### **Support Material**

## A. Definition MLCLSP-L-B with Probabilistic Demand

The MIP formulation of the MLCLSP-L-B with probabilistic demand is represented by a two-stage stochastic problem formulation. Many studies in the literature like Hu and Hu (2016) and Azizi et al. (2020) use that topology to model a two-stage stochastic programming formulation for lot size optimization. Scenarios are inserted into production, inventory, backorder, setup, and linked lot size decision variables as new indexes, whereby the total setup decision variable stays untouched. The total setup decision variable ensures that the model's outcome generates a unique setup plan across different scenarios. The model determines lot sizes so that setup, inventory, and backorder costs are kept at a minimum while demand has to be satisfied across several demand scenarios.

| $x_{s,p,t}^{su}$  | Equals 1, if $p \in \mathcal{P}$ is prepared for setup in $t \in \mathcal{T}$ and scenario $s \in \mathcal{S}$ , otherwise          |
|---|---|
| -77   | 0   |
| $x_{s,p,t}^l$   | Equals 1, if the production of $p \in \mathcal{P}$ is continued from $t$ to $t+1$ on period   |
| -77   | domain $\mathcal{T}_0$ and scenario $s \in \mathcal{S}$ , otherwise 0   |
| $x_{p,t}^{tsu}$   | First-stage total setup decision that equals $x_{s,p,t}^{su} + x_{s,p,t-1}^{l}$ for all $s \in \mathcal{S}$ , $p \in \mathcal{P}$ , |
| •   | and $t \in \mathcal{T}$   |
| $x_{s,p,t}^p$   | Production quantity of product $p \in \mathcal{P}$ in period $t \in \mathcal{T}$ and scenario $s \in \mathcal{S}$                   |
| $x_{s,p,t}^{inv}$   | Inventory quantity of a product $p \in \mathcal{P}$ in period $t \in \mathcal{T}_0$ and scenario $s \in \mathcal{S}$                |
| $x_{s,p,t}^p \ x_{s,p,t}^{inv} \ x_{s,p,t}^{bo} \ x_{s,p,t}^{bo}$ | Backorder quantity of a product $p \in \mathcal{P}$ in period $t \in \mathcal{T}_0$ and scenario $s \in \mathcal{S}$                |

Table 1: Decision variables of the MLCLSP-L-B with probabilistic demand

Let  $S, M, P, T \in \mathbb{N}$  be the number of scenarios, machines, materials, and planning periods, respectively. Each material is allocated to exactly one machine, but one machine can produce several materials. Thus, a machine index is not required for production-related decision variables and model parameters. Each finished good is requested by scneario- and period-specific deterministic demand. Probabilistic demand is expressed by the demand scenarios with equal probability. Moreover, a material can be stocked or backordered. For both cases, holding and backorder costs must be considered per unit at the end of each period. Each machine has a period-specific capacity. The production of materials requires variable production and fixed setup times. A setup operation is associated with product-specific setup costs. This paper assumes lead times to equal 0 periods, sequence-independent setups, and linked lot sizes' validity. If a material is produced, then several ingredients are issued. The set of issued ingredients can intersect with other sets of issued materials. Table 1 and Table 2 summarize model decision variables and parameters of the MLCLSP-L-B with probabilistic

```
S.
                Set of scenarios \{0, \dots, S\}
                Set of machines \{1, ..., M\}
\mathcal{M}
Ð
                Set of products \{1, ..., P\}
{\mathscr T}
                Set of periods \{1, \ldots, T\}
\mathcal{T}_0
                Set of periods including initial period \{0, ..., T\}
\mathscr{P}_p^{suc}
                Set of successors of a product p \in \mathcal{P}
\mathscr{P}_m
                Set of products that can be produced on machine m \in \mathcal{M}
\mathcal{P}^{Int}
                Set of intermediate products \{p \in \mathcal{P} | \mathcal{P}_p^{suc} \neq \emptyset\}
                Capacity of machine m \in \mathcal{M} in period t \in \mathcal{T}
b_{m,t}
\begin{array}{c} d_{s,p,t} \\ c_p^{su} \\ c_p^{inv} \\ c_p^{bo} \\ t_p^{su} \\ t_p^{p} \\ t_p^{as} \\ r_{p,q} \end{array}
                Demand of product p \in \mathcal{P} in scenario s \in \mathcal{S} and period t \in \mathcal{T}
                Setup cost for a product p \in \mathcal{P}
                Inventory holding cost for a product p \in \mathcal{P}
                Backorder cost for a product p \in \mathcal{P}
                Setup time for a product p \in \mathcal{P}
                Production time for a unit of product p \in \mathcal{P}
                Advanced shift for a product p \in \mathcal{P}
                Number of units of product p \in \mathcal{P} required to produce one unit of successor
                product q \in \mathcal{P}_p^{suc}
\begin{array}{l} \bar{x}_{s,p,0}^{inv} \\ \bar{x}_{s,p,T}^{inv} \\ \bar{x}_{s,p,T}^{bo} \\ \bar{x}_{s,p,0}^{bo} \end{array}
                Initial inventory quantity for p \in \mathcal{P} in scenario s \in \mathcal{S}
                Final inventory quantity for p \in \mathcal{P} in scenario s \in \mathcal{S}
                Initial backorder quantity for p \in \mathcal{P} in scenario s \in \mathcal{S}
               Initial setup state for p \in \mathcal{P}, such that \sum_{p \in \mathcal{P}_m} \bar{x}_p^l \le 1 for all s \in \mathcal{S} and m \in \mathcal{M}
               Large number, e.g. M_{s,p,t} = \min\{\sum_{\tau \in \mathcal{T}, \tau \geq t} d_{s,p,\tau}, b_{m,t}/t_p^p\} for s \in \mathcal{S}, p \in \mathcal{P}_m for a fixed m \in \mathcal{M}, and t \in \mathcal{T} whereby d_{s,p,\tau} represents primary demand in
                case of finished goods and is replaced by secondary demand for intermedi-
                ates
```

Table 2: Model sets and parameters of the MLCLSP-L-B with probabilistic demand

demand represented by scenarios. The correspondent MIP is based on the work of Quadt and Kuhn (2008), Helber and Sahling (2010), and Simonis and Nickel (2023b). Among this research, the MLCLSP-L-B with probabilistic demand is formulated as follows:

$$\min Z = \min \left\{ \frac{1}{S} \sum_{s \in \mathscr{S}} \left( \sum_{p \in \mathscr{D}} \sum_{t \in \mathscr{T}} c_p^{su} x_{s,p,t}^{su} + \sum_{p \in \mathscr{D}} \sum_{t \in \mathscr{T}} c_p^{inv} x_{s,p,t}^{inv} + c_p^{bo} x_{s,p,t}^{bo} \right) \right\}, \quad (1)$$

$$x_{s,p,t-1}^{inv} + x_{s,p,t}^{bo} + x_{s,p,t-t_p}^{p} = x_{s,p,t}^{inv} + x_{s,p,t-1}^{bo} + d_{s,p,t} + \sum_{p' \in \mathcal{P}_n^{suc}} r_{p,p'} x_{s,p',t}^{p}, \quad (2)$$

$$\sum_{p' \in \mathcal{P}_m} t_{p'}^{su} x_{s,p',t}^{su} + t_{p'}^p x_{s,p',t}^p \le b_{m,t}, \tag{3}$$

$$x_{s,q,t}^{p} \le M_{s,q,t} \left( x_{s,q,t}^{su} + x_{s,q,t-1}^{l} \right), \tag{4}$$

$$x_{p,t}^{tsu} = x_{s,p,t}^{su} + x_{s,p,t-1}^{l}, (5)$$

$$\sum_{p' \in \mathcal{P}_m} x_{s,p',t}^l \le 1,\tag{6}$$

$$x_{s,q,t}^{l} - x_{s,q,t}^{su} - x_{s,q,t-1}^{l} \le 0, (7)$$

$$x_{s,q,t}^{l} + x_{s,q,t-1}^{l} - x_{s,q,t}^{su} + x_{s,r,t}^{su} \le 2,$$
(8)

$$x_{s,p',t}^{bo} = 0,$$
 (9)

$$\begin{split} x_{s,p,0}^{inv} &= \bar{x}_{s,p,0}^{inv}, x_{s,p,T}^{inv} = \bar{x}_{s,p,T}^{inv}, x_{s,q,0}^{l} = \bar{x}_{s,q,0}^{l}, x_{s,p,0}^{bo} = \bar{x}_{s,p,0}^{bo}, \\ x_{p,t}^{tsu} &\in \{0,1\}, x_{s,q,t}^{su} \in \{0,1\}, x_{s,q,t}^{l} \in \{0,1\}, x_{s,p,t}^{bo} \geq 0, x_{s,q,t}^{p} \geq 0, x_{s,p,t}^{inv} \geq 0, \end{split}$$

