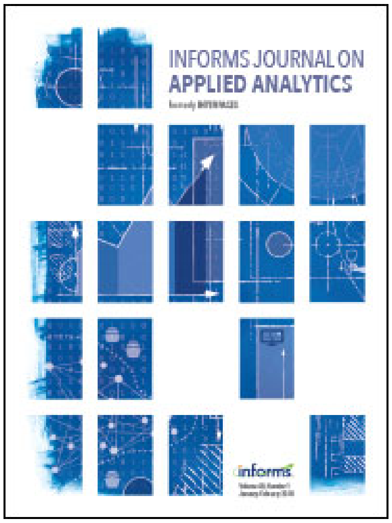

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ExxonMobil annually transports significant volumes of vacuum gas oil (VGO) from supply points in Europe to refineries in the United States. Optimizing these transportation costs by using modern mathematical programming technology can provide significant cost savings. We developed a mixed-integer programming formulation for VGO routing and inventory management, and we integrated it into a decision support tool to enable experienced traders and schedulers to further improve the performance of ExxonMobil's downstream supply chain.

Key words: inventory routing; maritime shipping; refinery feedstocks.
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ExxonMobil is an integrated petroleum and natural gas company operating in many countries. Its downstream affiliate companies provide clean fuels, lubricants, and high-value products and feedstocks through a global supply organization that optimizes both the supply of raw materials among its refineries and the supply of products to customers.

A refinery is a system of interconnected process units that transform crude oil into products for fuel and chemical markets. Some refineries also produce products, such as petrochemicals and lubricants, that other manufacturing plants use as raw materials. The first step in the refinery process is typically the separation of the complex mixture of hydrocarbons, i.e., crude oil, into fractions based on boiling-point temperatures using atmospheric distillation. Vacuum distillation is the process by which hydrocarbon mixtures with high boiling points are separated. The input to this process is residue or resid—the reduced crude from the bottom of the atmospheric distillation unit. The outputs of the vacuum distillation unit are gas oils and vacuum resid. In this paper, we consider the transportation of the vacuum gas oil (VGO) produced via this process.

VGO conversion processes include fluid catalytic cracking (FCC), hydrocracking, and thermal cracking. FCC is a conversion process used to crack large hydrocarbon molecules (primarily gas oils) into smaller, more useful molecules. The key outputs include light gases, gasoline blendstock, and cycle oils, which are later used to produce middle distillate fuels and fuel oil, with coke as a by-product. Hydrocracking is a higher-cost option that uses hydrogen to convert gas oils into light gases, naphthas, kerosene, and hydrocrackates. Thermal cracking, the lowest-cost option, converts vacuum resid and heavy gas oils into light gases, gasoline blendstocks, naphthas, lighter gas oils, and resid. Several introductory texts (Leffler 2008, Gary et al. 2007, Speight 2007) provide detailed overviews of refineries and refining processes and chemistry.

ExxonMobil Refining and Supply Company (R&S) has a Supply and Transportation (S&T) organization tasked with optimizing the allocation of bulk raw and intermediate feedstock petroleum products within ExxonMobil's global refining system. Efficiently using shipping vessels can lower transportation costs and substantially improve the effectiveness of the allocation effort. VGO, a primary feedstock used to manufacture gasoline, is actively traded in Europe and the United States. Arbitrage opportunities become available when the difference in VGO's value between the regions is greater than the prevailing shipping costs. This occurs because the demand for gasoline and the VGO used to produce it are greater in the United States than in other regions. Most of the 100 million barrels (approximately 15 million tons) of VGO that the United States imports each year come from or through Europe. ExxonMobil has an active program for transporting VGO from its European refineries to its US refineries that often includes chemical feedstocks and purchases from other suppliers. The program utilizes several sizes of shipping vessels and manages several grades of VGO, and it must operate within inventory and port constraints at both production and consumption facilities. In the academic literature, such inventory routing problems are known to be extremely challenging classes of optimization problems. For a recent review of inventory routing problems, see the section on inventory routing problems in Cordeau et al. (2007).

An integrated team of ExxonMobil research scientists and engineers, working jointly with R&S feedstock traders, developed a decision support tool to optimize the route scheduling of a bulk product from production locations to consumption locations while maintaining each location's inventory levels within capacity limits. This application considers very complex aspects of VGO inventory routing with the assumption that VGO is considered a single fungible product. As we discuss in Appendix B, it adds the optional capability to consider limited segregation of grades in the single-product model. The application significantly improves the analytical capability of traders and schedulers and yields both transportation cost savings and trading profit opportunities. Prior to implementing such analytical tools, ExxonMobil primarily performed the route scheduling using manual and spreadsheet calculations and analysis. The quality of the ship schedules developed was primarily a function of the feedstock trader's experience, skill, and available time.

In practice, ExxonMobil typically considers a shipping schedule for a range of 30 to 60 days of production rates and consumption requirements at several refineries in the United States and Europe. This typically requires chartering 5 to 10 voyages that use Panamax- and Aframax-class vessels (see Table 1). We define a voyage as a series of product loadings and subsequent discharges at various ports, and we consider a voyage to be finished when a ship has been completely emptied of its cargo. A decision support tool for optimizing the ship schedule while managing the inventory levels at the refineries may be run anywhere from a few times a week to several times per day depending on available volumes of VGO, the current state of the shipping market, and VGO values in both the United States and Europe. Usually after running and analyzing the model, ship chartering decisions are made for only the first few weeks of the time horizon, which leaves the flexibility to change the schedule and alter decisions further out into the future. Ships are typically chartered three weeks prior to loading, leading to using the tool to decide on the next ship to be chartered. Thus, the decision support tool is used in a somewhat rolling time-horizon fashion—perhaps approximating an infinite time-horizon model under uncertainty.

Although routing problems have been studied extensively in the open research literature, very little research addresses marine transportation problems. The comprehensive review of routing problems

Ship class	Maximum cargo	Part cargo minimum
Ultra-large crude carrier (ULCC)	420	350
Very large crude carrier (VLCC)	300	260
Suezmax	160	140
Aframax	80	75
Panamax	60	55
Handymax	30	25

Table 1: Typical ship size specifications are given in ktons (1 kton = 1,000 metric tons).

by Laporte and Osman (1995) cites over 500 references; however, only a few (Ronen 1983, 1993; Christiansen et al. 2004) focus on marine-vessel routing and scheduling problems. Christiansen et al. (2007) exhaustively review maritime transportation optimization research. However, marine-vessel transportation routing and logistics remains an open research area. The problem formulation we discuss in this paper shares many features of the models that Christiansen (1999) and Ronen (2002) propose. Christiansen (1999) considers the marine-inventory and time-constrained routing of bulk products and presents the complete formulation of the inventory pickup and delivery problem with time windows (IPDPTW) and a decomposition-based solution algorithm developed to manage the problem size. It involves a single bulk product and a heterogeneous pool of vessels. Unlike our work, Christiansen assumes fixed production and demand rates, thus permitting a continuous-time formulation that allows for a significant reduction in the size of the problem's mathematical formulation. She uses a simplified objective function that employs only fixed-leg costs. The port-visit time windows are determined based on a preprocessing procedure that considers the starting position of the vessels, routing information, inventory limits, and production and demand rates. Christiansen and Nygreen (1998a, b) develop methods for solving this problem using advanced decomposition and path-generation approaches. Ronen (2002) considers a multiproduct marine-inventory and time-constrained routing problem. Similar to our problem, the production and demands change daily, making it more natural to model in discrete time. The problem posed by Ronen (2002) also includes a more complicated objective function than the IPDPTW because it uses variable and fixed routing costs as well as penalties on inventory. However, unlike the problem we discuss, it allows only direct pickup to delivery routes. These assumptions can significantly limit the model's use in practice.

