Global Hydrocarbon Supply Model

Petroleum Refining Component Design Report

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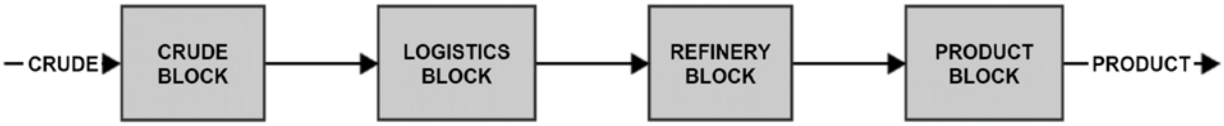
Executive Summary

The Office of Petroleum, Natural Gas, and Biofuels Analysis (PNGBA) of the EIA has been tasked to develop a dynamic representation (referred to here as *Global Hydrocarbon Supply Model*, *GHySMo*) of the global production, processing, transportation, distribution, and storage of natural gas and liquid fuels. The EIA suggests breaking GHySMo into sub-modules for 1) upstream oil and gas production operations; 2) logistics for transportation of primarily natural gas, crude oil, and petroleum products; and 3) transformational processes such as in refineries. The focus of this Component Design Report (CDR) is on Refining, which represents the conversion of crude oil into petroleum products.

The primary objective of the Petroleum Refining Component sub-module is to provide a reasonable representation of the world refining industry. The CDR discusses critical "Blocks" associated with the Refining model. Emphasis is placed on balancing model sophistication between the interactions of these Blocks with stakeholder objectives.



The Refining CDR will be viewed with consideration for the other sub-models, and the recommendations in this CDR will ultimately be recalibrated with the other sub-models for consistency in approach, design, and operations.

Key recommendations include the following:

- The refining model platform should be acquired commercially.
- Aggregating the World into approximately 30 regions and 15 crudes is reasonable.
- Defining clean products as either high or low quality for each unique region will facilitate modeling, while incorporating primary and secondary specifications.
- Crude production can be aggregated into Terminal Blocks, for downstream distribution.
- Regional Terminals will balance supply and demand every refining stream
- Product movements (imports and exports) are transported to and from terminals.
- Consideration should be given to developing a more inclusive Economics, Refining, and Logistics block which would rely on exogenous inputs from technical Refining LP results.
- "Robust" process technology is required for the refining process units to achieve stated objectives, including sulfur, weight, energy, volume, and emissions balances.
- Maintaining a balance of reasonableness with sophistication will form the foundation for a word-class global refining model.

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1. Introduction

The Office of Petroleum, Natural Gas, and Biofuels Analysis (PNGBA) of the EIA has been tasked to develop a dynamic representation (referred to here as *Global Hydrocarbon Supply Model*, *GHySMo*) of the global production, processing, transportation, distribution, and storage of natural gas and liquid fuels. The ultimate purpose of this project is to improve the EIA's capability to represent international markets for liquids and natural gas under a variety of assumptions. The primary function of the model will be to replace the existing upstream and midstream models of petroleum and natural gas within the World Energy Projection System Plus (WEPS+). GHySMo or its results will allow for a consistent international representation of the gas and liquids markets to be incorporated within the EIA's National Energy Modeling System (NEMS).

A secondary function of GHySMo is to operate in a standalone fashion to enable the targeted use of greater levels of detail to support certain topical analyses that may not critically depend on dynamic feedback from outside the liquids and gas markets. It is envisioned that a standalone GHySMo would be used to perform such analyses as deep-dive analyses of specific countries or World regions.

The EIA would like GHySMo to be broken into sub-modules to facilitate testing, maintenance, and model administration. As a starting point, the EIA suggests sub-modules for 1) upstream oil and gas production operations, including natural gas processing; 2) logistics for transportation of primarily natural gas, crude oil, and petroleum products; and 3) transformational processes such as in refineries.

The downstream representation will primarily include representations of petroleum refinery processing and the transportation of crude oil from production regions to refinery regions, and the transport of petroleum products from refinery regions to demand regions. GHySMo will include a mechanism for balancing supply and demand for each of the liquid products.

The focus of this CDR is on Refining, which represents the conversion of crude oil into petroleum products. The Refining process includes numerous processing steps to achieve this transformation, which will be discussed, but a more comprehensive approach is required. The Refining process requires crude input information including crude types and source of origin. The Refining process also produces products for consumption. The crude input, refinery processing, and product output must be balanced for all the regions of the World defined in the model. For all regions, every feed and product stream will balance on production, imports, consumption, and exports.

2. Methodology Overview

Model Objective

The primary objective of the Petroleum Refining Component sub-module is to provide a reasonable representation of the World refining industry. However, the definition of "reasonable" is wide, depending on an individual stakeholder's needs. Underneath the primary objective are layers of secondary objectives such as appropriate crude strategies, refining representations, product accounting, and country aggregating methods to name a few

This CDR will examine these secondary objectives, and make recommendations on their design strategies in order to fulfill the primary objective of developing a reasonable representation of the World refining industry.

The CDR recommendations will maintain the following fundamental design principles:

Flexibility

The model should be capable of converting to either higher or lower fidelity country analysis, as well as adding supplementary levels of technology, products, specifications, or crude types. A flexible model will require some degree of programming and analytical effort, but not a major "overhaul" of code.

The model will be developed with an "Evergreen" framework, since stagnant models quickly become undesirable and obsolete. As the hydrocarbon World changes (e.g., the technologies, specifications, geopolitics), so should the model. In the United States, the refinery models have had significant structural upgrades to better represent the changing refining requirements, such as:

- Reformulated Gasoline (Simple and Complex Model Phase 1 & 2),
- MSAT2,
- MTBE Ban,
- Renewable Fuel Standards (RFS),
- Ultra-Low-Sulfur Diesel (ULSD), and
- Low-Sulfur Gasoline Tier 1 & 2.

Long-term maintenance will improve if the developers have the foresight into future significant impacts to be analyzed with modeling efforts. Greenhouse gas emission predictions is an example where many existing models have limited capabilities, but is foreseen to be goal.

Robustness

In modeling vernacular, “robust” refers to specific characteristics in the model's structure that allow for a more thorough analysis that would otherwise be limited using more simplified techniques. As an example, a simplified FCC yield could have a low conversion mode making 55 percent gasoline and a high mode making 65 percent, without any adjustments for the feed quality, which do impact conversion. By adding feed quality adjustments, the model will make better yield predictions as a function of feed quality. Feed quality will change in the model because of the different crude types supplying the World.

There are some situations in modeling where the “Fixed Yield" or "Black Box” structure might be warranted. As will be emphasized throughout this report, a balance must be maintained between “robustness” and other model objectives.

Usability

Since a World Model will be complex, significant consideration to model design and usability is required. Organizationally, there are different types of model “users,” including:

- Model designers and developers who lay out the conceptual model requirements,
- Model programmers who transform conceptual design into a model,
- Data collection and maintenance specialists,
- Model analysts or “runners," and
- End-users who take model results for further analysis.

The model design should consider the organizational roles and responsibilities for model performance. Performance can mean many things, from speed of model, ease of data collection and pass-through, convergence and infeasibility analysis, or output results for end-user analysis.

Complex, sophisticated, and robust models have questionable long-term value if only a few people in the organization can work, modify, run, or analyze them. If the usability is so challenging that the EIA must always rely on outside expertise for minor adjustments, the design has failed.

Switches

A switch is a programming feature that can turn options on and off. For example, switches can:

- activate or turn off a country or region,
- activate or turn off a quality specification or product,

- activate or turn off a specific season, and
- allow a crude to a terminal or prevent the flow.

A switch will often prevent the data formulation from entering into the matrix code, and is fundamental to the design strategy and routinely used in refining planning models. These switches are fundamental to the World Model design. In one mode, the model can run summer and winter, and a switch can allow a single period run. Equally important is the developers adding the specifications for summer, winter, and average seasons in anticipation of these modes.

Rationale and Reasoning

This CDR attempts to provide rationale behind the recommendations. The World Model is a very important yet ambitious project. The stakeholders — inside and outside the EIA — come from many different backgrounds and experiences, and have different objectives. Some CDR recommendations can and should be challenged; some will ultimately require additional discussions. Providing the rationale can form the foundation for additional subject matter discussion.

Continuous Balance of Objectives with Technology

There are constant trade-offs associated with most aspects of World Model design. The technical items include regional aggregation, number and types of crudes and products, refinery configurations, and logistics. The objectives include model usability and maintenance, model speed, stability, and model analysis, to name a few.

Strategically, the trade-off is that higher resolution, detail, and fidelity will challenge the model performance, analysis, maintenance, and usability. Note, though, that sophistication, higher fidelity, and more complexity do not translate into better answers.

The need to balance data with complexity should be ongoing. Coupling unreliable or highly estimated data to sophisticated subroutines should be avoided.

When in doubt of the judgments and decisions associated with the model “balance,” one should go back to the fundamental objective of “reasonableness.”

Other

Numerical approximations are used throughout the document for demonstrative purposes. They illustrate points and examples behind the recommendations; there is no intent for these data to be used for model design or to extract the data for other uses.

Model Structure

The following requirements are fundamental to the Refining Sub-module:

- Receiving Crude
- Transforming Crude into Products (Refining)
- Distributing Products
- Logistics

These will be accomplished with the various sub-modules, or blocks, represented below:

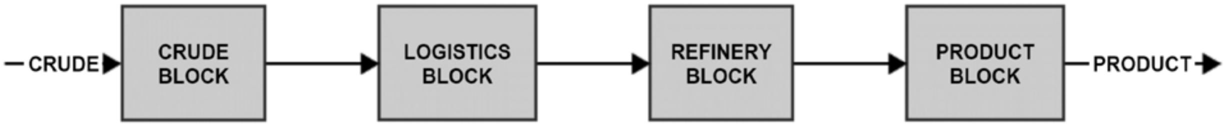

Figure 1. Block Methodology

Each of these blocks will be described in this CDR development. In addition, the inputs and outputs for each block will impact the other blocks. This is a critical concept because one goal of the CDR is to balance the sophistication of these modular components with the model goals. It would be a fundamental flaw to dramatically over-design one block, and substantially under-design another.

These blocks are briefly presented below:

- **Crude Block.** This module will collect and distribute the crudes to be used in the Global Model. This block is the foundation for the entire Global Model, and is where the number, types, transportation, and characterization of the crudes will be achieved. The data and characterization of this block will significantly impact the refinery block and the capability to globally balance World crudes and products.
- **Refining Block.** This module transforms crude into products. This block will have significant attention in the CDR to the development, operations, and rationale behind the recommendations. The World Model will simulate and balance the global crude and products supply and demand, and this block must have sufficient detail to properly represent the global operations. Not only will this block produce products, but will be tasked to generate weight, energy, and emissions balances. These additional tasks force an additional level of detail in the Block.
- **Product Block.** This sub-module will balance the World’s product supply. The number, type, transportation, and characterization (specifications) of products will be achieved in

this block. Movements of products from regions of the World to satisfy other regional demand requirements is fundamental to the Product Block.

- **Logistics Block.** This sub-module will interact with all the other blocks to receive, distribute, import, and export feeds and products with different modes of transportation. This is the module that connects every other module in this section of the Global Model. The Logistics Block will also be designed to capture regional material balances through the use of terminals and transportation vectors, which is fundamental to the Global balance.
- **Regional Block Characterization.** Each region represented in the World Model will have an independent set of Crude, Product, Refining, and Logistics Blocks. The World Model will contemplate how to define the regional blocks. For example, one could define a North American Block, or separate the countries and develop separate blocks for the United States, Canada, and Mexico.

3. Refining Block

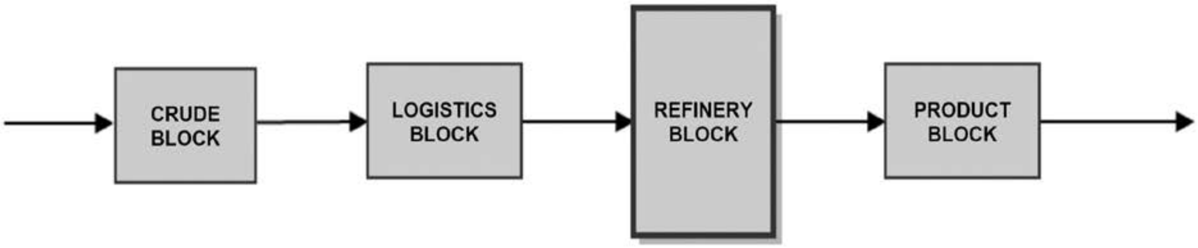

Figure 2. Refining Block

The Refining Block, central to the Global Model, must have sufficient complexity to:

- Receive, characterize, and process the regional crude slate
- Characterize, simulate, and utilize the refinery process units
- Produce global specification products
- Provide mass, energy, utility, and emissions balances

Within the Refinery Block are a number of sub-modules to represent process unit operations in a refining complex. If the complexity in the process sub-modules is too low, the following will be compromised:

- Capability to represent crude transformations on different types on crude inputs
- Capability to produce specification-grade products from different crudes and different unit operations
- Capability to provide mass, energy, utility, and emission balances

On the other hand, if the Refinery Block complexity is too high:

- model development, maintenance, and use-ability will suffer,
- model solving time will increase,
- model convergence and stability will be negatively impacted, and
- there will be a significant over-emphasis on this block compared to the other blocks.

In the Refining Block, “average operating conditions” is a term to reflect a yield prediction under an average condition. For example, the drum pressure of a coker has a range of operating pressure that can impact yields. A hydrotreater can be designed to operate under different pressures. The model will not simulate all the possible combinations of design variables, for which there are thousands across the globe. Rather, the model represents “average operating pressure.” In the end, the World Model does not simulate a pressure; instead, it simulates a representative yield pattern. One could simulate two different operating modes (e.g., high and low pressure), or a single mode at “average” conditions. Whether the process unit should be represented by an average condition or have different modes of operating condition will be discussed for each unit.

With these concepts in mind, the Refining Block begins with the refinery configuration. The configuration is fundamental to the transformation process, and it includes the types, capacities, and operations of refining process units.

The configuration must be defined for all regional or country models. One comprehensive and commercially-available data source for World refining capacity is *The Oil and Gas Journal Refinery Survey,* which defines common refinery process units and provides the capacity for these units. The capacities are listed on a Barrel Per Calendar Day basis (BPCD), not a Stream Day basis (BPSD). The BPCD should be chosen for the modeling basis, because this represents what the refinery can process over time, including planned and unplanned shutdowns.

Developing the configuration and throughputs is the first step in defining the Refining Block. The descriptive effort that follows is the characterization of the operations for each of the process units. These operations are the core for the Refining Block. The Block must be able to transform crude based on a wide range of crude qualities. The Block must be able to change operations to adapt to changing product demands. Finally, if mass, energy, and emissions balances are goals of the Global Model, sufficient operational detail to develop these balances is fundamental to the process sub-modules in the Refining Block.

In a refinery model, “sulfur balance” or “maintaining sulfur balance” means there is a quantity of sulfur in the feed that will distribute through the products. For instance, if 100 pounds of sulfur comes in, then 100 pounds of sulfur goes out, either in the form of H_2S, liquid products, or coke. Maintaining sulfur balance is fundamental and strongly recommended.

Similarly, “weight balance” or “maintaining weight balance” means there is a quantity of pounds in the feed that will distribute through the products. For instance, if 100 pounds come in, then 100 pounds go out as products. Maintaining weight balance is fundamental and strongly recommended.

Within the Refining Block, chemical reactions, kinetics, and operating variables are profoundly complex and impact process yields, qualities, and blending. The CDR focus is on the significant variables that impact these operations, and not the chemistry behind these factors, for which an abundance of reference materials exist.

The following sections list the types of technologies—or refinery “sub-modules”—commonly employed in refinery modeling.

Crude & Vacuum

The CDR decisions for the crude and vacuum tower are highly significant to the operation of the World Model. All the crude assays developed for the World Model will be “processed” at the crude tower. These assays will have pre-determined cutpoints, called the “cut set.”

In most modeling systems, each crude is developed and characterized in an outside crude assay program. The program often utilizes a template that is populated with data from each assay. This information subsequently inputs to the refining crude and vacuum tower.

The design, definition, and strategy of the cut set is fundamental. The products from the crude tower (crude assay) include: LPG, Naphtha, Jet/Kerosene, Diesel, Vacuum Gasoil (VGO), and Vacuum Resid (VR).

In the simplest form, the products of the crude tower—called straight run (SR) products—include SR naphtha, SR jet, SR diesel, Vacuum Gasoil (VGO), and VR. The combination of VGO and VR is called an atmospheric resid (AR) cut. Each crude has an initial boiling point (IBP) and an endpoint (EP). In refinery operations, the temperatures are not “fixed” because refineries have operational flexibility to change temperatures. The values below are typical, representative of the standard cuts.

Table 1. Simple Cuts

CUTS	IBP (F)	EP (F)
LPG	C1-C4	C5
Naphtha	C5	375
Jet/Kero	375	525
Diesel	525	650
VGO	650	1000
Resid	1000+	

This simple 5-cut representation will determine the volume of each cut. A user could re-cut the crude to adjust the volumes of each crude or region, if desired. While this method would greatly simplify the World Model representation, it would be overly constraining and overly simplified to simulate the Refining Block goals. Refineries have operational flexibility to adjust cutpoints. In refinery modeling, this is often represented utilizing swing cuts. Utilizing swing cuts would result in a cut set representation below:

Table 2. Advanced Cuts

CUTS		IBP (F)	EP (F)
LPG		C1-C4	C5
Lt Straight Run	LS	C5	160
Lt Naphtha	LN	160	220
Lt Lt Nap	LL	160	185
Lt Hvy Nap	LH	185	220
Hvy Naphtha	HN	220	350
Naphtha/Kero Swing	NK	350	400
Kerosene	KR	400	500
Kero/Diesel Swing	KD	500	550
Diesel	DS	550	650
AGO (Swing)	AG	650	680
LVGO	LV	680	800
HVGO	HV	800	1000
VGO/Vac Resid Swing	VS	1000	1025
Vacuum Resid	VR	1025+	EP
Atmospheric Resid	AR	680+	EP

Utilizing this technique, the model could, for example, move half of the naphtha/kero swing “up” to naphtha, effectively changing the naphtha EP from 350 to 375 (F) and swing the other half “down” to jet, effectively changing the IBP from 400 to 375 (F). This represents what a refinery can perform at an operational level and is justified to develop and calibrate yields to match regional refinery operations given the stated goals of the project.

The naphtha cut is often further sub-divided into a light and heavy portion to enhance the modeling for reforming qualities. Additional sub-sets on the light naphtha cuts include a benzene precursor cut.

The cutpoint set above is typical, but the IBP and EP temperatures can change during the model design. All refineries have different cutpoints based on crude qualities, downstream capabilities, and overall refinery economics. The cut set is intended to both reasonably reflect refinery operations and provide flexibility to achieve World balances.

When crudes are cut using commercially available software, there is often the capability to model “tails” by reflecting inefficiencies in tower operations. This is not required for World Model design. The basis of crude tower cutting—and downstream cutting—will be “perfect” cuts.

Developing the template from which all data are received and passed is critical, as it will establish the stream names, quantities, and downstream processing and blending. Re-cutting crudes to different cut-point temperatures is a very simple task with commercially available software. Redesigning the crude template after the model is developed presents challenges, and should be designed as best possible in anticipation of future Refining Block goals.

Any given crude assay brings in two types of data to the model: volumes and qualities. The volumes associated with the crude streams are more influential than qualities regarding balancing the World Model. This is not intended to minimize the importance of stream qualities, because the qualities “fine-tune” the operations. For example, the FCC feed is VGO, and the VGO cut will determine the throughput of the FCC. The VGO quality UOPK will also determine the gasoline production potential. Ultimately, the gasoline production is more influenced by **quantity** of VGO to the unit compared to the **quality** of the VGO. Restated, significant emphasis should be placed on balancing the distillation volumes at the crude tower using a well-developed crude assay.

The crude cut set is fundamental, but choosing the appropriate crude to the tower is equally influential. The resid content between a light crude and a heavy crude cannot be fully offset using cutpoint changes.

The stream qualities do play a valuable role in balancing the decisions on the cutpoint temperatures and swing cuts. For example, specification diesel is often constrained by cold flow properties. Since the AGO has poor cold flow qualities, and can swing up to diesel or down to VGO. The diesel cold flow specification can limit the AGO upward swing, effectively representing a lighter diesel cut. The swing cut can adjust both the volume and quality of the AGO SR cut. This capability will increase the success rate of the refining model goals.

Some comments regarding the streams and cutpoints are as follows:

- Separating full range VGO into Light and Heavy cuts is recommended
- Allowing a VGO/Vacuum Resid swing provides flexibility during design, and this option could be switched off later. Many refiners cannot cut a heavy crude to 1025 F or deeper, but this cutpoint could be achieved with a lighter crude. The refinery model will almost always choose the deeper cut option, so analytical judgments will have to be applied after the World Model is up and running.
- It is highly recommended that the template be consistent for all crudes. For instance, do not cut light crudes at a different temperature than heavy crudes; let the swing cuts do this work.
- Atmospheric Resid is typically produced in the atmospheric tower and processed in a separate vacuum distillation unit, which produces LVGO, HVGO, and vacuum resid. The crude assay will produce Atmospheric Resid either as a stand-alone stream for downstream operations, or for further distillation in the vacuum tower. The feed atmospheric resid will have other dispositions, as discussed later.

Regarding the World Model development, including three crude and vacuum towers in the model design (i.e., CD1/VT1, CD2/VT2, and CD3/VT3) is recommended. This will provide modeling flexibility and is an example of developing a simple design to code on the front end, and a challenge to rework on the back end. There may be future requirements to run sweet crude in one tower and sour crude in another.

Coking

Several different types of coking processes exist, including Fluid Coking, Delayed Coking, and Flexi-Coking. The primary coking technology in the World is overwhelmingly Delayed Coking, and will be represented in the model. As such, a critical model design decision must be made: should the World Model include Fluid and Flexi-Coking structure? In the context of designing a World Model, the recommendation is to aggregate all the various types of coking capacity and model all coking operations as Delayed Coking. It seems highly improbable that any decision from a World Model will be meaningfully impacted because a relatively small Fluid Coking capacity was aggregated with Delayed Coking capacity.

Coking yields are a strong function of Conradson Carbon (CCR), so all potential feeds should have a feed Concarbon quality. Some coker model predictions have shifts or yield adjustments based on the operating pressure. While this can impact yields, the recommendation for the World Model is to estimate the “average” operating pressure, and not develop multiple yields for different operating conditions. Rather, the single mode will have yield adjustments for feed quality.

The rationale for a single mode of operation follows: A low-pressure coke drum will have lower coke yields and higher liquid yields. In almost all circumstances, a model would choose the “better” economic yield pattern, which would be the lower pressure. With that in mind, adding a second high-pressure — “worse yield” — mode vector is impractical because it is highly unlikely the LP would choose this mode. Across hundreds of World coking operations, it is unlikely the data are available to estimate which are low-pressure versus high-pressure. In modeling language this is simply stated “model what is known,” and the design and operating pressure of all the global cokers are not known.

It is recommended that feed sulfur and gravity qualities be included. In addition, the coker produces gasoil that feeds an FCC, so the coker gasoil should have a prediction of the nitrogen quality.

The majority of feed to the coking process is vacuum resid. Some cokers have “Other” feeds, such as atmospheric resid, vacuum gasoil, visbreaker bottoms, FCC slurry, and SDA Tar. All of these feeds are processed at lower volumes compared to vacuum resid.

World Model design decisions must be made regarding the inclusion of these feeds into the coker. This does not apply to cokers alone, but to most refinery operations in the model. Each process model and stream mapping will have to be examined.

Products off the coker include C4-, naphtha, diesel, gasoil, and coke. The density of naphtha does not vary much and could be fixed for simplicity. Density of the diesel and gasoil will be calculated based on the feed density and the yields.

Coker naphtha is often split into fractions. In refinery modeling, this splitting can occur inside the coker unit, or in a separate outside unit such as a thermal naphtha splitter. For simplicity, the coker naphtha can be cut into a light C5 – 160 F (light SR) and a light and heavy naphtha. In a Global setting, many product qualities (e.g., octane and vapor pressure) can be fixed without adding substantial levels of code for enhanced predictions.

Fixing product qualities can be done judiciously throughout the model — not just in the coker — and must be examined on a case-by-case basis. If specification products are a goal of the model, the stream qualities impacting these blends must be reviewed. The following language describes the typical thought process for this discussion, and will be done for all process units:

> The coker gasoil sulfur and density should be predicted by the model based on feed quality, but the other specification blending qualities (e.g., cold, cetane, flash, and viscosity) can be fixed. Gasoil should have a prediction on nitrogen because nitrogen will

> have a negative effect on FCC cracking yields. If the FCC correlation uses UOPK as a feed quality, a coker gasoil UOPK quality prediction will be required.

Petroleum coke is generally sold as a product for production of power. The World Model should not have to consider gasification of coke, as in Flexi-coking. There are some situations where anode-grade coke production is significant at the refinery level, and other situations which feed significant volumes of atmospheric resid versus vacuum resid. It is not envisaged that anode-grade coke production should be in the World Model. If stakeholders consider this to be important, it would be logical to develop code for a second anode-grade coker.

Visbreaking

The visbreaker feed is predominately vacuum resid, although some locations feed small amounts of SDA Tar, FCC Slurry, and Atmospheric Resid, used to upgrade residual feeds.

Visbreaking modeling correlations are often done with a base yield mode and a shift on the NC5 insoluble content of the feed. Higher NC5 will result in more bottoms production.

The C5+ products include naphtha, diesel, gasoil, and bottoms. Since the gasoil can feed the FCC, quality predictions need to be made which impact the FCC yield. The model will need to balance both on weight and sulfur, so density adjustments based on feed will be required, as with most process units. It would be reasonable to have a fixed density on naphtha, and adjust diesel, gasoil, and bottoms to maintain weight balance.

