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Study of Different Formulations for the Multiperiod Blending Problem Applied to Lithium Recovery from Produced Water

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Abstract

Oil and gas production wastewater (i.e., produced water) may contain appreciable concentrations of rare-earth elements and critical minerals (REE/CMs), such as lithium, that can be recovered. However, each individual produced water source may have insufficient concentration or volume to meet the economic and operating requirements of the recovery facility. Therefore, there is the need to appropriately blend multiple sources to meet recovery and water reuse demands. Optimal stream mixing operation planning can be posed as a multiperiod blending problem (MPBP) to provide quantity and quality guarantees over time. We present several formulations to solve the MPBP for the recovery of REE/CMs from produced water and propose a decomposition approach that leverages strategies in general disjunctive programming to enhance its performance. We compare these proposed formulations/strategies via two illustrative case studies on recovering lithium from a network of produced water sources.

Keywords: Multiperiod Blending, Lithium Recovery, Mixed-Integer Nonlinear Programming, Decomposition

1. Introduction

Wastewater streams from oil and gas production (i.e., produced water) are expected to surpass 60 million barrels of water per day by 2030 in the U.S. alone (Wright, 2022). The treatment needed to mitigate the environmental impact of these wastewater streams is expensive due to high salinity and contaminant levels (Gaustad et al., 2021). Hence, a significant portion of produced water in the U.S. is simply disposed of via underground injection.

Notably, however, produced water sources may contain appreciable concentrations of critical minerals (CMs) such as lithium which are crucial for manufacturing electronics, pharmaceuticals, batteries, renewable energy generators, and more (Quillinan et al., 2018). Moreover, establishing a sustainable REE/CM supply chain is a critical concern of many industrial and governmental stakeholders. Thus, the recovery of REE/CMs from produced water has the potential to add sufficient economic value to incentivize the use of treatment technologies that mitigate the impact ofproduced water on the environment.

Operating a water network for the recovery of REE/CMs from multiple produced water sources is highly complex since REE/CM concentrations vary dynamically and geographically, there are limited storage locations, and treatment/recovery facilities have strict inlet-flow requirements (Gaustad et al., 2021). Such a system can be modeled as a classic multiperiod blending problem where source streams with time-varying compositions are blended in pooling tanks to satisfy quality and quantity demand requirements. Classic pooling formulations such as the one proposed in Haverly (1978) use bilinear terms to track compositions along the network. However, such formulations are often difficult to solve due to their inherent nonconvexity (Gounaris and Floudas, 2008). This difficulty is compounded by multiperiod models that incorporate binary variables.

In this work, we investigate several multiperiod blending problem (MPBP) formulations and solution strategies to optimally plan the delivery of lithium-rich streams for recovery and water reuse in development activities. In particular, we adapt the direct, generalized disjunctive programming, and decomposition MPBP approaches as described in Kolodziej et al. (2013) and Lotero et al. (2016) to a representative produced water network case study. It is shown that such strategies are key to guiding the treatment of a multi-enterprise produced water blending and determine whether such a system is feasible and economically viable.

2. Problem Formulation and Solution Strategies

2.1. Basic Problem Setup and Nomenclature

The multiperiod blending problem (MPBP) is defined over a set of supply tanks $\mathcal{S}$, blending tanks $\mathcal{B}$, and demand tanks $\mathcal{D}$ interconnected by a set of edges $\mathcal{A}$. The problem seeks to determine the optimal mixing schedule over a discretized time horizon $\mathcal{T}$ that maximizes the operation profit, while meeting flow and concentration specifications for each component $q \in \mathcal{Q}$. The initial conditions for each tank $n \in \mathcal{N} \coloneqq \mathcal{S} \cup \mathcal{B} \cup \mathcal{D}$ are specified via the initial level of every tank I_n^0 and its corresponding compositions C_{qn}^0. The incoming flow F_{st}^{IN} at each supply s is known with an incoming composition C_{qst}^{IN} that varies over t. The nodal inventories and flows are restricted by tank and pipeline capacities, which are denoted $[I_n^L, I_n^U]$ and $[F_{nn'}^L, F_{nn'}^U]$, respectively. Required demand varies with time and needs to satisfy specifications on the flow $[FD_{dt}^L, FD_{dt}^U]$ and concentration $[C_{qd}^L, C_{qd}^U]$. The MPBP formulations considered here assume that blending tanks do not operate at steady-state. Mixing requires that the tanks be charged at one period of time and discharged at another period (Lotero et al., 2016).