We pose a unique maritime inventory routing problem in which heterogeneous vessels are responsible for the transportation, production and consumption rates can change daily, multiple pickups and deliveries per vessel are allowed, and the objective function includes costs based on routes, timing, and load size.

Motivation and Development

Prior to the use of this tool at ExxonMobil, a primarily manual procedure by a single individual was used to schedule the voyages to transport VGO across the Atlantic. This scheduling involved the use of several customized spreadsheets and required that many individuals across the supply organization coordinate the sharing of information.

The combinatorial nature of the business problem and the special constraints and economic trade-offs related to factors such as draft (i.e., the depth of the ship below sea level) limits, port restrictions, vessel utilization, demurrage, and overage make manually generating an optimal schedule extremely complex. The dynamic nature of a constantly changing market places a premium on being able to quickly analyze new opportunities and provide decision support information for product trades and vessel chartering. Efficiently selecting vessels, shipping routes, and schedules heavily depends on user experience and skill.

Our goal in this project is to enhance the capabilities of the experienced ship schedulers by providing a decision support tool that can enhance the capabilities of an experienced ship scheduler by generating good, potentially nonintuitive, schedules quickly—not to create an application that replaces the schedulers. Such a tool can help a new scheduler to perform better while gaining invaluable experience; more importantly, it can enable experienced schedulers to easily verify the schedules generated and be able to devote substantially more time to analyzing other issues, thus significantly improving their performance.

R&S feedstock traders initially contacted ExxonMobil's research and engineering organization about developing a simulator to evaluate VGO's maritime routing and inventory management. After early discussions, it became evident that the business organization was interested in a decision support tool that uses optimization technology. This illustrates the common gap in the understanding of operations research that the business and technical organizations are trying to overcome.

A proof-of-concept application was developed to illustrate the potential for using mixed-integer programming technology to create a model of the business problem. During the discussion, development, and testing phases for the proof of concept, the research and engineering and S&T organizations formed an integrated team. The members from the research and engineering organization worked to understand the underlying business and operational aspects of transportation of refinery products and to educate members from the S&T organization about the potential use and current technological limits of optimization technology.

The team encountered several challenges. It took some time before the team determined that the objective posed in the model was unsuitable. The technical staff had initially assumed that the objective function would simply take the form of a cost minimization. Unfortunately, such an objective did not lead to solutions that were considered good by the business. After exploring penalties on inventory at the end of the scheduling time horizon, the team determined that since, in practice, the VGO shipping program is optimized on a cost-per-ton basis, the model should mimic this behavior. However, this cost-per-ton ratio could lead to a nonlinear objective and further complicate the model; therefore, the team applied a simple method to approximate this behavior (see Appendix D). In addition, efficiently solving the optimization model was more computationally difficult than initially anticipated and caused minor project delays. However, through teamwork, the researchers and engineers were able to work together to eventually achieve a viable model and solution method.

Problem Description

The objective of this optimization application is to find an optimal schedule for routing a heterogeneous pool of seagoing ships in the loading, transporting, and discharging of a single bulk product (i.e., VGO) to and from multiple ports and adhere to all inventory-related and port-specific capacities, constraints, and restrictions. This problem has the following characteristics:

- Production and demand projections that vary by day and by initial inventories;
- Minimum and maximum inventory constraints;
- A pool of heterogeneous vessels—both chartered and available for charter;
- Vessels that load and discharge at multiple ports;
- Both first-party (which must be managed, i.e., associated with ExxonMobil) and third-party (optional, i.e., non-ExxonMobil) supplies and ports;
- Complex transportation costs, including fixed-leg costs, variable overage rates, and demurrage rates; and
- Vessel size and draft limits for ports.

The problem's solution must determine the actual routes of specific vessels, the timing of each leg of a trip, and the quantities loaded and discharged. The overall planning horizon is determined based on the given production and demand profiles for each port, which are characterized by daily production or product consumption over some period. Careful consideration in the production and consumption data is needed to address the issue of the respective time horizons such that consumption can be met with production given known travel times between ports. In one VGO transportation example, all supply points are in Europe and all demand points are in the United States. The typical travel time for a transatlantic voyage is at least 17 days; thus, in practice, the consumption data must be offset by at least 17 days following the first day of production. Production and consumption horizons under consideration are generally the same length. In practice, product demand is often much greater than supply. If so, product consumption data are unavailable, and we assume that all product that can be physically discharged on a given day may be delivered—if other limits and constraints at the port are satisfied.

Several types of constraints and restrictions are imposed at each port. All ports have upper (and lower) limits on their inventory capacity in general or for specific days. They may also have general upper and lower limits on the amount of cargo that may be loaded or discharged and limits for a particular day. The inventory at each port is managed on a daily basis. Specific ships or general classes of ships may be restricted from visiting specific ports because of their size or other characteristics. Each port also has a limited number of berths available for different sizes or classes of ship. In the business case we present in this paper, only one ship per day may visit any given port. Draft limits play an interesting role in this optimization problem as they can affect the amount of product loaded onto ships or the order of ports visited. A ship's draft is a function of the amount of cargo loaded onto the ship. Clearly, ships with a draft greater than the port's maximum draft limit may not visit that port. Draft limits may be associated with a general class of ship or with specific ships at each port because the design and weight distribution of various ships can differ.

A heterogeneous (with respect to a ship's maximum cargo size, traveling speed, and parameters affecting its costs) pool of ships is used for transportation. After careful vetting of vessel, owner, and operator quality, vessels included as choices in our solution are primarily chosen from a pool of spot market ships of various classes available for hire. We do not consider long-term charter ships in our business case, and we hire all ships from the spot market; thus, we only hire ships to complete a single voyage. A ship is not typically loaded with product between discharges. In some cases, a ship will have been chartered prior to the optimization problem's time horizon, thus fixing its start date; however, its route can still be altered. In the VGO transportation-system case, Aframax- and Panamax-class ships are primarily hired. For our purposes, we assume that Aframax and Panamax ships travel at about the same cruising speed. Table 1 shows typical size specifications for various classes of ships used in the petroleum industry.

Based on port restrictions, user-defined rules, and other physical or geographic limits, a network of all possible transportation routes can be specified for each ship. The capability for a vessel to revisit a port multiple times is also allowed. The motivation to revisit a port is based on the possibility that a port inventory limit is lower than the cargo capacity of a ship, and thus a ship may load on some day, leave the port, and return to load again later after production increases inventory level. This concept presents significant challenges to solving our problem because it can substantially increase the combinatorial complexity.