The bottoms is usually routed to fuel oil blending, so fuel oil qualities need to be predicted, including density, sulfur, and viscosity.

FCC

The FCC representation is one of the most critical process units in the refinery model configuration. Here, a balance of sophistication and reasonableness must be maintained. The model should be able to make yield distinctions based on feed quality, and should be able to reasonably represent a range of FCC conversion potential from low conversion to high conversion. The model should have functionality to adjust product cutpoints, particularly between the Heavy Cat Naphtha (HCN) and the Light Cycle Oil (LCO).

In the context of World modeling, it is critical to emphasize that the FCC model is not being developed to analyze different technologies, catalyst types, revamps, or kinetic operational changes. Refinery LP models often have this level of sophistication, but it is not required for World or aggregate modeling. The World Model is not intended to design or fine-tune a specific refinery operation; rather, it is intended to reasonably reflect World FCC yields on representative feeds. It is, in principle, an average FCC technology across the World that is capable of adjusting to feed quality across a reasonable range of operations.

When designing the FCC correlation, there are two critical starting points:

1. Which feed qualities most greatly impact FCC yields?
2. What operating conditions greatly influence FCC yields?

The first point refers to the FCC feedstock characterization. Within the “FCC Expert” community, there are differing opinions on how best to characterize feed for FCC predictions. Experts typically focus on the need for highly specific feed characterization at a specific refinery, not generalized refinery modeling. It is also very important to remember the source of FCC feedstock qualities, which is crude assays. “Bulk” properties such as density are generally more reliable from an assay database than more technical qualities such as aniline point or refractive index.

One significant feed quality impacting the FCC yield is the “crackability” of the feedstock. Generally speaking, paraffins are more readily cracked compared to aromatics. Most models, however, do not directly quantify the paraffin or aromatic qualities; rather, UOPK is often employed. UOPK is a function of density and Mean Average Boiling Point (MABP). A feed with higher UOPK has better conversion potential than one with low UOPK. Some modelers choose to independently model both density and MABP.

Sulfur is a bulk quality that must be included in the representation. The structure must include a distribution of feed sulfur to the products, including H_2S, liquids, and coke. It is not essential to track and report the sulfur in coke, but it is essential that the sulfur pounds in coke are included in the sulfur balance.

Both Concarbon and Nitrogen qualities should be considered as feed input parameters, since both will negatively influence conversion. Nitrogen is typically reported as either Total Nitrogen or Basic Nitrogen.

Metals such as vanadium and nickel have negative impacts on operations and incur additional catalyst costs, which pale in comparison to other margin drivers. In the context of World economics, and that metals data in assays can be unreliable, it is not recommended to include metals as a variable in the FCC model.

FCC naphtha is the largest source of sulfur to the gasoline pool. Predictions of sulfur in the naphtha vary on a step change basis depending on whether the FCC feed has been hydrotreated or not. Hydrotreated feeds have a lower distribution of sulfur to the naphtha than unhydrotreated feeds. As an approximation, sulfur in naphtha from unhydrotreated feed is about 0.1 times the feed sulfur. Sulfur in naphtha from a hydrotreated feed is lower, around 0.06 times the feed sulfur. While this might seem to be a subtle difference, there are downstream implications. Higher FCC naphtha sulfur requires more downstream hydrotreating, resulting in higher octane loss, and shifts the octane balance.

The "Percent Hydrotreated" will also impact the overall FCC yield. Hydrotreated feeds will have better conversion potential than unhydrotreated feeds. This distinction creates a modeling dilemma: whether the model should have yields for hydrotreated and non-hydrotreated feeds. A hydrotreater will convert aromatics to paraffins, increasing the UOPK. One could conclude that using a UOPK feed quality will capture this impact to some extent. However, it is possible to have two feeds with identical UOPK which have different yields. This is because the two feeds can have different "types" of aromatics, based partly on the severity (pressure) of the upstream hydrotreater, which would influence the yields. However, this subject introduces considerable complexity and it is therefore not recommended to not separate yields based on hydrotreated and non-hydrotreated variables, with the simplifying assumption that the UOPK will capture this distinction.

The World Model should consider a "shift" to increase or decrease conversion. In operations, this could be achieved by increasing the Riser Temperature. In modeling terms, this could be achieved by a High, Medium, and/or Low mode. This range of operation could influence conversion by approximately 5 percent in the model to provide a wide range of operations.

When developing yield correlations, it is extremely important to avoid cross-correlating variables. In the FCC, it would be redundant and a poor modeling decision to characterize the feed using both UOPK and Aniline Point, or Refractive Index. UOPK is a function of density, so density and UOPK feed characterization should not be considered.

The decision of the final variables for the World Model FCC will be influenced by the data or method to establish the correlation. If publically available correlations are used, or if correlations are developed from literature, the variables will be set by the source. If commercial services are sought, and yields are regressed from a simulator, then the range of feed variables and operating conditions for the World Model FCC is wide.

The following are recommended to be included for feed and yield operations:

- Feed UOPK, Sulfur, Concarbon, and Nitrogen qualities and shifts
- Estimate FCC naphtha sulfur distribution using conservative "non-hydrotreated" relationships

- Develop a base yield vector with high and lower operational shifts, spanning ~5 percent conversion numbers. These details will be finalized during model development.

In “LP language,” the following is performed by: 1) Define a “base feed” yield including assumed UOPK, CCR, Nitrogen, and Sulfur, 2) Develop independent shift vectors for qualities, and 3) Develop independent shift vectors for high and low conversion.

FCC PRODUCTS

The products produced by the FCC include C4 and lighter, FCC naphtha, Light Cycle Oil (LCO), Slurry, and coke. The coke is not a saleable product and is consumed internally to heat balance the process, but is required in the yield model to properly predict overall yields while maintaining weight balance.

The FCC is typically the largest source for C3 and C4 olefins, which impacts alkylation potential and propylene production, so the yield correlations for both C3s and C4s need to be scrutinized. Some modeling representations include a shift vector for higher propylene production achieved through the use of specialty catalyst (often called ZSM-5). This can be accomplished “inside” the FCC structure or outside in a separate unit. While this is not necessarily a critical World Model impact, it would be reasonable to add this optionality while developing the model.

FCC naphtha is, in a cracking refinery, typically the largest blend component to the gasoline pool. Some of the FCC naphtha qualities can be predicted as a function of feed and operations, and others are well-suited to be “FIXED” to typical qualities. The density and sulfur will be predicted from the feed quality and process operations. The vapor pressure of FCC naphtha is generally in a sufficiently tight band that it can be fixed, around 7 psi. Paraffins, Olefins, Naphthenes, and Aromatics (PONA) qualities are reasonably consistent.

Often in operations, FCC gasoline RVP is higher than the approximate 7 psi mentioned. This is almost always the case of actual operations where C4s get mixed (carry over) with the C5+ FCC naphtha. In World modeling — in fact, most refinery modeling — the yields are expressed as “PERFECT” cuts, from the cuts off the crude towers and throughout the model representation. In individual refinery modeling, efforts are often employed to model tower and fractionating inefficiencies, to reflect that actual operations are **not** Perfect. These efforts are not required for the World Model because matching individual stream qualities is not required and these individual cuts are later recombined in the saleable product streams.

FCC naphtha octane is fairly constant although it will shift with conversion. It could be a reasonable strategy to develop octane changes as a function of operations. It would also be appropriate to FIX the octane because — in the context of World modeling as a reasonable representation — a FIX on the octane requires less code and less matrix structure.

In the final blend gasoline pool, the octane*Bbl is often dominated by the FCC naphtha in FCC cracking refineries. The octane*Bbl can be influenced by both FCC throughput and conversion to produce more barrels. In the end, one check for the reasonableness of the model is the ability to produce the World demand for octane*Bbl.

In terms of model challenges, it will be more critical to characterize the crude with an accurate volume of VGO from crude characterization and swing cuts, to properly fill the FCC versus a sophisticated octane prediction. This fact, coupled with operational modes to produce more octane*Bbls with conversion should be included. All combined, the model will have the design qualities to flexibly produce octane*Bbls. This is a reasonable strategy to support the use of a single average octane versus a more complex, predictive method.

FCC naphtha is often characterized as a C5 – 430 (F) cut. This wide cut needs to be re-cut into smaller fractions for modeling purposes. The most appropriate way to do this is using three separate and smaller cuts: Light Cat Naphtha (LCN), Medium Cat Naphtha (MCN), and Heavy Cat Naphtha (HCN). Some modeling programs produce LCN, MCN, and HCN off the FCC sub-module versus a wide C5/430 (F) cut. Another approach is to build a naphtha splitter, recommended for the Global Model. Here, C5/430 naphtha feeds a splitter that cuts the wide cut into LCN, MCN, and HCN. These cuts have unique quality features that should be developed appropriately for the model. For example, the cuts, in order of high octane to low octane, are HCN, LCN, and MCN. It would not be accurate to model all cuts with the same octane. As another example, the RVP between the cuts are substantially different.

A very important concept in modeling splitters is that they must quality balance. The volumetric sum of the products should equal the feed quality. The LP should not be able to identify and optimize on a splitter programming error which allows the products to have, for example, more octane from cutting the wide cut into smaller pieces.

A significant reason for splitting the FCC naphtha is to allow the HCN modeling option to swing up and stay in gasoline or drop to the LCO or distillate pool. This optionality is a critical operating lever for refiners shifting from a strong gasoline economy to a strong diesel economy. From the combination of FCC operating modes (low, medium, high) and the HCN swing cut, the model will be sufficiently robust to reflect a wide range of FCC operations.

LCO will have density and sulfur predictions based on feed quality. Many LCO qualities can be FIXED to typical FCC product qualities. LCO will often ultimately blend to diesel and will require a cetane quality.

Many strategic development paths must be considered for each process unit as it relates to quality predictions. This applies to most process operations. Within the FCC, there are two potentially significant issues:

- The determination to enhance FCC naphtha octane predictions
- The determination to enhance the cetane prediction of the LCO

FCC operations and catalyst formulations is an advanced subject. There exists an abundance of literature and commercial expertise on the subject, all of which could lead to enhanced FCC modeling code. Utilizing the expertise on this subject and the additional complexity that comes with it is likely inconsistent with global modeling objectives.

Global FCC modeling is attempting to capture representative FCC operations for about 300 FCCs in the World, all of which have different operating parameters, constraints, kinetics, technologies, and catalysts, to name a few. It is a challenging task, but adding dozens of vectors, shifts, quality predictions, and higher sophistication does not translate into a better model, given the goals of World modeling.

Using FIXED octane from a “typical” FCC operation would be sufficient for World modeling purposes. However, the recommendation is to allow FCC naphtha octane to shift with conversion, where higher conversion is higher octane. This higher level of fidelity is recommended due to the overall importance of balancing octane*Bbls in the World Model. Additionally, if sub-regions of the World Model are separated and run independently, this functionality will likely prove valuable. Most model results — and most refinery operations — blend to octane constraints. Since FCC naphtha is typically the largest volume to the gasoline pool, and octane is typically constraining, adding additional octane predictive capabilities is reasonable.

The recommendation is to use a single, fixed LCO cetane index. The rationale for this includes the fact that many regions of the World use deep hydroprocessing on LCO to blend to diesel, which results in a significant cetane gain across the unit. LCO is not typically the largest blendstock volume to diesel, and straight run crude diesel cetane will be more meaningful than the LCO cetane prediction. Additionally, some refiners are challenged on cetane. To this end, the recommendation to include cetane improver to the model structure will eliminate any infeasibility associated with diesel cetane.

Atmospheric Resid can feed a refinery FCC with appropriate process design. Atmospheric resid has more Concarbon than a VGO feed. This translates to higher heat generation when burning the coke off the catalyst, which further often translates to the need for the FCC to have additional cooling equipment, called *Cat Coolers*. There are a range of “clean” and “dirty” resids that will impact FCC operations.

In the end, this is a substantial challenge for the Global Model. First, there is limited information about which refineries process resid and which do not. In some data searches, it is possible to capture the capacity of “Resid Processing,” which can provide guidance on Resid to the Cat Cracker. Source data and literature searches can identify additional Resid FCC operations.

If the model allows Resid to FCC feed option, the resid will preferentially go there, because it is usually profitable to convert resid into valuable FCC products. The model doesn’t “know” if sufficient Cat Cooling investment is in place. This can be approximated by putting a Concarbon limit on the FCC feed. This becomes a bit “messy” from a modeling perspective, because the model will “cherry-pick” up to the CCR limit — as in, it will “find a way” to hit the CCR. If the CCR limit is set at 0.7, there might be zero resid to the feed pool, but setting a 1.2 CCR limit might allow 20 percent resid to the feed pool. Changing the CCR becomes arbitrary, because no aggregate knowledge of the actual CCR to the region is actually known.

Refiners processing clean light sweet crude often feed resids to the FCC; however, this does not likely show up in a typical capacity report. Resid feeds to the FCC will have to be done on a region-by-region basis.

Techniques will be discussed to develop, test, and analyze the model. One technique is “bottoms-up,” meaning balance the bottom of the barrel and work up. The bottom of the barrel is residual fuel production and heavy conversion processing such as Delayed Coking. The atmospheric resid option to an FCC can potentially create a significant bottoms imbalance, because the model destroys more resid than the region or refining center can actually perform.

Overall there are different modeling techniques to consider for the World Model. First, the model should allow a resid “switch” to the FCC, which is turned-off as the rule. Second, the model should capture the total CCR of the feed pool to place limits on the feed quality. Third, the model will need a separate and unique resid hydrotreating unit, for when a resid hydrotreater is identified, the product will be able to feed the FCC. Last, the model should have some vector or bound control limiting resid to the FCC. Atmospheric Resid controls and movements to the FCC will require analysis and interpretations on a region-by-region basis.

The Resid FCC could be represented as a separate and unique sub-module in the Word Model, but is unlikely required. The feed — as stated before — has more Concarbon, and other qualities are likely (but not necessarily) worse than traditional VGO. The robust code which will be developed for the FCC should reasonably reflect the appropriate yields for the RCC, because the FCC will have shifts for CCR and the other quality drivers. The global volume of Resid FCC is small compared to traditional FCC. This is fundamentally why the World Model might not need to include a separate Resid FCC as a sub-module: the aggregate volume of RCC is small, and there is uncertainty with the reporting of RCC capacity.

The potential exists for exceptions to the FCC modeling circuit. First, some regions of the World cut the FCC naphtha very light (~300F). The model will have an FCC naphtha splitter. An additional mode in the splitter could be developed with this light cut option which is generally “shut off” but can be activated with a switch. Also, some regions of the World process highly paraffinic crudes, and the LCO from FCC operations has very high cetane. Like many situations in the World Model, this must be examined on a case-by-case basis. It might be prudent to produce a high cetane LCO stream for these exceptions.

Reforming

Reformers are generally characterized into three types: Semi-regen, Cyclic, and Continuous. Semi-regen is high pressure and has lower C5+ yields compared to the low-pressure Continuous type. The Cyclic capacity can be approximated as the average of the Semi-regen and the Continuous. When aggregating countries, it is likely that the aggregate will have all three types, with the Cyclic capacity distributed equally to the other two technologies. With these assumptions, the World Model will include two unique sub-modules for the Semi-regen and the Continuous reformers.

Reforming correlations typically characterize feed using some combination of Paraffins, Naphthenes, and Aromatics (PNA). Whether an N+2A or P+A, or some other variation, the format of feed characterization is primarily driven by the source correlation data. All reforming feedstocks must be hydrotreated prior to feeding the reformer, which will be done in the naphtha hydrotreater unit. The reformer is the primary source of internally-produced hydrogen, so these yields should be well represented.

Reformer operations in refinery models generally have separate vectors representing severity. The vectors generally have 5 degrees of separation. The reformer yields are often represented by 90, 95, 100, and 105 severity. Continuous reforming is generally limited to 102, and Semi-regen reformers less — generally around 98 severity. The user can control the severity with a limit switch.

The reformers produce a full range reformate, which is often split into a light reformate and heavy reformate in a downstream splitter. Often, however, in modeling systems the light and heavy are produced in the reforming submodule, not in a separate unit splitter. Either approach is viable. From a coding perspective, it is often an easier approach to make the two types of reformate inside the unit. To capture the quantities and qualities of the light and heavy reformate, the feed characterization should include data on both the light and heavy naphtha feed. This is done back in the crude tower design, by separating the full range naphtha into a light and heavy fraction.

Reforming simulation has some unique challenges. If the reformer feed is a separate light and heavy naphtha, there will be a series of vectors at different severities for the light naphtha, and a similar set for the heavy. In addition to the base vectors there will be yield shifts based on feed quality. The shifts, as stated above, can be on N+A, P+N, or whatever source correlation is used.

Where the separate vector approach is chosen the model can, for example, run light in both a 90 and 95 severity mode, and the heavy in a 95 and 100 severity mode. If 50/50 is the activity, this would represent a 92.5 on the light and 97.5 on the heavy. Model behavior can become peculiar when the severities are not “side by side” — for example, running in a 105 and 90, which could represent the 100, rather than just selecting the single 100 vector. In the end, the model is competing for all the severity options by different feed types. In addition, allowing the model to run the light at one severity and heavy in another is not representative of operations at any given point of operation. In the overall perspective of global modeling, it is an over-optimization step that will not be overly significant.

In the end, this can be explained by interpreting these modes and choices as across the average operations. For instance, over a year there can be any combination of severities. In spite of some of the weakness in this method, it is commonly used.

There are other approaches, but these require a pooling methodology. This would allow a full range feed; however, this feed carries the light naphtha qualities and the heavy naphtha qualities in the total feed. So the pool is a single feed, with light and heavy quality distinctions.

With this approach, there is only a single severity that can be used, not a potentially separate severity on the light and heavy. Additionally, the light and heavy reformate can be produced inside the sub-module, because the feed contains light and heavy qualities. If the user does not want to produce separate light and heavy reformates, the two streams can be pooled off the unit to simulate a full range reformate.

The light naphtha is often characterized as a 160/220 F stream. The heavy naphtha is often characterized as a 220 F IBP, and the model can optimize on the endpoint. This is done with the swing cuts discussed earlier. If there is a 350 to 400 F swing cut, the model can effectively simulate any endpoint between 350 and 400 F.

The light naphtha contains the benzene and benzene precursor data used in the prediction of benzene. Benzene precursor data include methylcyclopentane (MCP) and cyclohexane. Rather than carry all the specific precursor qualities through the model, it is often convenient to carry a Benzene Precursor Index quality that will determine the benzene content of light reformate.

The prediction of benzene in a Global Model can be greatly simplified by using separate but fixed benzene data points for light reformate at each severity. The rationale for this simplified method begins with the fact that the Global Model will not — or at least should not — be equipped with detailed data to simulate the advanced prediction of benzene, nor the types of control strategies. Low benzene is the standard in the United States and many other regions of the World, but how this is achieved is challenging in a Global Model.

Generally speaking, there are two types of benzene control: Pre-treating (removing benzene and precursors, benzene saturation, and/or isomerization) and Post-treating (benzene saturation).

In the Global Model and other aggregate modeling efforts, the user often will not know which technology or combination of technologies might be employed. Going back to “The user cannot — or should not — model what is not known,” allowing both technologies in the model and allowing the model to choose or optimize is, quite frankly, random. The end result is similar: low benzene reformate. The consequence of benzene control is octane loss and hydrogen uptake. The qualities for either technology requires data characterization for both light and heavy naphtha.

If light reformate saturation is chosen, this is often easier from a coding strategy. Pre-treating has an extremely larger reliance on benzene and benzene precursor data, which is often mischaracterized in assays. Saturating light reformate is very straightforward from a modeling perspective. The light reformate will feed a reformate saturator, which would consume hydrogen and have an associated octane loss.

For the aforementioned reasons, the recommendation is to add a light reformate saturation unit for benzene control. The model developers should consider the option to use a fixed quality benzene, based on severity. This eliminates some fairly sophisticated code that is required to model benzene; would produce reasonable results; and can be switched or modified later, for more detailed modeling. For more advanced modeling, using a light naphtha benzene precursor index is reasonable. The index is determined at the crude assay level. If there is a strong argument for pre-treating technology, Benzene Saturation could be added at a later date.

Hydrotreating

The World Model will have a range of hydrotreaters, including:

- Naphtha Hydrotreater (NHT)
- FCC Naphtha Hydrotreater (CNT)
- Reformate Saturation

- Kerosene Hydrotreater (KHT)
- Diesel Hydrotreater (DHT)
- ULSD Hydrotreater (UHT)
- VGO Hydrotreater (VHT)
- Resid Hydrotreater (RHT)

All hydrotreaters will need to predict hydrogen uptake as well as quality changes across the unit. This is particularly important when accounting for emissions, specifically CO_2. Hydrogen production from a steam methane reformer will produce CO_2, which is one reason why hydrogen balances should be robust. Hydrogen produced outside the refinery limits incurs a CO_2 consequence. Additionally, hydrotreating units often change the output product qualities versus the feed input qualities. These changes impact downstream processing as well as direct blending. The API change across a hydrotreater impacts the energy content of the product. For these reasons, hydrotreating sub-modules need critical review to match the goals of the Refinery Block.

Naphtha Hydrotreater. This hydrotreater will have unique hydrogen uptake vectors for straight run naphthas and coker naphtha. The sulfur for the products will be zero, as well as olefins if applicable in the feed. The other product qualities leaving the NHT will be the same as entering. For example, if light naphtha has 12 RVP in the feed, the product will be 12.

FCC Naphtha Hydrotreater. This unit desulfurizes the FCC naphtha, which is typically the largest sulfur contributor to the gasoline pool. There are many types of technologies in practice to produce low-sulfur gasoline. For World modeling, it is best captured using a single process unit with different operational vectors.

The most significant quality to capture in the unit is the octane loss associated with hydrotreating. There is also a reduction in olefins that can be captured. The model should have a high and low severity mode, each with different levels of desulfurization, hydrogen consumption, and octane loss. In practice, the octane loss and severity is closer to an exponential curve as the severity approaches 100, versus a linear low/high severity. This is the balance of sophistication versus reasonableness in World modeling.

The FCC discussion included the recommendation to split the FCC naphtha into light, medium, and heavy. The heavy cut can swing down to LCO or remain in the gasoline pool. The 3-cut strategy is recommended because it provides flexibility for modeling. For example, the LCN could be routed to a merox unit which has lower desulfurization but minimal octane loss. The LCN can also be fed to a depentanizer if that unit is added to the World Model.
The recommended destinations include:

- LCN to Merox
- MCN + HCN to FCC Naphtha Hydrotreater

These units will likely only be operating in countries where ultra-low-sulfur gasoline is specified, and where FCC operations are in place. So, in the ultra-low-sulfur gasoline countries, the model can force 100 percent of the naphtha through the Merox and Hydrotreater, choose the severity based on the high and low vector, and produce low-sulfur naphtha. Here, there is no conflicting model decision associated with bypass streams.

Reformate Saturation. This unit feeds the light reformate off the reformer and destroys the benzene by converting the molecules to other non-benzene compounds. There is an associated hydrogen uptake and octane loss across the unit which should be captured.

This unit would only be in operations where low-benzene gasoline is specified.

Kerosene Hydrotreater. This unit is employed to desulfurize a kerosene fraction versus feeding a wider range kerosene/diesel cut to a distillate hydrotreating unit and fractionating the kerosene and diesel streams downstream. This can be simplified in the World Model using a single desulfurization vector, around 95 percent. This technique allows the jet feed pool to either bypass or go through the 95 percent mode. There are many crudes that can make jet without desulfurization; this bypass simulates this fact.

These units are relatively low 500 psi units, and do not have a significant impact on quality changes other than sulfur. With hydrogen consumption around 200 SCFB there is an API gain of less than 1. The low severity and operating conditions do not significantly change other qualities such as aromatics or smoke that need to be quantified in the World Model.

Distillate Hydrotreating. Not to be confused with higher pressure and severity Ultra-Low-Sulfur Hydrotreating units, these units operate around 700 psi. Hydrogen consumption is a function of the feed type, which includes Straight Run material and cracked stocks. Cracked stocks such as FCC LCO and Coker Distillate are high in aromatics and will consume more hydrogen. The desulfurization range can be wide, spanning from around 85 – 97 percent. Product sulfur ranges from under 500 ppm to under 1000 ppm, depending on the region of the World and diesel sulfur specifications.

From a modeling perspective, the code needs to reflect the different types of feeds. This can be reasonably accomplished by tracking the aromatic content of the feed pool, if pooling is the model strategy. The feed pool will consist of all the SR feed, cracked feeds, and any other intermediate streams as appropriate. Otherwise, separate vectors will need to reflect SR feed, FCC LCO, and Coker Distillate. While FCC LCO and Coker distillate aromatic quality is relatively consistent, SR has a wide aromatic quality. Consequently, if separate vectors are used, the model must adjust SR hydrogen from the base aromatic quality.

High and low severity vectors can be developed to capture the range of desulfurization anticipated in the World Model. This can, however, potentially create optimization cycling. The feeds to this unit will have the mapping to either run through the unit, or bypass the unit and blend directly to diesel products. Modeling two severities can create modeling “conflict” because the model can opt to bypass feed combined with a high severity on a low volume, or not bypass and run a lower severity.

This concept is demonstrated below in a simple example. While it is presented in this DHT discussion, conceptually it applies across all modeling strategies. In the first box, 100 lbs of sulfur enter a unit, and 50 percent goes through the 95 percent desulfurization vector and 50 percent through the 85 percent desulfurization vector, effectively representing 90 percent desulfurization.

Table 3. Two Mode DHT no Bypass

100 Lbs Sulfur with Two Vectors		
	Feed Lbs	Prd Lbs
Bypass	0.0	0.0
85% Desul	50.0	7.5
95% Desul	50.0	2.5
Total	100.0	10.0
DeSulf	90%	

In the next example, the same 100 lbs enter the unit, but about 95 percent goes through the 95 percent vector, and 5 percent is bypassed. The same 90 percent desulfurization occurs.