2.2. Direct MIQCP Formulation

We model the MPBP directly as a mixed-integer quadratically constrained program (MIQCP). The MIQCP formulation follows from extending steady-state pooling formulations to incorporate multiperiod scheduling. Here, binary variables $x_{nn't} \in \{0,1\}$ are introduced to indicate the existence of flow at each time period. This addition enables us to enforce a minimum flow in the pipeline, when the flow exists. We obtain the MIQCP formulation by adapting the formulation presented by Kolodziej et al. (2013) to handle time-varying concentration in the supply:

$$\max \quad \sum_{t \in \mathcal{T}} \left[\sum_{(n,d) \in \mathcal{A}} \beta_d^T F_{ndt} - \sum_{(s,n) \in \mathcal{A}} \beta_s^T F_{snt} - \sum_{(n,n') \in \mathcal{A}} \left(\alpha_{nn'}^N x_{nn't} + \beta_{nn'}^N F_{nn't} \right) \right] \tag{1a}$$

$$\text{s.t.} \quad F_{nn'}^L x_{nn't} \le F_{nn't} \le F_{nn'}^U x_{nn't}, \qquad (n,n') \in \mathcal{A}, t \in \mathcal{T} \tag{1b}$$

$$C_{qd}^L - M(1 - x_{bdt}) \le C_{qbt-1} \le C_{qd}^U + M(1 - x_{bdt}), \qquad q \in \mathcal{Q}, (b,d) \in \mathcal{A}, t \in \mathcal{T} \tag{1c}$$

$$C_{qd}^L - M(1 - x_{sdt}) \le C_{qst}^{IN} \le C_{qd}^U + M(1 - x_{sdt}), \qquad q \in \mathcal{Q}, (s,d) \in \mathcal{A}, t \in \mathcal{T} \tag{1d}$$

$$I_{st} = I_{st-1} + F_{st}^{IN} - \sum_{(s,n) \in \mathcal{A}} F_{snt}, \qquad s \in \mathcal{S}, t \in \mathcal{T} \tag{1e}$$

$$I_{bt} = I_{bt-1} + \sum_{(n,b) \in \mathcal{A}} F_{nbt} - \sum_{(b,n) \in \mathcal{A}} F_{bnt}, \qquad b \in \mathcal{B}, t \in \mathcal{T} \tag{1f}$$

$$I_{dt} = I_{dt-1} + \sum_{(n,d) \in \mathcal{A}} F_{ndt} - FD_{dt}, \qquad d \in \mathcal{D}, t \in \mathcal{T} \tag{1g}$$

$$x_{nbt} + x_{bn't} \le 1, \qquad (n,b), (b,n') \in \mathcal{A}, t \in \mathcal{T} \tag{1h}$$

$$I_{bt}C_{qbt} = I_{bt-1}C_{qbt-1} + \sum_{(s,b)\in\mathcal{A}} F_{sbt}C^{IN}_{qst} + \sum_{(b',b)\in\mathcal{A}} F_{b'bt}C_{qb't-1} - \sum_{(b,n)\in\mathcal{A}} F_{bnt}C_{qbt-1}, \quad q\in\mathcal{Q}, b\in\mathcal{B}, t\in\mathcal{T} \tag{1i}$$

$$I^L_n \le I_{nt} \le I^U_n, \quad n\in\mathcal{N}, t\in\mathcal{T} \tag{1j}$$

$$C^L_q \le C_{qbt} \le C^U_q, \quad q\in\mathcal{Q}, b\in\mathcal{B}, t\in\mathcal{T} \tag{1k}$$

$$FD^L_{dt} \le FD_{dt} \le FD^U_{dt}, \quad d\in\mathcal{D}, t\in\mathcal{T} \tag{1l}$$

$$F_{nn't} \ge 0, x_{nn't}\in\{0,1\}, \quad (n,n')\in\mathcal{A}, t\in\mathcal{T} \tag{1m}$$