Each possible travel leg has an associated distance, which can be converted into travel times between locations based on ship speed. Because of the precision of the data for the business problem, we discretize the time horizon into time intervals of one day and round travel times to integer values. We also assume that a ship may fully load or discharge in a single day; therefore, it can complete each port visit in one day. In some cases, restrictions are placed on the availability of a ship such that it can only be used within a specific time window. In addition, sometimes a port may not be permitted to be visited on specific dates or within specific date ranges.

The cost structure associated with ships hired from the spot market is a complex characteristic of the problem. Although the costs associated with long-term charter ships are based on fuel, staffing, and other fixed costs, spot market ship costs are based on the flat rates established by the Worldscale Association (2008). Shipping costs consist of three primary components—flat, overage, and demurrage—and are based on complete voyages. The cost for a voyage is the flat rate for a specific route multiplied by a Worldscale market rate multiplied by the part cargo minimum (PC) tons for the ship class. The Worldscale market rate is a negotiated multiplier used to adjust the annually updated flat rates based on current market conditions. Worldscale numbers vary based on ship class and the geographic regions that the ship visits. In our business case, we are interested only in Europe and the US Gulf Coast; therefore, the Worldscale numbers vary only based on ship class. However, they could vary among ships of the same class because of daily fluctuations in the shipping market. The flat rate is a cost per ton based on round-trip voyage distance, fuel-cost estimates, ship hire rates, and other factors. PC tons represent the minimum number of billable tons on a ship. For example, PC tons for an Aframax could be 80 ktons even though its maximum capacity is 90 ktons. The overage cost is based on the amount of cargo loaded onto a ship that exceeds the PC tons value. Overage costs apply to an entire voyage even if the ship exceeds the PC-ton value on only one leg of the voyage. Overage cost is calculated by multiplying the Worldscale number by the overage rate and highest cargo amount above the PC tons on the voyage.

Demurrage costs are based on waiting time. In this problem, demurrage time represents the time that a ship is idle, i.e., not traveling, loading, or discharging. For an already chartered ship, the first date from which to start consideration of demurrage is the date the charter begins. For ships to be chartered, the start date for consideration is the date of the first visit to a port. For all ships, consideration of demurrage ends after the final port visit. Because we approximate time by discretizing it into days, we can only estimate demurrage time. If a ship arrives, loads (or discharges), and immediately departs on the same day at all ports, its route includes no demurrage. Thus, we define demurrage time by subtracting the total travel time from the overall time of a ship's voyage. For example, consider a ship that travels from port A to port B and has a travel time of five days. If the ship arrives at port A on day 1, travels to port B, and departs from port B on day 6, the calculation that our demurrage definition specifies $(6-1-5=0)$ shows no demurrage days. Therefore, if the ship departs from port A on day 1 and does not depart from port B until after day 6, the voyage leg clearly has some waiting time.

In this section, we illustrate the concepts we have introduced by discussing examples of inventory profiles and a voyage. Figure 1 illustrates an inventory profile for two ports that produce VGO. It shows multiple loads by Pan1, a Panamax-size ship, and Afr1, an Aframax-size ship, and the dates the ships load VGO. Because the loads occur early in the period at each port, it takes some time for inventories to build up sufficiently for a second ship to load at each port. Table 2 illustrates a realistic voyage for Pan1, which is chartered for January 1; however, because its first load is on January 3, it waits for two days, thus incurring demurrage. If the ship is heavily loaded, it

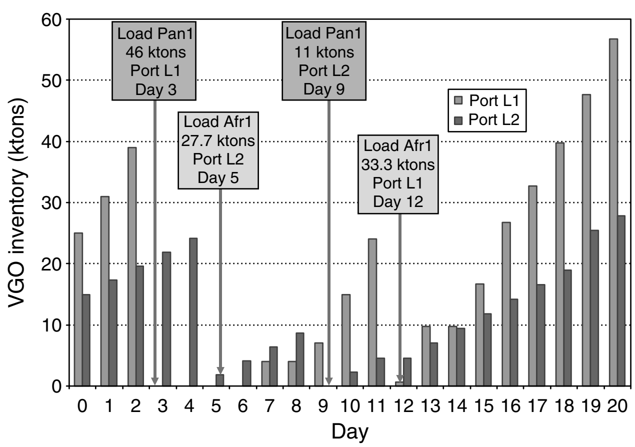

Figure 1: The inventory profiles for ports L1 and L2 are affected by ship loadings.

cannot enter the port because of L1's inlet draft limit of 30 ktons. After arriving at L2, Pan1 also waits at the port, allowing it to build up enough inventory to load 46 ktons. Pan1 does not leave D1 with more than 55 ktons because of D1's outlet draft limit. In addition, because of D2's inlet draft limit, Pan1 may not enter D2 with more than 50 ktons, essentially forcing the full ship to visit D1 prior to visiting D2 to offload some cargo to meet the draft limit. Pan1 spends 23 days traveling; therefore, we calculate the demurrage on this voyage as seven days $(31-1-23=7)$.

The flat cost is calculated by multiplying the Worldscale number by the flat rate by the PC tons for the entire voyage:

$$1.75 \times (1.9+11.1+1.2)\ (\$/\text{ton}) \times 55{,}000 \text{ tons}$$
$$= \$1{,}366{,}750.$$

The overage cost is calculated by multiplying the overage rate by the Worldscale number by the flat rate by the greatest overage amount on any particular leg of the voyage:

$$0.5 \times 1.75 \times (1.9+11.1+1.2)\ (\$/\text{ton}) \times 2{,}000 \text{ tons}$$
$$= \$24{,}850.$$

The demurage cost is calculated by multiplying the demurrage rate by the number of demurrage days:

$$\$24{,}000/\text{day} \times 7 \text{ days} = \$168{,}000.$$

In this example, the total voyage cost is $1,559,600. The costs for Aframax and Panamax voyages from Europe to the US Gulf Coast have historically ranged between $1.5 and $2.5 million in recent years.

In practice, a trader may impose other economic penalties and incentives, e.g., a hurdle for selecting certain vessel sizes. Inventory holding costs to adjust the balance of production-side and consumption-side inventory and encourage the use of first-party products over third-party products may be imposed. In addition, the opportunity to load or discharge cargo at third-party locations within some time window may arise, potentially improving the objective function when it is based on minimizing the cost per ton.