 $\forall s \in \mathcal{S}, m \in \mathcal{M}, p \in \mathcal{P}, q, r \in \mathcal{P}_m, q \neq r, p' \in \mathcal{P}^{Int}, t \in \mathcal{T}.$ 

(1) aims to minimize average setup, inventory, and backorder costs across all scenarios for each machine and material over the planning horizon. The material balance equation is covered by (2), capacity constraints are included by (3), and (4) binds a positive production quantity to a setup in the same or a linked lot size in the previous period. (5) sets the final setup decision  $x_{s,p,t}^{tsu}$  equal a setup operation  $x_{p,t}^{su}$  plus a linked lot sizes from previous period  $x_{s,p,t-1}^l$  for all scenarios. Thus  $x_{p,t}^{su}$  is the only decision variable set at time zero (scenario independent) while production, inventory, backorder, setup and linked lot size decision variables are decided within the scenario afterwards. (6) satisfies that at most one linked lot size per period on a specific machine can be operated, (7) guarantees that a linked lot size is only allowed when a setup in the same period or a linked lot size in the previous period take place, and (8) synchronizes production runs that continue over more than two periods on a machine  $m \in \mathcal{M}$  in scenario  $s \in \mathcal{S}$ . If  $x_{s,p,t}^l = x_{s,p,t-1}^l = 1$ , then either  $x_{s,q,t-1}^{su} = 0$  for all  $p, q \in \mathcal{P}_m$ ,  $q \neq p$  or for some  $q \neq p$ ,  $x_{s,q,t-1}^{su} = 1$  and  $x_{s,p,t-1}^{su} = 1$ . That is, either product p is produced exclusion. sively in period t-1 or product p is produced at the beginning of t-1, some other products were produced next, and the facility was reset to produce product p at the end of period t-1. (9) restricts the backorders to final products. This prohibits final products from being processed further if intermediate product shortages occur. Moreover, (10) sets the initial inventory and setup state and the initial and final backorder quantities, respectively.

## B. Modeling Background

This section presents the modeling background of the RDS applied on the MLCLSP-L-B with probabilistic demand. It focuses on the data representation for the MLCLSP-L-B with probabilistic demand provided by Simonis and Nickel (2023a). A detailed description of the mathematical formulation of the MLCLSP-L-B with probabilistic demand is provided by Appendix A. This section explains first the role of time-dependent value substitutions. Second, it summarizes the representation of probabilistic demand. Third, the section outlines the representation of multi-level production structures.

## B.1. Time-Dependent Values Substituted by Validity Horizons

| Machineld | ValidityDateFrom  | ValidityDateTo  | Total Capacity |
|-----------|-------------------|-----------------|----------------|
| Machine1  | 2021-01-01        | 2021-12-31      | 5200           |
|           | (a) Validity hori | izon representa | tion           |
| Machineld | Date              |                 | Capacity       |
| Machine1  | 2021-01-0         | )4              | 100            |
| Machine1  | 2021-01-1         | l1              | 100            |
|           |                   |                 |                |
| Machine1  | 2021-12-2         | 20              | 100            |
| Machine1  | 2021-12-2         | 27              | 100            |

(b) Multi period representation

Figure 1: Two different representations of time-dependent values for capacity data

Data in manufacturing processes (manufacturing costs, processing times, or production recipes) are updated yearly. Thus, planning parameters stay constant over a significant part of the planning horizon. The spreadsheets profit from that behavior by substituting time dependencies with validity horizons instead of periods as suggested by Dutta and Fourer (2008). A validity horizon has a start and an end date and represents a particular value for the entire horizon. Figure 1 illustrates this representation: A machine Machine1 might have a capacity of 100 for each week in 2021. In this example, a validity horizon represents a total capacity of 5200 in 2021 by one observation. At the same time, a multi-period representation consists of 52 observations with a capacity value of 100 per observation. Thus, validity horizons keep the data compact and easily maintainable in the spreadsheets. The price of this simplicity is that these time-dependent values mapped on validity horizons must be assigned to the correct planning period in the optimization model (part of the model formulation). Furthermore, the validity horizons are prohibited from overlapping for primary keys to avoid unique constraint issues (part of the business rules in the data storage).

### B.2. Probabilistic demand stored in simulation scenarios

| SimulationInstanceId | MaterialId | DeliveryDate | Quantity |
|----------------------|------------|--------------|----------|
| Sim1                 | Material1  | 2021-01-04   | 100      |
| Sim2                 | Material1  | 2021-01-04   | 110      |
| Sim1                 | Material1  | 2021-01-05   | 100      |
| Sim2                 | Material1  | 2021-01-05   | 90       |
|                      |            |              |          |

Figure 2: Storage of simulation scenarios for demand in spreadsheet Demand

Pharmaceutical tablets demand is uncertain. Almost all approaches from the literature simulate sufficiently many scenarios and search for efficient lot sizes across all scenarios. This data becomes large even on medium-sized problem instances since each demand scenario might increase the dataset by multiple. Demand scenarios are represented by a scenario instance identified by a unique ID in the developed spreadsheets. These instances are listed in spreadsheet *SimulationInstance* and referenced in spreadsheet *Demand*. Figure 2 illustrates the demand scenario storage in entity *Demand*. Simulation instances *Sim2* represent a demand shift of 10 units of material *Material1* from 2021-01-05 to 2021-01-04, while simulation instance *Sim1* assumes a constant demand of 100 across both months. The template supports demand scenarios stored in daily date buckets. Scenario representation becomes intuitive and easy for the endusers to fill out. However, the price for that is that daily demand has to be mapped and aggregated to model planning periods (part of model formulation).

## B.3. Multi-level BOM representation

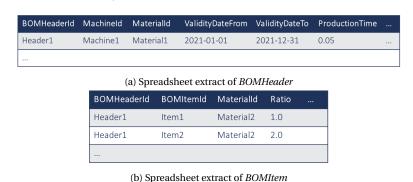


Figure 3: Representations of multi-level production structures

Multi-level production structures are complex and usually stored in a multi-level BOM in planning systems. They contain production-relevant information

and definitions of production relationships stored in the BOM header and BOM item entity, respectively. This representation provides a unified structure to describe different multi-level production processes. The developed spreadsheets follow this approach. They strictly separate production activities from product dependencies by the entities *BOMHeader* and *BOMItem*. Figure 3 shows that representation. A material *Material1* can be produced in the entire year 2021 on machine *Machine1*. For one production unit of *Material1*, the machine requires 0.05 days. If *Material1* is issued by *Header1*, then two ingredients *Material2* and *Material3* are issued by the production with 1.0 and 2.0 units, respectively.