Where β^T_d is the unit profit of demand d satisfied, β^T_s is the unit cost of supply stream s, $\beta^N_{nn'}$ is the unit transportation cost, $\alpha^N_{nn'}$ is the fixed transportation cost, F^{IN}_{st} is the incoming flow from supply tank s at time period t, $F_{nn't}$ is the flow between node n and node n' at time t, FD_{dt} is the flow directed to demand tank d at period t, and $M \in \mathbb{R}$ is a sufficiently large big-M constant. For simplicity in presentation, the edge set $\mathcal{A}$ can refer to a subset of edges depending on the indices being used where n refers to general nodes and s, b, and d refer to supply, blending, and demand nodes, respectively. The formulation allows flows to go directly from the supply to the demands without blending if and only if they meet the required specifications. Also note that Equation (1h) enforces that blending tanks cannot be charged, mixed, and discharged simultaneously. The key complicating factor of Problem (1) is that Equation (1i) involves bilinear terms.

2.3. Generalized Disjunctive Programming Formulation

Generalized disjunctive programming (GDP) is a framework for naturally posing mathematical programs that incorporate symbolic logic relationships between the variables (Grossmann and Trespalacios, 2013). In the MPBP, the bilinear mass balance shown in (1i) only needs to be considered when tanks are charging. Hence, this nonconvex equation can be omitted when a tank is discharging. Using GDP, we can define $Y_{bt} \in \{\text{True}, \text{False}\}$ to specify whether or not, at a given period, tank b is charging ($Y_{bt} = \text{True}$) or discharging ($Y_{bt} = \text{False}$). With this, we can replace Equation (1i) in Problem (1) with the following disjunction that accounts for the operational mode of the tank:

$$\begin{bmatrix} Y_{bt} \\ I_{bt} = I_{bt-1} + \sum_{(n,b)\in\mathcal{A}} F_{nbt} \\ I_{bt}C_{qbt} = I_{bt-1}C_{qbt-1} + \sum_{(s,b)\in\mathcal{A}} F_{sbt}C^{IN}_{qs} \\ + \sum_{(b',b)\in\mathcal{A}} F_{b'bt}C_{qb't-1}, \quad q\in\mathcal{Q} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{bt} \\ I_{bt} = I_{bt-1} - \sum_{(b,n)\in\mathcal{A}} F_{bnt} \\ C_{qbt} = C_{qbt-1}, \quad q\in\mathcal{Q} \end{bmatrix} \tag{2}$$

for each $b \in \mathcal{B}$ and $t \in \mathcal{T}$. Note that bilinear terms are only considered in the left disjunct. Also, the mass balances in both disjunctions have fewer terms since they leverage the tank operational mode to only consider active flows.

Formulation (1) has other constraints that enforce logical implications on variables, which are amenable for GDP reformulation. For instance, Equation (1b) activates the flow $F_{nn't}$ only if $x_{nn't} = 1$ during that period. Hence we can also redefine the flow existence as a Boolean variable $X_{nn't} \in \{\text{True}, \text{False}\}$ and rewrite Equation (1b) with the following disjunction:

$$\begin{bmatrix} X_{nbt} \\ F^L_{nb} \le F_{nbt} \le F^U_{nb} \end{bmatrix} \vee \begin{bmatrix} \neg X_{nbt} \\ F_{nbt} = 0 \end{bmatrix}, \quad (n,b)\in\mathcal{A}, t\in\mathcal{T}. \tag{3}$$

Equations (1c) and (1d) can be reformulated via similar GDP disjunctions. Moreover, Equation (1h) can be reformulated using GDP logical propositions:

$$X_{nbt} \Rightarrow Y_{bt}, \quad (n,b)\in\mathcal{A}, t\in\mathcal{T} \tag{4a}$$

$$X_{bnt} \Rightarrow \neg Y_{bt}, \quad (b,n)\in\mathcal{A}, t\in\mathcal{T} \tag{4b}$$

All these GDP equations are substituted into Formulation (1) to yield the GDP-based MPBP, which generalizes the GDP formulation proposed in (Lotero et al., 2016) to account for time-varying concentrations (prevalent in produced water constituents). Note that this formulation extends the one presented in (1) to account for the tank operating mode to yield fewer bilinearities after operating modes are determined.