We define the objective of this problem as minimizing the total cost per ton of the product (VGO) transported. The costs are based on the flat, overage, and

Worldscale rate (Europe to the United States)	1.75
PC minimum (Europe to the United States)	55 ktons
Ship capacity	60 ktons
Overage rate	0.5
Demurrage rate	$24,000/day
Charter date	January 1

Travel schedule

Source port	Departure date	Destination port	Arrival date	Travel time	Flat rate leg approx.	Overage on leg
—	—	L1	January 1	n/a	n/a	0 ktons
L1	January 3	L2	January 6	3 days	1.9 $/ton	0 ktons
L2	January 9	D1	January 27	18 days	11.1 $/ton	2 ktons
D1	January 29	D2	January 31	2 days	1.2 $/ton	0 ktons

Load/Discharge schedule

Destination port	Load/discharge date	Load (discharge) quantity	Inlet ship inventory	Inlet draft limit	Outlet ship inventory	Outlet draft limit
L1	January 3	46 ktons	0 ktons	30 ktons	46 ktons	80 ktons
L2	January 9	11 ktons	46 ktons	100 ktons	57 ktons	100 ktons
D1	January 29	(7 ktons)	57 ktons	60 ktons	50 ktons	55 ktons
D2	January 31	(50 ktons)	50 ktons	50 ktons	0 ktons	50 ktons

Table 2: This schedule represents an example of a voyage for Panamax Pan1.

demurrage costs and other penalties and incentives. In other problems discussed in the academic literature, the objective is typically based directly on a profit maximization of revenue minus cost; however, our selection of objective function is limited because determining the true value of first-party intermediate refinery products at each location is sometimes difficult.

Problem Formulation

The mathematical model takes the form of a mixed-integer linear programming (MILP) problem that can potentially be solved by using specialized algorithms or general commercial optimization software such as XpressMP or CPLEX. In this paper, we present a complete mathematical programming formulation for the routing, transportation, scheduling, and inventory management of a single bulk product (i.e., VGO) with production and demand profiles that change daily. We use the following assumptions to develop the mathematical formulation:

- Inventories are based on the end-of-day volume.
- A vessel can only visit each port once on a given day (although it may revisit a port).
- A vessel is limited to one day at each port per load or discharge.
- A vessel cannot travel from a discharge port to a load port.
- Ports are classified as either load-only or discharge-only.
- Only one ship may visit a port on a given day (berth limit).

We refer the reader to Appendices A through D for a detailed mathematical description of the model.

Solution Methodology and Implementation

We implement the problem formulation in a mathematical programming language and use a simple solution strategy. After calling a commercial solver and running it for some given time, our solution method keeps the best solution and terminates the process. The user typically determines the termination criterion by checking to see that the objective value of the incumbent solution has stopped improving. In practice, the solution is obtained in 10 to 15 minutes or less on a standard desktop workstation; however, there is no guarantee that it will find the globally optimal solution. In most (but not all) cases, it finds the globally optimal solution. We have found that adding many optional constraints, valid inequalities, and heuristic preprocessing techniques improves the performance of commercial solvers.

In our original implementation, we used Microsoft Excel as the user interface, GAMS for the problem formulation, and ILOG CPLEX, the commercial solver, to search for solutions. We developed VBA scripts to convert the Excel data into a format that could be read into GAMS. In a more recent implementation, we again use Excel as the data interface; however, macros import the data into the AIMMS modeling platform in which the model is formulated. Figure 2 shows screenshots of this implementation, which also uses CPLEX as the solver.

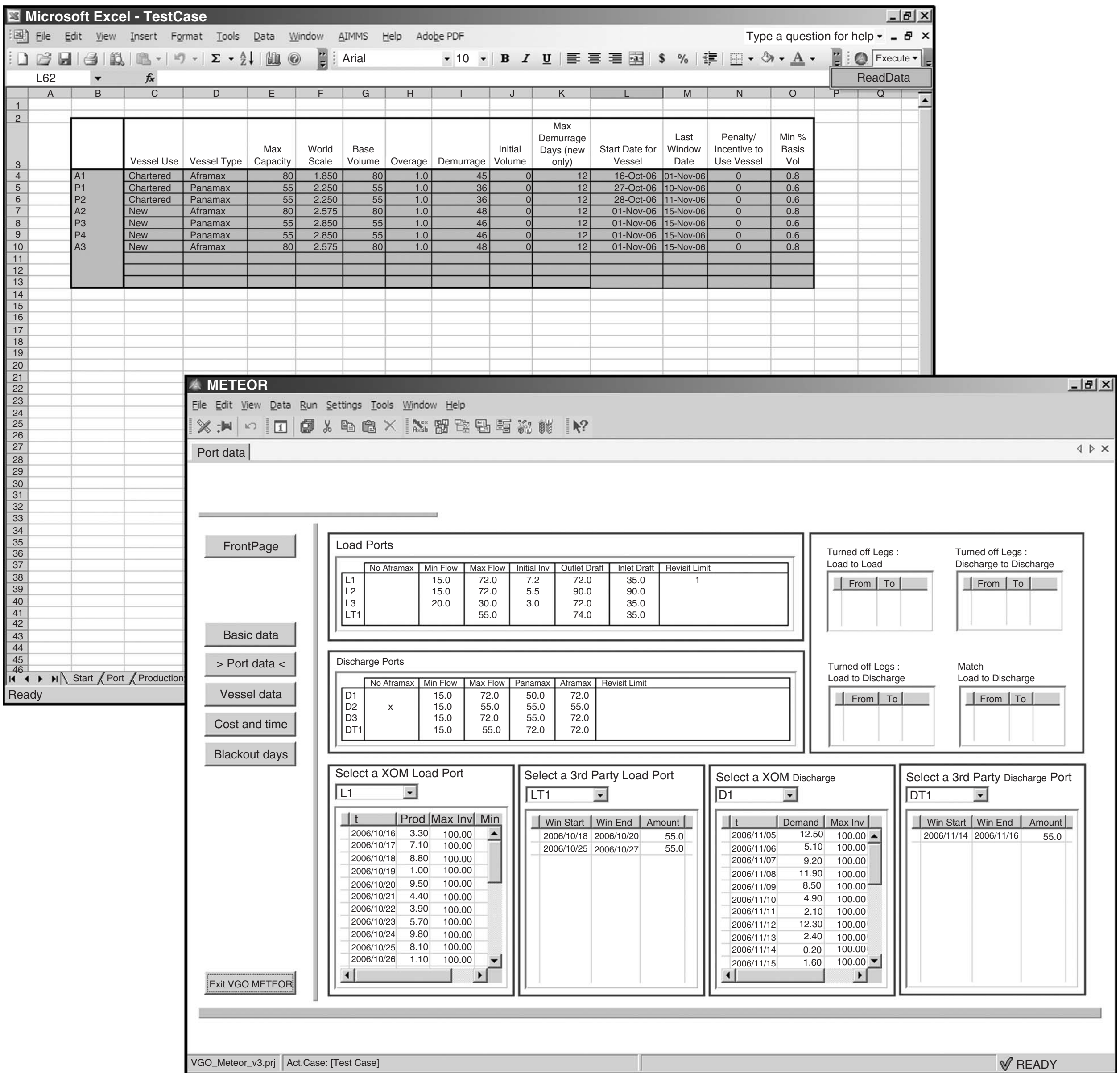

Figure 2: The graphical interface for the decision tool is implemented in Excel and AIMMS. Microsoft product screenshot reprinted with permission from Microsoft Corporation.