## C. Modeling Techniques

The MLCLSP-L-B is a complex MIP that relies on different data sources stored in a structured format, such as demand, capacity, material cost, production cost, setup matrix, and the BOM. A list of all developed entities and virtual tables is provided in repository documentation of Simonis (2024). Appendix E documents the mapping rules of the optimization model indices, sets, and coefficients to the RDS components This section organizes the applied modeling techniques as follows: First, it introduces the raw data template for the MLCLSP-L-B with probabilistic demand and how to build an Entity Relationship (ER) model. Second, it presents how to develop the Extended ER (EER) model to cover all required data preparation tasks.

## C.1. Entity Relationship Model

Simonis and Nickel (2023a) provided a data template developed in MS Excel spreadsheets to store the metadata information of the MLCLSP-L-B with probabilistic demand in 10 spreadsheets. They are named Material, Capacity, ProblemInstance, SimulationInstance, Demand, MaterialCost, SetupMatrix, BOM-Header, BOMItem, and InitialLotSizingValues. Complexity and hierarchy drivers of the data are the amount of data (machines, materials, and periods), demand scenarios, and multi-level production structures. Cunha et al. (2009) studied the relationship between non-hierarchical spreadsheets and RDS. A rule framework was created that defines the design of an ER model by the data representation of the spreadsheets. The authors created an ER model entity for each spreadsheet with primary and foreign keys. For each spreadsheet defined in Simonis and Nickel (2023a), a persistent table is created consistent with the spreadsheet's name, column names, column data types, and data relationships. An ER diagram of persistent tables in the ER model is shown in Figure 4. In terms of simplicity, not all relationships between production and simulation instances are listed. The entities ProblemInstance and SimulationInstance are the baseline of the relational data model. Each defined problem instance has multiple simulation

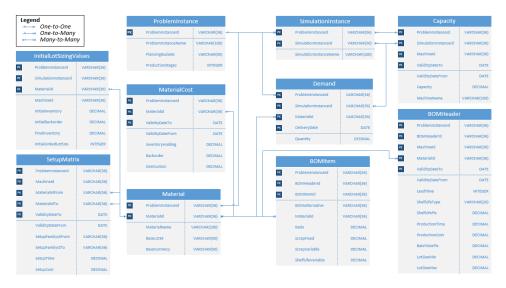


Figure 4: ER diagram of persistent tables

instances assigned. For each problem instance, materials (*Material*), material-related costs (*MaterialCost*), machines and product-to-machine assignments (*BOMHeader*), setup structure (*SetupMatrix*), and product structure (*BOMItem*) are set. Simulated scenarios are supported for demand (*Demand*), machine capacities (*Capacity*), and initial planning values (*InitialLotSizingValues*).

### C.2. Extended Entity Relationship Model

Based on the ER model from the previous section, the persistent entities of the ER model store only metadata information of the MLCLSP-L-B. Thus, data transformations must be executed to meet the requirements of MLCLSP-L-B instantiation while ensuring that data can be processed at scale. Data transformations are developed with virtual tables defined by Structured Query Language (SQL) queries. An overview of the EER model is shown in Figure 5. The EER model consists of the 10 persistent tables (blue shaded rectangles) outlined in the previous section and, in addition, 16 virtual tables (green shaded rectangles). The circles represent join operations whereby the letter "I", "L", and "R" represent inner, left outer, and right outer joins, respectively. Grouping operations are denoted by the "GROUP BY" label. In the following, the most essential virtual table modeling techniques are described: First, two essential virtual tables that transform validity horizons into a multi-period representation are described in detail. Second, the mapping and aggregation of demand scenarios into a multi-period representation are outlined. Third, the material cost mapping based on

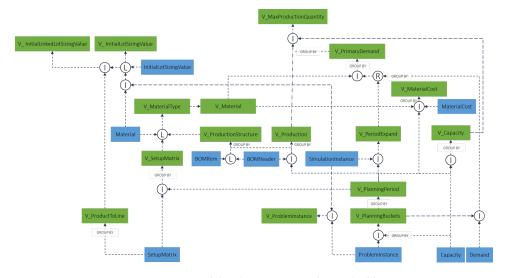


Figure 5: EER model with persistent and virtual tables

# validity horizons is explained.

Map Validity Horizons to Planning Periods. The following describes the transformation from validity horizons to multi-period representations in detail. These queries are a central transformation step on which almost all other virtual table definitions depend. The MLCLSP-L-B represents time by periods within the planning horizon. The planning horizon is determined by a start and end date, and each period has a particular duration (planning bucket). The query  $V_PlanningBuckets$  answers the question, "Which planning buckets, start and end date of the planning horizon are available for problem instance?". Figure 6 defines the virtual table. The planning horizon is determined by the minimum

```
CREATE VIEW "V_PlanningBuckets" AS

SELECT t_pi."ProblemInstanceId", t_pi."PlanningBuckets", j_c."PlanningEndDate", j_c."PlanningStartDate",

CASE

WHEN UPPER(t_pi."PlanningBuckets") LIKE '%DAY' THEN 'DAY'

WHEN UPPER(t_pi."PlanningBuckets") LIKE '%WEEK' THEN 'WEEK'

WHEN UPPER(t_pi."PlanningBuckets") LIKE '%MONTH' THEN 'MONTH'

WHEN UPPER(t_pi."PlanningBuckets") LIKE '%QUARTER' THEN 'QUARTER'

WHEN UPPER(t_pi."PlanningBuckets") LIKE '%YEAR' THEN 'YEAR'

ELSE 'DAY' END AS "PlanningBucketType"

FROM "ProblemInstance" AS t_pi

INNER JOIN (

SELECT t_c."ProblemInstanceId", MAX(t_c."ValidityDateTo") AS "PlanningEndDate",

MIN(t_c."ValidityDateFrom") AS "PlanningStartDate"

FROM "Capacity" AS t_c

GROUP BY t_c."ProblemInstanceId"

) AS j_c ON t_pi."ProblemInstanceId" = j_c."ProblemInstanceId";
```

Figure 6: Syntax definition of query *V\_PLanningBuckets* 

and maximum validity dates of the capacity for each problem instance from table *Capacity* (line 12-15). This information is merged with table *ProblemInstance* based on the identifier *ProblemInstanceId* (line 10, 11, and 16). Based on defined planning buckets, the type is derived by case-when statement. The query supports the types 'DAY', 'WEEK', 'MONTH', 'QUARTER', and 'YEAR' as duration of a period (line 3-9). Finally, the problem instance (*ProblemInstanceId*), planning buckets (*PlanningBuckets*), start and end horizon dates (*PlanningStartDate* and *PlanningEndDate*), and the planning bucket type (*PlanningBucketType*) are selected from the query.

The query *V\_PlanningPeriod* answers the question, "Which model period is mapped on which planning date for a problem instance within the planning horizon?". Figure 7a shows the syntax of the query. An illustrative example of the data transformations is summarized in Figure 7b. The nested query starts

```
CREATE VIEW "V_PlanningPeriod" AS

SELECT s_v_pb."ProblemInstanceId", s_v_pb."PlanningStartDate", s_v_pb."PlanningEndDate",

s_v_pb."PlanningBuckets", s_v_pb."PlanningDate",

DATE(s_v_pb."PlanningBuckets", s_v_pb."PlanningBuckets"::INTERVAL - '1 DAY'::INTERVAL) AS "PlanningDateIntervalEnd",

ROW_NUMBER() OVER(PARTITION BY s_v_pb."PlanningBuckets"::INTERVAL - '1 DAY'::INTERVAL) AS "PlanningPeriod",

FROM

SELECT v_pb."PlanningBuckets", v_pb."PlanningStartDate", v_pb."PlanningEndDate",

v_pb."PlanningBuckets", DATE(DATE_TRUNC(

v_pb."PlanningBucketType",

DATE(GENERATE_SERIES(

v_pb."PlanningBuckets", v_pb."PlanningBuckets",

v_pb."PlanningBuckets", v_pb."PlanningBuckets",

v_pb."PlanningBuckets", v_pb."PlanningBuckets",

v_pb."PlanningBuckets", v_pb.

FROM "V_PlanningBuckets", v_pb.

GROUP BY v_pb."ProblemInstanceId", v_pb."PlanningStartDate", v_pb."PlanningEndDate",

v_pb."PlanningBuckets", v_pb."PlanningBucketType"

) AS s_v_pb;

PanningBuckets", v_pb."PlanningBucketType"
```

