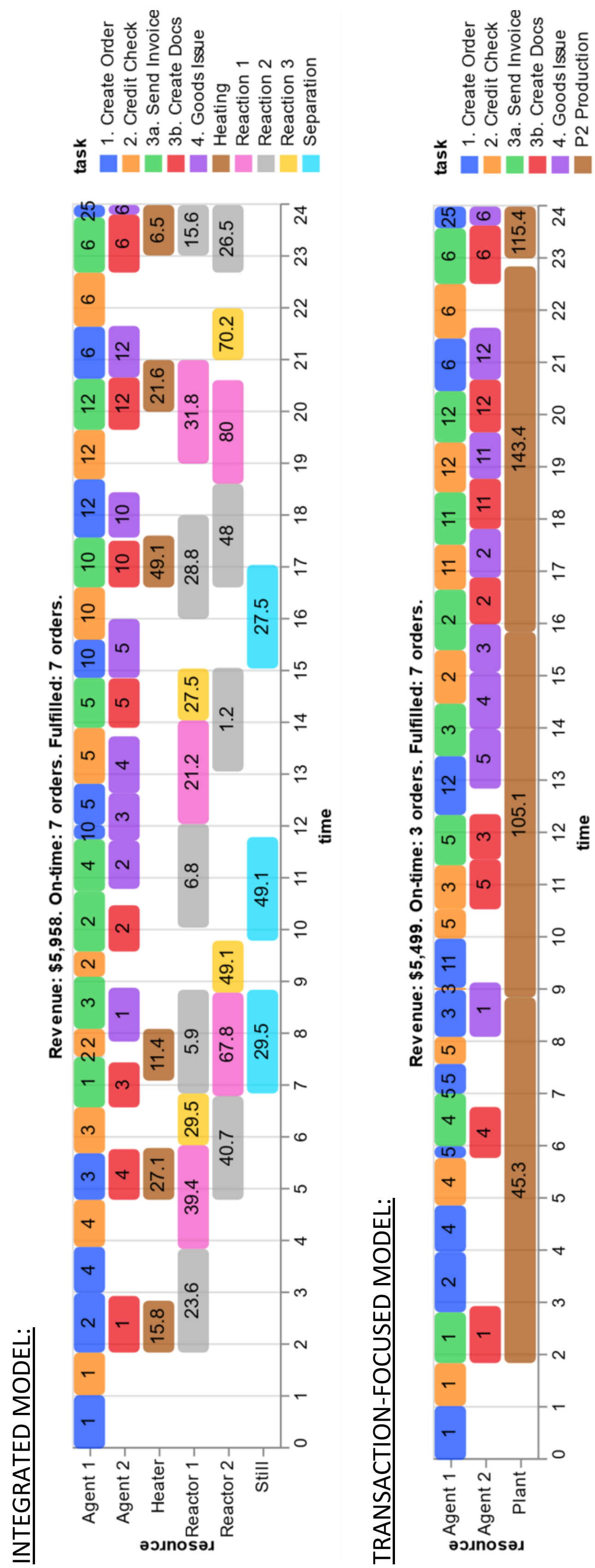

Figure 4.9. Gantt schedules for the integrated model (top) and transaction-focused model (bottom). Values inside bars in the agent schedules are order numbers. Values inside bars in the equipment schedules are batch sizes in kg.

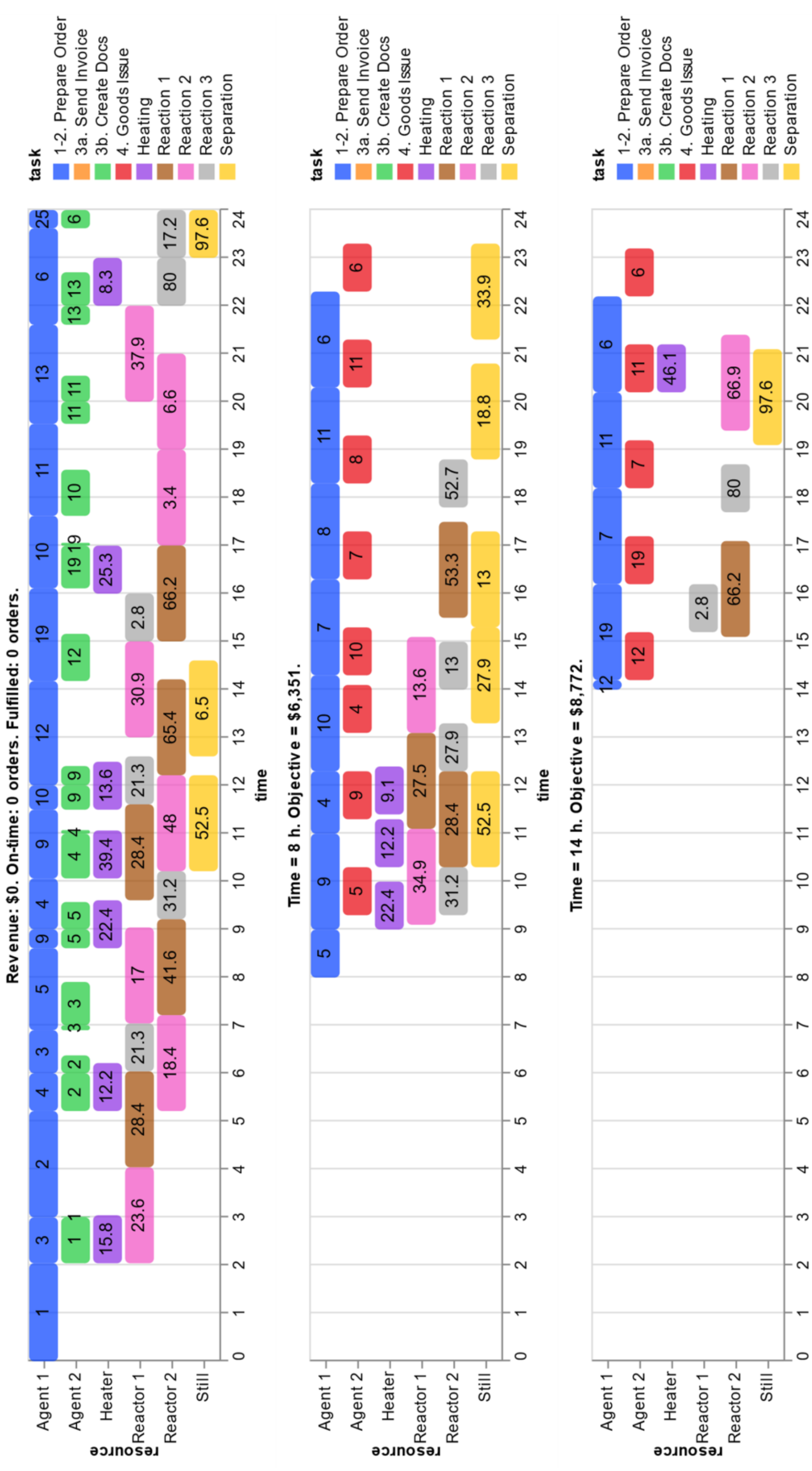

Figure 4.10. Gantt schedules for the material-focused simulation run (top), and the optimization models triggered at t = 8 h (middle) and t = 14 h (bottom). Values inside bars in the agent schedules are order numbers. Values inside bars in the equipment schedules are batch sizes in kg.

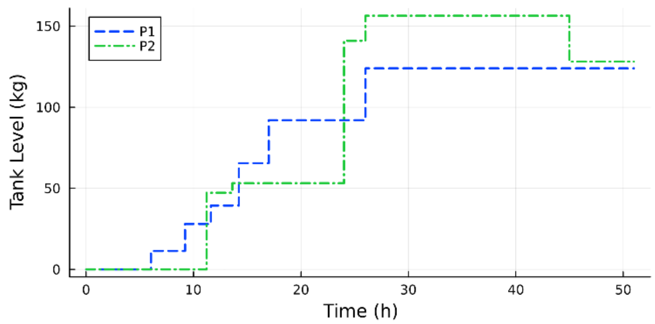

Figure 4.11. Product tank levels over time for material-focused model. The drop in P2 at t = 45 h is for the only order that gets shipped to the customer in the simulation (Order 26).