Impact

In a given year, ExxonMobil typically charters 60–70 ships to transport VGO from Europe to the United States. Transportation costs represent a substantial fraction relative to the value of VGO shipped. Introducing this decision support tool into the work process improved several key performance indicators; we list several indicators below and follow each with relevant factors.

Using shipping vessels more efficiently results in lower freight costs and reduced demurrage expense:

- Improved ship selection (i.e., Panamax versus Aframax);
- More optimal routing schedules, including the capability to look ahead and base the shipping program on a longer planning horizon;
- Higher utilization of vessel capacity;
- More accurate analysis of the trade-offs between waiting for the product to be produced versus dead freight (i.e., unused cargo capacity already paid) or visiting additional load ports;
- Decreased vessel waiting time at both load and discharge locations.

Feedstock traders are better able to manage inventories:

- Lower capital costs for holding inventory throughout the year;
- Attainment of inventory targets.

Feedstock traders are better able to adapt to a continuously changing environment:

- Optimization of previously chartered vessels to meet changed production and consumption plans;
- Adaptation of program to weather or operational delays.

Feedstock traders are better able to analyze and take advantage of short-notice trading opportunities:

- Purchase of third-party spot supplies;
- Leveraging of economies of scale resulting from a large transportation program.

Finally, incorporating other lines of business, e.g., chemicals feedstocks, into a common shipping program becomes possible.

The use of the tool has been described using a chess analogy as going from thinking 2 moves ahead to using a decision support tool to consider 12 moves ahead—essentially taking a proficient chess player to the master level. For example, in several instances a schedule that the tool generated seemed unreasonable to a feedstock trader because of a localized inefficiency such as an unusual amount of demurrage on a ship; however, after further review and analysis, the trader determined that the nonintuitive schedules created were accurate and economically attractive.

Using modern mathematical programming technology to optimize transportation costs permits substantial cost savings over previous methods. However, the incentives and credits realized are difficult to measure because we do not know how the program would have been structured without the optimization model. Based on conservative estimates, the annual transportation cost savings tend to range from 3 to 5 percent, in addition to significant benefits from trading opportunities.

Summary

Optimizing the transportation costs for routing intermediate refinery feedstocks from Europe to the United States using modern mathematical programming technology provides significant cost savings. We developed a novel mathematical programming formulation for VGO routing and inventory management. This model has several unique and complex characteristics that the literature does not typically discuss. The decision support system implementation uses spreadsheet and mathematical programming modeling platforms to enable experienced feedstock traders and schedulers to further improve the performance of ExxonMobil's downstream supply chain.

Current research and development efforts focus on expanding the system's capabilities. These efforts include exploring alternate mathematical formulations for improved performance using standard MILP solvers, developing sophisticated heuristics to reduce run times, and extending the system to consider multiple products for a marine shipping pool.

Appendix A. Nomenclature

Sets

G pairings of load ports to discharge ports for segregated product.

J all ports.

J^0 all original non-clone ports, $J^0 \subseteq J$.

J^3 all third-party ports, $J^3 \subseteq J$.
J^L all load ports, $J^L \subseteq J$.
J^D all discharge ports, $J^D \subseteq J$.
J^{LD} load ports with draft limits, $J^{LD} \subseteq J^L$.
J^{DD} discharge ports with draft limits, $J^{DD} \subseteq J^D$.
J_j^R all port clones for revisits of port j.
L^{JJ} allowed travel legs (jj') (edge set).
V all vessels.
V^{Chart} all previously chartered vessels, $V^{\text{Chart}} \subseteq V$.
T days (time intervals).

Indices

j port $j \in J$.
v vessel $v \in V$.
t day $t \in T$.

Parameters

B_v basis amount of product for vessel v.
$C_{jj'}$ flat rate for leg (jj').
C_v^{PEN} penalty cost or incentive for using vessel v.
D_{jt} product-lifting demand at port $j \in J^D$ on day t.
DW_v^{lim} demurrage days limit for vessel v.
DR_v demurrage rate of vessel v.
$\text{draft}_{vj}^{L,\text{in}}$ inlet draft limit of vessel v at loading port j.
$\text{draft}_{vj}^{L,\text{out}}$ outlet draft limit of vessel v at loading port j.
draft_{vj}^{D} inlet draft limit of vessel v at discharge port j.
$F_j^{\min}$ minimum flow rate at port j.
$F_j^{\max}$ maximum flow rate at port j.
I_j^0 initial inventory at port j.
$I_{jt}^{\min}$ minimum inventory at port j on day t.
$I_{jt}^{\max}$ maximum inventory at port j on day t.
$I_v^{V,\max}$ maximum amount of product on vessel v.
$\hat{I}_v^{V,\max}$ adjusted maximum volume of vessel v.
M minimum number of tons of product to be transported.
N^{LBV} lower bound on the number of vessels used.
N^{UBV} upper bound on the number of vessels used.
NT total number of days in time horizon.
OVR_v overage rate of vessel v.
pct_v minimum percent full PC tons for vessel v.
P_{jt} product amount produced at port $j \in I^L$ on day t.
$R^{\max}$ maximum cost-per-volume ratio.
T_v^{Chart} start day for demurrage calculation for chartered vessel $v \in V^{\text{Chart}}$.
$T_{jj'}$ minimum travel time for leg (j, j').
U maximum number of port stops plus legs in which both stops are in J^L or in J^D, $U \leq 2|J^L| + 2|J^D| - 2$.
WS_v Worldscale multiplier of vessel v.

Continuous Variables

DW_v demurrage days of vessel v.
f_{vjt}^L flow of product from load port j to vessel v on day t.
f_{vjt}^D flow of product from vessel v to discharge port j on day t.
$f_{vj}^{L,\text{tot}}$ total flow of product from load port j to vessel v.
$f_{vj}^{D,\text{tot}}$ total flow of product from vessel v to discharge port j.
first_v day vessel v starts its trip.
I_{jt} product inventory level at port j at end of day t.
I_{vt}^V product inventory level of vessel v at end of day t.
$I_v^{V,\text{tot}}$ total highest product inventory for vessel v.
last_v day vessel v finishes its trips.
OV_v overall overage volume of vessel v.
$OV_{vjj'}^{JJ}$ overage volume of vessel v on leg (jj').

Binary Variables

$h_v = 1$ if vessel $v \in V$ is used.
$u_{vjt} = 1$ if vessel v visits port j on day t.
$x_{vjj'} = 1$ if vessel v travels from port j to port j'.

Appendix B. Primary Constraints

The mathematical model takes the form of a MILP problem. We developed the model to minimize the number of discrete variables. Binary variables are introduced to represent (1) whether a ship visits a port on a particular day and (2) whether a ship traverses a leg from one port to another. We introduce a third auxiliary binary variable to represent whether a vessel is used at all.