2.4. GDP with Redundant Constraints (RC)

Typically, mixed-integer solvers employ continuous relaxations of the problem (by relaxing variable integrality) to iteratively obtain an optimal solution. Tight relaxations often provide high-quality solutions relative to the mixed-integer formulation, which can accelerate solver convergence. One way to tighten relaxations is to include additional constraints therefore redundant that provide no additional modeling information but further restrict the feasible region.

We derive redundant constraints for our GDP formulation by tracking component flow origins:

$$F_{nn't} = \sum_{r\in\mathcal{R}} \tilde{F}_{rnn't}, \quad (n,n') \in \mathcal{A}, t \in \mathcal{T} \tag{5a}$$

$$I_{bt} = \sum_{r\in\mathcal{R}} \tilde{I}_{rbt}, \quad b \in \mathcal{B}, t \in \mathcal{T} \tag{5b}$$

where $\mathcal{R} \coloneqq \mathcal{S} \cup \widehat{\mathcal{B}}$ is the set of possible initial origins, $\widehat{\mathcal{B}}$ is the set of blending tanks with nonzero initial inventory, and $\tilde{F}, \tilde{I}$, and $\widetilde{C^0}$ are the flows, inventories, and initial composition identified by origin, respectively. Following Lotero et al. (2016), we employ other redundant constraints to strengthen the GDP formulation, and we refer the reader to that work for more details and analysis on the tightness of the relaxation.

2.5. Two-Stage MILP-MIQCP Decomposition

We can pose a two-stage decomposition to the above GDP formulations for complex MPBPs that incur high computational cost. We define an upper-level problem that omits the bilinear species balances to obtain a linear formulation that provides an upper bound UB on the optimal solution and candidate operating states of Y_{bt}. Then we define a lower-level problem that fixes Y_{bt} in the full formulation to the values provided by the upper-level problem and removes the bilinear terms corresponding to idle/discharging tanks. When feasible, the lower-level problem provides a lower bound on the optimal solution. Integer cuts are added to the upper-level problem after each run of the lower-level problem as shown in (Lotero et al., 2016):

$$Z \leq -\left(UB - Z^i\right)\left(\sum_{b\in\mathcal{B},t\in\mathcal{T}|\hat{y}^i_{bt}=1} y_{bt} - \sum_{b\in\mathcal{B},t\in\mathcal{T}|\hat{y}^i_{bt}=0} y_{bt}\right) + \left(UB - Z^i\right)\left(\sum_{b\in\mathcal{B},t\in\mathcal{T}} \left(\hat{y}^i_{bt}\right) - 1\right) + UB, \quad i \in \mathcal{I}_O \tag{6a}$$

$$\sum_{b\in\mathcal{B},t\in\mathcal{T}|\hat{y}^i_{bt}=1} (1 - y_{bt}) + \sum_{b\in\mathcal{B},t\in\mathcal{T}|\hat{y}^i_{bt}=0} y_{bt} \geq 1, \quad i \in \mathcal{I}_F \tag{6b}$$

where Z is the objective of the upper-level problem, y_{bt} are the binary variables associated with Y_{bt}, $\hat{y}_{bt}$ are the fixed values of the tank modes at the i^{th} iteration, and $\mathcal{I}_O$ and $\mathcal{I}_\mathcal{F}$ contain the feasible and infeasible iteration indices, respectively. Here, Equation (6a) is added based on a feasible lower-level solution, and Equation (6b) is added based on infeasible solutions. Iterating between upper- and lower-level problems leads to convergence to a globally optimal solution of the MPBP. The gap of the decomposition is calculated between the upper and lower bounds (LB and UB) as shown in Equation (7) where ϵ is a small tolerance. A formal analysis is provided in (Lotero et al., 2016).

$$\text{Gap} = \frac{UB - LB}{LB + \varepsilon} \tag{7}$$

3. Case Study

We compare the formulations in Section 2 via two case studies focused on delivering a lithium rich stream from a network of produced water sources. Case 1 is a smaller system composed by a subset of the tanks considered in Case 2. Produced water with varied lithium concentrations is produced at different wells and a source of fresh water is available. Several demand nodes are considered with their respective schedules for feed quality and quantity. We choose parameters based on those reported by Dworzanowski (2019) and Figure 1 details the topology of Case 2.