(a) Syntax definition

| Problem<br>Instanceld | PlanningStartDate           | PlanningEndDate             | PlanningBuckets                | PlanningDate                     | PlanningDate<br>IntervalEnd                         | PlanningPeriod |
|-----------------------|-----------------------------|-----------------------------|--------------------------------|----------------------------------|---|----------------|
|                       | 2024 04 04                  | 2024 05 20                  | 2.14011711                     | 2021-01-01                       | 2021-02-28  | 1              |
| Problem1              | 2021-01-01<br>MIN(Capacity. | 2021-06-30<br>MAX(Capacity. | 2 MONTH<br>(V_PlanningBuckets. | 2021-03-01                       | 2021-04-30  | 2              |
|                       | ValidityDateFrom)           | ValidityDateTo)             | PlanningBuckets)               | 2021-05-01                       | 2021-06-30  | 3              |
|                       |                             |                             |                                |                                  |   |                |
|                       |                             |                             |                                | DATE_TRUNC(-) GENERATE_SERIES(-) | PlanningDate+<br>PlanningBuckets::Interval<br>1 Day | ROW_NUMBER(·)  |

(b) Illustration data transformations

Figure 7: Details for query  $V\_PlanningPeriod$ 

with "Get for each problem instance the planning buckets and types, and start and end date of the planning horizon." from virtual view  $V_PLanningBuckets$  (line 15). This view provides, for each problem instance, the planning start and end date and the date buckets. Next, this information is used by a sub-query that answers the question "Which planning dates are valid for associated planning buckets and a problem instance within the planning horizon?" (line 8-17).

It uses the *GENERATE\_SERIES* function (line 11). The function has the inputs *start* (start timestamp), *stop* (stop timestamp), and *step* (interval buckets of the time-series generation). It returns a set of timestamps from *start* to *stop* with frequency *step*. The output of the function *GENERATE\_SERIES* is formatted by the *DATE\_TRUNC* function (line 10). The function takes the inputs *field* (valid value for truncate) and *source* (set of timestamps). It returns a truncated set of timestamps (e.g., the start of day, week, month, quarter, or year). Finally, the virtual table *V\_PlanningPeriod* selects the problem instance (*ProblemInstanceId*), planning buckets (*PlanningBuckets*), start and end horizon dates (*PlanningStart-Date* and *PlanningEndDate*), and determines the planning end of each interval bucket (*PlanningDateIntervalEnd*) and planning period (*PlanningPeriod*) by the row number partitioned by the problem instances and ordered by the planning date (line 1-7).

Map and Aggregate Demand Scenarios to Planning Periods. The query V Demand answers the question, "How much demand of a material is expected per planning period for a problem and simulation instance?". Figure 8a shows the syntax of the query. Furthermore, code transformations are illustrated in Figure 8b and Figure 8c. The nested query starts with "How much demand of a material is expected in a particular delivery date truncated on date buckets" (line 11-18). The DATE TRUNC is used to format the column DeliveryDate in entity Demand against the PlanningBucketType provided by the view  $V_PlanningBuckets$ . After this operation, the demand quantity is summed over the problem and simulation instance ID, material ID, and the truncated delivery dates. Next, the demand per planning bucket is right-outer joined with the V PeriodExpand (equals the view V\_PlanningPeriod, but contains additionally the simulation instance and material id for all planning periods) view on the keys problem and simulation instance, planning date, and material id (line 20-22) whereby the DeliveryDate is joined with an BETWEEN condition on the interval PlanningDate and PlanningDateIntervalEnd. Suppose no demand quantity was defined for a particular planning period. In that case, the right outer join creates an observation that associates a delivery date and demand quantity of NULL with such a planning period. Thus, the resulting sub-query contains a demand quantity for each planning period, material, problem, and simulation instance. Base units and currencies are mapped from entity Material by an inner join on problem instance id and material (line 23-24). Next, this information is used by a sub-query that answers the question, "Which demand quantity per material is available for the planning periods across all problem and simulation instances?" (line 6-9). It transforms NULL values for the demand quantity to 0 and renames the mapped planning date from the multi-period grid to the delivery date. Finally, the origin question

```
CREATE VIEW "V_PrimaryDemand" AS

SELECT s_t_d."ProblemInstanceId", s_t_d."SimulationInstanceId", s_t_d."MaterialId",

s_t_d."DeliveryDate", SUM(s_t_d."Quantity") AS "Quantity", s_t_d."PlanningPeriod",

s_t_d."BaseUOM", s_t_d."BaseCurrency"

FROM (

SELECT j_pe."ProblemInstanceId", j_pe."SimulationInstanceId", j_pe."MaterialId",

j_pe."PlanningDate" AS "DeliveryDate", j_pe."PlanningPeriod",

j_v_m."BaseUOM", j_v_m."BaseCurrency",

CASE WHEN j_t_d."Quantity" IS NULL THEN 0 ELSE j_t_d."Quantity" END AS "Quantity"

FROM (

SELECT t_d."ProblemInstanceId", t_d."SimulationInstanceId", t_d."MaterialId",

DATE(DATE_TRUNC(j_v_pp."PlanningBucketType", t_d."DeliveryDate")) AS "DeliveryDate",

SUM(t_d."Quantity") AS "Quantity"

FROM

INNER JOIN "V_PlanningBuckets" AS j_v_pp ON t_d."ProblemInstanceId" = j_v_pp."ProblemInstanceId"

GROUP BY t_d."ProblemInstanceId", t_d."SimulationInstanceId", t_d."MaterialId",

DATE_TRUNC(j_v_pp."PlanningBucketType", t_d."DeliveryDate")

) AS j_t_d

RIGHT JOIN "V_PeriodExpand" AS j_pe ON j_t_d."ProblemInstanceId" = j_pe."ProblemInstanceId" AND

(j_t_d."DeliveryDate" BETMEEN j_pe."PlanningDate" AND j_pe."PlanningDateIntervalEnd") AND

j_t_d."MaterialId" = j_pe."MaterialId" AND j_t_d."SimulationInstanceId" = j_pe."SimulationInstanceId"

INNER JOIN "V_Material" AS j_vm

ON j_pe."ProblemInstanceId" = j_v_m."ProblemInstanceId" AND j_pe."MaterialId" = j_v_m."MaterialId"

) AS s_t_d

GROUP BY s_t_d."ProblemInstanceId", s_t_d."SimulationInstanceId", s_t_d."MaterialId" = j_v_m."MaterialId"

) AS s_t_d."PlanningPeriod", s_t_d."BaseCurrency";
```

#### (a) Syntax definition

| Problem<br>Instanceld | Simulation<br>InstanceId | MaterialId | DeliveryDate  | Quantity | PlanningBucketType                            | PlanningBuckets                                    |
|-----------------------|--------------------------|------------|---------------|----------|---|--|
|                       |                          | Material1  | 2021-01-01    | 100      |   | 2 MONTH<br>(V_PlanningBuckets.<br>PlanningBuckets) |
| Problem1              | Simulatio1               |            | 2021-01-01    | 100      | MONTH (V_PlanningBuckets. PlanningBucketType) |  |
| Problem1              | Simulation               |            | 2021-02-01    | 100      |   |  |
|                       |                          |            | 2021-06-01    | 400      |   |  |
| ,                     |                          |            | <u> </u>      | <u> </u> |   |  |
|                       |                          |            | DATE_TRUNC(·) | SUM(∙)   |   |  |