The inventory of bulk product at each port at the end of each day is equal to the inventory at the end of the previous day adjusted by any amount loaded on or discharged from vessels plus any product production or consumption. However, for the unlimited demand case for discharge ports, we set the inventories equal to the total amount discharged from a vessel on a given day because complete information about the product demand is not always available. We consider constraints for the case in which the demand consumption information is known as well as an alternate formulation for the case that assumes virtually unlimited demand. Alternate discharge port inventory constraints do not consider the demand of first-party ports; they limit the daily discharge based on the port capacity.

One primary concern is the possible infeasibility of the problem for a given production and consumption schedule. Because the inventory constraints are equalities requiring all products listed in production to be transported or stored and all consumption requirements to be met, the minimum and maximum bounds on the product inventory at each site could limit the possibility of finding a feasible solution; however, the reason for that infeasibility might not be obvious from casual observation. To account for this limitation, slack variables can be introduced into the inventory constraints. We place penalty costs on these slack variables as part of the objective function to make them very unattractive. They allow the MILP solution method to terminate with a "feasible" solution in all cases. However, if the slack variables have a nonzero value, then the solution provided will not fully meet the production and consumption schedule. Their values also give the specific information about which production or consumption data are causing the infeasibility.

The port inventory constraints require adjustment to allow for multiple visits to a port by some vessel. This ability to revisit a port is only needed on an occasional or very limited basis. We handle this revisiting capability by cloning a port—we add virtual port nodes into the network and consider all clones in the same inventory balance for the original port that is cloned.

At third-party ports, some amount of product is made available during a specific time range and inventory is tracked for that amount. No product production or consumption occurs at these ports; moreover, the window of availability is typically more limited than at first-party ports. These ports are represented by the same constraints as first-party ports with the production and consumption parameters fixed to zero.

The port inventory balance constraint set follows.

$$I_{jt} = I_{j,t-1} + P_{jt} - D_{jt} - \sum_{v\in V} f^L_{vjt} - \sum_{v\in V}\sum_{j'\in J^R_j} f^L_{vj't} + \sum_{v\in V} f^D_{vjt} + \sum_{v\in V}\sum_{j'\in J^R_j} f^D_{vj't} \quad \forall\, j\in J^0,\ t\in T,$$

$$I_{j0} = I^0_j \quad \forall\, j \in J^0.$$

The alternate discharge port inventory balance constraint set that does not consider the demands of first-party ports follows.

$$I_{jt} = \sum_{v\in V} f^D_{vjt} + \sum_{v\in V}\sum_{j'\in J^{DR}_j} f^D_{vj't} \quad \forall\, j\in J^D,\ t\in T.$$

Ship inventory at the end of each day is equal to the inventory at the end of the previous day adjusted by loads or discharges by the ship. We assume initial inventories to be zero. We require all vessels in this problem to have zero product inventory by the last day of the time horizon to ensure that all product that is loaded is also discharged within the given planning horizon.

$$I^V_{vt} = I^V_{v,t-1} + \sum_{j\in J^L} f^L_{vjt} - \sum_{j\in J^D} f^D_{vjt} \quad \forall\, v\in V,\ t\in T,\ t<NT,$$

$$I^V_{v0} = 0 \quad \forall\, v\in V,$$

$$I^V_{v,NT} = 0 \quad \forall\, v\in V.$$

"Flow rate" constraints require that products transferred to or from a vessel are to be treated as semicontinuous; i.e., loads or discharges are either zero or have a minimum amount greater than or equal to a practical minimum. These constraints also enforce upper bounds on cargo load or discharge amounts.

$$F^{\min}_j u_{vjt} \le f^L_{vjt} \le F^{\max}_j u_{vjt} \quad \forall\, v\in V,\ j\in J^L,\ t\in T,$$

$$F^{\min}_j u_{vjt} \le f^D_{vjt} \le F^{\max}_j u_{vjt} \quad \forall\, v\in V,\ j\in J^D,\ t\in T.$$

A number of logic constraints are necessary to enforce the assumptions as well as link the binary variables associated with travel legs to those associated with time. Only one vessel may stop at a particular load or discharge port on any particular day.

$$\sum_{v\in V} u_{vjt} \le 1 \quad \forall J \in J,\ t\in T.$$

In our formulation, we allow each vessel to stop at a particular load or discharge port node only once, thus forcing the need for the "clone" ports mentioned above.

$$\sum_{t\in T} u_{vjt} \le 1 \quad \forall v\in V,\ j\in J.$$

A vessel may only be at one port on any particular day.

$$\sum_{j\in J} u_{vjt} \le 1 \quad \forall v\in V,\ t\in T.$$

If a vessel does not stop at some port, then it may not have any travel legs to or from that port. Thus, travel leg binaries are forced to zero whenever the port-stop binaries are zero.

$$\sum_{\substack{j'\in J\\ (jj')\in L^{JJ}}} x_{vjj'} \le \sum_{t\in T} u_{vjt} \quad \forall v\in V,\ j\in J,$$

$$\sum_{\substack{j'\in J\\ (j'j)\in L^{JJ}}} x_{vj'j} \le \sum_{t\in T} u_{vjt} \quad \forall v\in V,\ j\in J.$$

Because we assume that no vessel will travel from a discharge port back to a load port, we infer that a vessel may only take one leg that goes from a load port to a discharge port. This assumption might not apply in other transportation scenarios.

$$\sum_{\substack{(jj')\in L^{JJ}\\ j\in J^L,\ j'\in J^D}} x_{vjj'} \le 1 \quad \forall v\in V.$$

Additional constraints ensure the following. If a vessel stops at a load port, then a travel leg for leaving the port exists; if a vessel stops at a discharge port, then a travel leg for entering the port exists; and a vessel may only stop at ports and travel between them if a load-to-discharge leg in the voyage exists.

$$\sum_{\substack{(jj')\in L^{JJ}\\ j\in J^L}} x_{vjj'} = \sum_{j\in J^L}\sum_{t\in T} u_{vjt} \quad \forall v\in V,$$

$$\sum_{\substack{(jj')\in L^{JJ}\\ j'\in J^D}} x_{vjj'} = \sum_{j\in J^D}\sum_{t\in T} u_{vjt} \quad \forall v\in V,$$

$$\sum_{j\in J}\sum_{t\in T} u_{vjt} + \sum_{\substack{(jj')\in L^{JJ}\\ j,\,j'\in J^L}} x_{vjj'} + \sum_{\substack{(jj')\in L^{JJ}\\ j,\,j'\in J^D}} x_{vjj'} \le Uh_v \quad \forall v\in V.$$

The constraints ensuring that travel times remain feasible are only activated if two ports are in a vessel's voyage and direct travel between the two ports is part of the ship's voyage.

$$\sum_{\substack{t'\in T\\ t'\ge t+T_{jj'}}} u_{vj't'} \ge 1-(2-u_{vjt}-x_{vjj'}) \quad \forall v\in V,\ (jj')\in L^{JJ},\ t\in T.$$

The draft constraints limit the total load a vessel may contain when it resides in a port that has a limiting water depth. These constraints are enforced both before (port inlet) and after (port outlet) loading has been completed and before discharge has begun. Draft limits are both port- and vessel-specific.