5. Example 2: Integrating business, financial, and physical processes throughout the supply chain network

This section illustrates how the different components in a real supply chain (see **Figure 3.1.1**) can be integrated in a holistic STN model. The model from **Section 4** for the integrated order fulfillment process at the Kondili batch plant is extended to model not just the material transformation site (plant), but also include three material suppliers for raw materials A, B, and C, as well as a distribution center downstream of the plant for storing finished good P1. Unlike Example 1, P1 is managed as a make-to-stock material. P2 remains as a make-to-order product. **Figure 5.1** depicts this supply chain topology with three external customers, one placing orders for P1 at the distribution center, another placing orders for P1 at the distribution center and P2 at the plant, and a third placing orders for P2 at the plant. This small supply chain allows capturing the four processes described in **Section 3**: material transformation processes at the plant; inventory processes between the suppliers and the plant, and the plant and the distribution center; order-to-cash between the demand facing nodes (plant and distribution center) and the customers, and source-to-pay between the suppliers and the plant; and financial modeling of accounts payable, accounts receivable, and cash.

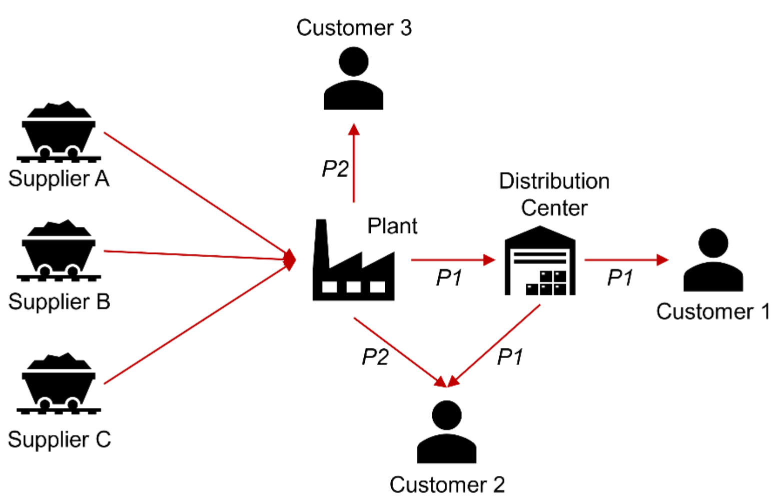

Figure 5.1. Supply chain topology used in Example 2.

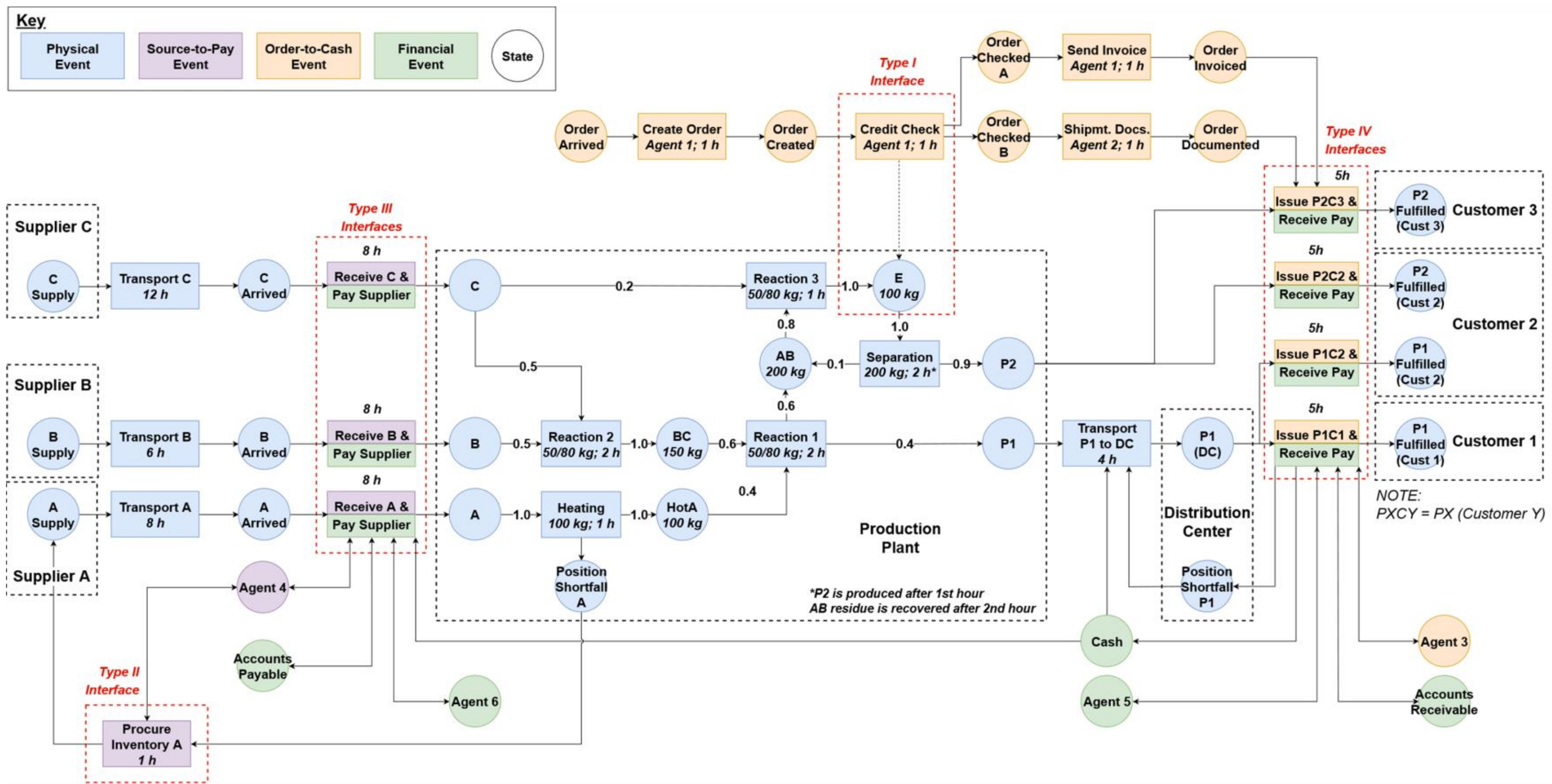

Figure 5.2. Integrated supply chain Task Network with physical, financial, order-to-cash, and source-to-pay processes.

The integrated Task Network graph for this process is illustrated in **Figure 5.2**. With this representation, the discrete event simulation model used in Example 1 can also be extended to simulate the entire supply chain with its associated processes if desired. However, this section focuses on developing an integrated scheduling model that accounts for each of these supply chain components. By including the financial elements in this representation, the objective of the optimization problem can be defined in terms of the *Cash*, *Accounts Payable*, and *Accounts Receivable* nodes.

To avoid cluttering the network representation, the following are not shown in **Figure 5.2**:

- Inventory processes for raw materials B and C. These processes are analogous to the one for raw material A. Note that since the enterprise is assumed to include the plant and distribution center, the inventory process for P1 at the warehouse does not require the source-to-pay transactions used in the procurement of raw materials. However, cash assets are consumed to cover transportation expenses.
- Connections between the *Order Invoiced* and *Order Documented* states and the *Issue & Receive Pay* transactions for Customers 1 and 2. These connections are identical to those used for Customer 3.
- Connections between *Issue & Receive Pay* and *Accounts Receivable*, *Cash*, *Agent 3*, and *Agent 5* nodes for Customers 2 and 3. These connections are identical to those used for Customer 1.
- Connections between the *Cash* state node (green) and the various processing steps in the plant, as is done with the transportation task for P1 between the plant and the distribution center. These connections represent how cash is consumed by the operating costs for the physical processes.