### (b) Illustration data transformations (line 11-18)

| Problem<br>InstanceId  | Simulation<br>InstanceId | MaterialId    | DeliveryDate | Quantity | PlanningDate | PlanningDateIntervalEnd | PlanningPeriod |   |  |
|--|--------------------------|---------------|--------------|----------|--------------|-------------------------|----------------|---|--|
|  |                          |               | 2021-01-01   | 200      | 2021-01-01   | 2021-02-28              | 1              |   |  |
|  |                          |               | 2021-02-01   | 100      | 2021-01-01   | 2021-02-28              |                |   |  |
| Problem1   | Simulation1              | 1   Material1 | Material1    | NULL     | O<br>NULL    | 2021-03-01              | 2021-04-30     | 2 |  |
|  |                          |               | 2021-06-01   | 400      | 2021-05-01   | 2021-06-30              | 3              |   |  |
| CASE [] WHEN [] V_PeriodExpand SUM(-) RIGHT OUTER DeliveryDate BETWEEN PlanningDateInterv. |                          |               |              |          |              |                         |                |   |  |

(c) Illustration data transformations (line 6-9, 20-22)

Figure 8: Details for query V\_PrimaryDemand

of  $V\_Demand$  is answered by summing the demand quantity overall problem and simulation instances, materials, delivery dates, planning periods, base units, and currencies.

```
CREATE VIEW "V_MaterialCost" AS

SELECT t_mc."ProblemInstanceId", t_mc."MaterialId", j_v_pp."PlanningDate", j_v_pp."PlanningPeriod"

AVG(t_mc."InventoryHolding") AS "InventoryHolding",

AVG(t_mc."Backorder") AS "Backorder"

FROM "MaterialCost" AS t_mc

INNER JOIN "V_PlanningPeriod" AS j_v_pp ON t_mc."ProblemInstanceId" = j_v_pp."ProblemInstanceId" AND

(j_v_pp."PlanningDate" BETWEEN t_mc."ValidityDateFrom" AND t_mc."ValidityDateTo")

INNER JOIN "V_Material" AS j_v_m ON t_mc."ProblemInstanceId" = j_v_m."ProblemInstanceId" AND

t_mc."MaterialId" = j_v_m."MaterialId"

GROUP BY t_mc."ProblemInstanceId", t_mc."MaterialId", j_v_pp."PlanningDate", j_v_pp."PlanningPeriod";
```

(a) Syntax definition

| Problem<br>Instanceld | MaterialId         | ValidityDate<br>From | ValidityDate<br>To | InventoryHolding | Backorder | PlanningDate  | PlanningPeriod |
|-----------------------|--------------------|----------------------|--------------------|------------------|-----------|---|----------------|
|                       |                    | 2021-01-01           | 2021-02-28         | 0.06             | 0.12      | 2021-01-01  | 1              |
| Problem1              | Problem1 Material1 | 2024 02 04           | 2021 06 20         | 0.075            | 0.15      | 2021-03-01  | 2              |
|                       |                    | 2021-03-01           | 2021-06-30         | 0.075            | 0.15      | 2021-05-01  | 3              |
|                       |                    |                      |                    | AVG(·)           |           | V_PlanningPeriod<br>INER PlanningDate BETWEI<br>ityDateFrom AND ValidityD |                |

(b) Illustration data transformations

Figure 9: Details for query V\_MaterialCost

Map Material Costs Based on Validity Horizons. Almost all MIP parameters are mapped from the data templates by validity horizons. As discussed in the previous sections, this keeps the raw data easily maintainable. The downside of validity horizons is that they must be mapped to the planning periods. This section explains this mapping based on the view V MaterialCost. However, analog transformations are implemented in the views *V\_Capacity*, *V\_Production*, and V ProductStructures. The query V MaterialCost answers the question, "Which inventory and backorder costs are associated with each material per planning period and problem instance?". Figure 9a shows the syntax of the query. Furthermore, code transformations are illustrated in Figure 9b. The entity MaterialCost is merged with the view *V\_PlanningPeriod* (line 6-7) on the problem instance id and the planning date that is between the validity horizon determined by columns ValidityDateFrom and ValidityDateTo. Next, the results are merged with the view V\_Material (line 8-9) on the problem instance and material id. Finally, the data is grouped by the problem instance, material ID, planning date, and planning period to average inventory-holding and backorder costs (line 2-4).

### D. Research Datasets

This paper consolidated the datasets of 4 important quantitative literature sources. The summary of established datasets across these research initiatives is shown in Table 3.

• TAB\_MAN: Simonis and Nickel (2023a,b) presented numerical experiments

| Dataset name | Linked<br>lot size | Backordering | Demand scenarios | Data availability | Problem instances | Scenarios per<br>problem |
|--------------|--------------------|--------------|------------------|-------------------|-------------------|--------------------------|
| TAB_MAN      | <b>√</b>           | ✓            | ✓                | ✓                 | 9                 | 451                      |
| C_1_6        | ✓                  |              | $\checkmark$     | on request        | 384               | 5                        |
| DATAB        | ✓                  |              |                  | $\checkmark$      | 60                | 1                        |
| MULTILSB     |                    | $\checkmark$ | ✓                | $\checkmark$      | 4                 | 30                       |

Table 3: Literature with structured published research data for capacitated lot-sizing problems

for pharmaceutical tablets packaging processes modeled by capacitated lot-sizing problems with linked lot sizes and backorders were provided. The authors developed a generalized uncertainty framework that embeds a variable neighborhood search (VNS) algorithm in a fix-and-optimize procedure to deal with probabilistic demand. The performance of the developed solution approach was evaluated in terms of costs and service-level metrics based on 4 problem instances, including 451 simulation scenarios per problem instance from real-world tablets manufacturing processes.

- DATAB: Suerie and Stadtler (2003) and Stadtler (2003) introduced the MIP formulation for the multi-level capacitated lot-sizing problem (MLCLSP) with linked lot sizes (MLCLSP-L). The authors applied a time-oriented decomposition heuristic in combination with Cut-and-Branch (C&B) and Branch-and-Cut (B&C) algorithms to solve small- and medium-sized simulated test instances. The author's formulation of the MLCLSP-L became a standard in capacitated lot-sizing literature. To evaluate their heuristic, they solved 60 simulated problem instances. Demand scenarios were not included in the MLCLSP and MLCLSP-L datasets.
- C\_1\_6:Tempelmeier and Buschkühl (2009) solved the MLCLSP-L with a slightly modified Lagrangean heuristic of Tempelmeier and Derstroff (1996). The Lagrangean heuristic applies a Lagrangean relaxation in each iteration on several constraints of the MLCLSP-L and solves resulting subproblems by dynamic programming (DP) to improve terminated solution quality. 1920 problem instances with demand scenarios were simulated and used to evaluate the performance of the heuristic in terms of optimization time and costs.
- **MULTILSB**: Akartunalı and Miller (2009) applied a heuristic framework with valid inequalities (VI) and a relax-and-fix (R&F) procedures on the MLCLSP with backorders (MLCLSP-B). The authors solved 120 simulated problem instances with demand scenarios.