Table 4. Two Mode DHT with Bypass

100 Lbs Sulfur with One Vector + Bypass		
	Feed Lbs	Prd Lbs
Bypass	5.3	5.3
85% Desul	0.0	0.0
95% Desul	94.7	4.7
Total	100.0	10.0
DeSulf	90%	

When the World Model is developed, there will not be sufficient data intelligence to determine the desulfurization capabilities for the global DHTs. Allowing the model to optimize across the range of two severities, coupled with bypassing, will create a push and pull effect on the process optimization.

In addition, the top example used 100 lbs of capacity, while the bottom used about 95 lbs (bypassing 5 lbs). Clearly, this will change the throughput for the models, but given the range of accuracy of the reporting of DHTs, these differences should be acceptable.

This is the prevailing reason why a single severity is recommended for the Global Model. To be clear, this is a simplifying assumption that might not be recommended for more advanced simulations. The base desulfurization should be set around 97 percent.

Diesel Hydrotreating will result in an API gain and an improvement in cetane because of aromatic saturation. Sulfur and hydrogen adjustment vectors should shift the yields as a function of feed quality. These details will be sorted out once final modeling strategies are clarified (specifically table versus pool format). There will be a small amount of naphtha produced which will recombine to the naphtha circuit.

ULSD Hydrotreating. This unit produces ultra-low-sulfur diesel off the unit, operating around 1,000 psig. The operations are more severe than the traditional distillate hydrotreater. In order to achieve the ultra low specification, the unit must be of sufficient pressure and hydrogen to “open-up” aromatic rings to remove sulfur molecules.

The amount of hydrogen uptake is a strong function of feed aromatics. This can be represented as a feed pool, or in a table structure where there would be separate vectors for SR diesel, coker diesel, and FCC LCO. Higher feed aromatics will consume more hydrogen.

With the conversion of aromatics to paraffins, there can be a substantial cetane improvement across the unit that needs to be reflected in the model operation. The desulfurization is high — 99.9 percent in some cases. Rather than allowing a model to choose between a high and low severity, the approach should be to produce a target sulfur, for instance, 10 ppm.

Like the FCC Naphtha Hydrotreater, this unit would only be in operation when the country has an ultra-low (10 – 15 ppm) specification on the finished diesel.

Between the FCC naphtha hydrotreater, the ULSD hydrotreater, and the Benzene Saturation, the reporting on the capacities is extremely unreliable. The ULSD hydrotreater is often reported as a diesel hydrotreater, and the FCC naphtha hydrotreater and Benzene saturation is often not reported.

If a country produces ULSD, LSG, or low-benzene gasoline, there will be sufficient capacity to produce the product, regardless of the reporting. As a first step in developing the model, allow unlimited "Clean Fuel" capacity, and zero-in afterwards.

VGO Hydrotreating. These units prepare the feed for an FCC, and operate around 1,200 psig, consuming around 500 SCFB. The feeds generally include SR VGO and Coker Gasoil. Since the product from the unit goes to the FCC, the VHT must track and predict the FCC input qualities, likely to be UOPK, SUL, NIT, and CRC.

There will be quality improvements associated with pre-treating: UOPK goes up while SUL, NIT, and CRC go down. These changes are a function of the unit design, operating pressure, feed types, and hydrogen uptake.

Similar to the discussion on the DHT, the recommendation is to use a single base vector and shift yields and qualities based on feed qualities. The base operation should be around 90 percent desulfurization, and additional relationships can be developed for de-nitrification, UOP and API gain, and CCR reduction. These quality predictions will impact the FCC operation.

Resid Hydrotreating. The amount of reported Resid Hydrotreating units is extremely small. For World modeling — because of the aggregating methodology — and for simplicity, the reported resid capacity could be aggregated with the VGO pool to the VGO Hydrotreater. In other words, if VHT is 100 and RHT is reported as 5, the VHT could be a revised capacity of 105, while allowing 5 resid to feed the VHT.

On an individual modeling or country basis, the need for a separate Resid Hydrotreater might be appropriate, but can only be determined after the countries are aggregated and the amount of resid hydrotreating as a percent of other operations can be examined.

If more sophistication is deemed appropriate for residual desulfurization, the RHT would be developed similar to the VHT described above.

Hydrocracking

Modeling generalized hydrocracking is a great challenge in generalized refinery modeling. The operating pressures, severities, technologies, catalyst types, and feedstocks to the units — conditions that impact yields and hydrogen uptake — are broad and the reliability of the reported data is wide.

Even if a robust modeling technology is employed — which, among other variables, might include high, medium, and low severity — the operations and product yields are highly dependent on the feedstock characteristics. Restated, it is challenging to develop a generic medium severity vector when the feed can range from light distillate to SR or Cracked VGO to Deasphalted Oil (DAO). Moreover, reported data for VGO hydrotreating might be mild hydrocracking, or vice-versa.

As a starting point, World hydrocracking capacity in *The Oil & Gas Journal* lists two types of hydrocracking: Mild and Severe.

There are many technical approaches to hydrocracking modeling. Part of the technique will be determined by the methods used to develop and correlate the data, which could be internally or externally developed.

Recommendations include developing two units, one for Mild HYK and the other for Severe HYK. Within each unit, there can be two severities, high and low, and for each severity there can be three types of feed: Light (diesel), Cracked (LCO and coker distillate), and Heavy (VGO and Coker Gasoil and DAO). The Coker Gasoil and DAO typically have worse qualities compared to VGO, but could be pooled to the Heavy Pool. This is shown below:

Table 5. Example Hydrocracking Matrix

	Mild HYK		**Severe HYK**	
	Low Sev	Hi Sev	Low Sev	Hi Sev
Light				
Cracked				
Heavy				

The individual yields would have shift offsets to feed qualities (e.g., UOPK). Hydrogen balance needs to be adjusted to feed quality.

Yields from the HYK can be equally challenging from a modeling perspective, because different severities produce large changes in volume change or total C3+ liquid yield and refineries have different fractionating objectives. Jet material might stay in the diesel pool and not be separated.

Often in modeling, a HYK has swing cuts, similar to the crude tower. The HYK can produce Jet, a Jet/Diesel swing, and a Diesel draw, as an example. Similarly, the HYK naphtha needs to have all the product cuts and qualities represented in the crude tower, because these HYK naphtha cuts go to the same destinations.

For most of the product qualities, fixed quality might be reasonable; again, this will be a function of the correlation and data development. Density will likely change to maintain weight balance.

For example, it might be reasonable to assign a single cetane number to the diesel stream, regardless of mode of operation. If the cetane varies significantly, then separate diesel products for each mode can be used (with different cetane or other quality), and pooled outside the unit.

Resid hydrocracking is another subset of hydrocracking. Compared to other hydrocracking technologies across the globe, its use is small. Depending on the volume of resid processed in a defined region, it might be reasonable to allow a relatively small volume of resid to the traditional hydrocracking technologies.

SDA

This unit is not often reported, but might be captured in other investigative methods. For World modeling, the structure can be simplified by having a low (60 percent) and high (75 percent) lift. Lift refers to the amount of liquid (called *Deasphalted Oil*, or *DAO*) which is pulled from the feed vacuum resid. With more lift comes more contaminates from the feed resid, which becomes a worse-quality feed to a downstream FCC unit, the typical destination of the DAO. Having the two lift vectors allows for better optimization. For additional simplification, a single lift vector (e.g., 65 percent) could be assumed. Since limited information on SDA will be available, fixing the lift to this number would be very reasonable.

The term “quality balance” was discussed earlier. The SDA should attempt to quality balance, although some discretion can be made as to the “important” qualities. If Quality A is feed to the unit, and 60 percent DAO is lifted with Quality B, the remaining Tar will have a quality that will balance the Feed and DAO quality.

DAO prediction has higher priority because it is higher volume and it feeds to a unit that produces higher valued products. The bottoms of the SDA unit, called *Tar* or *Pitch*, usually blends to fuel oil. The Tar can quality balance on sulfur and density. The viscosity prediction can be a function of the feed viscosity.

The DAO should have quality predictions for all the qualities used in the FCC, including UOPK, CRC, SUL, and NIT, all of which will be a function of feed quality.

Aromatics (BTX, Hydrodealkylation, Cyclohexane, Cumene)

The inclusion of these models in the World Model will be challenging, and will not be finalized until the GHySMo stakeholders discuss the merits and downfalls of including petrochemicals.

From a modeling perspective, the level of detail needs to be determined before finalizing the design. The BTX unit uses reformate as a feedstock and extracts benzene, toluene, and xylenes, while producing by-product raffinate. These recoveries are a function of the feed reformate. Consequently, the product yields are “only as good as” the feed reformate predictions. Certainly, sophisticated kinetic reformer models are available to produce this information, but the trade-off is complex code to capture this information.

Approximations could be well suited for this unit without the need for more robust calculations. These decisions will also be a function of the type of reformer protocols designed in the model. At even a high level, the model can sell reformate as an approximation of the extraction of BTX.

One important concept to keep in mind when modeling the unit is to maintain an octane balance. The full reformate comes to the unit with an octane quality. The product “pieces” should volumetrically balance on octane. For example, a high octane reformate will produce more C8/C9 aromatics than a low octane.

Overworking these units would be a mistake, as the desire to enhance these relatively small aggregate volumes leads to complex code decisions upstream in the naphtha and reformer models.

Fixed Yield Models

Some process units have simple, fixed yield models, with fixed output qualities that are easily input to a refinery model. These units include:

- Sulfuric Alkylation (C3, C4, and C5 modes)
- HF Alkylation (C3, C4, and C5 modes)
- Cat Poly (C3 and C4 modes)
- Dimersol
- C4 Isomerization
- C5/C6 Isomerization
- MTBE
- ETBE
- TAME
- Saturates Gas plant
- Unsaturates Gas plant

The C5/C6 isomerization has two types: once-through or single pass, and recycle. The recycle option produces higher octane, but also has higher vapor pressure. In the reporting of isomerization, there is no reporting by type. The Global Model could include both, or one, or an average of the two. The quality of isomerate will change with feed quality (amount of C5s versus

C6s and distribution of iso-paraffins and n-paraffins), but a typical "fixed" octane can be a reasonable approach for global modeling, and eliminates additional code for enhanced octane predictions.

Alkylation in C5 mode (both HF and sulfuric) will require a generation of a C5 olefin feed stream from the FCC naphtha. This is one reason why the full range cut is split into an LCN, MCN, and HCN. The LCN feeds a depentanizer which recovers the C5s to send to the TAME Unit.

Gas and LPG Recovery

Many of the submodules will produce a range of C4 and lighter (C4-) material that will include: methane, ethane, ethylene, propane, propylene, isobutane, n-butane, and butylenes. The methane and ethane will be routed to the fuel gas system, where the contained BTUs will balance the fuel gas requirements, coupled with purchased natural gas. The C3s and C4s will route to a gas plant. The C3s can have a recovery factor, where about 10 – 20 percent goes to fuel gas, and the balance goes to LPGs. C4 losses are typically less than 2 percent. Often, two gas plants are employed in the models: one for the saturates gas and the other for the unsaturates units such as the FCC and coker. Often a single model is put in the refinery model block.

The C4s produced off the units will be individually predicted. For example, the FCC will produce NC4, IC4, and C4 olefins, not a combined C4 steam. This is because the C4 olefins will need to be routed to an alkylation unit. Nor will the C3s be aggregated for the same reasons as the C4s.

Also included here is the collection of H_2S throughout the refinery processes. The H_2S is collected in the Sulfur Block where a fixed yield model will convert H_2S into sulfur, which is a product output.

Utilities

The utilities section in the refinery model is critical for achieving credible results on operations and predictions of energy use and efficiency, to name a few. When an energy balance is calculated across the refinery (or specific process units), the utility predictions and consumptions are critical. The calculation of CO_2 is a strong function of fuel gas combustion and electricity.

Every process sub-module will have various utility demands, usually expressed as a consumption per barrel of feed, or per barrel of product:

- Fuel (000 BTU/Bbl)
- Electricity (KWH/Bbl)
- Cooling Water Circulation (000 Gal/Bbl)
- Steam (000 Lb/Bbl)
- Catalyst & Chemicals ($/Bbl)

The utilities sub-module will perform the accounting of all the utility uptakes and balance the demand with a combination of refinery-generated utilities or purchased utilities.

Many individual models allocate different types of steam by pressure group (High, Medium, and Low pressure). This level is not warranted for World modeling, and a single pressure can be used. Cooling water circulation is tracked to 1) estimate the requirement for make-up water, and 2) estimate the power required to circulate the cooling water through the refinery.

Fuel will be satisfied by the combustion of refinery-produced fuel, purchased fuel (natural gas) or burning of fuel oil. It is through this combustion process that one significant source of CO_2 will be calculated. This combustion will also be the source for the NOx calculation which will be based on the average rather than LoNOx burner technology.

In all likelihood, the model will have to develop average utility uptakes. In reality, it is well known that some refineries are efficient in energy management and some are not. The model developers will not have that level of detail, and any attempt to define a region or country as being more or less energy efficient would be difficult unless reliable data is obtained.

Electrical power can be produced at the refinery, purchased, or a combination of both. Often, high pressure steam is topped in a condensing turbine to generate electricity. These details will not be known by country. The modeler should choose a consistent approach for all refinery configurations.

Energy Balance

The model representation will provide robust refinery inputs and outputs, representing the refinery material balance. Every process unit will be designed to maintain weight balance, model volume balances, and estimate energy balances. There are two approaches that will accomplish this task:

- Develop volume-based yields and make density predictions to maintain weight balance
- Develop weight-based yields and develop specific volume predictions to predict volume gain/loss

Both methods (weight-based and volume-based) are used in refinery models throughout the World. Neither system is right or wrong; it often comes down to user preference. Both systems have their advantages: crude is traded in volume; many blending specifications are volume-based (e.g., octane, vapor pressure); weight-based process yields easily maintain refinery weight; and many World balances are often reported in weight. The final decision will also depend on the upstream and downstream conventions, such as the upstream crude feed to the refinery will likely be in volume (barrels). Ultimately the volume-based model must be weight balanced as a fundamental accuracy check, and any weight-based model must be converted to barrels to track crude and refined products volumes.

Maintaining weight balance in the model is critical in developing the model energy balance. In a volume-based model, energy content of streams can be correlated to density. If a reasonable energy balance is to be maintained in the model, the refinery yield predictions need to be solid, for it is these predictions that impact the energy content distribution of the products. This reason supports the need for robust base and quality shift vector calculations in critical process units, compared to an overly-simplified yield representation.

Energy density of each whole crude and all of the crude fraction streams will be provided in the assay data. All of the finished products will contain energy content based on the component stream energy qualities predictions. The “other input” streams such as VGO, resid, and LPG become part of the energy input balance. The refinery models will have predictions of utility uptakes such as fuel and electricity. The refinery will produce fuel gas, and to the extent required will purchase outside natural gas to balance the system. Other energy inputs such as hydrogen and electricity might be required.

With these model requirements, the overall refinery energy balance can be calculated. The refinery efficiency, defined as energy of the products divided by energy inputs, can be calculated. Often this calculation is performed outside of the refinery model, while the “pieces” of the calculation are provided from the model.

The overall refinery energy balance in a Global Model should be sufficient for most energy applications. The “energy” box could be tightened to include the energy efficiency of each process unit. Energy balances across all the process units within the refinery become extremely complex and are not recommended for World modeling applications. The energy “information” from the model could feed outside programs for more complex, higher resolution calculations which could include product efficiency and burden calculations.

The functional design specifications, process sub-model specifications, and product blending have all been designed and contemplated with energy and emission strategies in the World Model.

Refinery models are not kinetic simulators and will not provide precise energy balances. The models are designed as yield models based on weight and volume, and the energy is calculated from these yields as secondary correlations. This emphasizes that the sub-module process yield predictions and the process sub-module utility requirements need a higher level of detail. Restated, poor process yield predictions coupled with poor process utility predictions ensure poor energy balance calculations.

This is also critical in the hydrogen balance. The hydrotreating units discussed in the sub-modules requires attention because of the impact on the energy balance. Aside from energy balance, hydrogen via steam methane reforming produces CO_2, which is discussed later. Hydrogen impacts the energy balance from the input and output side of the process unit. Energy is required to produce feed hydrogen, whether from the reformer, a hydrogen plant, or purchased hydrogen. On the product side, hydrogen consumption will result in an API gain (density reduction) which will impact the product volume, i.e., lower density equals lower energy. The amount of net energy change is related to both the amount of hydrogen consumed and the heating value of the products produced.

Clean fuels products require more energy to produce. Generally speaking, clean fuel specifications are produced from additional hydrotreating, such as a ULSD hydrotreater, or an FCC pre-treater, or an FCC naphtha hydrotreater. Using the ULSD hydrotreater as an example, it requires extra hydrogen consumption which is directly related to aromatics. As such, the process sub-modules need to reasonably track aromatics, which is called for in the Functional Design Specifications.

If the Global Model specification calls for a single grade of gasoline, this could potentially be an over-simplification as it relates to energy balance, compared to the high-quality clean fuel gasoline. Countries or regions that produce higher percentages of clean fuels will require more energy for these specific products compared to non-clean fuels.

CO_2, GHG, Utilities

The LP will make a prediction of CO_2 produced inside the refinery module battery limit. The elements of CO_2 production in the refinery include:

- CO_2 from the combustion of fuel
- CO_2 from the burning of FCC coke
- CO_2 from Hydrogen Plant (not the reformer)

Balancing the CO_2 from the combustion of fuel comes from the following considerations:

- Logical assessment of all the process sub-module definitions and utilizations which are strongly based on the correct crude feed definitions
- Reasonable predictions of fuel gas production from the process sub-modules, which includes C1s, C2s, and unrecovered C3s
- Realistic estimates of all utility uptakes in the refinery

The logical accounting mechanism for the fuel gas balance is BTUs. On the process side, the BTUs represent the demand. The fuel gas production, coupled with burning of purchased natural gas or burning of residual fuel, represents the BTU supply. Other components can enter the BTU supply such as hydrogen or C4s, depending on how the model is constructed.

Every Btu supplied by a stream has an associated CO_2 produced from the combustion. These factors are readily available in reference materials, and likely already standardized in DOE/EIA models. This accounting ultimately balances CO_2 from fuel gas combustion.

FCC coke burn is another source of CO_2 in refineries. The accurate prediction of FCC coke is directly linked to the FCC sub-module correlations. While a simplified yield correlation on FCC yields might be achieved with a UOPK factor, these yields — including the FCC coke yield — are better represented with the additional variables recommended in the FDS section. Once the FCC coke is estimated, this can be multiplied by a factor to calculate the CO_2 from this combustion.

Last, hydrogen production from the hydrogen plant will generate CO_2. This CO_2, coupled with the CO_2 from fuel gas combustion and FCC coke burn, will provide the CO_2 generated inside the refinery battery limit.

Every refinery region or country will have fuel balances and CO_2 balances that are calculated and reported as output from the model. These outputs can be used on a stand-alone basis or passed to other outside models for additional calculations. Some of this information includes:

- Fuel production by type (C1s, C2s, C3s, hydrogen, unrecovered hydrogen, others as defined in the model design). These are defined by type, not aggregated as “Still Gas,” for example
- Liquid fuel burn (residual fuel oil, plant fuel oil)
- Purchased fuel (natural gas)
- FCC coke burn

- Summary of utilities by unit and overall. Include fuel (BTU), electricity, steam, and cooling water.

SOx emissions from the FCC are generally calculated from the FCC feed sulfur and FCC coke production. The feed sulfur to an FCC is distributed to the products, including H_2S, liquids, and FCC coke. Proper characterization of FCC sulfur distribution is required to estimate the sulfur in the FCC coke. Additionally, SOx from sulfur plants can be included in the refinery SOx balance.

It was previously discussed that the refinery combustion of fuel oil will also be the source for the NOx calculation.

A modeling decision needs to be made on the accounting of CO_2, SOx, and NOx, whether to calculate inside the model or in external models, based on output from the Refinery model. Either method can be used. Performing the CO_2 and NOx calculations within the Refinery model can be achieved, provided the model has been developed with accurate fuel and utility balances. If the SOx calculation is performed inside the model, accurate FCC yields, weight balance, and sulfur distribution are critical. Often the refinery CO_2, SOx, and NOx values — or the basis for the calculations, such as FCC sulfur and coke production — are used as input to other external GHG emissions models for more sophisticated calculations, such as Well-to-Wheel, refinery efficiency, or product burden.

Other Refining Block Inputs

Aside from crude inputs, the refinery model will be designed for other types of typical inputs. These inputs include but are not limited to:

- Purchased Vacuum Gasoil (VGO)
- Purchased Atmospheric Resids
- Purchased Condensates or Natural Gasoline
- C4 LPGs

The VGO and Resid feeds, often characterized as low-sulfur or high-sulfur, would likely come from other refinery locations, and be part of the overall global material balance. In the United States, for example, the source of these feeds is known. In the rest of the World, this data is likely difficult to know the source and destinations. As such, it will be difficult to model all these potential sales and purchase nodes. If the source is known (e.g., the United States receiving topped Urals), then sales from Russia of topped Urals to the United States can be implemented. This method would maintain the World material balance more appropriately. For other areas of the World, if the feed is required and the source is not known, a simple vector purchase of Resid or VGO would suffice.

Another input to the refinery can include Natural Gasoline, which is typically a C5/C6 stream from the upstream production of oil and gas. These volumes might be quantified in the upstream sub-module and can transfer as inputs to the refinery sub-modules for processing or blending. Other refinery (country or region) transfers that could occur include naphtha and distillate range materials. The model can be designed to produce these intermediates, transport to another location, and consumed at the receiving location. Implementing this code is straightforward, but populating this code with reliable production, movements, and consumption will likely prove difficult. On a World Model basis, these volumes are small compared to World crude movement.

Another source of inputs includes C4s, specifically Iso-butane and N-butane. Iso-butane is often moved to balance alkylation requirements. Normal butane is significant to the gasoline blending pool. Often, refinery-produced NC4 is transferred to storage or underground salt domes during the summer and pulled out for blending in the winter. The World Model, while designed for potential summer and winter modes, will most often be used in an average mode. C4 imbalances can be satisfied from mid-stream production. Balancing C4s to the refinery will need to be reconciled with other World sub-modules, including downstream and midstream.

Functional Design Specifications

The Refining Block development is often conceived and outlined using Functional Design Specifications (FDS). The goal of this CDR is not to provide a comprehensive FDS set. The FDS will be developed at a later step, following additional clarification of the upstream, downstream, and other critical sections of the Global Model.

This section is intended to provide strategic recommendations on several key FDS categories:

- Crude Tower cutting and pooling
- Crude stream quality requirements
- SR Blending Destination
- Product Blending
- Sub-module development

The following table provides crude cutting definitions as well as qualities to be carried in the model. These qualities also form the basis for specification blending.

Table 6. Refining Model Qualities

		GASOLINE QUALITIES						DISTILLATE STREAMS								
	C4-	LSR	Lt Nap	LN Front End	LN Back End	Hvy Nap	Nap / Jet	Jet	Jet / Dist	Dist	Dies/ VGO	LVGO	HVGO	Vac Swing	VR	AR
		LS	LN	LL	LH	HN	NK	KR	KD	DS	AG	LV	HV	VS	VR	AR
TBP, degF		49	160	160	185	220	350	400	500	550	650	680	850	1000	1025	680+
EP degF		160	220	185	220	350	400	500	550	650	680	850	1000	1025	EP	EP
**** ALL STREAMS***																
Density, SpGr	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q
Sulfur, Wt%	0	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q
Sulfur, ppm	0	P	P	P	P	P	P	P	P	P	P	P	P	P	P	P
Heat Content	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q
**** Distillation***																
% Off at 200 F		Q	Q	Q	Q	Q	Q									
% Off at 300 F		Q	Q	Q	Q	Q	Q									
Deg (F) @ 10%		P,S	P,S	P,S	P,S	P,S	P,S									
Deg (F) @ 50%		P,S	P,S	P,S	P,S	P,S	P,S									
Deg (F) @ 90%		P,S	P,S	P,S	P,S	P,S	P,S									
Driveability Index		P,S	P,S	P,S	P,S	P,S	P,S									
V/L		P,S	P,S	P,S	P,S	P,S	P,S									
**** Reforming qualities***																
Benzene		Q	Q	Q	Q	0	0									
Aromatics		Q	Q	Q	Q	Q	Q	Q	Q	Q	Q					
Paraffins		Q	Q	Q	Q	Q	Q									
BZ Precursor Index		P,S	P,S	P,S	P,S	0	0									
N+A		P,S	P,S	P,S	P,S	P,S	P,S									
**** Typical gasoline qualities***																
RVP		Q	Q	Q	Q	Q	Q									
Olefins		Q	Q	Q	Q	Q	Q									
RON		Q	Q	Q	Q	Q	Q									
MON		Q	Q	Q	Q	Q	Q									
(R+M)/2		Q	Q	Q	Q	Q	Q									
Oxygen Wt%		0	0	0	0	0	0									
Alcohol, Vol%		0	0	0	0	0	0									
**** Distillate qualities***																
Flash Point							Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X
Pour Point							Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X
Freeze							C	C	C	C	C	C	C	C	C	C
Cloud							C	C	C	C	C	C	C	C	C	C
CFPP							C	C	C	C	C	C	C	C	C	C
Viscosity, cst @ 122F							Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X	Q,X
Smoke Pt							Q	Q	Q							
Cetane Index							Q	Q	Q	Q	Q					
**** Conversion Qualities***																
UOPK Factor									Q	Q	Q	Q	Q	Q		Q
Wt % Concarbon											Q	Q	Q	Q	Q	Q
Basic or Total N2											Q	Q	Q	Q	Q	Q
NC5 Insolubles														X	X	X
Metals (Ni+Van)												M	M	M	M	M

Q is quality to be carried from Assay data
P is "pseudo" quality, calculated from other qualities
S is a "switch" to add code and implement later as deemed appropriate
0 is always a "zero" quality for the stream
X is quality to be calculated with Index Methodology
C is Cold Flow Quality that could be calculated with PPT, or separate Index Method. Not required for Global model, but "place holders" could be added in the design
M is combined Nickle + Vanadium.