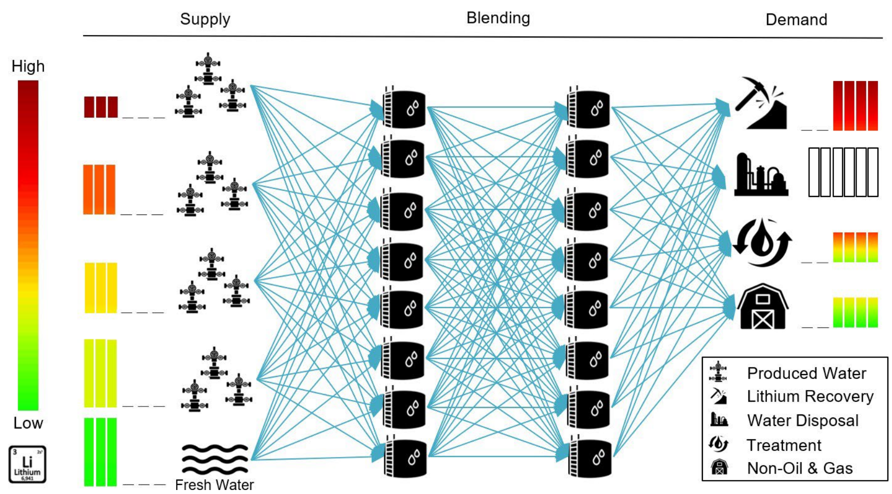

Figure 1: Topology of Case Study 2. Edges that connect sources with demands directly are considered in the case study but are not shown in the figure for simplicity.

GDP problems are often solved via big-M reformulation (BM) or Hull reformulation (HR) (Grossmann and Trespalacios, 2013; Lee and Grossmann, 2000). Previous work conducted by Lotero et al. (2016) and Ovalle Varela et al. (2021) only use BM reformulations. We explore solving these formulations using both BM and HR to study their impact on solution performance. We implement all approaches in Pyomo.GDP on a Linux machine with 8 Intel® Xeon® Gold 6234 CPUs running at 3.30 GHz with 128 hardware threads and 1 TB of RAM with Ubuntu. We use Gurobi v9.5.1 and BARON v22.7.23 as appropriate to solve all formulations. We impose a target optimality gap of 1% and 3% for case studies 1 and 2, respectively; moreover, we set a wall-time of 3600s.

Table 1: Approach comparison for the lithium recovery case studies

		Case 1		Case 2	
Upper-level	**Lower-level**	**Time [s]**	**Gap[%]**	**Time [s]**	**Gap[%]**
MIQCP	-	843.87	0.77	3,600	20.02
GDP (BM)	-	3,600	61.10	3,600	47.91
GDP (HR)	-	3,600	-	3,600	-
RC (BM)	-	69.05	1.00	3,600	26.33
RC (HR)	-	3,600	1.30	3,600	-
RC (BM)	RC (BM)	160.57	**0.03**	3,600	-
RC (HR)	RC (BM)	**12.54**	0.08	**54.1**	**1.08**

Table 1 shows the solution time and final optimality gap of each solution method and case study. The columns corresponding to the levels indicate the selected formulation and GDP reformulation (BM or CH) when applicable. Rows without an entry in the lower-level column are solved directly without the two-stage decomposition. Note that the two-stage decomposition using RC (BM) and RC (BM) was originally proposed by Lotero et al. (2016), and decomposition using RC (HR) and RC (BM) is proposed in this work. The results from Case 2 suggest that the monolithic formulations readily become intractable, which justifies the use of decomposition strategies. In fact, only our proposed decomposition is able to achieve an optimal solution for Case 2 within the wall-time. Hence, we observe that the choice of GDP reformulation strategy can significantly affect solution performance.

4. Conclusions

The multiperiod blending problem is a nonconvex mixed-integer quadratically constrained program that is challenging to solve for real life applications such as lithium recovery from produced water. We observe that the previous solution approaches considered in this work are extremely expensive computationally for this problem class. Moreover, our adaptation of the two-stage decomposition approach to use hull reformulations significantly enhances scalability. These results motivate further investigation into how combinations of possible formulations, GDP solution techniques, fixing strategies, and solver tunings can accelerate the convergence of the two-stage decomposition strategy considered in this work. Future work also includes integrating these formulations within the PARETO framework (Drouven et al., 2022) for REE-CM recovery extensions.

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