The integrated model is a hybrid of a STN and a RTN. The network is defined as a STN for all nodes and tasks except for the Interfaces of Type III and Type IV (enclosed in red rectangles in **Figure 5.2**), which are modeled as RTN super-transactions. The interface regions are modeled as follows:

5.1 Type I Interface

The first interface region is the interface between the order-to-cash process and the plant, which links the *Credit Check* transaction and material state *E*. This interface point differs from the way in which the order fulfillment and material transformation processes were integrated in Example 1. Since raw materials are supplied from an external supplier now and an inventory policy is in place, a state limit balance analogous to the resource limit balance from Wassick and Ferrio (2011) is used instead. The state limit balance is formulated as shown in (5.1), where the upper bound on a make-to-order (MTO) material $k \in K^{MTO}$ (e.g., material E) becomes a variable that is indexed over time. This upper bound is updated at t from its value at $t-1$ by adding the amount of upper bound produced when the interface transaction L_k^{pred} (e.g., *Credit Check*) completes and deducting the amount of material consumed by all downstream (successor) physical processes $i \in I_k^{succ}$ (e.g., *Separation*). The production ratio used is $q_{o,k}$, which is the amount of material *E* required to execute order o. (5.1) ensures that no more P2 can be produced until another order passes its respective credit check.

$$S_{k,t}^{max} = S_{k,t-1}^{max} + \sum_{o \in O} q_{o,k} \cdot \sum_{l \in L_k^{pred}} \sum_{a \in A_l} B_{o,l,a,t-\tau_{o,l,a}} - \sum_{i \in I_k^{succ}} \rho_{i,k}^{cons} \cdot \sum_{j \in J_i} B_{i,j,t} \qquad \forall k \in K^{MTO}, t \in T \tag{5.1}$$

5.2 Type II Interface

The second interface region is the source-to-pay interface linking the plant and the raw material suppliers. The *Procure Inventory* transaction includes the replenishment triggering and an order placement steps. This transaction and the state nodes connected to it can be treated with the traditional STN formulation for physical processes.

5.3 Type III Interfaces

The third interface regions occur at the *Receive Material & Pay Supplier* super-transactions, which link the source-to-pay, physical, and financial processes and flows upstream of the plant. This super-transaction includes three sub-transactions that are assumed to occur in tandem when receiving a raw material supply: *Receive Raw Material* (performed by *Agent 4* with a duration of 1 h), *Wait for Accounts Payable Terms* (duration of 6 h), and *Pay Supplier* (performed by *Agent 6* with a duration of 1 h). Because the nodes connected to the *Receive Material & Pay Supplier* task are consumed/produced at various points in the 8 h duration of the super-transaction, the RTN model is better suited for this task.

The levels of the resource nodes involved are controlled by the resource balance in (5.2), where $N_{i,t}$ signals that task i has been triggered at t, $B_{i,t}$ is the batch size of the task, $\rho_{i,k,\theta}^{fixed}$ is the fixed production/consumption ratio, and $\rho_{i,k,\theta}^{var}$ is the variable production/consumption ratio. These parameters are defined in **Table 5.1**. A time offset parameter θ is used to indicate the time relative to when a task is triggered, which allows for production/consumption at different time points during the task duration. Disjunction (5.3) is similar to (3.1.2) with the addition of N for the fixed consumption and production of the agent resources. The variable domains for the new variables introduced are given in (5.4) – (5.6). Note that since the processing units (agents) are nodes connected to the task node, the equipment index j is dropped from W and B.

$$S_{k,t} = S_{k,t-1} + \sum_{i \in I_k} \sum_{\theta=0}^{\tau_i} (\rho_{i,k,\theta}^{fixed} \cdot N_{i,t-\theta} + \rho_{i,k,\theta}^{var} \cdot B_{i,t-\theta}) \qquad \forall k \in K^{super}, t \in T \qquad (5.2)$$

$$\begin{bmatrix} W_{i,t} \\ N_{i,t} = 1 \\ V_i^{min} \le B_{i,t} \le V_i^{max} \end{bmatrix} \vee \begin{bmatrix} \neg W_{i,t} \\ N_{i,t} = 0 \\ B_{i,t} = 0 \end{bmatrix} \qquad \forall i \in I^{super}, t \in T \qquad (5.3)$$

$$B_{i,t} \in \mathbb{R}: 0 \le B_{i,t} \le V_i^{max} \qquad \forall i \in I^{super}, t \in T \qquad (5.4)$$

$$N_{i,t} \in \mathbb{R}: 0 \le N_{i,t} \le 1 \qquad \forall i \in I^{super}, t \in T \qquad (5.5)$$

$$W_{i,t} \in \{True, False\} \qquad \forall i \in I^{super}, t \in T \qquad (5.6)$$

Table 5.1. Temporal scaling factor, ρ, for the *Receive & Pay* tasks. All values are for variable consumption/production, except for the Agent resources, which are fixed consumption/production ratios.

	Time Offset, θ			
Resource/State	0[a]	1[b]	7[c]	8[d]
A Arrived	-1	-	-	-
A (Plant)	-	1	-	-
Agent 4	-1	1	-	-
Agent 6	-	-	-1	1
Accounts Payable	-	p_A	-	$-p_A$
Cash	-	-	-	$-p_A$

[a]Start *Receive A sub-process*
[b]Start *Wait for Payment Terms sub-process*
[c]Start *Pay Supplier A sub-process*
[d]Payment Complete

5.4 Type IV Interfaces

The fourth interface regions occur at the *Issue Product & Receive Pay* super-transactions, which link the order-to-cash, physical, and financial processes and flows downstream of the plant. This super-transaction includes three sub-transactions that are assumed to occur in tandem when fulfilling a customer order: *Issue Goods to Customer* (performed by *Agent 3* with a duration of 1 h), *Wait for Accounts Receivable Terms* (duration of 3 h), and *Receive Payment for Invoice* (performed by *Agent 5* with a duration of 1 h). Once again, the RTN model in (5.2) – (5.6) is used. Since each of these super-transaction tasks i is order specific, the indices o, l should be used in place of i. The $\rho_{o,l,k,\theta}^{fixed}$ and $\rho_{o,l,k\theta}^{var}$ parameter values are given in **Table 5.2**. Note that for *Accounts Receivable* and *Cash* nodes, the ρ parameters are not constant because the order revenue z_o changes with time. To avoid introducing bilinear terms, z_o can be precomputed for all $t \in T$. Thus, $\rho_{o,l,k,\theta}^{var}$ is replaced with $z_{o,l,t,\theta}$, which is defined in (5.7). This ensures that when the *Issue Product & Receive Pay* task is triggered in this example at t' ($N_{o,l,t'} = 1$), the *Accounts Receivable* (AR) increases by $z_{o,t'+1}$ when $t = t' + 1$ and $\theta = 1$ (1 period into the *Issue & Collect* task, which is when the *Issue Goods* sub-transaction completes and the order revenue value is set), and then decrease by $z_{o,t'+1}$ when $t = t' + 5$ and $\theta = 5$ (5 periods into the *Issue & Collect* task, which is when the invoice payment is received).

$$\rho_{o,l,k,\theta}^{var} = z_{o,l,t,\theta} = \begin{cases} z_{o,t-\theta+1} & \text{if } k = AR, \theta = 1 \\ -z_{o,t-\theta+1} & \text{if } k = AR, \theta = 5 \\ z_{o,t-\theta+1} & \text{if } k = Cash, \theta = 5 \\ 0 & \text{otherwise} \end{cases} \quad \forall o \in O, l \in L_o^{lim}, k \in \{AR, Cash\}, \theta \in \{0, \dots, \tau_l\}, t \in T \tag{5.7}$$

Table 5.2. Temporal scaling factor, ρ, for the *Issue & Receive Pay* tasks. All values are for variable consumption/production, except for the Agent resources, which are fixed consumption/production ratios.

	Time Offset, θ

Resource/State	0[a]	1[b]	4[c]	5[d]
P1 (DC)	$-q_o$	-	-	-
P1 Shortfall	q_o	-	-	-
P1 Fulfilled (Cust 1)	-	q_o	-	-
Agent 3	-1	1	-	-
Agent 5	-	-	-1	1
Accounts Receivable	-	z_o	-	$-z_o$
Cash	-	-	-	z_o

[a]Start *Issue P1 to Customer 1 sub-process*
[b]Start *Wait for Payment Terms sub-process*
[c]Start *Collect Payment P1 (Customer 1) sub-process*
[d]Payment Collected

Of the states connected to the aggregated boundary tasks I^{lim}, the *Cash* node is the only one that is also connected to other processing tasks in the network (*Heating*, *Reaction 1*, *Reaction 2*, *Reaction 3*, *Separation*, and *Transport P1*). Each time one of these processing tasks is performed, there is a fixed and variable operating cost, which consumes the *Cash* inventory. Instead of modeling these costs via *Accounts Payable*, we assume that these operating costs are paid immediately from the *Cash* asset at the end of each processing task. This means that the consumption/production ratios for the *Cash* node are all zero except for $\theta = \tau_i$ for each cost-incurring processing task i. However, in practice, these costs can be modelled via *Accounts Payable* with specified payment terms (e.g., utility bill payment dates) as is done in this model with the raw material sourcing costs (see Type III interfaces in **Section 5.3**).