| Class          | Coefficient             | EER model component            | Column mapp              | ing rule              |
|----------------|-------------------------|--------------------------------|--------------------------|-----------------------|
| Class          |                         | •                              | Value                    | Index                 |
| Index sets     | 8                       | V_ProblemInstance              | SimulationInstanceId     | -                     |
|                | M                       | V_Capacity                     | MachineId                | -                     |
|                | P                       | V_Material                     | MaterialId               | -                     |
|                | $\mathcal{T}$           | V_PeriodExpand                 | PlanningPeriod           | -                     |
|                | $\mathcal{T}_0$         | V_PeriodExpand                 | PlanningPeriod           | -                     |
|                | P <sub>p</sub> suc      | V_ProductionStructures         | GoodsReceived            | GoodsIssued           |
|                | $\mathscr{P}_m$         | V_ProductToLine                | MaterialId               | MachineId             |
| Capacity       | $b_{s,m,t}$             | V_Capacity                     | CapacityPerPeriod        | SimulationInstanceId, |
|                |                         |                                |                          | MachineId,            |
|                |                         |                                |                          | PlanningPeriod        |
|                | $t_{p,t}^p$             | V_Production                   | ProductionTimePerBaseUOM | MaterialId,           |
|                | "                       |                                |                          | PlanningPeriod        |
|                | $t_{p,t}^{su}$          | V_SetupMatrix                  | SetupTime                | MaterialId,           |
|                | "                       |                                |                          | PlanningPeriod        |
| Demand         | $d_{s,p,t}$             | V_PrimaryDemand                | Quantity                 | SimulationInstanceId, |
|                | "                       |                                |                          | MaterialId,           |
|                |                         |                                |                          | PlanningPeriod        |
| Costs          | $c_{p,t}^{inv}$         | V_MaterialCost                 | InventoryHolding         | MaterialId,           |
|                | "                       |                                |                          | PlanningPeriod        |
|                | $c_{p,t}^{bo}$          | V_MaterialCost                 | Backorder                | MaterialId,           |
|                | "                       |                                |                          | PlanningPeriod        |
|                | $c_{p,t}^{su}$          | V_SetupMatrix                  | SetupCost                | MaterialId,           |
|                | "                       |                                |                          | PlanningPeriod        |
| Production     | $r_{p,q}$               | V_ProductionStructures         | Ratio                    | GoodsReceived,        |
|                | ' '                     |                                |                          | GoodsIssued           |
|                | $t_p^{as}$              | V_Production                   | LeadTime                 | MaterialId            |
|                | $M_{s,m,p,t}$           | V_MaxProductionQuantity        | BigM                     | SimulationInstanceId, |
|                | ,.                      |                                |                          | MachineId,            |
|                |                         |                                |                          | MaterialId,           |
|                |                         |                                |                          | PlanningPeriod        |
|                | $\bar{x}_{s,p,0}^{inv}$ | V_InitialLotSizingValues       | InitialInventory         | SimulationInstanceId, |
| Initial values | -,,,,                   |                                |                          | MaterialId            |
|                | $\bar{x}_{s,p,0}^{bo}$  | V_InitialLotSizingValues       | InitialBackorder         | SimulationInstanceId, |
|                | 3, p,0                  |                                |                          | MaterialId            |
|                | $\bar{x}_{s,p,T}^{inv}$ | V_InitialLotSizingValues       | FinalInventory           | SimulationInstanceId, |
|                | s, p, 1                 |                                |                          | MaterialId            |
|                | $\bar{x}_{s,p,0}^l$     | V_InitialLinkedLotSizingValues | InitialLinkedLotSize     | SimulationInstanceId, |
|                | s, p,u                  |                                |                          | MachineId,            |
|                |                         |                                |                          | MaterialId            |
|                |                         |                                |                          |                       |

Table 4: Mapping rules for MLCLSP-L-B instantiation for a given problem instance

# E. Documentation of Optimization Model Instantiation

The mapping of model coefficients with their value representation from the EER model instantiates the MLCLSP-L-B with probabilistic demand. Table 4 shows a summary of mapping rules. The group index sets, capacity, demand, costs, production, and initial values are used to classify all coefficients. Then, the EER model component that contains the mapping values is listed. Next, the mapping value is derived from the referenced technical column name. A referenced column reads the index value if the model coefficient has an index. Thus, the instantiation is executed in two steps: First, index sets are created.

Required indices for scenarios, machines, products, periods, product successors, and machine allocations are read from *V\_ProblemInstance*, *V\_Capacity*, *V\_Material*, *V\_PeriodExpand*, *V\_ProductionStructures*, and *V\_ProductToLine*. Second, model coefficients are defined. Capacity-related model coefficients are read from views *V\_Capacity*, *V\_Production*, and *V\_SetupMatrix*. Demand data is collected by virtual tables *V\_PrimaryDemand*. Cost-related coefficients are mapped by *V\_MaterialCost* and *V\_SetupMatrix*. Production-related model coefficients are set by the virtual tables *V\_Production*, *V\_ProductionStructure*, and *V\_MaxProductionQuantity*. Finally, initial values are read from the virtual tables *V\_InitialLotSizingValues* and *V\_InitialLinkedLotSizingValues*. Mapping rules instantiate the MLCLSP-L-B with probabilistic demand. Afterward, it can be used by a solver API to run optimization procedures on the instantiated model.

## F. Numerical experiments with real-world data

This section evaluates the defined EER model for tablets manufacturing processes. Appendix D provides the source definition of the used research data for the numerical experiments. First, an evaluation of the data entry is presented. Second, a discussion on the performance of RDS is provided. Third, the impact of RDS on the optimization procedure is outlined.

### F.1. Data storage efficiency

This section briefly discusses the data entry of the RDS outlined in Section C.1 in terms of simplicity, generalization, and required disk storage. The research datasets listed in Table 3 are used for evaluation. In the following, simplicity

|              |         | ion   |                      | After      | migrati | on    |       |              |
|--------------|---------|-------|----------------------|------------|---------|-------|-------|--------------|
| Dataset name | Folders | Data  | Data File Disk stora |            | Folders | Data  | File  | Disk storage |
|              |         | files | types                | types [KB] |         | files | types | [KB]         |
| TAB_MAN      | -       | -     | -                    | -          | 1       | 3     | XLSB  | 17000        |
| C_1_6        | 18      | 1104  | TXT                  | 4400       | 1       | 1     | XLSB  | 1700         |
| DATAB        | 60      | 960   | PRN                  | 1012       | 1       | 1     | XLSB  | 92           |
| MULTILSB     | 128     | 124   | TXT 4000             |            | 1       | 1     | XLSB  | 244          |

Table 5: Data entry characteristics before and after data model migration

is measured by the number of required data files, folders, and used file types. Generalisability is measured by the used file types and the ability to store information in a consolidated data format. Table 5 summarizes these measures and the disk storage in kilobytes (KB) for the raw data (before migration) and the data spreadsheets (after migration). The bash command du -h "research\_data/" >  $logs/storage\_analysis/output.txt$  collects this information from the datasets in

directory *research\_data* with their blocked disk storage and writes the information in the file location *logs/storage\_analysis/output.txt*. Furthermore, Table 5 uncovers the following data template behavior: First, binary Excel workbooks (XLSB) can store only 1048576 rows per spreadsheet.

Dataset TAB\_MAN represents large real-world tablets manufacturing datasets. 3 binary workbooks are required to store all problem instances properly. All other research datasets fall below the row limitation so that they can be stored in one binary workbook. Second, the data entry is kept as simple as possible for C\_1\_6, DATAB, and MULTILSB. Only one file and one folder are required to store all information for the MLCLSP-L-B. Third, the required disk storage is reduced by 61.36%, 90.91%, and 93.90% for C\_1\_6, DATAB and MULTILSB, respectively. Finally, all research data could be stored in one data template structure and file format. Thus, RDS consolidate the data structure into a generalized data entry that is easily consumable. Hence, the data spreadsheets significantly impact simplicity, maintainability, and stored disk size across all considered research datasets. Moreover, it defines a generalized data entry for the relation database structures.