The crude tower and assay data are the foundation to the model.

The model will predict density and sulfur throughout, and assay data coupled with predictions throughout the sub-modules and blending will ensure the model stays in both sulfur and weight balance. To be sure, maintaining weight and sulfur balance will require significant coding and correlation development, but it is fundamental to credible modeling efforts.

Another requirement of the model is energy reporting. This begins with the SR energy density off the crude tower and downstream predictions throughout the model. The SR energy density is readily available in assays. The strategy on intermediates will have to be determined after more discussion on the topic.

Heat content on intermediate streams can be correlated to density. Adding heating value correlations as a function of density will require a substantial effort because density must first be predicted at the process units, which is then used to calculate energy. Often, the correlation is a polynomial fit, which would be challenging in many modeling platforms. It should, however, be sufficient to assume an average product density and use a fixed heating value for that product or stream. Whether low heating value (LHV) or high heating value (HHV) is used can be determined by the stakeholders.

Density, Sulfur, and Energy will be reported for every stream generated off the crude tower. The units of sulfur should be decided by the model development team. Sulfur in Wt% or ppm is appropriate. Sulfur in ppm can be defined as a pseudo quality equal to Wt% X 10,000. Sulfur prediction across units should only be done once, so do not make separate code for Wt% and PPM. If the other can be readily calculated using a pseudo quality, then carrying both qualities should be acceptable.

The FDS reference “P” as a pseudo quality. These are qualities that can be predicted using other qualities. For example, T90 can be predicted using E300 and T50 can be predicted using E200, and these correlations are provided in the EPA’s Complex model spreadsheet. Distillation should be blended using “Percent Evaporated” data. For example, E200 represents percent evaporated at 200 F. The blending components into a gasoline pool should blend the E200 quality – the “Percent Evap’s.” The final E200 quality can be used to calculate the blended gasoline T50. Alternatively, a pseudo T50 can be blended for each component. Finally, the gasoline specification could be restated in terms of E200 and not T50. As such, there are different alternatives to distillation blending. The capability of using pseudo qualities may be ultimately be determined by the capabilities of the modeling platform.

Note that the distillation qualities also have an “S” prefix, which means this should be modeled with a switch to turn on and off. Distillation blending might be turned off for a strategic World Model.

There are numerous cold flow quality specifications associated with distillate blending: Freeze, Pour, Cloud, and Cold Flow Plug Point (CFPP). The Global Model only needs to carry a single cold flow quality, for which Pour is recommended. There are reasonable relationships between these qualities. As such, if the user wishes to model Cloud, the Cloud can be converted to an equivalent Pour Point, and the model will capture the cold flow in terms of Cloud.

The “X” in the FDS refers to index methods. Many qualities (e.g., Viscosity, Pour, and Distillation) do not blend volumetrically. There are methods — called *index methods* — in which the base quality is converted to an index, and the index can be volumetrically blended. Depending on the model platform, the index blend can be re-calculated as a non-index quality, or the specification can be expressed as the index and not the quality.

As stated previously, some qualities are defined with an “S,” meaning a recommendation of developing with a “Switch” to provide additional flexibility in the future, or turning off when the quality is not required.

The above qualities defined in the assay data will be the qualities carried throughout the model. In other words, there will not be a new quality generated downstream of the crude tower. The final qualities will be defined will be determined during model development.

The following tables define crude stream blending to pools, downstream units, and products.

Table 7. Crude Swing Cut Mapping

		LSR	LT NAP	HVY NAP	KERO	DIESEL	LVGO	HVGO	VAC RES	ATM RES
POOLS ===>		**LS$**	**LN$**	**HN$**	**KR$**	**DS$**	**LV$**	**HV$**	**VR$**	**AR$**
CRUDE TOWER										
LSR	**LS**	**1**								
LT NAPHTHA	**LN**		**1**							
HVY NAPHTHA	**HN**			**1**						
NAPHTHA/KERO	**NK**			**1**	**1**					
KERO	**KR**				**1**					
KERO/DIESEL	**KD**				**1**	**1**				
DIESEL	**DS**					**1**				
AGO	**AG**					**1**	**1**			
LVGO	**LV**						**1**			
HVGO	**HV**							**1**		
VAC SWING	**VS**							**1**	**1**	
VAC BTMS	**VR**								**1**	
ATM RES	**AR**									**1**

Table 8. Crude Cut Mapping to Units

	LSR	LT NAP	HVY NAP	KERO	DIESEL	LVGO	HVGO	VAC RES	ATM RES
POOLS ===>	**LS$**	**LN$**	**HN$**	**KR$**	**DS$**	**LV$**	**HV$**	**VR$**	**AR$**
DOWNSTREAM PROCESSING									
CRUDE TOWER	X	X	X	X	X	X	X	X	X
NHT	X	X	X						
NHT - ISOM	X								
NHT - REFORMING		X	X						
KERO HDT				X					
DSL HDT				X	X				
VGO HDT						X	X		
RESID HDT									X
FCC						X	X		X
VGO HDT						X	X		X
COKER								X	X
SDA								X	
VISBREAKER								X	

The first table provides some examples of swing cuts. For example, the NK (Naphtha/Kero) can blend up to Naphtha or down to Kerosene. The NK cut does not go downstream for further processing. The destination of NK occurs at the crude tower based on the optimization of the case.

The data above are reasonable recommendations. The final blending strategies will be confirmed during the model development. The above information does not capture all the required blending destinations, also called “blend mapping.” There will be many intermediate streams generated that will require mapping. These cannot be defined until the final process modeling sub-modules and techniques are determined.

Allowing the model to produce a “DUMP” stream is a modeling technique to minimize infeasibilities. If the “DUMP” is priced sufficiently low to dis-incentivize the production, the model will only use it as a product of last resort, and could prevent infeasible solutions. When the product is produced, the user should investigate further.

4. Product Block

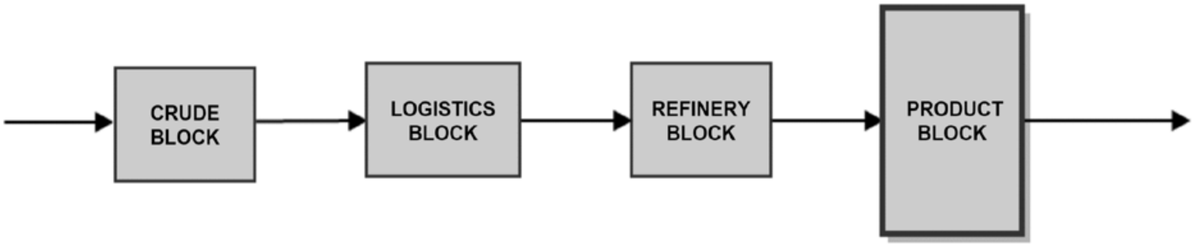

Figure 3. Product Block

Another significant module in the Global Model is the Product Block, which defines many variables such as the number and types of products and the specifications for products. This Block is critical for correctly balancing product supply and demand, which includes production, imports, consumption, and exports. If the Refining Block is inadequately designed to produce the appropriate volumes and qualities of steams, the Product Block will not function.

The definition of products for a World Model can be challenging. The data sources for most World balances define a single product grade. For example, the product “Gasoline” is reported, not Premium and Regular grades. The United States has detailed data on gasoline types: Premium versus Regular, Conventional versus Reformulated, BOBs versus Final Blends. Other counties have limited definition of product grades.

Grades. In the United States, production of gasoline grades is approximately 80 percent conventional versus 20 percent RFG, and approximately 90 percent regular versus 11 percent premium (Midgrade is a small percent that is usually split 50/50 to premium/regular for modeling purposes). This range of options (CG, RFG, Regular, Premium) would be represented by programming 4 grades of US gasoline.

Seasons. Product specifications also vary by season, for which consideration has to be given in the World Model development.

Regions. In the United States and other countries, there are regional specifications for grades, including Northern and Southern grades and CARB to name a few.

Developing dozens of product ID codes for different grades, regions, and seasons is simple from a coding perspective. There are, however, significant requirements in the model for each grade, including collecting and maintaining data, producing each grade in the Refining Block, imports and exports (or movements between PADDs) of each grade by source and destination, and consumption by grade. In other words, knowledge of the full supply/demand balance is required for every produced grade in the World Model, and multiple grades will complicate the balance.

Because regular (lower octane) gasoline dominates most gasoline demand, the definition of a single grade of gasoline could be used as a simplifying assumption, with a blended octane set at the estimated grade volumes. For example, if 85 percent regular at 87 octane is blended with 15 percent premium at 93 octane, the model could produce an average gasoline at 87.9 octane.

Table 9. Average Gasoline Grade

Simplifying Grades		
	Vol %	**(R+M)/2**
Regular	85%	87.0
Premium	15%	93.0
Blend		87.9

In the United States, the distinction of Conventional and Reformulated has become less critical from a modeling perspective. Conventional gasoline, with low sulfur and low benzene, has recipes similar to RFG. In the summer, RFG has a lower vapor pressure, usually around 7 psi. The World Model is not envisioned to routinely run seasonally (although it will have the capability), so an annual average specification can be defined. The volumes, specifications, and grades for all the states and regions are known, so with volumetric and normalized calculations, a single generic US gasoline (although not necessarily recommended) could potentially be developed for the World Model. This standard will likely change if the United States is run in a stand-alone mode or a Global Model.

The discussion points out that a single gasoline grade could be utilized in a World Model, and would provide a reasonable material balance and global representation. While true that the model could in fact have an average single gasoline grade, the developers should have foresight to include code that provides the flexibility to separate the grades by region, quality, and season.

As an example, US gasoline can be separated by region and grade. The following regions will be used:

- PADD 1
- PADD 2
- PADD 3
- PADD 4
- PADD 5, Excluding California
- California

It is not recommended to further divide the PADD regions into sub-districts (e.g., Texas Gulf Coast, Louisiana Gulf Coast). If that level of fidelity is required, a separate US model should be developed.

The grades of gasoline in each region include: CG Regular, CG Premium, RFG Regular, RFG Premium, and CARB, which could be used later if the model is further subdivided. Each grade can be defined with a summer, winter, and average specification. The model can be run in an average mode, with the flexibility to run in a seasonal mode.

Below is an example of defining gasoline grades, which can be used for any region in a country. If a country produces a high volume of a single grade, aggregating might be a reasonable assumption.

Table 10. High, Low, Average Gasoline

	Summer	Winter	Average
Prem (High Quality)			
Volume Percent	15%	15%	15%
RVP	9.0	13.0	11.0
(R+M)/2	93.0	93.0	93.0

	Summer	Winter	Average
Reg (Low Quality)			
Volume Percent	85%	85%	85%
RVP	9.0	13.0	11.0
(R+M)/2	87.0	87.0	87.0

	Summer	Winter	Average
Avg Quality			
RVP	9.0	13.0	11.0
(R+M)/2	87.9	87.9	87.9

The model will contain unique code for three grades of gasoline: Premium (High Quality), Regular (Low Quality), and Average Quality. The model can run in a summer, winter, or average mode.

Table 11. High, Low Average Gasoline Codes

Summary	Summer	Winter	Average
Prem (High Quality)	MHS	MHW	MHA
Reg (Low Quality)	MLS	MLW	MLA
Avg Quality	MVS	MVW	MVA

M = Mogas
V = Avg Quality, H = High Quality, L = Low Quality
S = Summer, W = Winter, A = Average

This same technique can be used for diesel production.

Table 12. High, Low, Average Diesel

	Summer	Winter	Average
High Quality Diesel			
Volume Percent	60%	60%	60%
Cetane	48.0	48.0	48.0
Pour Pt	10.0	0.0	5.0
Sulfur	15	15	15

	Summer	Winter	Average
Low Quality Diesel			
Volume Percent	40%	40%	40%
Cetane	42.0	42.0	42.0
Pour Pt	15.0	5.0	10.0
Sulfur	500	500	500

	Summer	Winter	Average
Avg Quality Diesel			
Cetane	45.6	45.6	45.6
Pour Pt	12.0	2.0	7.0
Sulfur	209	209	209

Summary	Summer	Winter	Average
High Quality	DHS	DHW	DHA
Low Quality	DLS	DLW	DLA
Avg Quality	DVS	DVW	DVA

D = Diesel
V = Avg Quality, H = High Quality, L = Low Quality
S = Summer, W = Winter, A = Average

In a World Model, product imports/exports require special consideration. The United States, for example, exports three grades of distillate: low sulfur less than 15 ppm, medium sulfur between 15 and 500 ppm, and high sulfur over 500 ppm. The United States exports all three grades to Mexico and the Netherlands (although the high sulfur volume is small). Keeping the distillate resolution at this detail for all global regions would be overly complex in a World Model.

The following guidelines can be used for grade development. In most situations, three grades should be adequate, but can change based on the above-mentioned points

Single Grade. This grade will be used for initial product development, model calibration, and model vetting. This grade can be used to simplify the global material balance. The single grade will likely be required if the Refinery Block does not have sufficient detail to produce multiple grades. For example, if a regional Refinery Block does not have a ULSD hydrotreater, Ultra Low Sulfur Diesel cannot be produced.

Multiple Grades. This can be used for regions where there is a clear delineation of separate product grades. Multiple grades will be particularly useful when separating a region from the World Model and in developing enhanced energy and emission balances. Clean products require more energy intensity than low quality products, and multiple grades will provide enhanced resolution on these emissions.

The Product Block can have different definitions for different regions. While this CDR offers representative examples for the Product Block, the final determination is a function of many variables:

- How will the regional product consumption be defined?
- How will the regional product flows (imports/exports) be defined?
- Specific data resolution and granularity on regional or country products.
- Refinery Block model details and process sub-module capabilities to produce the specification grade products.
- Stakeholder requirements.

These variables (and potentially others) must be considered before a final product slate is defined for each region. One region might define high and low quality by octane, and another region might define the quality distinction by sulfur level. Still yet, the model developer team might find it absolutely necessary to produce four variations: Hi Octane Low Sulfur, Hi Octane High Sulfur, Low Octane High Sulfur, and Low Octane Low Sulfur. Flexible model code can accommodate these decisions, and there are many variations, hybrid examples, and strategies that can be implemented — the code does not have to be limited to high, low, and average quality.

Initially, the World Model could only produce, consume, and transport major hydrocarbon products, with no grade distinction. The specifications should be “loose” during model prototype and development. After the preliminary World Model is further calibrated, tested, and vetted, additional product segregation can be done.

During the initial phases of the model development, coding for different grades of products can be developed. These can be turned off until the modeler chooses otherwise. Adding specification grade products to model code requires minimal effort. The final number of products can — and probably will — change as the model evolves. If the model is used to “zero-in” on a specific country on a stand-alone basis, the requirement for more grades becomes more likely.

Below is an example of the production and movements of two grades of gasoline, or a single grade.

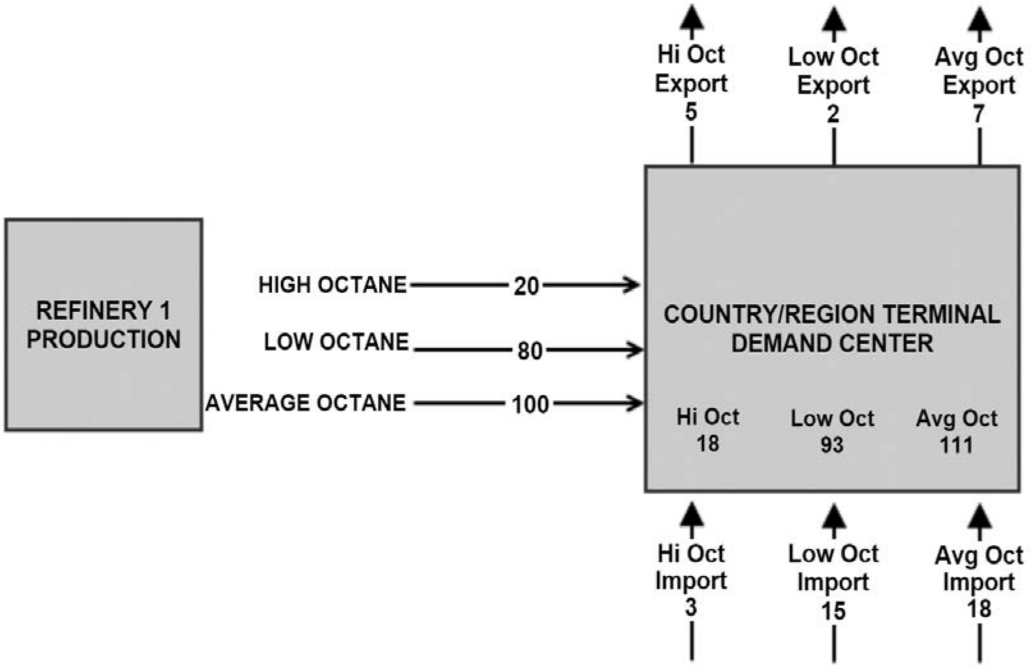

Figure 4. Gasoline Production and Movements

The refinery can be specified to produce a high + low octane, and an average octane. Transportation node vectors will be defined for all three grades:

- Hi Octane From Refinery 1 to Terminal 1
- Low Octane from Refinery 1 to Terminal 1
- Average Octane from Refinery 1 to Terminal 1

- Six more transportation vectors are required for Imports and Exports (these should be netted out, but shown for illustrative purposes)

Even in this simple example, it should be clear that a Refinery Block producing multiple grades is straight-forward. The great challenge is movements of multiple grades to and from regions. Above, three vectors describe the production, while potentially six vectors are required for imports and exports of product. For World modeling and product balancing, a single average grade for many regions may be adequate. For additional resolution, every additional grade creates challenges.

- Data collection
- Transferring the raw data to the model
- Run time, convergence, and infeasibility increases
- Analysis of the runs
- Refinery Block must be designed to produce the grade
- Separate vectors must move the products around the World

Product Movements. Imports and exports of product grade are a significant decision. For example, some regions might have three or more grades of diesel: on road, off road, ULSD, and Home Heating Oil. If the demand is known by grade, and the Refinery Block can produce each grade, then the Product Block can be filled by the Refinery production. Below, there is a direct linkage from the refinery to the demand center. Three grades are produced and three vectors move the products to the demand center to satisfy three demands.

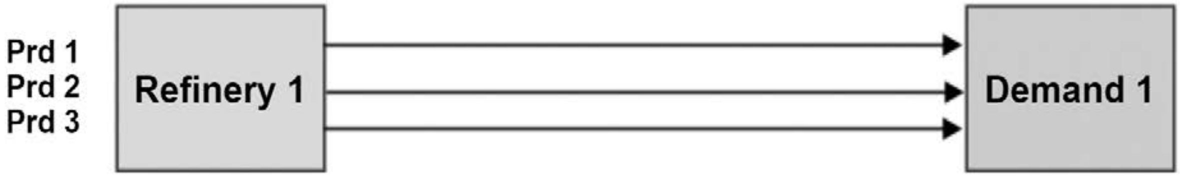

Figure 5. Product Movements: Single Location

If Demand Center 1 cannot be satisfied by the internal production and requires imports, the situation becomes more complex. Additionally, the production of a certain product from Refinery 1 might be an export to another region. The code and model sophistication increases dramatically.

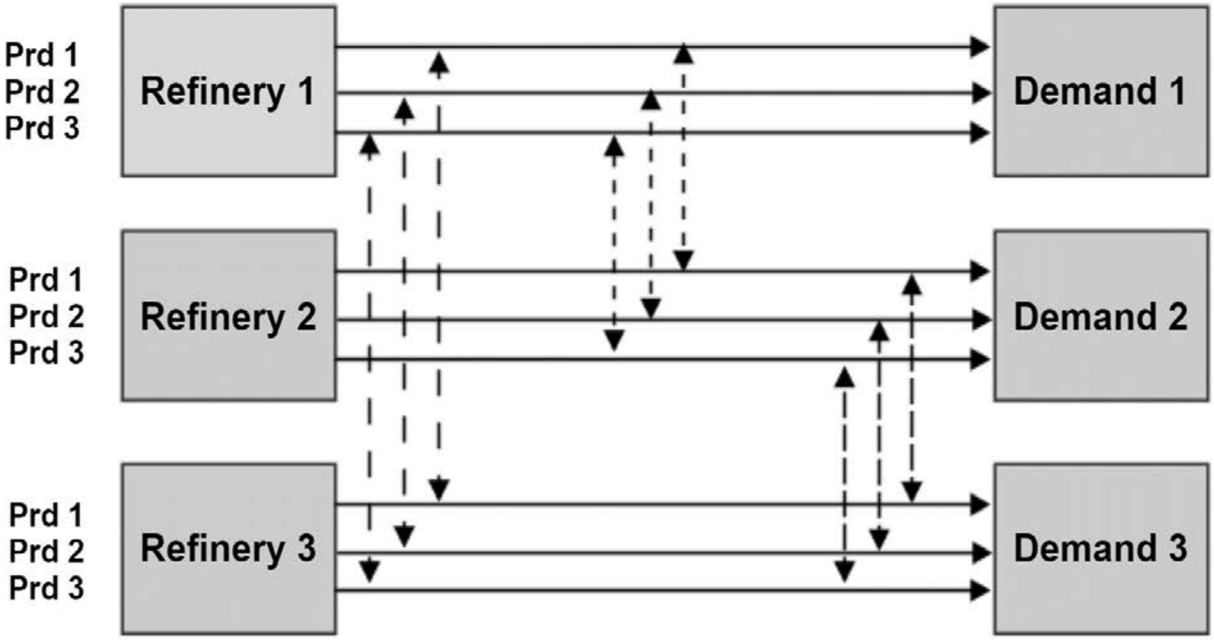

Figure 6. Product Movements: Multi-Location

The above situation allows Products 1, 2, and 3, produced from Refinery 1, 2, and 3, to import and export to Demand Centers 1, 2, and 3. This situation can be further compounded because this diagram assumes that each refinery makes a fungible, matching grade of product to the region which it is importing from or exporting to. In other words, Product 1, 2, and 3 are fungible grades across the regions. If Product 1 from Refinery 3 does not match Product 1 from Refinery 1, then the model will have to make even more grades (e.g., Refinery 3 would have to make another grade to export to Refinery 1).

The number of combinations of regional production to satisfy both internal needs and export requirements can become chaotic from a modeling perspective. The level of complication is clearly related to the Product Block fundamental assumption for how many grades. Producing multiple grades from a refinery to satisfy an internal demand is much less complex than the logistics movements of these grades across the World.

World Model transportation flows and vectors can become very large, very quickly when multiple grades are incorporated. Aside from the model code development, maintaining this data in a meaningful, useable form is challenging. In 2013, the United States exported approximately 145, 13, and 8 MBPD of USLD, <500 ppm and > 500 ppm sulfur diesel, respectively, to the Netherlands, for a total 166 MBPD. One solution would be aggregating all three grades and exporting approximately 166 MBPD ULSD. After all, 87 percent of the export volume is ULSD. Another solution would be to export 87 percent ULSD and 13 percent 500 ppm sulfur by combining the <500 ppm with the >500 ppm. Part of the decision-making process must include the receiving party (the Netherlands), which might have a total country demand of 95 percent ULSD and a very small demand requirement for higher sulfur. In this example, it would be reasonable to simplify the target of 166 MBPD of ULSD export from the United States to the Netherlands, which can be represented by one vector.

The Netherlands example has another layer of modeling decisions. The diesel from the United States might have a cold flow Pour Point specification of 5 F and the Netherlands might be 0 F. So while the sulfur specification is matched, the ULSD cold flow specification does not match. The US Refinery block could be coded to make ULSD with Netherlands cold flow specification. This is not practical if this logic is extended to all the regions represented in the model. Rather, a logical solution would be to assume the US ULSD and the Netherlands ULSD are reasonably consistent. Although the cold flow specification is different, it is a reasonable simplifying assumption.

One assumption is to allow regions to produce a HI, LOW, and/or AVG quality grade of gasoline and diesel (where, HQD = High Quality Diesel). Remember, if a specific region produces the majority of a HQ product, the need for a LQ or AVG is minimized — it is a model developer's decision. Each country will produce these grades with regional specification from its home Refinery Block. The simplifying assumption is that the HI Quality specs from Country 1 will be reasonably consistent with Country 2. With this approach, **one** product ID code is used for both countries for the HI quality grade. The specs will “follow” the home country specifications: HQD exported from the United States to the Netherlands will blend to US specs and transfer to the Netherlands to satisfy HQD volume demand.

The programming logic for the CDR will define a HI, LOW, and/or AVG quality gasoline and diesel using the same product ID code. Each region can have a different specification set and still retain the product ID. Each region will carry a specific country code, and each season will have a unique period code. The tables below show two countries (1, 2) with three products (HQM, LQM, AQM) that can run in three different seasons (S, V, W). If HQM exports from 1 to 2, the transferred specifications will be consistent with 1. If LQM transfers from 2 to 1, the transferred specifications will be consistent with 2.

Table 13. Product Vectors

Refinery 1	Summer	Winter	Average
Period	**S**	**W**	**V**
Spec Set	**a**	**b**	**c**
Refinery	**1**	**1**	**1**
Hi Qual Grade	**HQM**	**HQM**	**HQM**
Low Qual Grade	**LQM**	**LQM**	**LQM**
Avg Qual Grade	**AQM**	**AQM**	**AQM**
Hi Qual Vector	**1SHQMa**	**1WHQMb**	**1VHQMc**
Low Qual Vector	**1SLQMa**	**1WLQMb**	**1VLQMc**
Avg Qual Vector	**1SAQMa**	**1WAQMb**	**1VAQMc**

Refinery 2	Summer	Winter	Average
Period	**S**	**W**	**V**
Spec Set	**a**	**b**	**c**
Refinery	**2**	**2**	**2**
Hi Qual Grade	**HQM**	**HQM**	**HQM**
Low Qual Grade	**LQM**	**LQM**	**LQM**
Avg Qual Grade	**AQM**	**AQM**	**AQM**
Hi Qual Vector	**2SHQMa**	**2WHQMb**	**2VHQMc**
Low Qual Vector	**2SLQMa**	**2WLQMb**	**2VLQMc**
Avg Qual Vector	**2SAQMa**	**2WAQMb**	**2VAQMc**

For the Hi/Low mogas specification quality option, a multi-region model can be defined with two product ID codes: HQM and LQM. These product ID codes do not change from summer, winter, or average periods, on the specification changes.