5.5 Objective Function

The objective function of the integrated system modeled is given in (5.8), which maximizes the change in shareholder equity across the scheduling horizon, which is the difference between the change in assets (Cash and Accounts Receivable, AR) and the change in liabilities (Accounts Payable, AP). While the initial values for AR and AP can be set to 0, an initial cash level must be set. Otherwise, production at the plant cannot occur until cash is collected from sales at the distribution center. The objective function also includes penalties for the following:

- The slack between the level on the inventory holding tanks (K^{Inv}) *A*, *B*, *C*, and *P1 (DC)* at the end of the scheduling horizon ($t = |T|$) and the initial inventory levels (full tanks). The slack is weighted by parameter w_k. This encourages the optimizer to restore the inventory levels by the end of the scheduling horizon.
- The state levels for the *Material Shortfall* ($K^{shortfall}$) and *Raw Material Arrived* ($K^{arrived}$) states, weighted by parameter w_k. This encourages continuous replenishment of inventory holding tanks *A*, *B*, *C*, and *P1 (DC)* and immediate receipt of raw materials as they arrive at the plant.

$$\begin{aligned}\max Z = &\left(S_{Cash,|T|} - S_{Cash,0}\right) + \left(S_{AR,|T|} - S_{AR,0}\right) - \left(S_{AP,|T|} - S_{AP,0}\right) \\ &- \sum_{k \in K^{Inv}} w_k \cdot \left(S_{k,0} - S_{k,|T|}\right) - \sum_{t \in T} \sum_{k \in K^{shortfall} \cup K^{arrived}} w_k \cdot S_{k,t}\end{aligned} \tag{5.8}$$

For Example 2, a monolithic scheduling optimization is performed on the integrated system described in this section (see **Figure 5.2**). Since Example 1 already showed the benefits of an integrated model over single-focused model, this comparison is not made in Example 2. Instead, this example is used to present an instance of the fully integrated model that accounts for the major flows involved in supply chain operations. To the best of our knowledge, such a model has not been reported in the literature of supply chain management. The major assumptions of such a model are (in addition to those described in the model for Example 1 in **Section 5**):

- Invoice payment terms are fixed and invoices are paid/collected when the payment terms expire. In other words, the model does not consider late payments on invoices.
- Shipping times are fixed and replenishment orders can be shipped immediately after they are processed. Explicitly accounting for limited shipping resources (e.g., trucks) could be accommodated in the model if desired. Raw material supply limitations could be accounted for by introducing an additional task at the supplier to prepare the amount of material that needs to be shipped.

In Example 2, 43 customer orders enter the system at random during a 48 h horizon with interarrival times sampled from the $Poisson(\lambda = 1\ h)$ distribution, meaning that approximately 1 order enter the system each hour. The characteristics of the customer orders are given in **Table 5.3**. The prices used for raw materials are $p_A = \$5.00\ /\ kg$, $p_B = \$3.75\ /\ kg$, $p_C = \$4.75\ /\ kg$. For the weighting parameters in the objective function (5.8), $w_k = 2 \cdot p_k$. Although the price of P1 is order specific, a fixed weighting parameter $w_{P1\ (DC)} = \$20.00\ /\ kg$ is used in (5.8). The inventory parameters used for the inventory holding tanks *A*, *B*, *C*, and *P1 (DC)* are given in **Table 5.4**. Each of these tanks operates under a *basestock* policy (order-up-to) with continuous review. The initial tank levels for these tanks are set to the inventory position targets (full tanks). All other tanks are assumed to be empty at t = 0 h. The fixed and variable cost parameters for the processing tasks at the plant and the shipping of P1 from the plant to the distribution center are given in **Table 5.5**. An initial *Cash* level of $3,000 was selected to ensure that physical processes can be executed before cash enters the system from the orders fulfilled. The exact initial investment required to avoid running out of cash is discussed later. For the raw material supply nodes, the maximum state level is set to 0, to ensure that any inventory requested by the plant is immediately shipped once the plant performs the necessary procurement task.

Table 5.3. Customer order characteristics for each material type

Parameter	P1	P2
Number of Orders	22	21
Customer 1	16	0
Customer 2	6	9
Customer 3	0	12
Material Quantity (kg)	Normal(μ=40, σ=10)	Normal(μ=50, σ=10)
Revenue ($ thousands)	Uniform(0.5, 1.0)	Uniform(1.0, 1.5)
Early Fulfillment Incentive	20%	20%
Fixed Late Penalty	10%	10%
Late Fulfillment Depreciation	10%	10%
Due Date – Early Date	Uniform(4, 12)	Uniform(7, 12)

Lost Sale Date – Due Date	Uniform(1, 6)	Uniform(1, 6)

Table 5.4. Safety stocks and inventory position targets for Example 2.

Parameter	Safety Stock (kg)	Position Target (kg)
A (Plant)	34.8	174.1
B (Plant)	37.2	186.1
C (Plant)	20.6	164.4
P1 (Distribution Center)	20.0	100.0

Table 5.5. Fixed ($\rho_{i,Cash,\tau_i}^{fixed}$) and variable ($\rho_{i,Cash,\tau_i}^{var}$) cash consumption ratios for operating tasks.

Task	Fixed Cost ($)	Variable Cost ($/kg)
Heating	10.00	1.50
Reaction 1	10.00	1.37
Reaction 2	10.00	1.28
Reaction 3	10.00	1.38
Separation	10.00	1.38
Transport P1	10.00	3.00

The scheduling problem was solved with the same hardware and software versions used in Example 1. The model and solution statistics are given in **Table 5.6**. The problem is solved to a 4.3% relative optimality gap tolerance in 58 min. Gurobi presolve significantly reduced the model size by 59%, 90%, and 76% for the number of discrete variables, continuous variables, and constraints, respectively.

Table 5.6. Model sizes and computational statistics for Example 2.

Parameter	Value
MIP Solution	
MIP Solution	$9,754
Optimality Gap	4.3%
Nodes Explored	88,757
Cuts Applied	3,180
CPU Time (s)	3,482
Original Model Size	
Binary Variables	11,417
Integer Variables	0
Continuous Variables	15,096
Constraints	16,174
Reduced Model Size	
Binary Variables	4,655
Integer Variables	1
Continuous Variables	1,543

Constraints	3,950

The best feasible schedule found is given in **Figure 5.3**. The Gantt chart shows that 19 of the 43 customer orders are fulfilled with fulfillment statistics reported in **Table 5.7**. The resulting schedule yields the following observations,

- The most congested resources are Agents 1, 2, and 4. Adding additional resources for the order-to-cash steps and procurement tasks can potentially enable fulfilling more orders throughout the horizon.
- Most of the reaction and heating batches at the plant are performed at or near the equipment capacity with some idle slots in the plant operation.
- Replenishment of A, B, C, and P1 (at the distribution center) are performed with 1, 1, 4, and 2 trucks respectively.

Table 5.7. Order fulfillment statistics for Example 2.

Fulfillment Status	**P1**	**P2**
Early	7	8
Customer 1	5	0
Customer 2	2	4
Customer 3	0	4
On-time	1	2
Customer 1	1	0
Customer 2	0	0
Customer 3	0	2
Late	1	0
Customer 1	0	0
Customer 2	1	0
Customer 3	0	0