# F.2. Performance of RDS

RDS divide data storage and processing from optimization runtime. This section evaluates a model instantiation based on the relational database and analog processing in the optimization runtime environment. Database queries are executed with the sqlAlchemy module while the pandas module executes all data transformations directly in the optimization runtime. For all following analyses, analysis is executed per problem instance listed in Table 3 and averaged over the mapped simulation instances for the datasets TAB MAN, C\_1\_6, DATAB, and MULTILSB. The analysis uses processing time and memory consumption as performance indicators. Table 6 summarizes the results for all considered research datasets grouped by problem classes. The bash command sh run\_instantiation\_experiments.sh executes the experiment (takes approx. 4 hours). The script stops the processing time of model instantiation and logs memory usage with Pythons memory profiler module in the directory /logs/instantiation. A problem class contains several problem instances. The EER instantiation dominates the Python runtime instantiation regarding processing time and memory usage for the datasets TAB MAN and C 1 6. The EER instantiation required 95.30% (352.91 seconds) and 86.78% (100.47 seconds) less processing time and 45.60% (152.05 MB) and 23.46% (32.26 MB) less memory on average than the runtime instantiation for TAB\_MAN and C\_1\_6, respectively. The situation could be clearer for dataset DATAB. 11.14% (1.29 seconds) more processing time was required, but 2.9% (3.30 MB) less memory was used. The

|               |               | Instantiate from    | disk and runtime  | Instantiate from    | relational database |
|---------------|---------------|---------------------|-------------------|---------------------|---------------------|
| Research data | Problem class | Processing time [s] | Memory usage [MB] | Processing time [s] | Memory usage [MB]   |
| TAB_MAN       | MODEL001      | 368.96              | 288.00            | 17.08               | 135.10              |
|               | MODEL002      | 369.30              | 282.30            | 17.07               | 131.80              |
|               | MODEL003      | 369.57              | 316.40            | 19.56               | 154.10              |
|               | MODEL004      | 372.99              | 322.60            | 20.55               | 176.60              |
|               | SET1          | 372.03              | 307.70            | 18.71               | 161.20              |
|               | SET2          | 378.81              | 299.80            | 18.91               | 156.10              |
|               | SET3          | 394.55              | 365.70            | 23.80               | 231.70              |
|               | SET4          | 401.25              | 412.60            | 25.89               | 247.00              |
|               | SET5          | 339.54              | 405.70            | 27.70               | 263.20              |
| C_1_6         | 1             | 120.00              | 137.80            | 13.20               | 110.10              |
|               | 2             | 118.82              | 138.00            | 13.06               | 110.20              |
|               | 3             | 114.18              | 137.90            | 15.07               | 110.20              |
|               | 4             | 113.73              | 137.80            | 16.36               | 111.00              |
|               | 5             | 114.33              | 135.90            | 17.20               | 110.60              |
|               | 6             | 113.57              | 137.60            | 16.66               | 111.20              |
| DATAB         | 1             | 11.58               | 113.50            | 12.87               | 110.20              |
| MULTILSB      | SET1          | 15.07               | 120.60            | 16.80               | 126.10              |
|               | SET2          | 15.33               | 129.30            | 16.87               | 129.80              |
|               | SET3          | 15.12               | 120.50            | 16.63               | 120.60              |
|               | SET4          | 15.08               | 125.90            | 17.16               | 128.50              |

Table 6: Average performance of model instantiations

runtime dominates the EER instantiation by 11.32% (1.72 seconds) less processing time and 3.71% (4.61 MB) less memory usage for MULTILSB. DATAB and MULTILSB are less complex than TAB\_MAN and C\_1\_6. Thus, RDS might not bring advantages in processing speed and efficient memory usage on more minor problem instances. Nevertheless, they dominate runtime data processing when datasets are more complex. However, complex data sets are usually expected in practice, so RDS are an efficient tool to utilize data processing at scale for industrial applications.

## F.3. Impact on optimization procedures

The last section observed that RDS significantly reduce processing time and RAM within the optimization runtime. This section analyzes the impact of these two influencing factors on solver performance. All presented results focus on the real-world dataset TAB\_MAN. It is important to note that the authors of this paper used the commercial solver Gurobi, which is often used in industrial applications. Open-source solvers do not have full parameter support and cannot reach commercial solvers' performance (e.g., CBC solver does not allow the setting of RAM limitations to the solver heuristics). That is why the authors used Gurobi instead of an open-source solver. Execution of the code would require a commercial Gurobi license, and hence, a solver program can not provided in the Docker environment. All problems were solved with Gurobi 10.0 software license on a laptop with an AMD Ryzen 7 PRO processor with 8 GB CPU and 32 GB RAM. The standard optimization procedure of Gurobi includes branch-and-bound

| Problem instance | Stages | Machines | Products | Periods | Model coefficients | Decision variables | Constraints |
|------------------|--------|----------|----------|---------|--------------------|--------------------|-------------|
| MODEL001         | 1      | 1        | 3        | 50      | 18,262             | 38,100             | 50,650      |
| MODEL002         | 1      | 1        | 3        | 50      | 18,262             | 38,100             | 50,650      |
| MODEL003         | 1      | 1        | 7        | 50      | 39,278             | 88,900             | 181,450     |
| MODEL004         | 1      | 1        | 9        | 50      | 49,786             | 114,300            | 276,850     |
| SET1             | 2      | 2        | 6        | 50      | 36,527             | 121,800            | 311,600     |
| SET2             | 2      | 2        | 6        | 50      | 36,527             | 121,800            | 311,600     |
| SET3             | 2      | 2        | 15       | 50      | 83,818             | 304,500            | 1,438,850   |
| SET4             | 2      | 2        | 20       | 50      | 110,096            | 406,000            | 2,415,100   |
| SET5             | 3      | 5        | 22       | 50      | 128,115            | 948,200            | 7,349,050   |

Table 7: Size of problem instances from TAB\_MAN

(B&B), VI, B&C, and C&B heuristics to solve a MIP. Based on the instantiated model, the Gurobi API is called with the Python module *gruobipy*. The MIP gap is a key performance indicator for the solution quality of the MLCLSP-L-B, as determined by Gurobi. It is derived by the incumbent objective value (Z) and the lower bound (LB) of the MLCLSP-L-B derived by the solver. The MIP gap stays at Gurobi's standard value of 1e-4 so that a solution of the MLCLSP-L-B is optimal if the MIP gap falls below this threshold.

Before the MLCLSP-L-B can be sent to a solver, the model coefficients must be mapped to constraints, decision variables, and the objective based on the mapping rules from Appendix E. Table 7 summarizes the model sizes of TAB\_MAN. All problem instances have a planning horizon of 50 periods. MODEL001 to MOLDEL004 are single-level and single-machine problems with 9 products at most. SET1 to SET2 are multi-stage and multi-machine problems with at most 5 machines and 22 products. The number of model coefficients, decision variables, and constraints increases from MODEL001 to SET5. The range of model coefficients, decision variables, and constraints increase by the factors 7.01,

24.89, and 145.09, respectively. Thus, TAB\_MAN contains an ordering in the model size (from MODEL001 to SET5) with a significant range of mid- and large-size problems.

|                  |          | Inst | antiate | from di | sk and r | untime |       | Instantiate from relational database |       |       |       |       |       |  |
|------------------|----------|------|---------|---------|----------|--------|-------|--------------------------------------|-------|-------|-------|-------|-------|--|
| Environment      | RAM [MB] | 2000 |         |         |          |        |       |                                      |       |       |       |       |       |  |
| Elivirollillelit | CT [min] | 1    | 10      | 60      | 240      | 420    | 1440  | 1                                    | 10    | 60    | 240   | 420   | 1440  |  |
|                  | MODEL001 | Inf  | 4.25    | 0.00    | 0.00     | 0.00   | 0.00  | 72.47                                | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |  |
|                  | MODEL002 | Inf  | 26.66   | 3.41    | 0.48     | 0.00   | 0.00  | 94.73                                | 8.66  | 3.09  | 0.33  | 0.00  | 0.00  |  |
|                  | MODEL003 | Inf  | 75.03   | 1.44    | 0.00     | 0.00   | 0.00  | Inf                                  | 55.32 | 0.84  | 0.00  | 0.00  | 0.00  |  |
|                  | MODEL004 | Inf  | 1.44    | 0.00    | 0.00     | 0.00   | 0.00  | Inf                                  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |  |
| SET1             |          | Inf  | 43.19   | 6.82    | 1.39     | 0.00   | 0.00  | 54.05                                | 28.02 | 6.82  | 1.39  | 0.00  | 0.00  |  |
| SET2             |          | Inf  | 60.14   | 52.29   | 14.78    | 14.01  | 12.01 | 68.50                                | 53.42 | 52.29 | 14.78 | 14.01 | 12.01 |  |
| SET3             |          | Inf  | Inf     | Inf     | 96.85    | 96.85  | 65.95 | Inf                                  | Inf   | Inf   | 96.85 | 96.85 | 65.95 |  |
|                  | SET4     | Inf  | Inf     | 87.52   | 87.52    | 79.22  | 15.19 | Inf                                  | 95.10 | 87.52 | 87.52 | 79.22 | 15.19 |  |
|                  | SET5     | Inf  | Inf     | 63.39   | 57.58    | 57.58  | 42.93 | Inf                                  | Inf   | 63.39 | 57.58 | 57.58 | 42.93 |  |