The following examples can form the foundation for the Global Model. It should be noted that each aggregated region or country can have separate specifications or multiple grades.

The tables show initial recommended product blending specifications for gasoline and distillates. The model will have switches to run an annual average specification or a summer and winter specification. The tables have primary and secondary specifications. The primary specifications are typical limiting production constraints. The secondary drivers could be set at very loose limits, or turned off for simplification. The code is recommended for flexibility. The World Model might have little need to simulate gasoline distillation, but a “break-out” mode of a specific country might require this detail.

Table 14. Gasoline Products and Specifications

GASOLINES	PRIMARY SPECIFICATIONS						SECONDARY SPECIFICATIONS				
	DEN	SUL	RVP	ARO	OXY	OCT	BTU	DIST'L	OLE	N+A	PFF
Grade Subsets											
High Quality	X	X	X	X	X	X	X	X	X		
Low Quality	X	X	X	X	X	X	X	X	X		
Average Quality	X	X	X	X	X	X	X	X	X		
Regional Subsets											
Specific Country	X	X	X	X	X	X	X	X	X		
Aggregate Regions	X	X	X	X	X	X	X	X	X		
Naphtha Subsets											
Full Range Naphtha	X	X	X	X			X			X	
Lt Naphtha	X	X	X				X				X

Table 15. Distillate Products and Specifications

DISTILLATE FUELS	PRIMARY SPECIFICATIONS					SECONDARY			
	DEN	SUL	PPT	ARO	CET	BTU	SMK	FLS	VIS
Jet									
Jet	X	X	X	X		X	X	X	X
Kero or No.1	X	X	X	X		X	X	X	X
Diesel									
Grade Subsets	X	X	X	X	X	X		X	X
High Quality Diesel	X	X	X	X	X	X		X	X
Low Quality Diesel	X	X	X	X	X	X		X	X
Average Quality Diesel	X	X	X	X	X	X		X	X
Heating Oil	X	X	X			X		X	X
Regional Subsets	X	X	X	X	X	X		X	X
Specific Country	X	X	X	X	X	X		X	X
Aggregate Regions	X	X	X	X	X	X		X	X

The following tables are for residual fuels and recipe blends. Residual bunker fuel specifications are consistent across the World but movements are small compared to gasoline and distillates. A recipe blend has no specification; rather, it is a volume. For example, asphalt can have a recipe of 100 percent vacuum resid without any specification. The "DUMP" product allows any steam in the refinery model to "leave the system," and is a modeling technique to prevent infeasibilities. The World Model should initially be set to produce a single mix of C3 and C4 LPG. As the model evolves, and as data resources are improved, more detail can be implemented. The developer is not "locked-into" producing multiple grades of residual fuel oil at any location, for example. Any given country can produce a single grade determined by a variety of factors.

Table 16. Other Products and Specifications

RESIDUAL FUELS	**PRIMARY**			**SECONDARY**		
	DEN	**SUL**	**VIS**	**BTU**	**PPT**	**FLS**
RFO Grade Subsets						
LS RFO 380 cst	X	X	X	X	X	X
HS RFO 380 cst	X	X	X	X	X	X
LS RFO 180 cst	X	X	X	X	X	X
HS RFO 180 cst	X	X	X	X	X	X
Plant Fuel Oil	X	X		X		

INTERMEDIATES	**PRIMARY**		**SECONDARY**				
	DEN	**SUL**	**BTU**	**CCR**	**UOPK**	**VIS**	**PPT**
VGO (LS & HS)	X	X	X	X	X		
ATM RES (LS & HS)	X	X	X	X	X	X	X

RECIPE BLENDS
World LPG (C3 & C4)
LPG Grade Subsets
C3/C4 Mixed LPG
Refy Grade Propane
Refy Grade Propylene
Mixed C3's
Mixed C4's
Specialty Chemicals
Solvents
Asphalt
Lubes
Waxes

DUMP STREAM
Dump Stream

The model must volumetrically balance on the product slate. While some data balances include the definition of “other” products, there is no production of “other” in the World Model. The model will produce a full range of products and will maintain weight balance.

There are no inventory adjustments or inventory draws to balance the system, which would be a questionable strategy to allow when evaluating future, predictive scenarios.

5. Crude Block

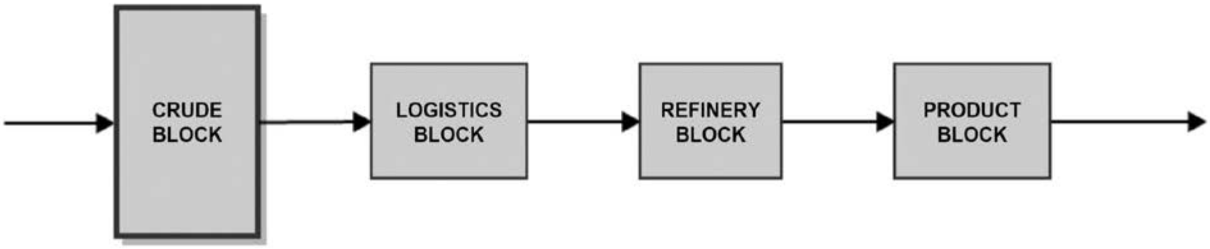

Figure 7. Crude Block

This section discusses strategies for Crude Selection. While the Refining Block and Product Block are critical in any modeling system, the crude methodology is also highly influential on the outcome of the World Model operations. The quality of Product Block outputs is strongly correlated to the Refining Block, and the quality of Refining Block outputs is strongly correlated to the Crude Block. Whether the World Model is developed with simplistic assumptions or advanced simulation representation, one variable is consistent: the Crude Block.

The Crude Block strategies need to capture two fundamental goals:

- Sufficient fidelity for refinery operations
- Sufficient fidelity for World balancing

On the refinery operations side, the concept of aggregate modeling should be re-examined. For example, if 10 individual refineries are aggregated, this essentially creates a large, single refinery. When the estimated crudes from these refineries are volumetrically combined into a single crude, the aggregate crude will reasonably “fill-up” the configuration. When the configuration and crude are matched, a representative product yield will follow.

The concept of aggregation might imply an overly simplistic approach — it is not. The aggregate crude calculation is based on significant data collection and analysis. As much effort goes into developing a 5-crude slate input to a refinery model as a single aggregate crude slate.

The aggregate approach for both the Refining Block and Crude Block is standard for large multi-refinery applications. The crude types, configuration data, or production data will almost always be the weakest link, not the aggregation methodology. Regardless of an aggregation method, the World Model will solve to a material balance, a standard which data sources do not have to maintain.

A bottoms-up analysis is a strategy to develop and analyze the Crude Block assumptions and suitability for a region. In the Refining Block, data exist for all the bottoms conversion units (e.g., coker, visbreaker) and heavy production (e.g., residual fuel oil, asphalt), collectively called *bottoms potential*. The United States has about 20 percent bottoms potential; if the proposed crude slate vacuum resid is substantially different, a potential mismatch can be easily identified without even running a model. The average US API is about 31, and Saudi Medium is about 32 API with a vacuum resid content of about 21 percent —certainly a reasonable starting point.

As another Crude Block strategy, the reported vacuum tower capacity can be used as an initial start to estimate the atmospheric resid content of the crude slate. Russian Urals has about 43 percent atmospheric resid, and Russian reported vacuum capacity is about 38 percent of crude.

The US bottoms potential and Russian Urals atmospheric resid are presented to strongly reiterate that the correct characterization of the crude input — regardless of a single blend or individual crudes — into an aggregate region is fundamental to the success of the World Model.

With that fact established, it should also be accepted that a single aggregate crude could be successfully implemented to balance aggregated regions at a strategic level. This is not, however, the final recommendation for this CDR or World Model strategy. The final recommendation will ultimately be a “hybrid” solution, where some regions could be characterized by a single crude, and others by multiple crudes.

The next example compares the flows and strategies between separate crude feeds and an aggregate crude feed.

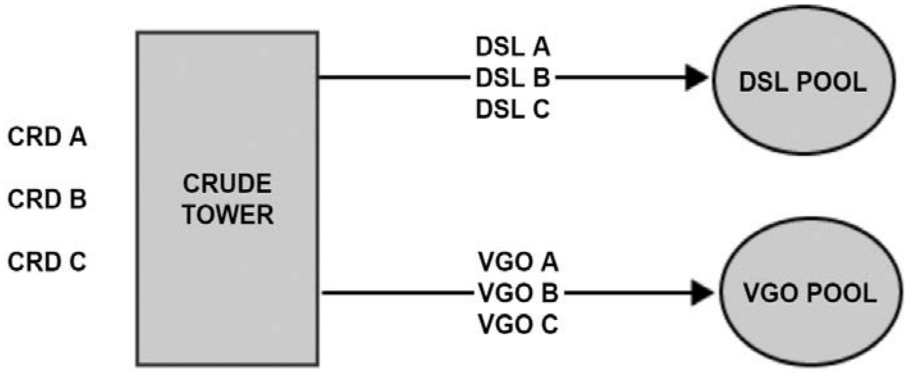

Figure 8. Three Crude Feeds to Downstream Pools

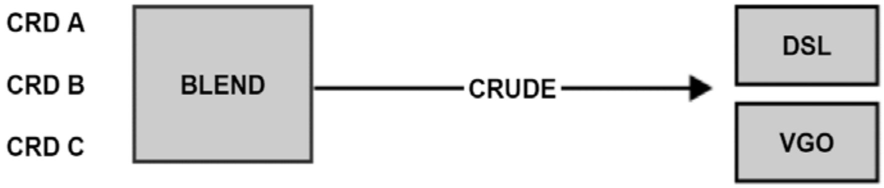

Figure 9. Aggregate Crude Feed

At the top are three crudes entering the aggregate model, producing two streams (i.e., diesel and VGO) from each crude**. If pooling — an important detail — is implemented, and a single tower is used,** the diesel from each crude will combine into single pool. The same occurs with the VGO pool. In the aggregate system, the three crudes are pooled to create a single aggregate crude (volumetrically blended identical to the ratios in the top diagram). The aggregate crude runs through the crude tower to produce a DSL and VGO pool. The end result is essentially identical.

The three-crude system has potential benefits. For example, if Crudes A, B, and C are Saudi Light, Mars, and WTI, this provides some modeling advantages:

1. Reasonable limits can be applied to specific crudes. If Saudi Light is estimated to be 25 percent of the crude slate, a minimum can be set at 20 percent and a maximum can be set to 30 percent. This provides tremendous modeling flexibility versus aggregating the crude to an exact 25 percent. After all, the data sources will never be reported to this rigor.
2. If pricing and marginal value analysis is being performed, transparent prices are available for Saudi Light, Mars, and WTI. This is a significant benefit in model analysis. Differentials, crude values, and marginal values can be more easily quantified because of the separate crudes and the unique price sets. There is no such transparent pricing in an aggregate crude mix.
3. There could be a quality in the Saudi Light crude that is extremely detrimental to the system. This will show up as a strong disincentive (marginal value) on the Saudi Light crude, or a stream from the Saudi Light crude. This would be extremely challenging to determine in an aggregate crude.

There are also arguments that a crude blend can be a rational approach. For example, Nigeria has significant production of Medium Sweet crude: Bonny Light, Forcados, and Escravos. These are all relatively consistent in quality and could be blended up volumetrically by actual production, to develop a Nigerian MDSWT. The blended Nigerian MDSWT could be balanced among all export destinations. The difference is this example versus the Saudi Light, Mars, and WTI example above is that all components of the Nigerian blend come from the same country/regional source, and all have very similar whole crude qualities (API, Sulfur).

If the Nigerian crude blend technique is not used, the model developer can choose the “best” crude to represent Nigerian MDSWT using a logical rationale. Here, Bonny Light is the highest volume production, and could be chosen on this basis. Another logical test is analyzing the individual APIs from the production sources and choosing based on the “best” match.

So, while the answers from a single aggregate region would be similar to those from the multiple crude stream, the analysis on a multiple crude system is enhanced. This is especially significant when attempting to balance all of the Saudi Light production, for example. A simple balance row of Saudi Light to all the regional refineries equals the estimated production. This simple concept is challenging when Saudi Light is a component of a crude blend.

In the crude tower discussion, it was recommended to develop the structure for two crude towers, possibly three. If two crude towers are added to an aggregate system, a hybrid system can be envisaged:

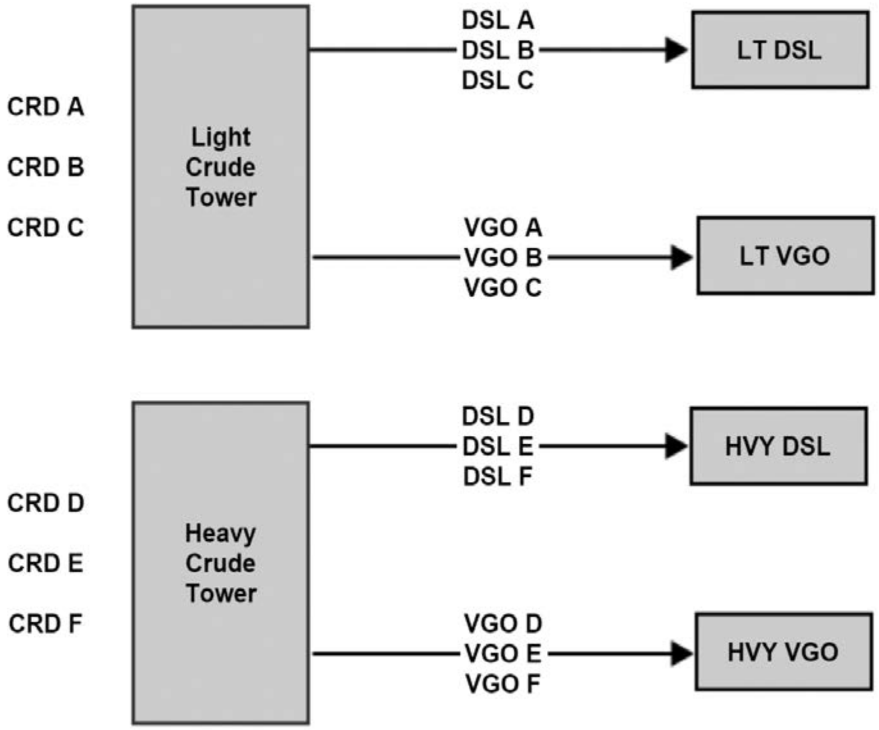

Figure 10. Two Tower Methodology

Two crude towers could be used to designate Light and Heavy, or Sweet and Sour. Limits can be added to the tower that would prevent crudes with a sulfur higher than 1.0 percent (or whatever value is selected) to process through the Light / Sweet tower. This hybrid provides additional benefits over the single aggregate system. As an example, the light VGO might bypass the VGO HDT and go directly to the FCC, while the Heavy VGO could be routed to the VGO HDT. Similar strategies could be utilized throughout the aggregate configuration.

This provides rationale that sufficient fidelity for crude operations can be achieved with a single aggregate crude, or a single representative crude. The fidelity of the single crude tower will be enhanced—but is not required—using a hybrid approach, whereby an additional level of refinery operations can be achieved, coupled with the use of multiple crude types. While the single aggregate methodology is likely easier for convergence and optimization, it does have less model flexibility, which can be an acceptable consequence, depending on the region being modeled.

If a single crude tower is utilized in a specific region, the user may benefit from having the code for a second crude tower. This allows additional resolution if the region is separate from the World Model for additional studies, or enhanced analysis.

There is no generic rule to establish a singular protocol for the World Model. These decisions will be made after stakeholder input, modeling discussions, and weighing the benefits and weaknesses for each aggregate region. The end result should be a hybrid approach and a function of region definition, domestic production, imports, range of crude quality, and potential necessity to “drill down” on specific locations or sub-regions.

Crude Selection. There are many variables that go into the definition of crude selection for the model. A generalized rule does not exist to define the crude characterization for the model. As with all Blocks, hybrid approaches will prevail and still be consistent with model design, stakeholder requirements, and the overall balance of complexity with reasonableness.

General guidelines and strategies follow. The ability of the model to properly characterize World operations has many variables. One of the significant variables relates to vacuum resid (bottoms up) balancing. The amount of resid destruction is critical for balancing conversion units and RFO production. This in turn drives issues such as hydrogen balances, other unit operations, efficiency calculations, and emissions to name a few.

Resid balancing begins with the appropriate crude methods. As a rough rule of thumb, every API degree is “worth” a little over 1 percent of vacuum resid. As a representative example below, the difference between a 28 API crude and a 38 API crude is about 12 percent vacuum resid.

Table 17. API and Vacuum Resid Content

	Approximate Relationship of Crude API and Vacuum Resid					
	Heavy		Medium		Light	
CRUDE API	25.5	28.0	30.5	33.0	35.5	38.0
VAC RESID	27%	24%	21%	18%	15%	12%

It will be challenging to meet a reasonable material balance tolerance for an aggregate country if the model’s vacuum resid is 12 percent different than actual.

For illustrative purposes, the average API of the World crude production is approximately 33 API, a medium crude. Using a 5 degree separation between grades, the World’s heavy and light would be around 28 and 38 API. In these terms, a representative 33 API blended crude would probably be a reasonable fit for a World Model represented as a single aggregated refining system. Obviously, this has insufficient resolution, so additional fidelity is required.

The next logical option would include aggregating all the heavy into a blend, and creating a blend of light, resulting in a two-crude methodology. An extension of this is to aggregate into a Light, Medium, and Heavy blend. This resolution makes perfect sense from a strategic level, but additional information is required:

- The volume of the crude production
- The country origin of crude production

The following table has World crude production volumes from the EIA. The table also includes representative crudes for the country, and is not intended to be a complete set, nor does it contain the production volumes by grades or types. It would be reasonable to define some level of aggregation blending based on the region of production, shown here as Middle East (ME), North Sea (NS), West Africa (WAF), North Africa (NAF), South America (SA), Eastern Europe (EE), and Asia Pacific (AP). The term “blend” does not necessarily translate to a formal blend by assays; it could imply aggregating all similar crudes as a representative crude (e.g., Saudi Light for all ME medium sour crude).

The table represents volumes of countries over 500 MBPD. These aggregates could be further separated, such as Middle East Light and Middle East Heavy using crude blenders or terminal techniques. Volume of crude could be a reasonable criteria to separate the crude from a blend, such as modeling Saudi Light, and blending the remaining light Middle East into a blend. Geopolitical and anticipated modeling scenarios might warrant separation as well.

There are many considerations that will go into the final crude selection criteria, such as:

- Mexican Maya and Isthmus have about 13 API degree separation; Venezuela BCF and Mesa have about 15 API degree separation. All crudes have different export destinations.
- Australia (and others) has crudes ranging from 20 API to 60 API.
- The United States might require more or less crudes depending on anticipated disaggregating.
- Canadian crude decisions will be a strong function of the fidelity developed within both Canadian and US aggregate models.
- Should World marker crudes such as Brent and Dubai be individually modeled?

Table 18. Crude Production Volume and Blending

Country Production Volume (EIA 2010)			**Potential Crude Blends**						
COUNTRY	**000 BPD**	**Typical Crude**	**ME**	**NS**	**WAF**	**NAF**	**SA**	**EE**	**AP**
Saudi Arabia	10,642	Saudi Lt, Saudi Hvy	ME						
Russia	10,157	Urals						EE	
United States	9,685	WTI (LLS); WTS (Mars); ANS; Shale							
China	4,363	Daqing							AP
Iran	4,243	Iran Hvy, Iran Lt	ME						
Canada	3,442	WCS, Long Lake, Lt Swr Bld							
Mexico	2,979	Maya & Isthmus							
UAE	2,813	Murban	ME						
Brazil	2,712	Marlim					SA		
Kuwait	2,460	Kuwait	ME						
Nigeria	2,459	Bonny Lt			WAF				
Venezuela	2,405	BCF 17 and Mesa					SA		
Iraq	2,403	Basrah	ME						
Norway	2,155	Ekofisk		NS					
Angola	1,948	Cabinda			WAF				
Algeria	1,881	Saharan				NAF			
Libya	1,789	Es Sider				NAF			
Qatar	1,788	Qatar Marine	ME						
Kazakhstan	1,609	CPC Blend						EE	
United Kingdom	1,406	Forties		NS					
Azerbaijan	1,045	Azeri						EE	
Indonesia	1,042	Indonesia Blend							AP
India	965	Bombay							
Oman	870	Oman	ME						
Colombia	806	Cusiana, Cano Limon					SA		
Argentina	791	Candon Seco; Medantino							
Egypt	735	Suez				NAF			
Malaysia	683	Tapis							AP
Australia	604	Gippsland							AP

While the number of crudes contained in the model is a significant decisions, the emphasis should first be on whether the model has sufficient choices to capture the goals of the World Model, not a specific target number. It would be incorrect to generalize that the model will solve quicker and be more stable because the number of crudes was held to “X.” In fact, carrying a few additional crudes could potentially make the model more stable because the extra crudes were a better fit to the constraints placed in the model.

In the United States, for example, the type of crude quality import is known (e.g., Saudi Light and Saudi Heavy). This will not be known in most regions of the World and will be a factor in crude selection. If a country receives 100 MPBD of Total Saudi Crude, and Saudi has been defined by Light and Heavy, the model can carry a group code so that SAL + SAH equals approximately 100 MBPD.

The following additional points should be considered:

- Use actual, representative crudes such as Bonny Light as first approximation.
- If a country has high API variation on product fields (e.g., BCF and Mesa), a blend may be required, and should be blended on a volumetric basis. The blend will dilute the modeling impact to export light to one region and heavy to another, because the total blend will move as a single crude.
- Develop crude representations on a regional basis — do not blend light sweet North African with North Sea to produce a Light Sweet.
- Crude destinations should be considered. North African and West African should not be consolidated as Africa, because the export destinations are unique.
- Imports and Export transportation vectors are to be considered. Defining a Middle East Light and a Middle East Heavy will require approximately twice the vectors.
- Over 80 percent of the World’s crude production is defined in 20 countries, and within these countries there are numerous aggregation potentials (e.g., Middle East Light Sour).
- A World Model with more country segregation will likely require more crudes; this should be balanced. A model with 30 countries and 3 crude types is likely imbalanced similar to a 5-country model with 10 crudes.
- The knowledge base will accumulate data on production, import, export, net movements, and quality. The LP model will be designed with reasonable constraints to match known movements. The selected crudes will not have large degrees of “float.”
- The crude decision in the prototype model can change during development and testing; the World Model does not have to be “locked-in” and can be designed with additional crude typing for situations where disaggregating is envisioned.
- Crude selection will be designed with consideration for the Upstream and Logistical Blocks strategies.

- It would be reasonable to identify around 15 crudes as an initial point for the Global Model using a combination of blends or a single representative crude (e.g., West African Blend or Bonny Light).
- Develop model with up to three crude towers per region. If only a single tower is used, the capacity for the other two is **fixed** to zero. The flexibility remains to run a single crude train, or multiple crude trains, and the effort to code three towers is minimal.

6. Logistics Block

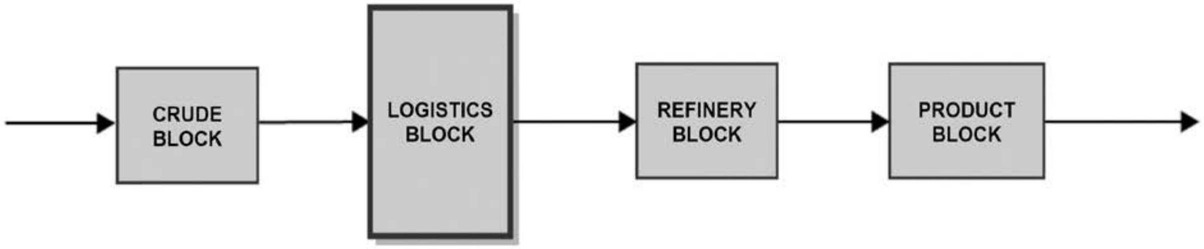

Figure 11. Logistics Block

The movement of feeds and products through the Crude, Refining, and Product Blocks is accomplished with the Logistics Block. This definition includes the regional balancing of supply and demand for all feeds and products to and from these blocks.

Transportation and logistics routes and costs can be developed within the World Model, and do not have to be separated from the other Blocks. In the World Model, crude supply and product demand regions can be represented as Terminals. All of the inputs and outputs are balanced in the Terminals. Each regional configuration will have a Terminal for refining crude, producing products, importing products, exporting products, and consuming products.

Each upstream crude supply location will have a unique crude terminal. The upstream crude model will impact the design of the downstream refining modules. Below is an example of how the upstream crude production module could interact with the downstream system.

In this example, there are three fields producing light crude and three fields producing heavy crude. The crude is aggregated by type and characterized as Saudi Light and Saudi Heavy. As such:

- Three light crudes feed crude Terminal A, resulting in a Saudi Light crude
- Three heavy crudes feed crude Terminal A, resulting in Saudi Heavy crude

The option will remain if the model produces an actual “blend” of the crudes (Middle East Light and Middle East Heavy) or uses a specific crude assay (SAL or SAH) as the representative produced crude.