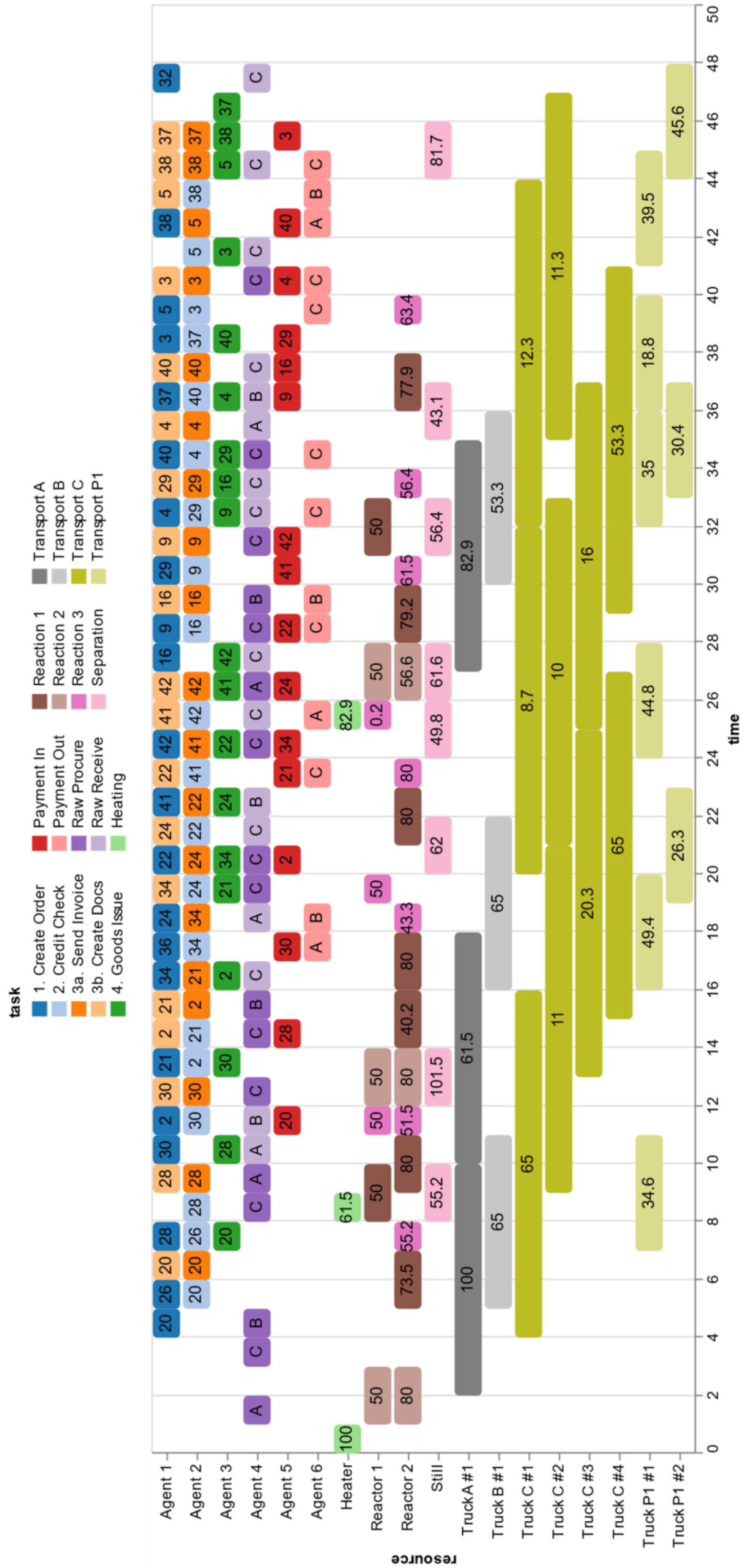

Figure 5.3. Gantt schedule obtained for Example 2. Values inside bars in the agent schedules are order numbers or material involved. Values inside bars in the production and transportation schedules are batch sizes in kg.

The inventory levels for the storage tanks operating with *basestock* inventory policies are given in **Figure 5.4**. The level in Tank A drops below the safety stock between t = 8 h and t = 11 h, but has no stockouts. The level in Tank B is well above the safety stock throughout the scheduling horizon, indicating that a lower inventory target could be used for this tank. Tank C stocks out between t = 12 h and t = 17 h, suggesting that the inventory target should be increased for this tank. P1 at the distribution center stays at or above the safety stock for most of the horizon, except for period 45. Inventory levels are restored to their initial values for all tanks except Tank C, which is 92% full at the end of the horizon.

The dynamic accounting ledger for the supply chain is shown in **Figure 5.5**. The cash assets decrease during the first 12 periods, until enough revenue enters to offset the operating expenses. After t = 12 h, the cash levels have a general upward trend. The accounts payable are maintained below $1,053 and the accounts receivable do not exceed $3,604. The proposed schedule expects a net increase in cash of $8,247, with $365 in accounts payable and $3,368 in accounts receivable at the end of the simulation horizon. The dynamic cash profile in this integrated model can be used to gain valuable financial insights on the system being modeled. These include,

- An initial investment of at least $1,099 is required to avoid the system from becoming cash constrained at t = 14 h. If the initial cash level is below this value, the solution provided will no longer be feasible. This type of information is valuable in determining the amount of initial cash required to maximize shareholder equity.
- The rate of cash consumption in the system is $228/h on average (see **Figure 5.6**). At this rate of cash out-flow, the system would become cash constrained at t = 18 h if no payments are received for outstanding customer invoices. Since the first order is fulfilled at t = 8 h, the longest payment delay that the system can handle is 10 h. This type of information can be used to evaluate the payment terms a company has agreed to with its customers to ensure that the system does not become cash constrained.
- The rate of cash creation in the system is $511/h on average (see **Figure 5.7**), which is substantially greater than the rate of cash consumption. This results in a net cash flow of $283/h on average. The return on investment (ROI) in this system is 3.75, which makes the system attractive from a financial point of view. This ROI corresponds to an average interest rate of 21% for each of the 48 periods. Another valuable metric is the net unit return, which is approximately $14 per kg of product on average. For orders with an average of 45 kg of material, this results in a margin of $645 per order. For a system with these high margins, the focus can shift from minimizing costs to maximizing yield and throughput while ensuring that quality specs are met.

These financial metrics give valuable insights when it comes to assessing the value of holding inventory in the supply chain. Financial departments in companies often view holding inventory as a problem because capital is tied up in storage. However, when the expected interest rates from the supply chain operations are greater than the interest rates obtained from other financial activities (e.g., buying government bonds), holding inventory can be more easily justified. The model can also be used to understand the impact of reducing inventory levels by quantifying the impact of inventory reductions on shareholder equity. If reductions in inventory result in greater stockouts, lost sales, and loss in revenue, such decisions can be identified as financially undesirable. Note that the model can be augmented to include other financial flows (e.g., taxes, time value of money, and bank loans for the initial cash investment) if desired. Doing so will give more accurate financial metrics.