$$I^V_{v,\,t-1} \le \mathrm{draft}^{L,\,\mathrm{in}}_{vj} + (I^{V,\,\max}_v - \mathrm{draft}^{L,\,\mathrm{in}}_{vj})(1-u_{vjt}) \quad \forall v\in V,\ j\in J^{LD},\ t\in T,$$

$$I^V_{vt} \le \mathrm{draft}^{L,\,\mathrm{out}}_{vj} + (I^{V,\,\max}_v - \mathrm{draft}^{L,\,\mathrm{out}}_{vj})(1-u_{vjt}) \quad \forall v\in V,\ j\in J^{LD},\ t\in T,$$

$$I^V_{v,\,t-1} \le \mathrm{draft}^{D}_{vj} + (I^{V,\,\max}_v - \mathrm{draft}^{D}_{vj})(1-u_{vjt}) \quad \forall v\in V,\ j\in J^{DD},\ t\in T.$$

A slightly alternate form may be used for the draft limits on discharge ports.

$$I^V_{vt} + f^D_{vjt} \le \mathrm{draft}^{D}_{vj} + (I^{V,\,\max}_v - \mathrm{draft}^{D}_{vj})(1-u_{vjt}) \quad \forall v\in V,\ j\in J^{DD},\ t\in T.$$

We use overage constraints to calculate the total load volume and overage tonnage (tons above PC tons) for any given vessel on any given leg of its voyage. If any leg of a vessel's voyage incurs overage, the overage rates apply to all legs of that voyage.

$$OV_v \ge I^V_{vt} - B_v \quad \forall v\in V,\ t\in T, \tag{B1}$$

$$OV_v \le \hat{I}^{V,\,\max}_v \sum_{\substack{(jj')\in L^{JJ}\\ j\in J^L,\ j'\in J^D}} x_{vjj'} \quad \forall v\in V, \tag{B2}$$

$$OV^{JJ}_{vjj'} \ge OV_v - (\hat{I}^{V,\,\max}_v - B_v)(1-x_{vjj'}) \quad \forall v\in V,\ (jj')\in L^{JJ}. \tag{B3}$$

In this model, the approximate number of demurrage days for a particular vessel's voyage is calculated based on the first and last days of the voyage and considers the travel times for each leg; however, we should note that in practice, demurrage is based on the amount of time the vessel exceeds the allowed time in port as agreed in the contract.

$$\text{first}_v \le t + NT(1-u_{vjt}) \quad \forall v \in V,\ u \in J^L,\ t \in T, \tag{B4}$$

$$\text{last}_v \ge t - NT(1-u_{vjt}) \quad \forall v \in V,\ j \in J^D,\ t \in T, \tag{B5}$$

$$DW_v = \text{last}_v - \text{first}_v - \sum_{(jj')\in L^{JJ}} x_{vjj'} T_{jj'} \quad \forall v \in V. \tag{B6}$$

In the alternate scenario in which demand is assumed to be unlimited at the discharge ports, the number of demurrage days for a particular vessel's voyage is calculated based only on the first and last day of loading, and the equations below replace Equations (B5) and (B6).

$$\text{last}_v \ge t - NT(1-u_{vjt}) \quad \forall v \in V,\ j \in J^L,\ t \in T,$$

$$DW_v = \text{last}_v - \text{first}_v - \sum_{\substack{(jj')\in L^{JJ}\\ j,\, j'\in J^L}} x_{vjj'} T_{jj'} \quad \forall v \in V.$$

A binary variable h_v is added to the formulation to represent whether or not a vessel is used. Previously chartered vessels are vessels that have already been hired and therefore must be used; however, their voyage remains unspecified. Because chartered vessels have already been hired, the demurrage calculation start date is known.

$$h_v = \sum_{\substack{jj'\in L^{JJ}\\ j\in J^L,\, j\in J^D}} x_{vjj'} \quad \forall v \in V,$$

$$h_v \in \{0, 1\} \quad \forall v \in V,$$

$$\sum_{t\in T}\sum_{j\in J} u_{vjt} \ge 1 \quad \forall v \in V^{\text{Chart}},$$

$$\text{first}_v = T_v^{\text{Chart}} \quad \forall v \in V^{\text{Chart}}.$$

Some valid inequalities are applied as an attempt to tighten the linear programming relaxation.

$$I_v^{V,\,\text{tot}} = \sum_{j\in J^L}\sum_{t\in T} f_{vjt}^L \quad \forall v \in V,$$

$$I_v^{V,\,\text{tot}} \le h_v \hat{I}^{V,\,\max} \quad \forall v \in V,$$

$$0 \le I_v^{V,\,\text{tot}} \le \hat{I}^{V,\,\max} \quad \forall v \in V.$$

Several constraints are optional and may be included in the model at the user's discretion. These optional constraints may be added when the user wants to impose additional restrictions on the solutions that are provided. VGO grade-segregation constraints allow for specifying that all products loaded at some particular subset of load ports on a vessel must be discharged at a specific discharge port. Using these constraints, multiple grades or products may be considered in this single-product model—at least to some limited extent.

$$f_{vj}^{L,\,\text{tot}} = \sum_{t\in T} f_{vit}^L \quad \forall v \in V,\ j \in J^L,$$

$$f_{vj}^{D,\,\text{tot}} = \sum_{t\in T} f_{vjt}^D \quad \forall v \in V,\ j \in J^D,$$

$$\sum_{\substack{j'\in J^L\\ (j'j)\in G}} f_{vj'}^{L,\,\text{tot}} = f_{vj}^{D,\,\text{tot}} \quad \forall v \in V,\ j \in J,$$

$$0 \le f_{vj}^{L,\,\text{tot}} \le \hat{I}_v^{V,\,\max} \quad \forall v \in V,\ i \in I,$$

$$0 \le f_{vj}^{D,\,\text{tot}} \le \hat{I}_v^{V,\,\max} \quad \forall v \in V,\ j \in J.$$

Limits on the minimum and maximum number of ships to hire are achieved through bounds on the number of ships used.

$$N^{LBV} \le \sum_{v\in V} h_v \le N^{UBV}.$$

Another constraint may set a minimum percent total loading for any newly hired or previously chartered vessels used.

$$\sum_{j\in J^L}\sum_{t\in T} f_{vjt}^L \ge \text{pct}_v B_v h_v \quad \forall v \in V.$$

A minimum amount of product transported in the time horizon may be specified.

$$\sum_{v\in V}\sum_{j\in J^L}\sum_{t\in T} f_{vjt}^L \ge M.$$

A maximum cost-per-ton ratio may also be optionally specified.

$$\begin{aligned} R^{\max}\sum_{v\in V}\sum_{j\in J^L}\sum_{t\in T} f_{vjt}^L \ge{} & \sum_{v\in V} B_v WS_v \sum_{(jj')\in L^{JJ}} C_{jj'} x_{vjj'} \\ & + \sum_{v\in V} OVR_v WS_v \sum_{(jj')\in L^{JJ}} \cdot C_{jj'} OV_{vjj'}^{JJ} \\ & + \sum_{v\in V} DR_v DW_v. \end{aligned}$$

Many other additional optional restrictions can be applied in practice to reduce the size of problem instances before solving the problem, which can reduce computational run times. Examples of manually adjustable options include port blackout days, windows of availability for ships, requirements for use of specific ships, restrictions on specific ships at specific ports, and disallowed legs of travel. These do not typically require new constraints; they simply restrict the domain range for the decision variables.