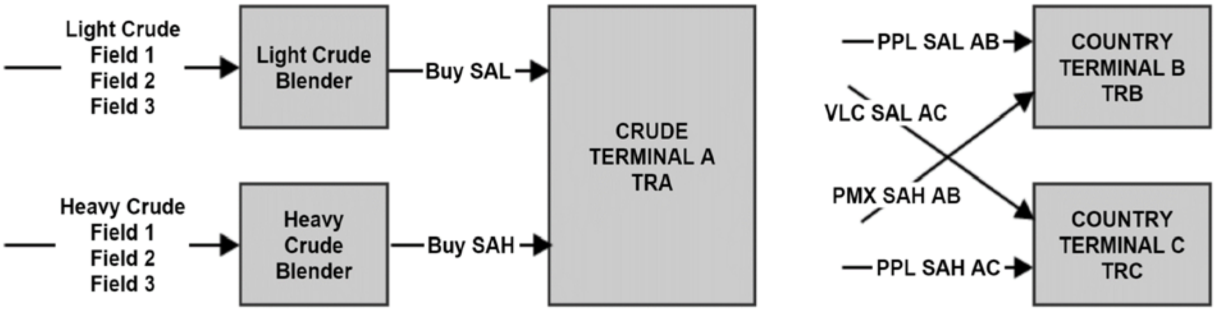

Figure 12. Crude Terminal Methodology

After the crude is collected in Crude Terminal A, the movements can be coded. If SAL is transferred from the Country A terminal to the Country B terminal via pipeline, that could be represented by a vector: PPL SAL AB. This movement will have a specific price. Additionally, this movement can have volume constraints, so that limits can be placed on the vector (MIN and/or MAX).

In this simple example, there are four movements, and each can have a unique price and volume constraint:

SAL via Pipeline from A to B:	PPL SAL AB
SAL via VLCC from A to C:	VLC SAL AC
SAH via Panamax from A to B:	PMX SAH AB
SAH via Pipeline from A to C:	PPL SAH AC

Group constraints can be defined to limit the total number of movements. For instance, if Country B can only take 10 MBPD of crude from Terminal B:

- PPL SAL AB + PMX SAH AB < 10

Country Terminal A & B will need a cost to purchase and receive the crude. Each mode above has an associated movement cost; here, for example, PPL SAL AB is $2.00/Bbl. The FOB price for SAL defined in the model is $100.00, making the purchase price of SAL to Country B $102.00 for this mode of transportation. This represents the delivered CIF price.

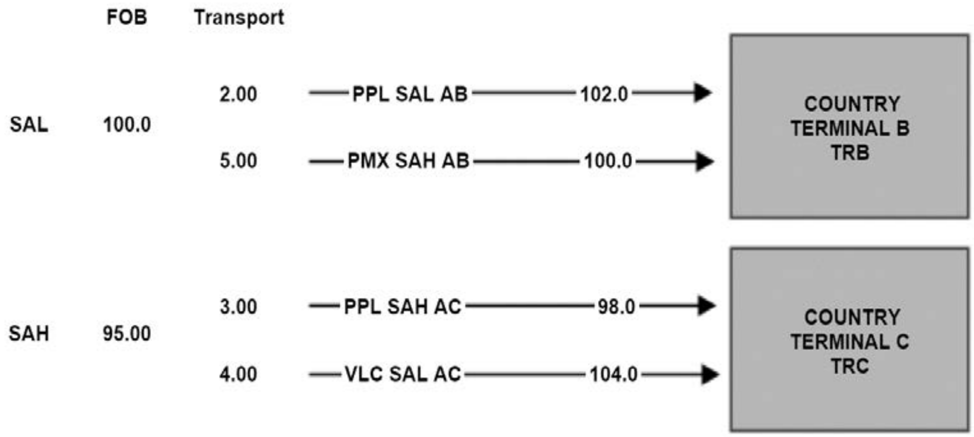

Figure 13. Crude Purchase at Country Level

Alternatively, the following mechanism can be used to allocate the costs for the World Model. Below, Terminal A purchases the SAL crude for $100.00. This cost could represent cost of production, which is the FOB price of the crude. The PPL SAL AB vector costs $2.00/Bbl, which represents a delivered CIF price of $102.00.

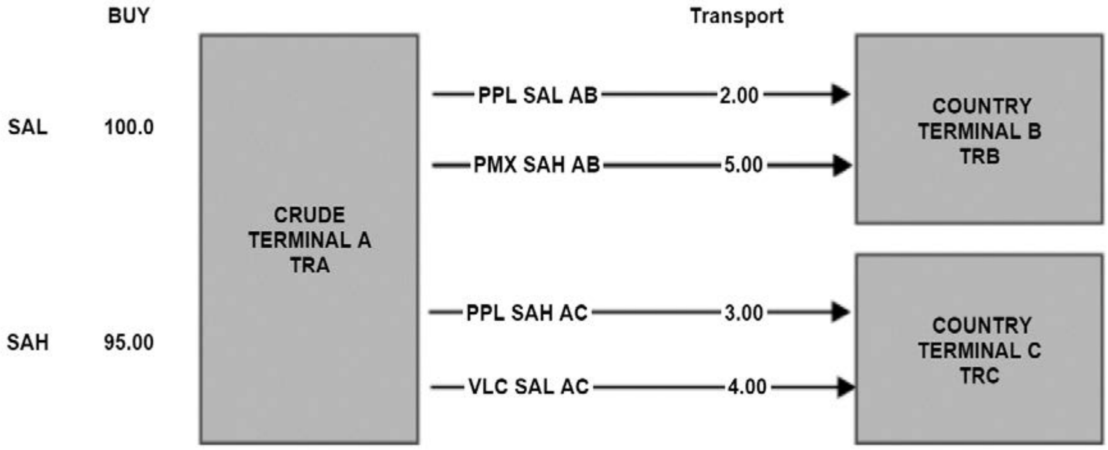

Figure 14. Crude Purchase at Field Location

From the above example, the following can occur:

- Multiple crude terminals throughout the World that can export throughout the World.
- Crude terminals do not have to match the country or regional terminals, but do have to balance on volume (input = output), unless an inventory option is added to the crude terminals.

- Crude terminals can match the region; for example, the Russia crude terminal would match the Russia region.
- Complete flexibility on modes of transportation between terminals, including the number of modes, the cost of mode movements, and the source and destinations.
- Additional groupings such as total SAL, total Port, or total Pipeline constraints can be developed.
- If desired, Crude Terminals can be combined. For instance, Nigeria Crude Terminal can combine with Angola Terminal to equal West Africa Terminal.

Terminal B and C above represent a region or country in the World Model. Once the crude(s) are input to the terminals, they move to the regional or country Refinery. The B Terminal feeds Refinery b, and the C Terminal feeds Refinery c. Each Refinery produces Product 1 and Product 2. The movement of crude to the refinery and product from the refinery is represented as a transportation vector. The refinery and terminal are assumed to be at the same location (same region or same country), and the cost to move crude and products between the refinery and terminal should be considered zero. However, a vector must be added to the model to perform the supply/demand accounting at the terminal level.

The hydrocarbon supply and demand balance for each country or region will occur at the Terminal level. It is at the terminal that imports, exports, production, and consumption occur for all feeds and products. The regional production is represented by the movement from the refinery to the Terminal.

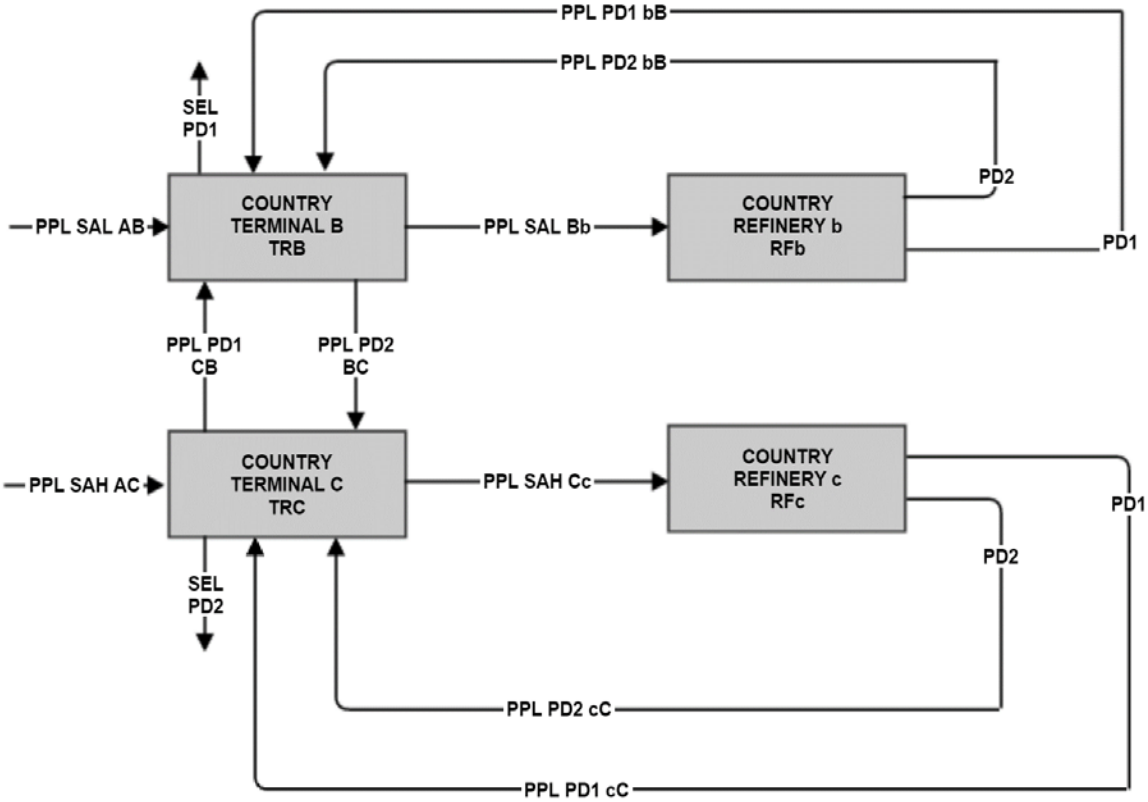

Figure 15. Country Refining and Terminal Overview

The above example is on Country B and C, Refinery b and c, and Products 1 and 2. For simplicity, all movements are defined as pipeline (PPL) movements. Imports and exports of the products occur at each terminal. Here, Product 2 exporting from Country B to C is represented as: PPL PD2 BC. Product 1, exporting from C to B is represented as PPL PD1 CB.

The consumption of a product is represented as a sale of the product from the Terminal.

Terminal B sells Product 1 , and Terminal C sells Product 2. Here, if Country B has a 10 MBPD demand on Product 1, this would be represented as selling 10 MBPD of Product 1.

The balance row on each product in all regions of the World Model will equal zero. The supply is imports + production. The demand is sales (consumption) + exports. For Product 1 (PD1) at Refinery b, the following vectors are formed:

- Production: PPL PD1 bB (Produced at Refy b, Transported to Terminal B)
- Imports: PPL PD1 CB (Transported from Terminal C to Terminal B)
- Exports: PPL PD1 BC (Transported from Terminal B to Terminal C)
- Consumption: SELL PD1 TRB (Sale from Terminal B)

This method allows for flexibility throughout the World Model with respect to products. Multiple transportation modes, costs, and volumes can be defined to and from all Terminals.

Terminals are the balance point for all products, above Product 1 and 2. However, a simplifying technique can be used. There will be many situations where there is no need to balance a product at a terminal. For example, if asphalt is produced and there is no transfer between terminals, the product can be sold directly off the refinery. This saves a transportation vector. Restated, the Terminal is used to balance imports and exports with production and sales. If there are no imports or exports, the demand equals production.

Intermediates and blending components require specific consideration. This is best exemplified using ethanol-based E10 gasoline. There are at least two methods to model this:

- Produce BOB as a refinery product, transfer the BOB to the terminal, bring ethanol to the terminal, and blend the finished gasoline
- Bring ethanol to the refinery, produce the finished gasoline with ethanol, and transfer the finished gasoline to the terminal

The latter is recommended, although there could be unique situations to model otherwise. The terminal points “notionally” serve as supply demand points, not technical points of blending. The gasoline specification blending occurs in the refinery bounds, and carrying specification requirements to the terminal can create confusion. Yes, in this example, a specification E10 BOB can be produced at the refinery and blended at the terminal without terminal specifications. However, if another bio-component is brought as a diesel blending stream, there is no equivalent “biodiesel-BOB” to produce at the refinery that blends to a fungible diesel at the terminal. This would force specification blending at the Terminal. Ultimately, these decisions have user preference issues, but final considerations will be determined during prototype design whereby a specific requirement might force the decision one way or the other.

Note that the “pipeline” movement from the crude terminal to the regional terminal PPL SAL AB could bypass the terminal and go directly to the refinery. The value of sending the crude through the terminal is that a regional material balance is better represented across the terminal. The solution does not change. Movements of crude from the terminal to the refinery and from the refinery products back to the terminal are often expressed as a “zero” cost, assuming the locations are the same.

From the above discussion, the World Model will have the following characteristics:

- Flexibility on the number of crude supply and demand regions that can be the same or different from the refining regions. This is accomplished with the use of terminals and transportation vectors.
- Product flexibility similar to crude system
- Flexibility on the number of transportation modes with different routes and costs for both crude and products
- Combined limits can be placed on transportation modes and terminals
- Transportation expansion costs can be approximated in the World Model
    - Example: Existing Pipeline A to B costs $1.00/Bbl up to 10 MBPD, and incremental capacity up to 20 MPBD costs $2.00/Bbl
- Crude terminals can be defined to receive data from the upstream model and transport to the downstream refining models, via Country Terminals
- Crude types and prices can be developed by countries and aggregated to a region, and further transported to other countries or regions
- Crude types can be expressed as an aggregated crude blend, or by individual grades of crudes

Biofuels, Downstream Gas, and LPG

There are other World sub-models that are envisioned to interact with the Refining module, including biofuels, natural gas, and LPG market drivers. A natural mechanism for these impacts is in the terminals, or country supply/demand centers.

These interactions can take on different forms depending on the types of streams involved. For example, a biodiesel product can be produced and transferred into any regional terminal. The total diesel product can be specified at 100, but can be combined with a grouping that includes both hydrocarbon-sourced and bio-sourced diesel.

If a bio-stream is a blending component to a hydrocarbon-based pool, the stream can enter the refinery block — where hydrocarbon-based diesel is produced — and blended in the Refining Block to produce diesel. It was previously discussed that bio-components could be modeled at the refinery block or the supply/demand terminal, but the former appears to be a more logical strategy.

Terminal movements as supply/demand centers can be extended to natural gas and LPGs. Data can transfer from these modules, to the Refinery module, and back. Similar consideration on where the streams flow must be applied. If natural gas is supplied to the supply/demand terminal, then a vector must be used to move the gas to the refinery for consumption. It seems more logical to send the gas directly to the Refining Block.

Logistics External to the Refinery Block

While logistics can be modeled within the framework discussed above, modeling logistics in a separate model should be evaluated. In this scenario, crude (quantity and quality) would be passed from the Crude sub-module to the Logistics model, which is separate from the Refinery Block. The separate Logistics Block transfers crude to the Refinery Block. The Refinery Block products would transfer to the separate Logistics Blocks where the supply/demand balances occur.

Below, when logistics is modeled inside the Refinery Block, the crude model feeds the crude terminal (inside the Refinery Block), where it is distributed to the country terminals (inside the Refinery Block). The Refinery Block receives and transforms crude into products. The products flow back to the country terminal whereby all the supply/demand balances occur (inside the Refinery Block). The crude model is separated, but all the other “transactions” are in the Refinery Block

When the logistics is modeled outside the Refinery Block, the movements are similar, but the data “hand-offs” occur at different locations. The Logistics Block sends the crude information to the Refinery Block for transformation. The Refinery Block sends production information to the Logistics model for supply/demand balancing. In essence, the Refinery Block becomes a “Refinery Gate”-based model. The Logistics model sends data to the Refinery Gate, and the Refinery Gate products go to the Logistics model.

The Logistics model (either inside or outside of the Refinery Block) will have fundamental characteristics for marine movements: ship size, port restrictions, world-scale rates, and other information that might be required to optimize freight movements. Pipeline vectors will also populate the Logistics model.

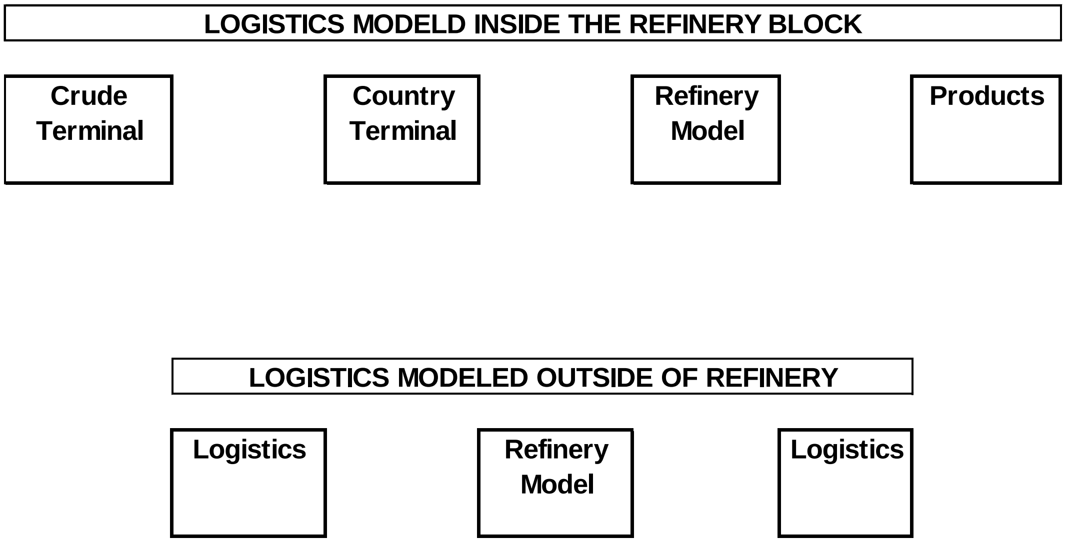

Figure 16. Logistics Model Inside & Outside of Refinery Block

The decision of where to model logistics (inside or outside of the Refinery Block) is critical. The decision will fundamentally be developed based on the type and architecture envisioned in the Logistics model, and how the Logistics model will interact with other sub-models used in the World model. Data transfers and strategic protocols need to be assessed. Logistics — whether inside or outside the model — will include critical data such as product demands, crude availability to achieve these demands, and prices of feeds and products.

For all practical purposes, with respect to **ONLY** material balance movements, positioning the Logistics Block inside or outside the model will have similar outcomes. The most critical decision in influencing model behavior is **HOW** economic data such as price and quantity are passed "back and forth" between Logistics and Refining, and **HOW** the optimization and solving routines are established and linked. These issues will drive the decision process on where the logistics model resides, which is the subject of the next section.

Linking the Blocks (Logistics, Refining, Economics)

In this CDR, considerable discussion has been devoted to the technical aspects of the Refining Block. The Refinery Block is typically represented in an LP application. LP methods are significantly embedded throughout the refining industry; however, these refinery LP techniques are not advanced economic models in the sense of relating supply and demand curves with prices, or economic equilibrium models.

The LP results represent a single point solution for the given conditions and constraints of the model. Consider a scenario which has a WTI crude supply curve as below. At 50 MBPD the price is $90/Bbl, and price increases as WTI purchases increase. One LP run at $90/Bbl will produce a single point solution. Another LP run at $95/Bbl will produce another single point solution. This curve is not embedded in the LP procedure, and is not part of the optimization process. An analyst could run a series of single point cases to evaluate this curve and the refining response on production and operations.

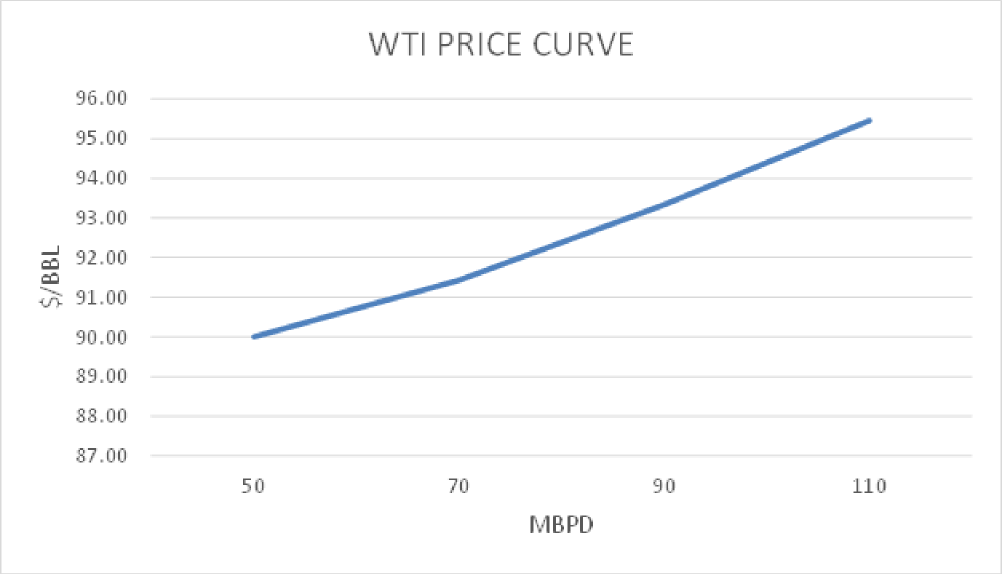

Figure 17. WTI Price Curve

Alternatively, the LP model could be developed using a series of "Tiered" purchases. This is represented in the table below:

Table 19. Tiered Purchase Strategy for WTI Purchases

TIERED PURCHASE STRATEGY FOR WTI PURCHASES						
	$/BBL	Max MBPD	$000/D	Total MBPD	Cumulative $/D	AVG $/B
CRUDE						
WTI_A	90.00	50.00	4,500	50.00	4,500	90.00
WTI_B	95.00	20.00	1,900	70.00	6,400	91.43
WTI_C	105.00	20.00	2,100	90.00	8,500	94.44
WTI_D	120.00	20.00	2,400	110.00	10,900	99.09

In the "Tiered" purchase approach, the model could purchase up to 50 MBPD of WTI_A at $90/Bbl, but the next tier of 20 MBPD WTI_B would cost $95/Bbl, which would average to $91.43 for the total 70 MBPD WTI. Both WTI_A and WTI_B are identical crude assays, each with a different name. With this Tiered strategy, a single LP run with these 4 WTI price and volume points can be used to represent the graphical curve above.

A Tiered approach is often used for products modeling, especially when the destination markets have a wide geographic range. Markets far from the refining center typically have lower netback prices. Overall, the “selective” use of the tiered strategy for feeds and products provides a reasonable approach in a single refinery model representation.

As an illustrative example, consider a matrix with 10 crude choices and 10 products that has 100 elements (combinations). If 4 tiers of prices are added to both crude and products, the matrix increases to 40 crudes and 40 products, or 1600 elements. If this single region was expanded to 30 regions, it is clear that this Tiered methodology in a Global LP environment with full transportation and terminal demands would become extraordinarily challenging in size and solving potential.

If a World Global LP model is developed with crude terminals, transportation and logistics, refinery blocks, and country supply/demand balancing terminals, the LP will provide an optimal solution to a single “point” scenario. In this example, the Refining LP Block will require either a series of price inputs to optimize on quantities, or a series of quantity requirements to calculate prices, using the cost of production. These inputs to the Refinery LP would be from a separate submodel, or economic model. Using two modeling techniques (LP and economic) appears to set up an overly complex mathematical dilemma of “competing” optimization routines: one routine solves economic algorithms to feed the refinery LP algorithms, which then sends results back to the economic model. Sending data back and forth from vastly different optimization pathways would appear significantly more challenging if a single algorithm would suffice.

The economic model is “broad” in the ability to analyze global economic supply, demand, and economic equilibrium across the globe, but is “narrow” specific to technical Refinery operations. The Refinery LP is technically “deep” to analyze refinery operations, but “narrow” in global economics of supply, demand, and economic equilibrium.

It seems prudent to analyze how to best fit the strengths of each modeling system to create a synergistic modeling platform for the World model. The World model has more emphasis on global supply and demand balancing and economic analysis than it does for technical goals such as optimizing the reformer severity in China.

In one scenario, the economic model would perform the “heavy lifting” of the global economics and supply/demand (pricing). If a 35-region model is developed in the economic platform, there would be 35 exogenous LP models. The data on operations, product yields, operating costs, and key parameters would be established with technical LP solutions and used as a starting point operation to populate the economic model.

Under this scenario, the economic model is not as "technically" accurate as the refinery LP, but it is reasonably accurate because it was populated with LP operating parameters. The refinery LP is "off-line" with respect to the economic model. Restated, the off-line LP was run in a "refinery gate" operation to populate refinery gate approximations in the economic model. The logistics would reside in the economic model. Actually, the Logistics Block has transformed into an Economic, Refining, and Logistics Block. The Refinery Block representation has transformed from a highly technical LP to a reasonable representation in the Logistics and Economic model. Moreover, there are no competing optimization platforms with vastly different mathematical distinctions.

The Economic, Refining, and Logistics model will develop all the price & quantity definitions in all the locations around the World. There is no transfer of prices to the LP Refinery Block because the LP block is non-existent — it is now embedded in the Logistics and Economic Block. All the price and quantity as well as supply and demand relationships are performed in the Economic model. The LP Refinery Block has significant exogenous use after the initial data populating to the Economic Model. The outputs from the economic model on 35 regional locations — primarily price and quantity — can be input to the 35 regional LPs. The LPs will be run and analyzed in a more sophisticated and technical LP in areas such as blending, marginal values, and capacity incentives to name a few. This is the critical sanity check and will be iterative. With these validation steps, if the economic model incorrectly approximated some blending conditions, the technical LP would find these conditions, which could then be resolved.

Developing and maintaining the LP models in an external fashion will allow the EIA the ability to drill down "deep" on technical issues for a refinery, country, or region. The regulatory cost of a regional clean product specification would be calculated on the technical LP models, not the Global economic model.