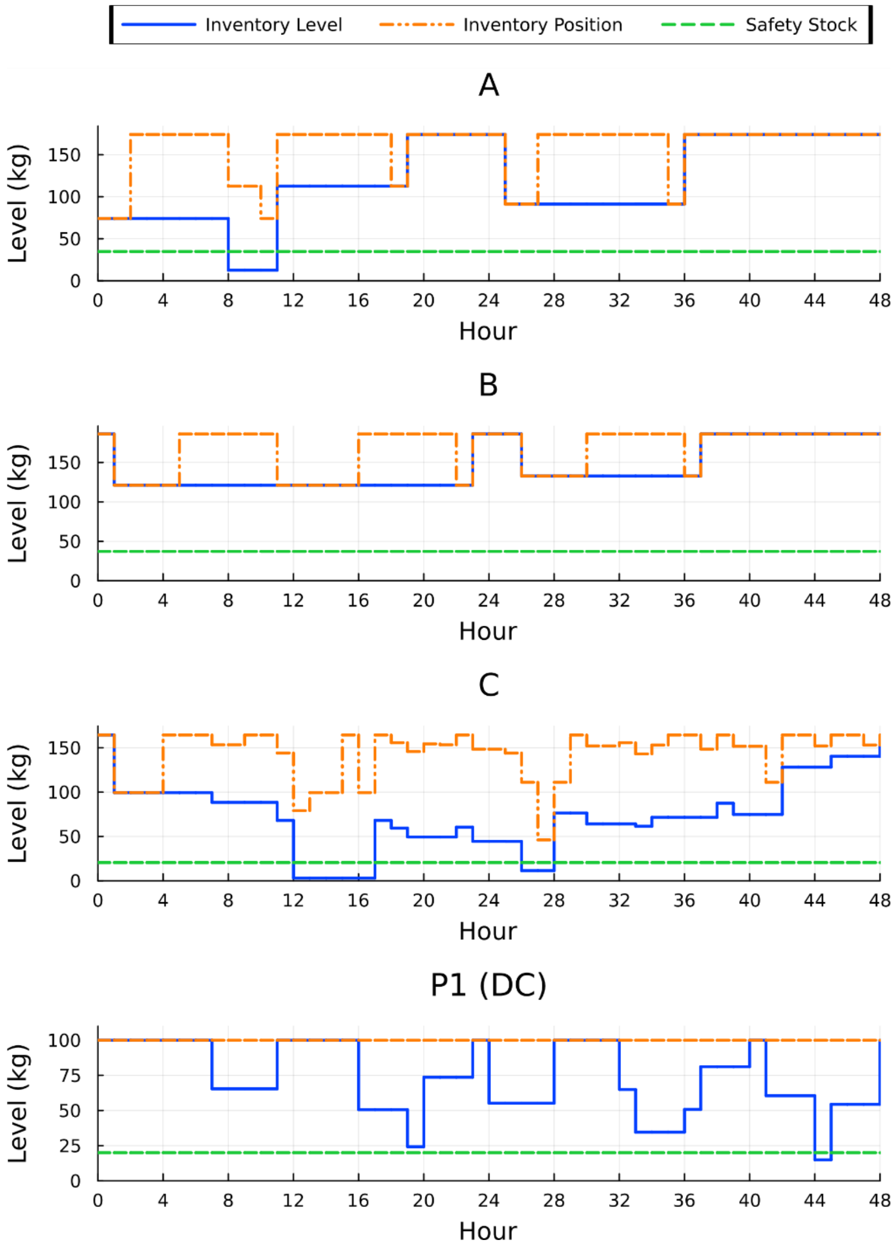

Figure 5.4. Inventory profiles for A, B, C, and P1 (Distribution Center) storage tanks in solution found for Example 2.

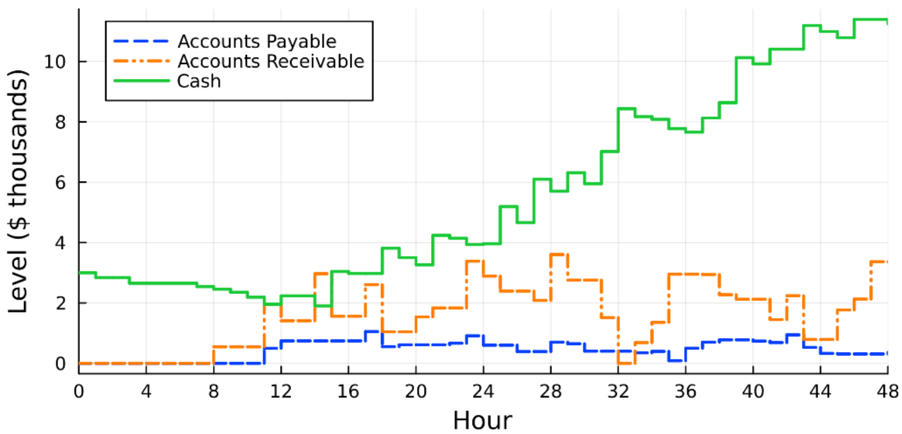

Figure 5.5. Dynamic accounting ledger for solution found in Example 2.

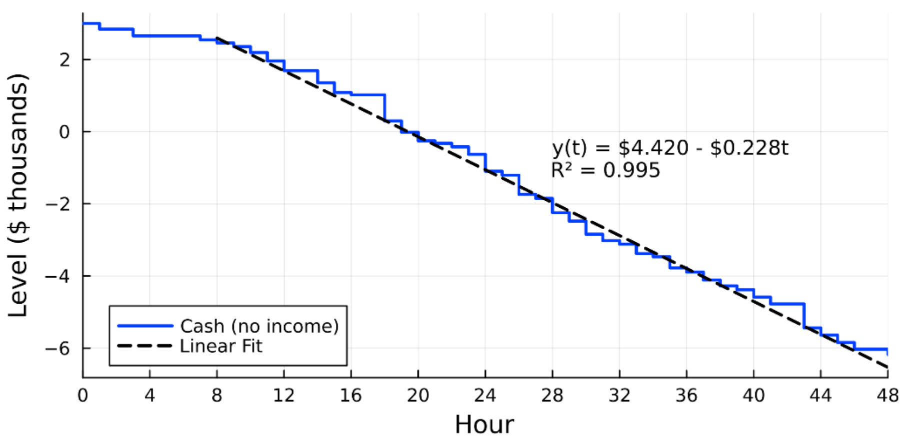

Figure 5.6. Cash levels if no income is received (assuming no accounts receivable are closed) in Example 2.

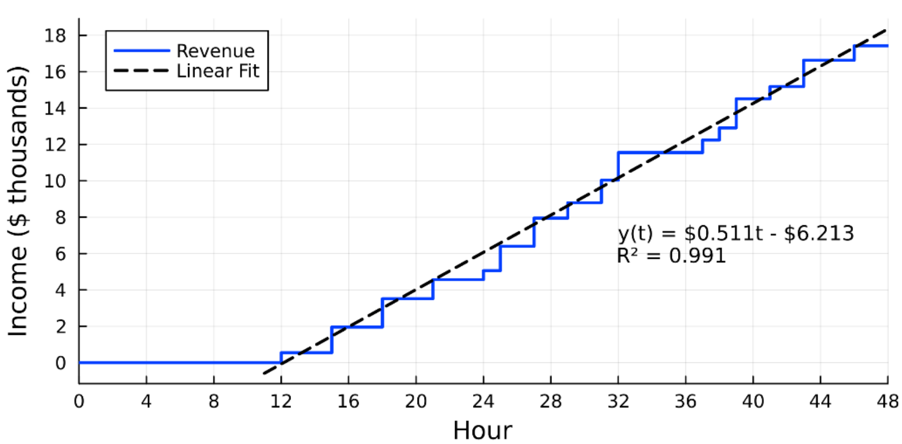

Figure 5.7. System income in Example 2.

6. Conclusions

This work presents a novel approach to integrating material, information, and financial flows in a supply chain. The enabling technology for such an integration is the novel application of the State-Task Network and Resource-Task Network scheduling models to model the key components and flows in the supply chain. Among these is a STN representation of inventory policies in a supply chain, which allows encoding commonly used policies such as order-up-to and fixed-order-quantity policies with either continuous or periodic review of inventory levels. The key in modeling such policies is to introduce an artificial state that represents the amount by which the inventory position is below its target. This allows controlling inventory not by the on-hand level, but by the inventory position, which accounts for in-transit inventory as is traditionally done in inventory control policies. Another novel application of Task Network models is in representing the financial processes occurring in a supply chain via a RTN that allows tracking the major resources in a financial balance sheet: assets, liabilities, and shareholder equity. The STN model for the order-to-cash process used in prior work is also extended to apply it to the source-to-pay business process for raw material procurement in connection with the inventory control model.

By representing the different components of a real supply chain using Task Network-based models, these can be linked to obtain integrated models that account for the relationships between the components in a supply chain. Two examples of this integration were presented. In the first example, the order-to-cash process is linked with the STN model of a batch chemical plant in a make-to-order supply chain. In this example, the interaction between the order-to-cash process and the manufacturing plant is in the availability of raw materials, which are enabled once an order has been cleared for manufacturing in the enterprise resource planning (ERP) system. The draining of finished goods is then linked to the Goods Issue transaction of the order-to-cash process. This integrated transactional-physical scheduling model is compared against a transaction-focused model that lumps the physical processes into one task node for each product, and a material-focused model that only considers upstream and downstream transactions to the plant. Each of these models is used for online scheduling in a DES that captures uncertainty in order processing times, order arrivals, and order characteristics, as is the case in a real supply chain. The single-focused models underperform the integrated model because they either ignore intermediate storage at the plant and the relationships between the different production pathways, which yields suboptimal solutions, or they ignore the resource limitations and transactions that must occur in parallel to manufacturing, which results in solutions that are infeasible in practice. The infeasibility demonstrated in the illustrative example is indicative of actual circumstances encountered in industrial supply chains. The lack of rigorous coordination between manufacturing scheduling and order processing often leads to telephone calls and email exchanges between schedulers and customer service representatives to ultimately resolve conflicts between their respective domains. The proposed modelling approach is a first attempt to integrate the information and material involved in a digital supply chain.

The second example extends the model from the first example to introduce material sourcing from upstream suppliers, which includes both the procure-to-pay business process and the inventory control processes. Material distribution at a downstream warehouse is also added with customers placing orders directly at the plant or at the downstream distribution center. A dynamic accounting ledger is also included in this integrated model, allowing for a more complete representation of cash flow in a supply chain. The objective function of the model is to maximize shareholder equity, referring to the difference between assets and liabilities in the supply network. This model combines elements from the STN and RTN formulation to reduce the network model complexity and decrease the number of discrete variables.