Capacity constraints and general bounds follow.

$$
\begin{gathered}
I_{jt}^{\min} \le I_{jt} \le I_{jt}^{\max} \quad \forall j \in J^0,\ t \in T,\\
0 \le I_{vt}^{V} \le I_{v}^{V,\max} \quad \forall v \in V,\ t \in T,\\
0 \le f_{vjt}^{L} \le F_{j}^{\max} \quad \forall v \in V,\ j \in J^L,\ t \in T,\\
0 \le f_{vjt}^{D} \le F_{j}^{\max} \quad \forall v \in V,\ j \in J^D,\ t \in T,\\
0 \le \mathrm{first}_v \le NT \quad \forall v \in V,\\
0 \le \mathrm{last}_v \le NT \quad \forall v \in V,\\
0 \le OV_v \le \hat{I}^{V,\max} - B_v \quad \forall v \in V,\\
0 \le OV_{vjj}^{JJ} \le \hat{I}^{V,\max} - B_v \quad \forall v \in V,\ (jj') \in L^{JJ},\\
0 \le DW_v \le DW_v^{\lim} \quad \forall v \in V.
\end{gathered}
$$

Appendix C. Symmetry Breaking

Port Revisit Order and Timing Constraints

Symmetry-breaking constraints based on revisit order and timing can be added to the mathematical model. A visitation-order constraint ensures that original ports must be visited before a clone port is visited and that clone ports are prioritized based on the order of elements in the set.

$$
\begin{gathered}
\sum_{t\in T} u_{vjt} \ge \sum_{t\in T} u_{vj't} \quad \forall v \in V,\ j \in J^0,\ j' \in J_j^R,\\
\sum_{t\in T} u_{vj't} \ge \sum_{t\in T} u_{vj''t} \quad \forall v \in V,\ j \in J^0,\ j' \in J_j^R,\ j'' \in J_j^R,\ j' < j''.
\end{gathered}
$$

The timing of the visitation constraint requires that original ports are chronologically visited before clone ports and that clone ports are prioritized chronologically by the order of elements in the set.

$$
\sum_{\substack{t'\in T\\ t'\le t}} u_{vjt'} \ge \sum_{\substack{t''\in T\\ t''\le t}} u_{vj't''} \quad \forall v \in V,\ j \in J^0,\ j' \in J_j^R,\ t \in T,
$$

$$
\sum_{\substack{t'\in T\\ t'\le t}} u_{vj't'} \ge \sum_{\substack{t''\in T\\ t''\le t}} u_{vj''t''}
\qquad \forall v \in V,\ j \in J^0,\ j' \in J_j^R,\ j'' \in J_j^R,\ j' < j'',\ t \in T.
$$

Removing Redundant Legs When Revisiting Ports

To prevent redundant binary variables and to break symmetry and cycles, various pairs of port-to-port legs can be removed when allowing ports to be revisited and thus "cloned" in the model. The constraints described in this section can potentially conflict with the constraints described above.

The following legs are not generally allowed in the leg set L^{JJ}:

$$\{(j'j) \mid j \in J^0,\ j' \in J_j^R\}.$$

Under the more limiting assumption, which is typical in practice, in which port revisits may only occur directly from the same port, the following legs may alternatively be removed.

$$\left\{ (j'j) \mid j \in J,\ j' \in \bigcup_{\substack{j''\in J^0\\ j''\ne j}} J_{j''}^R \right\}.$$

In addition, when a port has multiple clones, the following legs are removed.

$$
\begin{gathered}
\{(j''j') \mid j \in J^0,\ j' \in J_j^R,\ j'' \in J_j^R,\ j' > j''\},\\
\{(j''j) \mid j \in J^0,\ j'' \in J_j^R,\ \exists j' \in J_j^R \text{ s.t. } j' < j''\}.
\end{gathered}
$$

Appendix D. Objective Function

The total transportation cost is a combination of voyage flat rate calculated based on legs traveled, the overage penalties, demurrage penalties, and optional penalties and incentives that the user can impose for costs associated with usage of various ships. If the objective function were to be set simply as minimizing transportation costs with potentially additional inventory holding penalties, problem solutions would result in boundary effects such that inventory levels are left at either maximum or minimum levels at the end of the time horizon.

The ideal objective function as per our analysis and the users' request is to minimize the total cost per ton of products transported, thus avoiding the boundary effect problems; however, it results in a nonconvex nonlinear objective function. To maintain the linearity of the problem, we approximate this cost-per-ton ratio in the objective. It is modeled as the total cost minus a weighting parameter multiplied by the total product amount transported. Theoretically speaking, if we set the weighting parameter to the optimal cost per ton, assuming it is known before trying to solve the problem computationally, the solution to the MILP problem should be exactly equivalent to the solution using the ideal nonconvex cost-per-ton function as the objective. When the weighting parameter is set to an approximate value for the optimal cost-per-ton ratio, the "true" optimal solution is likely to be achieved with this heuristic objective. The choice of this parameter relies on the business experience of the user to estimate an expected optimal cost per ton. The objective function could also be treated as a netback (revenue minus transportation costs) if some way to estimate arbitrage for the product is available.

As previously mentioned, the Worldscale number is typically a function of the regions of the world in which a ship travels during a voyage. In this formulation, we assume that this number is a fixed parameter. This assumption is reasonable for our business case because we are considering only two geographic regions, Europe and the US Gulf Coast. In reality, flat rates are based on a complete round-trip voyage. However, experience has shown us that in many practical cases, these can be accurately approximated based on decomposing the flat rate into additive components per leg of a voyage.

The objective function can be posed in a number of ways. The following is only one example of a function used in practice:

$$\begin{aligned}\min \sum_{v\in V} B_v WS_v \sum_{(jj')\in L^{JJ}} C_{jj'} x_{vjj'} \\ + \sum_{v\in V} OVR_v WS_v \sum_{(jj')\in L^{JJ}} C_{jj'} OV_{vjj'}^{JJ} \\ + \sum_{v\in V} DR_v DW_v - \eta \sum_{v\in V}\sum_{j\in J}\sum_{t\in T} f_{vjt}^{L} + \sum_{v\in V} C_v^{\text{PEN}} h_v.\end{aligned}$$

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Janice K. Kane, Global Manager – LPG/Feedstocks, Commercial Trading, ExxonMobil Sales and Supply LLC, 3225 Gallows Road, Fairfax, VA 22037, writes: "We have implemented a feedstocks transportation routing and inventory management model (METEOR), developed by ExxonMobil Research and Engineering (EMRE). Although incentives and credits are difficult to capture, conservative analyses consistently indicate about 3%–5% annual transportation cost savings and significant benefits from trading opportunities."