When separated, the economic model becomes "smarter" from the inputs and operations from the Refinery LP to better predict the supply, demand, and price functions. The Refinery LP becomes "smarter" because of the price and quantity inputs from the economic model to check and validate the technical operations from the economic model. De-coupling the two solving algorithms should have significant "mathematical" advantages. The Refinery LP Block, while off-line from the Global model, will serve as the superior method for technical analysis and "deep dive" refining analysis, and the Economics, Refining, and Logistics model carries the "heavy burden" of world economics and balancing.

If this de-coupling did not occur, and the Refinery LP was integrated, the economics model would pass prices to the LP, and the LP would calculate quantities, cost of production, and margins, which feed back to the economic model. In some scenarios, the LP can feed back marginal values for the economic valuation. This iterative function from a refinery LP to an economic or similar platform introduces challenging modeling issues.

Conceptually, the Economics, Refining, and Logistics model would provide the "envelope" to wrap separate models such as Refinery LP and Crude Production under a single Economics model. This is shown below:

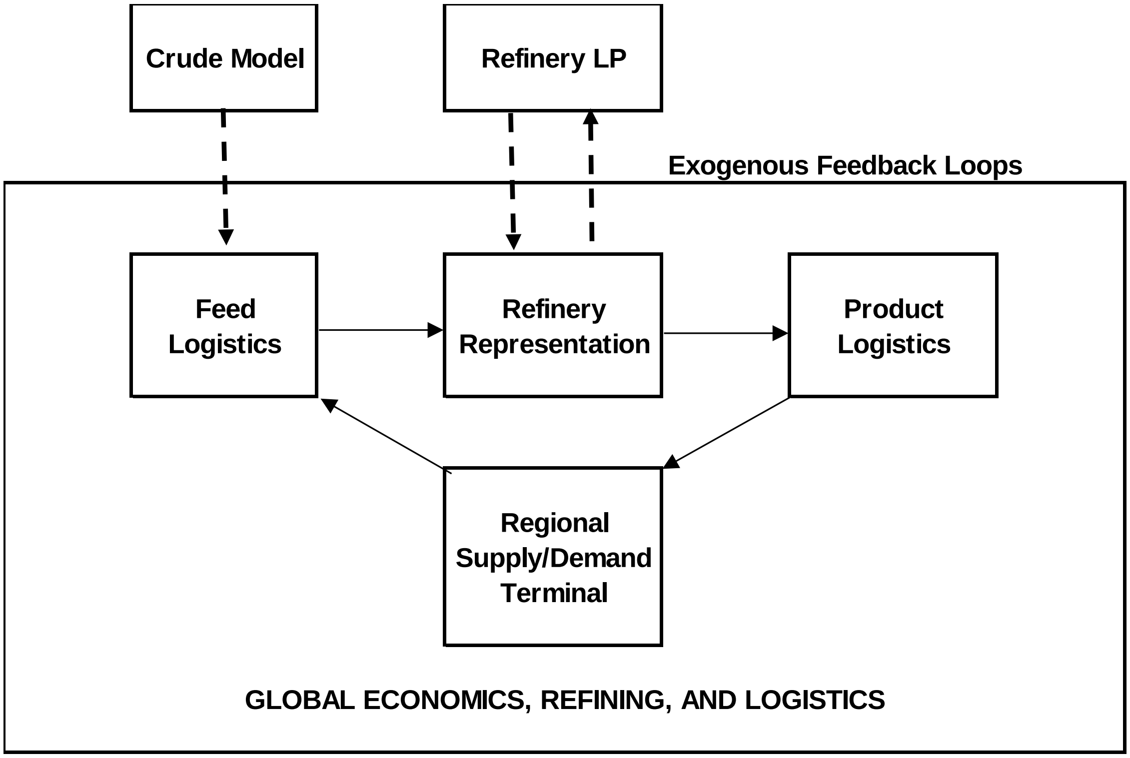

Figure 18. Economics Model

To be clear, the Author is not an expert in Economic modeling. The discussion on combining the Economic, Logistics, and Refining Block under a single "umbrella" seems to be a reasonable technique to discuss during this phase of the World model development. It could ultimately lead to an enhanced operational World model, or be ruled out if appropriate. Clearly, the Economics model would require sufficient sophistication to handle the goals of the EIA. Conceptually, the strategy should be investigated and vetted.

7. Regional Blocks (Country Aggregation)

The CDR has divided the discussion topics into the Refining Block, Crude Block, and Product Block. Proper model development for these blocks is critical to the success of the World Model. This section discusses how the blocks are regionally defined. Each region will have its "own" set of blocks. A North American region (block) can be defined, or there can be separate US, Canada, and Mexico blocks.

The strategies recommended for the Refining, Crude, Logistics, and Product Blocks are sufficiently robust to capture the operations of a refinery, a country, or an aggregated region. These blocks should not have to change, regardless of the regional definition, whether the model design is for North America or the United States, Mexico, and Canada, for example. Obviously, data inputs and vector nomenclature will change, but the fundamental building blocks are consistent regardless of the aggregation. This requirement must receive a high priority because the ability to separate the World Model into higher fidelity regions or countries is a goal.

Developing the regional blocks has many variables for consideration. At the core of these variables is to define at what point a country is modeled independently or aggregated with other countries. Some considerations include:

- Crude Block Inputs
    - Crude supply & demand, imports, exports, and volumes
    - Whole crude and specific crude types, qualities, and volumes
- Product Block Outputs
    - Petroleum products production, imports, exports, and consumption
- Refinery Operations and Configurations
    - Aggregate size and complexity

Some countries have large crude production with relatively small refining, while other countries have small crude production and large refining capacity.

Degrees of aggregation will be fundamental to the World Model. The EIA identifies 217 countries in the International Statistics. Defining levels of aggregation for the model is critical to the World Model. For the examples below, presented for representative purposes, the basis is 2010 EIA International Statistics. As the model develops, more current data will be used going forward.

The first level of aggregation—or disaggregation—should consider volume. Generally speaking, large volume countries should be represented as a unique country in the model.

The definition of large volume needs to be elaborated. Volume in the World Model can consider the following data (all of which are tracked by the EIA):

- Crude Production
- Crude Imports
- Crude Consumption
- Crude Exports
- Refining Capacity (BPD of Crude)
- Petroleum Products Consumption

The country crude supply and demand balances are very simply stated as:

- Crude Production + Imports = Consumption + Exports
- No inventory modeling adjustments should be included in the model

For a country to meet the “large volume” criteria, the volume can be production, imports, exports, consumption, or any metric deemed appropriate. It simply represents a country with a “large” volume of crude movements.

To be clear, the recommendations in this CDR will have to be processed with the various stakeholders for the model. Techniques and strategies will have to be discussed and vetted. The metric of “large volume” will have different meanings to different people.

Stakeholders for the World crude balances will likely have different objectives than those for hydrocarbon product distribution, ultimately leading to different country aggregation philosophies. It is highly recommended that:

- There should be reasonable consistency between country and aggregated regions through the hydrocarbon blocks. Each regional block (Russia, for example) will have its unique Crude, Refining, Product, and Logistics Block. Russia should not have an independent Crude Block with a Refining Block aggregated with Eastern Europe.
- This consistency is recommended for use-ability, maintenance, and overall “packaging” of the data and operations into independent blocks.
- This consistency recommendation is not definite. Some judgments can be applied. For example, Angola exports almost 2 million BPD of crude, but has less than 50 MPBD of crude capacity. It would be reasonable to model Angola with a West African Crude terminal, but combine its small refinery capacity with all of Africa.
- Resist the urge to keep adding countries to the model. This can make the model overly complex.

Kyrgyzstan, with petroleum consumption of around 30 MBPD and 10 MBPD of crude capacity, would unlikely be defined as a separate country in the World Model. Kazakhstan has strong crude production capacity, but relatively weak crude processing. Ukraine has relatively strong crude processing, but relatively weak crude production. The recommendation for this example is to aggregate Kyrgyzstan, Kazakhstan, and Ukraine (and others) into an aggregate “CIS region.”

However, if there is a need to have higher fidelity in the CIS aggregation, the CIS can be stripped out from the World Model and simulated with separate and unique CIS countries. The CIS can be disaggregated for higher fidelity analysis, and if desired, any additional knowledge gained from this specific analysis can be transferred back to the World Model.

Modeling strategies and techniques for Import and Export volumes need to be defined. For example, data show Russia imported about 32 MPBD and exported about 4.9 million BPD of crude. Netting out volumes is a strategic decision. The Russia example is an extreme, where imports are about 0.6 percent of exports. Imports should be ignored at this level, and reduce code.

There is another consideration when developing these strategies. Often the data on “Import To” and “Export From” do not match. For example, the “UK Export Volume to France” will not match the “France Import Volume from UK.” If possible, a standard should be established, and generally speaking, the Import data are often more reliable than the Export data.

The definition of a “large” country ultimately provides a basis to contemplate whether an individual country should be in the World Model versus aggregating. As discussed previously, the definition of a significant “large” country can be ranked according to different categories: 1) Producer, 2) Consumer (refining), 3) Importer or Exporter, or 4) Petroleum Products Consumption.

These category rankings tend to move together, but there are exceptions. Canada, for instance, ranks #7, #6, and #11 for crude consumer, producer, and exporter, respectively — a tight grouping. Nigeria, meanwhile, is #4 exporter and #68 consumer — a wide grouping.

The first volumetric analysis identifies significant crude producers by country. These data are provided by the EIA and are a logical starting point for defining World regions. For the tables that follow there are four columns of data:

- The BPD of category (e.g., import, export, production)
- Country rank
- Percent of the World
- Rolling percent

The rolling percent is an important metric to follow. If 80 percent of the World movement can be captured with the top 20 countries, that becomes compelling evidence of which countries to carry separately, and which to aggregate.

The tables below rank the top crude-producing countries on the Supply side, which is Production + Imports. The table provides the absolute BPD, the percent of the World Production, and the cumulative percent. Of the 87.5 MMBPD production, about 75 percent of this is captured in the top 15 countries. About 90 percent of the World crude import countries is captured in the top 25 countries. On the import side, about 80 percent of imports is captured in the top 15 cumulative countries.

Table 20. Crude Production and Crude Imports

COUNTRY	CRUDE PRODUCTION			
	Crd Prd'n	Rank	Pct	Roll'g
Russia	9,694	1	13%	13%
Saudi Arabia	8,900	2	12%	25%
United States	5,471	3	7%	32%
Iran	4,080	4	5%	38%
China	4,078	5	5%	43%
Canada	2,741	6	4%	47%
Mexico	2,621	7	4%	51%
Nigeria	2,455	8	3%	54%
UAE	2,415	9	3%	57%
Iraq	2,399	10	3%	60%
Kuwait	2,300	11	3%	63%
Venezuela	2,216	12	3%	66%
Brazil	2,055	13	3%	69%
Angola	1,899	14	3%	72%
Norway	1,869	15	3%	74%
Libya	1,650	16	2%	76%
Algeria	1,540	17	2%	78%
Kazakhstan	1,525	18	2%	81%
Qatar	1,459	19	2%	83%
United Kingdom	1,233	20	2%	84%
Azerbaijan	1,035	21	1%	86%
Indonesia	953	22	1%	87%
Oman	865	23	1%	88%
Colombia	786	24	1%	89%
India	751	25	1%	90%
Argentina	626	26	1%	91%
Egypt	568	27	1%	92%
Malaysia	563	28	1%	92%
Sudan	486	29	1%	93%
Ecuador	486	30	1%	94%

COUNTRY	CRUDE IMPORTS			
	CRD IMP	Rank	Pct	Rolling
United States	9,213	1	21%	21%
China	4,754	2	11%	32%
Japan	3,473	3	8%	40%
India	3,272	4	8%	47%
S. Korea	2,372	5	5%	53%
Germany	1,876	6	4%	57%
Italy	1,592	7	4%	61%
France	1,298	8	3%	64%
Singapore	1,137	9	3%	66%
Spain	1,061	10	2%	69%
Netherlands	1,027	11	2%	71%
United Kingdom	965	12	2%	73%
Taiwan	886	13	2%	75%
Thailand	848	14	2%	77%
Canada	770	15	2%	79%
Belgium	668	16	2%	81%
Australia	477	17	1%	82%
Poland	452	18	1%	83%
Greece	405	19	1%	84%
Virgin Islands	402	20	1%	85%
Sweden	398	21	1%	86%
Indonesia	388	22	1%	87%
South Africa	385	23	1%	87%
Brazil	344	24	1%	88%
Turkey	339	25	1%	89%
Belarus	295	26	1%	90%
Aruba	229	27	1%	90%
Bahrain	225	28	1%	91%
Portugal	222	29	1%	91%
Israel	221	30	1%	92%

The chart shows the number of countries that capture the cumulative World percent for Crude Production and Crude Imports.

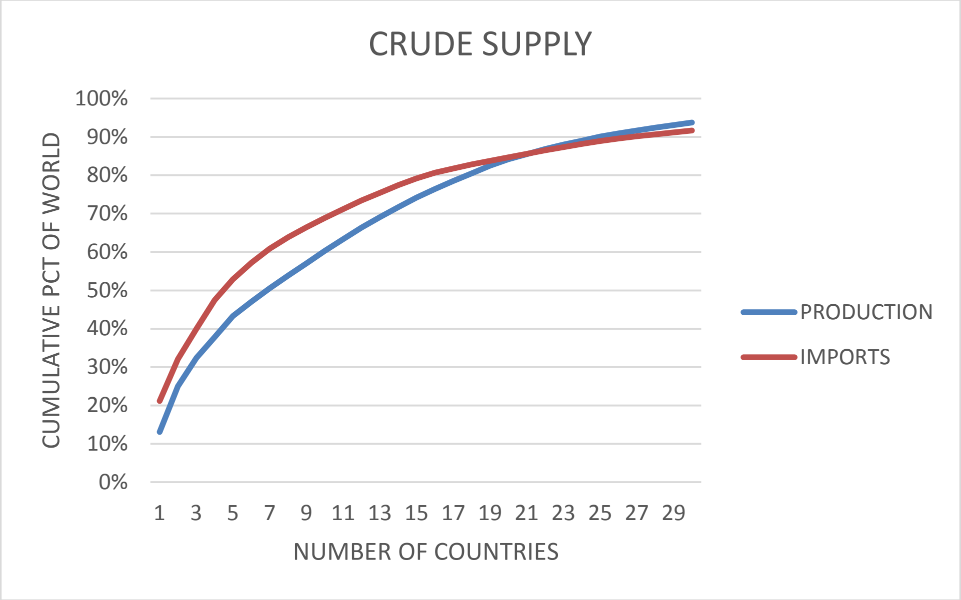

Figure 19. Cumulative Crude Production

The graphical representation clearly shows the diminishing returns associated with additional country representation. On the production side of supply, 43 percent of the World crude supply is captured with Countries 1 – 5, while 4 percent is captured in Countries 25 – 30.

From a strategic level on volumetric production volume alone, the World crude supply can be well represented using around 25 countries. Once crude production drops below 1 percent of the World or less than 500 MBPD, the relative volume of the country becomes less significant. The metric used to decide on aggregation could be any country with production or imports greater than 500 MBPD. Every aggregating decision will be unique. There will not be an absolute methodology for country definition. To be clear, even top producing countries can be aggregated. For example, Angola and Nigeria might be deemed to be aggregated with West Africa.

The following table lists the top countries for Consumer and Exports of Crude.

Table 21. Crude Consumption and Crude Exports

COUNTRY	CRUDE CONSUMPTION			
	CRD Consumed	Rank	Pct	Roll'g
United States	14,642	1	19%	19%
China	8,771	2	12%	31%
Russia	3,478	3	5%	36%
India	4,023	4	5%	41%
Japan	4,838	5	6%	48%
Korea, South	1,779	6	2%	50%
Canada	1,911	7	3%	52%
Saudi Arabia	2,056	8	3%	55%
Germany	2,372	9	3%	58%
Brazil	2,062	10	3%	61%
Iran	1,161	11	2%	63%
Italy	1,316	12	2%	64%
United Kingdom	1,719	13	2%	67%
France	1,459	14	2%	69%
Mexico	1,681	15	2%	71%
Singapore	1,003	16	1%	72%
Spain	1,063	17	1%	74%
Thailand	1,137	18	2%	75%
Netherlands	647	19	1%	76%
Indonesia	1,037	20	1%	77%
Kuwait	1,062	21	1%	79%
Taiwan	886	22	1%	80%
Belgium	532	23	1%	81%
Australia	571	24	1%	81%
Venezuela	485	25	1%	82%
Argentina	668	26	1%	83%
Egypt	387	27	1%	83%
Iraq	535	28	1%	84%
Malaysia	273	29	0%	84%
Poland	479	30	1%	85%

COUNTRY	CRUDE EXPORTS			
	CRD EXP	Rank	Pct	Roll'g
Saudi Arabia	6,844	1	16%	16%
Russia	4,888	2	11%	27%
Iran	2,377	3	6%	33%
Nigeria	2,341	4	5%	38%
UAE	2,142	5	5%	43%
Angola	1,928	6	5%	48%
Iraq	1,914	7	4%	52%
Venezuela	1,645	8	4%	56%
Norway	1,602	9	4%	60%
Mexico	1,460	10	3%	63%
Canada	1,449	11	3%	67%
Kazakhstan	1,406	12	3%	70%
Kuwait	1,395	13	3%	73%
Libya	1,378	14	3%	77%
Qatar	1,106	15	3%	79%
Algeria	1,097	16	3%	82%
Azerbaijan	908	17	2%	84%
United Kingdom	740	18	2%	86%
Oman	705	19	2%	87%
Brazil	619	20	1%	89%
Colombia	484	21	1%	90%
Sudan	389	22	1%	91%
Ecuador	342	23	1%	92%
Indonesia	338	24	1%	92%
Equatorial Guinea	319	25	1%	93%
Australia	314	26	1%	94%
Congo	310	27	1%	95%
Malaysia	245	28	1%	95%
Gabon	225	29	1%	96%
Vietnam	215	30	1%	96%

The next tables show crude capacity and petroleum consumption. The petroleum consumption is a different technical indicator, as the previous ones were related to crude.

The discussion on country aggregation should not just consider crude supply and demand, but also include petroleum consumption.

Table 22. CDU Capacity and Petroleum Consumption

COUNTRY	CDU CAPACITY			
	Crude Twr	Rank	Pct	Roll'g
United States	17,584	1	20%	20%
China	6,806	2	8%	28%
Russia	5,428	3	6%	34%
Japan	4,624	4	5%	40%
India	2,836	5	3%	43%
S. Korea	2,702	6	3%	46%
Germany	2,411	7	3%	49%
Italy	2,337	8	3%	51%
Saudi Arabia	2,080	9	2%	54%
Canada	2,039	10	2%	56%
France	1,984	11	2%	58%
Brazil	1,908	12	2%	61%
United Kingdom	1,866	13	2%	63%
Mexico	1,540	14	2%	65%
Iran	1,451	15	2%	66%
Singapore	1,357	16	2%	68%
Taiwan	1,310	17	2%	69%
Venezuela	1,282	18	1%	71%
Spain	1,272	19	1%	72%
Netherlands	1,206	20	1%	74%
Indonesia	1,012	21	1%	75%
Kuwait	936	22	1%	76%
Ukraine	880	23	1%	77%
Belgium	798	24	1%	78%
United Arab Emirat	773	25	1%	79%
Egypt	726	26	1%	80%
Australia	725	27	1%	80%
Turkey	714	28	1%	81%
Iraq	638	29	1%	82%
Argentina	627	30	1%	83%

COUNTRY	PETROLEUM CONSUMED			
	PET CONS	Rank	Pct	Roll'g
United States	19,180	1	22%	22%
China	9,330	2	11%	33%
Japan	4,455	3	5%	38%
India	3,255	4	4%	41%
Russia	2,992	5	3%	45%
Brazil	2,622	6	3%	48%
Germany	2,470	7	3%	51%
Saudi Arabia	2,371	8	3%	53%
Korea, South	2,269	9	3%	56%
Canada	2,265	10	3%	59%
Mexico	2,080	11	2%	61%
France	1,833	12	2%	63%
Iran	1,726	13	2%	65%
United Kingdom	1,621	14	2%	67%
Italy	1,544	15	2%	69%
Indonesia	1,466	16	2%	70%
Spain	1,441	17	2%	72%
Singapore	1,380	18	2%	73%
Australia	1,060	19	1%	75%
Netherlands	1,020	20	1%	76%
Thailand	1,011	21	1%	77%
Taiwan	972	22	1%	78%
Egypt	738	23	1%	79%
Venezuela	718	24	1%	80%
Iraq	662	25	1%	81%
Belgium	655	26	1%	81%
Turkey	650	27	1%	82%
Argentina	620	28	1%	83%
United Arab Emirat	618	29	1%	83%
Malaysia	598	30	1%	84%

Region Definitions

World Model definition will include specific countries and an aggregation of other countries. The aggregation and separation is a **strong** function of the data availability and the reliability of data. The IEA provides comprehensive World energy data; the IEA's country definitions and aggregation are a logical starting point to define the World Model regions.

Below are examples of reasonable structures for the World Model. The table below is the Base Level Aggregation, the lowest level of fidelity recommendation. This level is similar to 16 WEPS+ regions and IEA designations. From a modeling perspective, building 16 or 20 regions is not a significant difference. With all the various stakeholder influences and opinions, this CDR does not attempt to define which aggregation method is "best," because it does not exist. All stakeholder opinions are important, and must be weighed with what best matches—or compromises—the integrity of the model. This CDR will make recommendations on the number of regions the World Model should contemplate, but the final definitions will have to be developed. The example definition below combines IEA definitions with WEPS definitions to create a 22 aggregated regional model.

Table 23. Base Level Country Aggregation

BASE LEVEL AGGREGATION	
USA	N. Africa
Canada	W. Africa.
Mexico	China
Venezuela	Indonesia
Brazil	India
S. America- Other	Other Asia
Northern OECD	OECD Asia
Southern OECD	Singapore
Non-OECD Europe	Saudi Arabia
Russia	Iran
CIS - Other	Middle East - Other

Total Regions = 22

The next level includes all of the OPEC countries, including Ecuador which is a relatively small producer and exporter of crude. Recognition of all OPEC countries in the World Model might be a significant delineation for the DOE. **The inclusion of OPEC is only a representative illustration of how the EIA might choose to delineate countries, and is not a specific recommendation.** This example contains 31 regions.

Table 24. Base Level plus OPEC Locations

BASE + ALL OPEC			
USA		N. Africa - Other	
Canada		W. Africa - Other	
Mexico		China	
Venezuela	OPEC	Indonesia	
Brazil		India	
Ecuador	OPEC	Other Asia	
S. America- Other		OECD Asia	
Northern OECD		Singapore	
Southern OECD		Saudi Arab	OPEC
Non-OECD Europe		Iran	OPEC
Russia		UAE	OPEC
CIS - Other		Iraq	OPEC
Nigeria	OPEC	Kuwait	OPEC
Angola	OPEC	Qatar	OPEC
Libya	OPEC	Middle East - Other	
Algeria	OPEC		

Total Regions = 31

The last level of aggregation includes other "large" countries, whether defined by production, consumption, imports, or exports. The definition of "large" will clearly have to be identified, discussed, and finalized, as there is significant room for interpretation. This is shown as an example, that the model can be developed with a flexible number of regions and that individual countries can be aggregated or separated. The development of a 46-country model is not recommended, however.

Table 25. Base plus OPEC plus Large Countries

BASE + OPEC + "Large"	
USA	Singapore
Canada	Saudi Arabia
Mexico	Iran
Venezuela	UAE
S. America- Other	Iraq
Northern OECD	Kuwait
Southern OECD	Qatar
Germany	Middle East - Other
France	Brazil
Non-OECD Europe	Ecuador
Russia	Colombia
CIS - Other	Argentina
Nigeria	Japan
Angola	Korea, South
Libya	Italy
Algeria	United Kingdom
N. Africa - Other	Norway
W. Africa - Other	Spain
China	Netherlands
Indonesia	Australia
India	Netherlands
Other Asia	Taiwan
OECD Asia	Thailand

Total Regions = 46

There are many external factors driving the decision for regional definitions for this CDR. This CDR will make the recommendation that with strategic thinking, defining the regions for today, the future regions, and expert mapping of the systems—and potential systems—the World Model will have tremendous flexibility.

The example below shows how the mapping and model development philosophy can provide this flexibility. The example has Country 1, 2, 3, and future 4 not yet defined. Each country will have a unique supply/demand pattern. These data can reside as individual country-level operational data.

If there is a need to combine Countries 1 & 2, this would be New Region 5. Region 5 refinery capability is the sum Production, Import, Export, and Consumption for Countries 1 & 2. The data should build up from the country level and then be aggregated.

Table 26. Aggregating Countries

SUPPLY/DEMAND	**ID**					
Country 1	1	Ref'y 1	Prod'n 1	Import 1	Export 1	Consume 1
Country 2	2	Ref'y 2	Prod'n 2	Import 2	Export 2	Consume 2
Country 3	3	Ref'y 3	Prod'n 3	Import 3	Export 3	Consume 3
Future 4	4	Ref'y 4	Prod'n 4	Import 4	Export 4	Consume 4
Aggregate						
Region 1-2	5	Ref'y 5	Prod'n 5	Import 5	Export 5	Consume 5
Country 3	3	Ref'y 3	Prod'n 3	Import 3	Export 3	Consume 3

Transportation and flows must be critically thought out. In the example below, Country 1 receives imports from A and exports to a. Country 2 receives imports from B and exports to b. In this transportation the code is “Source – Destination,” so A1 is from Country A to Country 1, and 1a is from Country 1 to Country a.

If it is envisaged to aggregate Country 1 and 2 into Region 5, the transportation flows must be updated. The imports into 5 come from A (to Country 1) and B (to Country 2). Now two separate countries can import into 1 and 2, so two separate nodes must be defined for Region 5, which become A5 and B5.