The integrated models presented in this paper represents an important step towards integrating the approaches to supply chain management discussed by Shapiro (1999), and attaining the vision for holistic supply chain management promoted by Laínez and Puigjaner (2012). Future directions that can be taken with the integrated RTN/STN model presented include developing case studies that rely on industrial data. This will create opportunities to address potential issues with varying time scales between business process transactions and material flow processes, as well as potential challenges with modeling large scale systems. The former can be addressed by extending modeling approaches that integrate systems with varying time scales as those discussed by Brunaud *et al.* (2019). The latter can be addressed via model decomposition, such as decomposing by the customer order or type of process (business, physical, and financial) in a Lagrangean decomposition approach (Guignard and Kim, 1987). Other methods that can be considered for dealing with the curse of dimensionality are to look to reinforcement learning methods (Hubbs *et al.*, 2020) and distributed decision making via multi-agent systems (García-Flores and Wang, 2002; Lara and Wassick, 2023). These can be trained on simulation models that are built upon the Task Network modeling abstraction of the integrated supply chain processes presented in this work.

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Appendix A: Inventory Policy Dynamics

Figure A shows the temporal evolution of inventory throughout several replenishment cycles under an (s, S) order-up-to policy. Consider a demand of A modeled by the $Normal(\mu = 70kg, \sigma = 10kg)$ distribution. With a lead time of 8 periods, the expected demand over the supply lead time is 560 kg. For a 96% service level target, a safety stock of 50 kg is used, resulting in a total stock of 610 kg, which is enough to satisfy 96% of the demand over the supply lead time on average. These values are used to define the (s, S) policy with a reorder point of 610 kg and a target inventory position of 1,170 kg. At t = 8 h, the inventory position of A has dropped below the reorder point and the position shortfall has exceeded the 560 kg threshold ($TIP_A - ROP_A$), triggering a replenishment order from the upstream supplier. When the replenishment order is triggered, the inventory position target is restored, and the position shortfall drops to 0 kg. This replenishment order is received at t = 16 h (after the 8 h lead time). Note that the on-hand inventory replenishment observed at t = 8 h is for the order placed at t = 0 h.

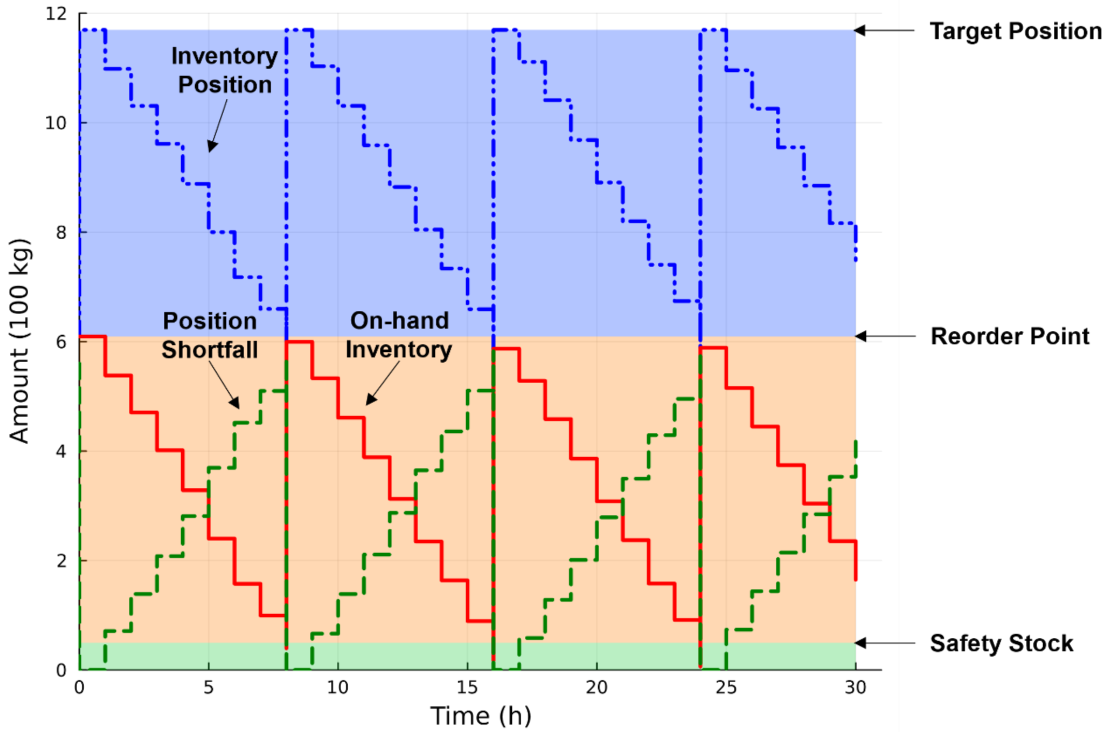

Figure A. Inventory position, inventory level, and position shortfall for material A in each period at the Plant over 30 periods. Quantities are in multiples of 100 kg.

Appendix B: Business Process STN Model

The business process STN model is an extension of the GDP STN model from **Section 3.1**. The equivalent mixed-integer linear programming (MILP) model is given in Perez *et al.* (2022). Using the notation from **Section 3.1**, the set of states is defined as $K = \{(o,s): o \in O, s \in S\}$, where O is the set of orders and S is the set of information states. The set of processing steps is $I = \{(o,l): o \in O, l \in L\}$, where L is the set of process transactions. The set of processing equipment is $J = \{a: a \in A\}$, where A is the set of agents in the business process. Since information flows in discrete quantities from one state to another, the states are bounded between 0 and 1 and are consumed/produced in their entirety. This results in "batch sizes" of 1 and production/consumption ratios of 1. Although this seems to violate mass conservation in tasks with more than one input states, this is not a concern since information is not conserved in the same sense as mass is. This is analogous to how moles are not conserved in a chemical reaction. External supply of information to states only occurs at the starting information state ($s = 1$) of each order when the order enters the system ($t = t_o^r$, where t_o^r is the release time of order o). External demand of information from the system only occurs at the final information state ($s = |S|$) of the business process when the variable $S_{o,t}^{exit} = 1$. Thus, (3.1.1) – (3.1.3) becomes (B.1) – (B.5).

$$S_{o,s,t} = S_{o,s,t-1} + \sum_{l \in L_s^{pred}} \sum_{a \in A_l} B_{o,l,a,t-\tau_{o,l,a}} - \sum_{l \in L_s^{succ}} \sum_{a \in A_l} B_{o,l,a,t} + S_{o,s,t}^{supply} - S_{o,s,t}^{demand} \quad \forall o \in O, s \in S, t \in T \tag{B.1}$$

$$S_{o,s,t}^{supply} = \begin{cases} 1, & \text{if } s = 1, t = t_o^r \\ 0, & \text{otherwise} \end{cases} \quad \forall o \in O, s \in S, t \in T \tag{B.2}$$

$$S_{o,s,t}^{demand} = \begin{cases} S_{o,t}^{exit} & \text{if } s = |S| \\ 0 & \text{otherwise} \end{cases} \qquad \forall o \in O, s \in S, t \in T \qquad \text{(B.3)}$$

$$\begin{bmatrix} W_{o,l,a,t} \\ B_{o,l,a,t} = 1 \end{bmatrix} \vee \begin{bmatrix} \neg W_{o,l,a,t} \\ B_{o,l,a,t} = 0 \end{bmatrix} \qquad \forall o \in O, l \in L, a \in A_l, t \in T \qquad \text{(B.4)}$$

$$\Gamma\left(1, W_{o,l,a,t'} \ \forall o \in O, l \in L_a, t' \in \{t - \tau_{o,l,a} + 1, \dots, t\}\right) \qquad \forall a \in A, t \in T \qquad \text{(B.5)}$$

The delivery of an order is modeled with the disjunction in (B.6). There is a direct mapping between the Boolean variable $D_{o,t}$, which *True* if the order is fulfilled (delivered) at t, and the continuous variable $S_{o,t}^{exit}$. Therefore, when reformulating to a MILP, the continuous variable $S_{o,t}^{exit}$ can be replaced by the binary variable obtained from $D_{o,t}$. This disjunction also fixes the time an order is fulfilled t_o^{exit} to the timepoint in which $D_{o,t} = True$.

$$\begin{bmatrix} D_{o,t} \\ S_{o,t}^{exit} = 1 \\ t = t_o^{exit} \end{bmatrix} \vee \begin{bmatrix} \neg D_{o,t} \\ S_{o,t}^{exit} = 0 \\ 0 \leq t_o^{exit} \end{bmatrix} \qquad \forall o \in O, t \in T \qquad \text{(B.6)}$$

The disjunction in (B.7) allows distinguishing if the order is one of the following:

- Fulfilled on-time ($OT_o = True$), which occurs when the order is fulfilled between the early due date t_o^e and the final due date t_o^d,
- Backlogged ($BL_o = True$), which occurs when the order is fulfilled after the due date and by the lost sale date t_o^{ls}, or
- Lost-sale ($LS_o = True$), which occurs when the order is not fulfilled.