Table 8: MIP gap [%] of best found solution with rather limited calculation time

Next, the impact of processing time on the MIP performance is analyzed. Table 8 presents the best-found solution's MIP gap of Gurobi's standard MIP solver with a fixed RAM limit of 2000 MB and varying calculation times (CT) (1 minute to 1 day) for the problem instances MODEL001 to SET5. If Gurobi runs out of time, the optimization procedure terminates with the best-found solution. All optimization runs were executed with a fixed random seed. Thus, Gurobi started for all problems with the same initial optimization values. If the MIP gap is Inf, no solution could be found within the predefined RAM and CT restrictions. Remarkably, this study analyses the effect of faster processing times on standard MIP procedures. It will not further expand the discussion on decreasing high MIP gaps. The data from Table 8 shows that Gurobi profits from the faster processing time of RDS. Better solutions were found in 5 cases (CT < 10 minutes). This effect also leads to an improvement in average solution quality. If both approaches find a solution, then the relational database processing leads to an average MIP gap improvement of 7.37% in 9 cases. A positive effect of faster processing time affects problem instances MODEL001 to MODEL004, SET1, SET2, and SET4 with a calculation time of less than 240 minutes. SET3 and SET5 are the most challenging problems for the MIP solver. Long calculation times are required to find even an adequate solution. The effect of faster processing time is vanishing on long calculation times for these problem instances. Hence, the MIP solver can not take advantage of the faster processing time for the variations of the CT. However, faster processing time significantly reduces the MIP gap on TAB MAN if the CT is limited (CT < 420 minutes) and small and medium-sized problem instances are considered.

| Instantiate from disk and runtime |          |      |       |       |       |       |       | Instantiate from relational database |       |       |       |       |       |  |
|-----------------------------------|----------|------|-------|-------|-------|-------|-------|--------------------------------------|-------|-------|-------|-------|-------|--|
| Environment                       | CT [min] | 1440 |       |       |       |       |       |                                      |       |       |       |       |       |  |
|                                   | RAM [MB] | 250  | 500   | 750   | 1000  | 1500  | 2000  | 250                                  | 500   | 750   | 1000  | 1500  | 2000  |  |
|                                   | MODEL001 | Inf  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00                                 | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |  |
|                                   | MODEL002 | Inf  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00                                 | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |  |
|                                   | MODEL003 | Inf  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00                                 | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |  |
|                                   | MODEL004 | Inf  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00                                 | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |  |
|                                   | SET1     | Inf  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00                                 | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |  |
| SET2                              |          | Inf  | 12.01 | 12.01 | 12.01 | 12.01 | 12.01 | 12.01                                | 12.01 | 12.01 | 12.01 | 12.01 | 12.01 |  |
| SET3                              |          | Inf  | 65.95 | 65.95 | 65.95 | 65.95 | 65.95 | 65.95                                | 65.95 | 65.95 | 65.95 | 65.95 | 65.95 |  |
|                                   | SET4     | Inf  | 66.55 | 15.19 | 15.19 | 15.19 | 15.19 | Inf                                  | 57.64 | 15.19 | 15.19 | 15.19 | 15.19 |  |
|                                   | SET5     | Inf  | 42.93 | 42.93 | 42.93 | 42.93 | 42.93 | Inf                                  | 42.93 | 42.93 | 42.93 | 42.93 | 42.93 |  |

Table 9: MIP gap [%] of best found solution with rather limited RAM

Next, assume that the CT is fixed and the assigned RAM of the solver becomes a limiting factor. If Gurobi runs out of memory, the solver heuristics search for high-quality solutions with less depth or even terminate with the best-found solution. Table 9 presents the best-found solution's MIP gap of Gurobi's standard MIP solver with a fixed CT limit of 1440 minutes (1 day) and varying RAM (250

MB to 2 GB) for the problem instances MODEL001 to SET5. Gurobi benefits in 7 cases from more assigned RAM by finding a feasible solution (MODEL001 to MODEL004 and SET1 to SET3). Nonetheless, the advantage vanishes with 500 MB or more RAM assignment to the runtime. The first solution was found with at least 500 MB RAM assignment for SET4 and SET5. The advantages of RDS lead to a reduction of the MIP gap of 8.91% and 0.00% for SET4 and SET5 with RAM assignment of 500 MB, respectively. For more RAM assignments, there is no improvement for SET4 and SET5. Thus, more RAM assignments to the solver positively impact the ability to find initial solutions on TAB\_MAN if the RAM runtime is limited (RAM < 750 MB).

### References

- Akartunalı, K., Miller, A.J., 2009. A heuristic approach for big bucket multi-level production planning problems. European Journal of Operational Research 193, 396–411.
- Azizi, V., Hu, G., Mokari, M., 2020. A two-stage stochastic programming model for multi-period reverse logistics network design with lot-sizing. Computers & Industrial Engineering 143, 106397.
- Cunha, J., Saraiva, J., Visser, J., 2009. From spreadsheets to relational databases and back, in: Proceedings of the 2009 ACM SIGPLAN workshop on Partial evaluation and program manipulation, pp. 179–188.
- Dutta, G., Fourer, R., 2008. Database structure for a class of multi-period mathematical programming models. Decision Support Systems 45, 870–883.
- Helber, S., Sahling, F., 2010. A fix-and-optimize approach for the multi-level capacitated lot sizing problem. International Journal of Production Economics 123, 247–256.
- Hu, Z., Hu, G., 2016. A two-stage stochastic programming model for lot-sizing and scheduling under uncertainty. International Journal of Production Economics 180, 198–207.
- Quadt, D., Kuhn, H., 2008. Capacitated lot-sizing with extensions: a review. 4OR 6, 61–83.
- Simonis, M., 2024. PostgreSQL: Relational database structures application on capacitated lot-sizing for pharmaceutical tablets manufacturing processess. https://github.com/MichaelSimois/mlclsplb\_eerm/blob/software\_impacts.doi:https://github.com/MichaelSimois/mlclsplb\_eerm.vl.l.

- Simonis, M., Nickel, S., 2023a. Generalized data model for real-world capacitated lot-sizing problems with linked lot sizes and backorders. Data in Brief 49, 109440.
- Simonis, M., Nickel, S., 2023b. A simulation–optimization approach for a cyclic production scheme in a tablets packaging process. Computers & Industrial Engineering 181, 109304.
- Stadtler, H., 2003. Multilevel lot sizing with setup times and multiple constrained resources: Internally rolling schedules with lot-sizing windows. Operations Research 51, 487–502.
- Suerie, C., Stadtler, H., 2003. The capacitated lot-sizing problem with linked lot sizes. Management Science 49, 1039–1054.
- Tempelmeier, H., Buschkühl, L., 2009. A heuristic for the dynamic multi-level capacitated lotsizing problem with linked lotsizes for general product structures. Or Spectrum 31, 385–404.
- Tempelmeier, H., Derstroff, M., 1996. A lagrangean-based heuristic for dynamic multilevel multiitem constrained lotsizing with setup times. Management Science 42, 738–757.