In the lost-sale disjunct, the fulfillment time is set to 0, which forces (B.6) to select $D_{o,t} = False \ \forall t \in T$ (note that $T = \{1, \dots, |T|\}$), meaning the order is not fulfilled. It is assumed that $t_o^e < t_o^d < t_o^{ls}$. If $t_o^d = t_o^{ls}$, then the backlog disjunct should be excluded from (B.7), indicating that orders become lost sales after their due date. Depending on which disjunct is selected from (B.7), a different function ($f_{1,o}$, $f_{2,o}$, and $f_{3,o}$) is used to determine the profit of the order z_o. These functions can take different forms, but for the purposes of this work, they are assumed to be linear as discussed in (Perez *et al.*, 2022). The cardinality clause in (B.8) ensures that exactly 1 of the disjuncts is selected, where $\Xi(n,\cdot)$ is the *exactly n* predicate (Perez and Grossmann, 2023). The propositional logic constraints in (B.9), (B.10), and (B.11) link disjunction (B.7) with disjunction (B.6), so that the order fulfillment Boolean variable $D_{o,t}$ is aligned with the appropriate final order condition (OT_o, BL_o, or LS_o) depending on the timepoint in which it occurs. Note that the double implications in (B.9) and (B.10), and the forward implication in (B.11) are redundant as a result of the relationships between the fulfillment time variable t_o^{exit} and the Boolean variables in (B.7) and (B.6). Nonetheless, they are included to explicitly represent these links and provide clarity.

$$\begin{bmatrix} OT_o \\ t_o^e \leq t_o^{exit} \leq t_o^d \\ z_o \leq f_{1,o}\left(t_o^{exit}\right) \end{bmatrix} \vee \begin{bmatrix} BL_o \\ t_o^d + 1 \leq t_o^{exit} \leq t_o^{ls} \\ z_o \leq f_{2,o}\left(t_o^{exit}\right) \end{bmatrix} \vee \begin{bmatrix} LS_o \\ t_o^{exit} = 0 \\ z_o \leq f_{3,o}(0) \end{bmatrix} \qquad \forall o \in O \qquad \text{(B.7)}$$

$$\Xi(1, \{OT_o, BL_o, LS_o\}) \qquad \forall o \in O \qquad \text{(B.8)}$$

$$OT_o \Leftrightarrow \bigvee_{t \in \{t_o^e, \ldots, t_o^d\}} D_{o,t} \qquad \forall o \in O \tag{B.9}$$

$$BL_o \Leftrightarrow \bigvee_{t \in \{t_o^d+1, \ldots, t_o^{ls}\}} D_{o,t} \qquad \forall o \in O \tag{B.10}$$

$$LS_o \Leftrightarrow \bigwedge_{t \in T} \neg D_{o,t} \qquad \forall o \in O \tag{B.11}$$

For scheduling business processes, the objective used is that of maximizing system profit given in (B.12).

$$\max \sum_{o \in O} z_o \tag{B.12}$$

The domains and bounds for the variables used in this GDP model are given in (B.13) – (B.20). The full GDP model is given by (B.1) – (B.20).

$$B_{o,l,a,t} \in \mathbb{R}: 0 \le B_{o,l,a,t} \le 1 \qquad \forall o \in O, l \in L, a \in A_l, t \in T \tag{B.13}$$

$$S_{o,s,t} \in \mathbb{R}: 0 \le S_{o,s,t} \le 1 \qquad \forall o \in O, s \in S, t \in T \tag{B.14}$$

$$S_{o,t}^{exit} \in \mathbb{R}: 0 \le S_{o,t}^{exit} \le 1 \qquad \forall o \in O, t \in T \tag{B.15}$$

$$t_o^{exit} \in \mathbb{R}: 0 \le t_o^{exit} \le t_o^{ls} \qquad \forall o \in O \tag{B.16}$$

$$z_o \in \mathbb{R} \qquad \forall o \in O \tag{B.17}$$

$$D_{o,t} \in \{True, False\} \qquad \forall o \in O, t \in T \tag{B.18}$$

$$BL_o, LS_o, OT_o \in \{True, False\} \qquad \forall o \in O \tag{B.19}$$

$$W_{o,l,a,t} \in \{True, False\} \qquad \forall o \in O, l \in L, a \in A_l, t \in T \tag{B.20}$$

Appendix C: Optimization results from Example 1

The duration of the optimization runs triggered for each model within the discrete event simulation are shown in **Figure C**. The time to solve the model grows as more orders enter the system, as expected. The integrated model, generally takes longer to solve, followed by the transaction-focused model, and then by the material-focused model. This trend is expected and is supported by the number of binary variables in each model as given in **Table 4.2**, which indicates the size of the largest model in each case. The largest model size corresponds to the model run at t = 23 h, which is when the last order enters the system during the 24 h simulation run. For the optimization runs that reach the allotted time limit of 360 s, the relative optimality gap is less than 4% for the integrated model, and less than 2% for the transaction-focused model. The expected system profit with each of the models is shown in **Figure C**, which also increases with each consecutive optimization run. This is expected because more orders in the system create a greater opportunity for making profit. The exception is the material-focused model, which sees a decline in the expected profit after t = 14 h due to the infeasible schedules produced by this model. The expected profits exceed those from the simulation because the optimization has an adaptive rolling horizon that runs the scheduling until the last lost sales date for the orders in the system, which exceeds the 24 h simulation horizon. This extends the scheduling horizon up to 51 h, which occurs in the last optimization run and corresponds to the lost sales date for the last order (Order 26).

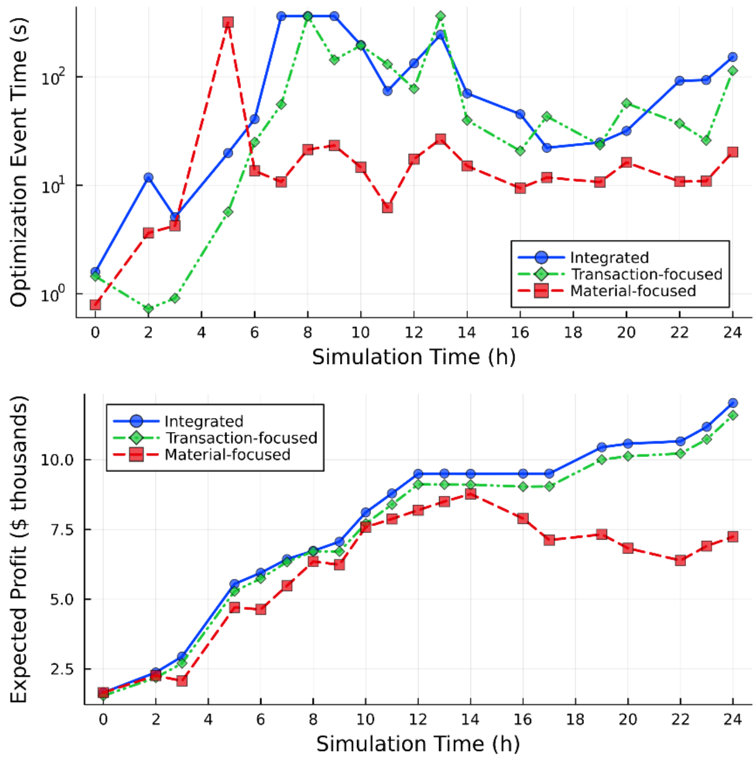

Figure C. Time to build and solve the scheduling model (top) and expected profit from the scheduling models (bottom) obtained each time a new order enters the system in Example 1.