Table 27. Aggregate Country Node Definitions

IMPORT/EXPORT FLOWS	ID	Import From	Export to	Import Node	Export Node
Country 1	1	A	a	A1	1a
Country 2	2	B	b	B2	2b
Country 3	3	C	c	C3	3c
Future 4	4	D	d	D4	3c
Aggregate					
Region 1-2	5			A5	5a
				B5	5b
Country 3	3			C3	3c

Some commercial software can allow up to 99 locations, so “size or number” of regions is technically feasible to develop a large model with considerable fidelity. Software can activate or deactivate (turn on/off the switch). In other words, Country 1 and 2 can be modeled independently, while Country 5 is turned off. On the other hand, Country 5 can run, while Country 1 and 2 are turned off.

Some countries such as the United States, Canada, Russia, and China can be further subdivided (PADDs 1 – 5, for example). While technically feasible, these decisions should be approached cautiously. Simply because the technology exists to do detailed aggregation, there could be a strong argument to maintain a very sophisticated US model outside—and independent of—the World Model. This would have more sophistication than the “pieces” of the World Model, and might be challenging to link to the World. The detailed US Model, for example, will make at least 4 grades of gasoline and 4 more grades of BOBs by seasons and regions (i.e., CG Regular & Premium, and RFG Regular and Premium), potentially E15, and E85.

With every aspect of this World Model, there is a trade-off. The recommendations for the Refinery Block Technology and operations are relatively advanced for a World Model application. However, to perform other desired World Model operations such as GHG or Energy calculations, this detail will be required to achieve credible results on those topics. The modeling downside is that more code and convergence issues surface with more advanced structure. This fact, coupled with a high number of regions, can potentially negatively compound modeling performance, so the number of regions needs to be held in “check” with the sophistication of refinery yield methods.

Another trade-off when contemplating regional aggregation is the Crude Block. If a single crude is used from each country (e.g., Saudi Crude) versus multiple grades (e.g., Saudi Light, Medium, and Heavy), the crude movements in the multiple crude case, coupled with more regions and three crude towers per refinery, is a recipe for more modeling challenges.

In non-technical terms, the following guidelines should be considered when defining regional aggregation:

- 16 WEPS+ Regions are very doable with robust refinery operations specified and multiple product grades
- 20 – 25 Regions is a reasonable, achievable goal
- 30 – 35 Regions is reaching the limits of model management, not technical code
- 40 Regions—while technically feasible—becomes challenging to manage, run, and analyze model results
- 40 + Regions—while technically feasible—becomes overwhelming to manage, interpret, and find any meaningful results other than “the model solved.”

The developers of the World Model must take significant steps that the results produced from the World Model can be effectively analyzed to make informed project decisions. The point above regarding "the model solved" emphasizes this need. In model development, the model builders (programmers), model runners (analysts), and model interpreters (project leads) are often separate people or organizations. A model builder can develop a 50-region model that is technically sound. Model runners can populate data to the 50 regions, and run to a converged solution and provide output. The model builder and runner are satisfied because "the model solved." There is a point where the input and output is so complex, intertwined, premise-laden, and assumption-driven, that the model interpreter cannot perform a comprehensive analysis, and is more beholden to "this is **how** the model solved," instead of "this is **why** the model solved." This would be a tremendous disappointment if the Global Model crossed into this territory. Reiterating the point at the beginning of the CDR, neither a bigger nor more sophisticated model ensures a better model.

8. Pooling vs. Table Structure

This CDR assumes the reader is familiar with the term *pooling*. Below is a very simple example of pooling:

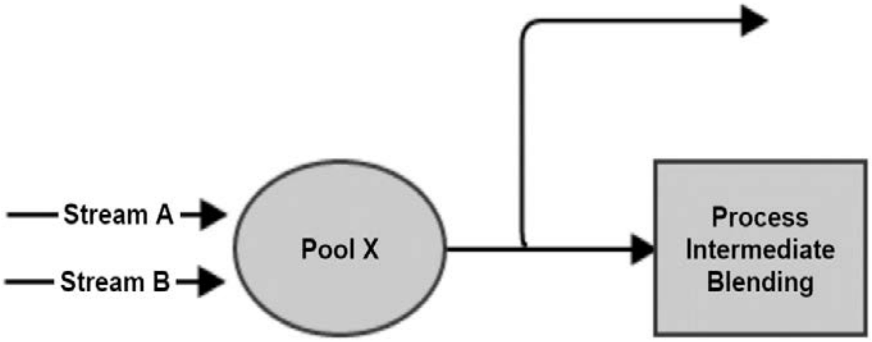

Figure 20. Pooling

In the example above, two streams are blended and the qualities of the pool are the volumetric blend qualities of the individual streams. The pool can go to a process unit; an intermediate stream that is further refined downstream; or to product blending. If a portion or all of the pool is optimized by by-passing the operation, the entire pool must move. The qualities of the pool come from two potential sources: crude assay, or prediction from a process operation.

The next example is a representation of how a table format would potentially translate into a flow process. Here, both Stream A and B can act independently. The optimization could route a portion or all of either Stream A and B to the operation, or bypass the operation entirely.

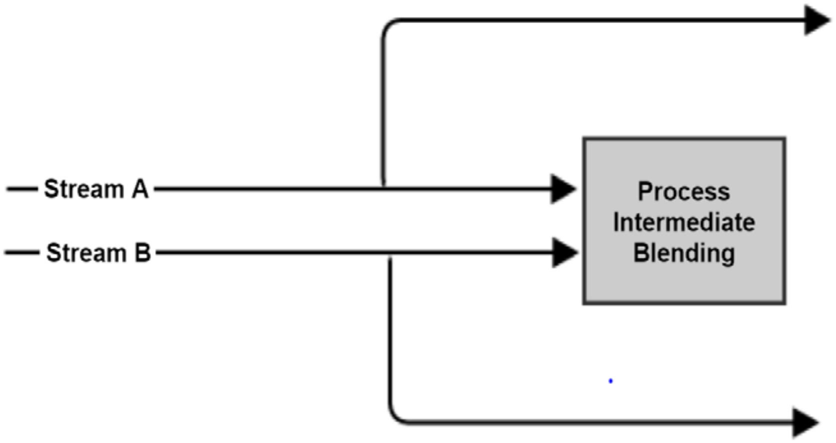

Figure 21. Non-Pooled Flows

As an example, if the model structure is more complex and has 10 streams, the optimization options become more complex. With 10 streams (e.g., A – J), the combination of potential movements greatly increases. With the pool structure, Streams A – J blend to a single pool that still has only two destinations: the operation or bypass. Even in the simple 2-stream example, if there is 50 BPD of Stream A and B, the Pool will have 100 BPD, and there are two destinations (i.e., through or around the unit). In a table structure there are thousands of options (e.g., 75 MBPD to Unit, 25 MBPD to bypass; 50 MBPD to Unit, 50 MBPD bypass; 25 MBPD to Unit and 70 MBPD to bypass); this is further compounded by the options for Stream B.

The table structure can lead to what is commonly called “cherry picking,“ in which the model can grab the “best” streams and qualities to one location, and the “worst” streams and qualities to another. In practice—and certainly in actual operations—the ability to cherry pick is limited. For example, there could be a sweet crude tank and a sour crude tank; a refinery can choose to run one or both.

One could correctly deduce that a table structure creates numerous over-optimization potential. Over-optimization in general means the model can operate in a method that is superior to actual operations. However, across an aggregate region with 10 refineries, the model could be intentionally developed to be over-optimized. In these 10 locations, Stream A could go to a different operation at Refinery 1 versus Refinery 2.

A pooled structure also has over-optimization potential in an aggregate method. If Refinery 1 with an FCC is aggregated with Refinery 2 with a HYK, the aggregate of Refinery 1 + Refinery 2 has both an FCC and HYK. LCO in Refinery 1 actually routes to the ULSD HDT in a stand-alone operation. However, since the aggregate model has a HYK, the LCO can also go to the

HYK. This is over-optimization. Furthermore, if the modeler wants to make these distinctions — such as a HYK refinery versus an FCC refinery — then why not just model Refinery 1 – 10 as unique models, which of course goes against the purpose of aggregate modeling.

The distinctions between over-optimization and under-optimization are minimized in an aggregate World Model situation, when the models are used in a differential method. This method is the strength of refinery modeling, where a Base Case is developed, a Scenario situation is performed against that Base Case, and the differential results are analyzed. If the Base Case is over-optimized, the model has the same “opportunities” as the Scenario Case for most instances, and the same holds true for under-optimized models. The differential results are likely to be extremely consistent from either starting point.

With pooling and table structure there is a fundamental difference on how operations and data are passed through for operations. Using an FCC example, where each stream might carry qualities for UOPK, NIT, CRC, and SUL, the pool is created with a weighted average (volume or weight, whichever is appropriate) for the qualities. Many commercial software packages allow the option of defining each specific quality on a weight or volume basis for blending.

In the pooling example, the pool quality “enters” the sub-module, and the yields are predicted on the pool. In this example, the qualities are passed through the model beginning with the assay data, to the pools.

There are different methods to the table structure. In one example, every crude will have an FCC yield prediction, which can be generated during the assay generation step with a formula file that represents the FCC prediction. This can become complicated quickly, because the yield needs to be defined for all potential streams such as LVGO, HVGO, AGO, and ATM RES. In another example, each stream is defined in the permanent data structure for predictions external of a crude assay/formula file method.

Regardless of the table format, the following holds true: table structure can create significant challenges for model maintenance. If a correlation is changed, each vector must be regenerated and modified. In the pooling example, the crude assay qualities are the same, and no modifications are required. The correlation update is on a few vectors inside the sub-module.

The table structure is also difficult for new or intermediate model users to understand. The code is dramatically increased and often difficult to follow. Seasoned model experts will understand the table structure, certainly if they are the developers. In most organizations, however, this detailed expertise lies with a select few people, which is a potentially dangerous situation organizationally.

The above discussion leads to the recommendation to abandon table structure methods and move to pooling strategies. A pooling strategy will satisfy the requirements of the reasonableness objective.

9. Input / Output / Data Requirements & Knowledge Management

To some extent, the input/output and knowledge management will be governed by the software platform for the model. This would include decisions such as data warehousing in a database format or a spreadsheet format. If the refinery platform can read in, or export to, these applications will impact the input/output strategies.

The experience of the author is grounded in commercial-based refinery LP packages, primarily GRTMPS. To this end, the recommendations on code and structure in the CDR incorporates some degree of knowledge of the capability of these applications.

Commercial software platforms or internally generated programs should not be considered singularly, because the software platform works in conjunction with other critical components of the refinery modeling system. These components include:

- The refinery LP modeling platform
- The refinery database technology
- The crude assay database manager

The refinery database defines many of the segments discussed in this CDR, including but not limited to:

- All process yield and material predictions for the sub-modules
- Stream qualities and definitions
- Blending and stream mapping
- Transportation vectors and mapping

Additionally, the refinery database technology and software platform work in conjunction with crude assay technology. Crude assay information can be purchased commercially or manually developed. Aside from the crude assay data, a mechanism must be implemented to “cut” the assays, described in the Crude Block. Crude cutting software is also commercially available.

This CDR does not attempt to make a recommendation for the specific refinery modeling platform, whether commercial based or internally developed. It is fully understood that the Global Hydrocarbon Module is an ambitious project. It seems logical for the DOE/EIA to strongly consider the use of an industry-proven commercial refinery modeling platform system to tie the knowledge base to a refining modeling system.

The user requirements to develop, run, and analyze this model are great — and errors and infeasibilities will be part of the prototype, calibration, and scenario development. This requirement is ongoing, for the life of the project. The use of an industry recognized platform will first ensure that the techniques and strategies are consistent and proven. Second, it will allow the DOE/EIA to concentrate their efforts and expertise on data development and model design without undue consideration if it is a “fit” for the model platform. Third, the commercial support would include “behind the scenes” analysis for matrix development, solution paths, and stability issues — all of which are critical to the success of this World Model.

Run time is another point to include in the Software design considerations. Model developers, unfortunately, will not be able to estimate run time during model development. The number of variables that impact run time are great, and the impact of these variables is intertwined. Examples of these variables include the number of: regions, process units, product grades, specifications, crudes, and terminals. These are examples that will influence the matrix size. Matrix size, however, does not necessarily correlate to run time. Poor design of process units or methodologies can overwhelm solution time and stability. A small, unstable, difficult-to-converge refinery matrix can have much worse run time issues than a large, stable matrix. Outside expertise from the commercial technology platform vendor will be an invaluable advantage, because they provide essential knowledge and experience to analyze the model “at the matrix level.”

Passing, Prices, Quantities, and Other Data between Submodules

Technically speaking, passing data to and from the refining module to other sub-modules is feasible. This requirement supports the consideration of commercially available software in which specialized techniques may require development for specific transfers — whether database-driven or spreadsheet-driven, for example. Within a refining platform this is routinely performed such as passing crude data to external cut-point optimization programs, process data to external process simulators, or refinery LP input/output data to scheduling packages.

One challenge of this application is determining what data to pass, specifically the fidelity of the data. As an example, consider an aggregate region that produces a high and low quality of gasoline. The developers must consider the merits of passing the total volume of gasoline to outside models, or passing the individual grades of gasoline. Producing two grades of gasoline may be appropriate for the regional analysis, but in the scheme of a fully integrated World energy model, the total volume may be appropriate.

Information flows to and from the refining module can be structured to support the goals of the World Model. The developers will need to rigorously contemplate which information flows are iterative (determined during model execution) or derived from external models in input as static values. To be clear, a static input can be updated and “re-tuned” as part of a project study.

Model stability is clearly influenced by the time period for data transfers. Obviously, running a model on an annual basis for 10 years is more challenging than running two 5-year cycles. A tighter time period is more practical if the Refining model is performed on a stand-alone basis, not fully integrated with the Global Model. In commercial applications, developing a 12-month multi-period model for refinery annual planning is common.

Outputs from the model can include some of following data as inputs to other models:

- Material Balance data
    - Imports, Exports, Production
- Refinery Operations
    - Emissions, Crude consumption, Volume Gain, Unit Throughputs

Iterative inputs to the model can include some of the following data points:

- Product Demands by regions
- World crude production
- Prices (discussed below)

Non-iterative, static, exogenous data can include the following:

- Variable and operating cost data
- Capital Investment factors
- Product specifications
- Transportation costs by product, mode, and routes
- Initial configuration data (before investment)

The use of data curves as a pass-through mechanism would be achieved similar to techniques of transferring process operational yield curves (non-linear representations as well) from the refinery LP to outside simulators and back, during model execution.

Marginal Value Price Pass-Through. Using marginal value pass-through data as a basis for price forecasting is not a technique used within the experience of the author. Price forecasting can be performed in an external model and statically input to the refining model. A static input, as the name implies, is a fixed number, not an iterated or optimized calculation derived from pass-through marginal values.

An externally derived price forecast can take many forms. In an abbreviated example, the forecaster will make a “call” or scenario price on marker crudes and gasoline and diesel relationships. Using other forecasting techniques, a refined products price set can be coupled with specific refinery configuration yield patterns derived from LP runs, leading to gross margins. Variable margins then form the basis for operating margins, which form the basis for financial returns on specific refinery configurations. The forecaster will analyze the input “calls” to specific regional financial returns and perform external iterations and analysis to produce regional forecasts. Fundamentally, the method is grounded in refinery operations and financial returns, with full capability to run external models and analysis to tune and adjust the forecast.

It seems intuitive — for lack of a specific citation — that a Global Model which passes dozens of price marginal values across potentially dozens of refinery regions, working within the definitions and constraints of thousands of matrix variables, will dramatically and negatively impact solving potential and analysis.

This topic has fundamental implications to the Global Model, and undoubtedly generates strong opinions and refinery economic modeling philosophies and methodologies between stakeholders. This CDR fully supports the use of external pricing models as static inputs to the refining module.

Knowledge Management (KM) System Design

The Knowledge Management system design begins with a strategic review of the input and output requirements of the Refining module. Clearly, the input and output requirements are closely related to the final design of the model. In many situations, data collection will be challenge, because there is no transparent reporting of such data. This will lead to design estimates and assumptions as inputs to models. As such, the model design must take into account what information is readily available, what can be reasonably estimated, and what data are "guessed."

Refinery Configuration. Each region will have a unique refinery configuration design. The process sub-model blocks have been defined in a previous section. *The Oil & Gas Journal* is a reasonable starting point for “today’s” operation. Additional data can be obtained from source information, such as website information from oil and refining companies.

The KM system should monitor announced new and expanded capacity additions. While this information can be “announced” it can also never actually be constructed, and should be used cautiously, not as a certainty.

Product Specifications. Once in place, the initial specifications will serve as the model basis. Many countries have transparent specifications which form the model basis, but scanning the trade publications will be an ongoing KM activity. Going to the future, countries and regions typically announce plans to change product qualities, usually increasing clean-fuel shares. The CDR is recommending that most countries have a HI and LOW quality gasoline and diesel fuel, as a reasonable assumption for World modeling. The developers will have to make judgments on developing this strategy. For example, US midgrade gasoline can be allocated to premium and regular. High quality and Low Quality US gasoline is Unleaded Premium and Regular.

If a country is planning on a major clean fuels initiative, the model must have the appropriate process sub-modules to produce the new grades. A country model without the ULSD HDT structure in the database will go infeasible when directed to make ULSD.

Feed and Product Prices, Logistics. The crude prices into the model are CIF, the delivered costs plus insurance and freight. These prices are often derived from source FOB locations. It is envisioned that the model will have Crude Terminals, representing the fields or regions of production. This would be the FOB "buy" point for the model. The regions will receive the crudes via transportation routes and vectors. Developing and maintaining this information is challenging. The developers will need to construct modes (pipeline, VLCC, Panamax), costs, and combined limits as required.

Crude segregation by type (e.g., Bonny Light) will allow KM to monitor published data. There may be situations where the crude has been aggregated or blended (West African Light Sweet) for which a proxy price will be reasonably estimated.

Product prices will be a KM task. It is envisioned that each country will have a specific terminal for a sale or consumption. This is the product price. Imports and exports will move from countries using transportation modes and prices, similar to the structure for crudes.

The market pricing and transportation logistics inputs will likely require specific expertise to develop and populate the model. After implemented, the KM will be responsible for monitoring.

Regional Material Balance Blocks. This will be a significant effort for KM to develop and maintain. Over two hundred countries will be condensed down to approximately 30 regions. This clearly implies over 200 countries' data must be aggregated to the specified regions.

For crude and major product, the balance will include: production, imports, consumption, and outputs. During this compilation, there will be challenges primarily because all the pieces will not "flange-up." There will be exports from a country that do match the reciprocal import from the receiving country. This and other data will require developer and KM assumptions. Often, the data inconsistencies tend to balance-out across the aggregated regions.

The data collection does not have to be a "perfect" balance, only reasonable. The model will balance, not necessarily the outside data. The model will neither be required to match the data, nor run freely without the "guidance" of the data. The data gathered from KM will guide the model. This will be the critical step of a model calibration effort. The model should use the KM data target coupled with a reasonable tolerance. These tolerances will be used throughout the model.

Defining tolerance thresholds will change for each vector, and should certainly be anticipated to change over time. Initially, the tolerances will be wide, say +/- 50 percent during development, to allow for feasible solutions, and subsequently tightened. Tolerance strategies can be hybrids, for example “FIX” the amount of High Quality Gasoline, and use +/- 10 percent for the Low Quality. Tolerances should be implemented for unit operations. If the expected FCC operation is 100 MBPD, a minimum should be applied, as it represents an operational turn-down limit. Tolerances will change by region based on data certainty and impact to the overall result.

Variable Costs. The Refining Module will calculate the fuel, power, water, and steam requirements. KM will develop the cost for these components (e.g., $/KWH). Catalyst and Chemicals use will also be an input to the model, such as $/Bbl of feed.

Refining Outputs. KM will be tasked with receiving the model outputs and providing analysis on the reasonableness of the run(s). This analysis is time-consuming and requires specific training and expertise. Some specific items include:

- Material Balance Analysis for each region
    - Production, Imports, Consumption, and Exports
    - Crude, Other Inputs, Products
- Refining Outputs
    - Material Balances across units, and regions (weight and volume)
    - Refinery throughputs and capacity additions through investment
    - Capital expenditures
- Refinery Energy and CO_2 emissions (including off-line calculations)
- Logistics and movements of crude and products

Summary. The inputs to the model are significant. The data needs will align with model development and should be developed in parallel. Almost every input data can impact the resulting output. Judicious efforts should be utilized during model design to reflect the data uncertainty, which will be significant. Overdesigning any component of the model that requires data which is difficult to obtain, or has questionable accuracy, should be avoided. For example, in most cases, it would be reasonable to transfer crude to/from a region using a single vector, not separate vectors for different DWT vessels.

10. Investments

A refining model designed for operations and scenarios in the future will require some level of investment design. Investments are also challenging modeling functions to design and implement.

Investments require input data for specific process units. The first level is grassroots investment for process units. This is often done using a "cost-curve" approach. The cost for an investment is specified for a "standard" size unit. This is based on a specified year (Base Year), so that the investment can be escalated for future investment. The investment calculation has an exponential factor to account for a specific throughput investment that is not the same size as the standard size. The standard investment also has a regional basis, often USGC, so that other regions can have a location factor that multiplies off the 1.0 USGC factor.

Investment in a regional, aggregated model requires additional strategic design considerations. The region will have a capacity much greater than any single refinery capacity, so code can be implemented to limit the investment to any size, but allow for multiple units. This is called the largest single train factor. Instead of building 240 MBPD of FCC capacity, the model will be three units, each with 80 MBPD as an example.

An OSBL factor is required for investment. This factor has significant variability based on investment, location, age of unit, and complexity of unit to name a few factors. Choosing a single OSBL factor (e.g., 1.5) should be sufficient for almost all applications because any additional fidelity likely brings in too much uncertainty.

The new investment can include the number of operators for the unit, which will impact the fixed cost and overall investment decision. With this definition, the cost for wages per operator must be estimated for all regions.

Once the process sub-module investments factors are determined, the financial requirements are input. This is the hurdle rate and can be defined as ROI, Payback, or NPV. This input will should also require the project life in years and/or a discount rate.

Investment models in the World Model will not likely have the level of detail that can be input for more sophisticated techniques. For example, across the World regions, depreciation techniques, government or local taxes, other fixed costs such as insurance, or tax credit will unlikely be known at any level of certainty. And, to carry this information in some regions, but not others seems arbitrary.

The capital investment challenge is increased because there is often a potential to retrofit a number of refinery and regional specific capacities versus a single grassroots unit. Sufficient knowledge of this distinction will carry great uncertainty. With the use of exponents described above, the calculated investment of a small unit will have a higher cost per barrel than a large unit, but lower overall cost in absolute dollars. Defining a separate set of retrofit or reconfiguration inputs is not recommended; rather, let the exponent methodology make this distinction.

The model carries one mathematical objective value and all the regions operate to achieve that point. Restated, all the regions will invest optimally for the “greater good” of the World. Clearly this is a modeling limitation that must be overcome, and it is unlikely that mathematical algorithms will prevail. This limitation is best dealt with through the use of sound analytical principles, after a solution has been met. The question to answer is whether the investment is rational and logical.

Known investments or announced investments (with reasonable certainty of being developed) can be analyzed exogenously. It would be reasonable for the stakeholders to estimate some degree of anticipated World investments and input this to the model. It is also logical to adjust model inputs if the investment solutions seem inappropriate.

11. Uncertainty and Limitations

There are both uncertainties and limitations with any single refinery model representation. A large Global Model is no exception, perhaps prone to higher degrees of uncertainties.

One area of uncertainty will be data acquisition and its use in the model. One principal requirement is the material balance of all feed and products in the World. This will be done for all countries (or aggregated countries) in the model. Data development begins from the country level and is “worked-up” to an aggregate level. On a country level, data exist (e.g., the IEA) for production, imports, consumption, and exports. The production and consumption data is typically more reliable than imports and exports. The exporting country data can be a different volume than the receiving country import data. When aggregating many countries, there is a significant challenge to manage all the movements between the aggregated countries.

The recommendation is to perform as much “netting-out” as practically possible. This task will require significant judgments based on data, experience, and assessments on the potential impacts on the World Model. There are no definitive rules. Netting out crudes of similar quality is highly recommended. While the type of crude (e.g., LT Sweet, MD Sour) import/export is unlikely known, reasonable judgments can be applied. For example, UK and Norway movements could be considered similar crude types. As another example, the model does not need to export 100 MBPD of Medium Sour to one country, and import 50 MPBD Medium Sour from the same. The model should be netted to export 50 MPBD Medium Sour. Additionally, large volume differences between import/export locations can facilitate the netting out decision, because a large volume will tend to override the impacts. These decisions, while not arbitrary, will create uncertainty.

This information is required for one of the single most important requirements of the model: the model must be calibrated. There is no single source of data to calibrate this World Model, so the model calibration will be against this data collection effort, including all netting-out decisions, refinery operations, regional aggregation, and supply/demand balances. Additionally, while the model can be calibrated to the off-line data, the reverse can be true: the model can provide the basis for “filling the caps” for data scarcity.

The calibration is perhaps the single largest mitigating factor for model uncertainty. The most common use of refining models is a differential analysis to a base, calibrated case. In strategic analysis, there is a base case and scenario cases. For the EIA, this could be the current year case, and future 2020 and 2040 cases. A well-calibrated model provides a higher level of confidence of future modeling scenarios. With LP, the model solves to an optimal solution, and while the World does not operate “optimally,” it is the basis from which to compare the base, calibrated case to future cases.

The development, case set-up, and model execution is based on significant model and industry experience. While the model is calibrated to current conditions, more judgment will be applied for future cases. The model will not be allowed to “do what it wants,” nor will it be required to carry unreasonable base case constraints into the future. These decisions will be part of the analysts’ experience and model execution strategies.

The Refinery Block will have uncertainties associated with the process configurations and capacities. Maintaining this data will be an ongoing task for the knowledge base. The reporting of “clean fuels” units is typically mis-reported. If a country is producing clean fuels (ULSD, Low Benzene, LSG) the assumption should be made that process capacities are located at the country, even if these units are not reported. Clean Fuels units include benzene and reformate saturation, FCC naphtha hydrotreating, and ULSD units. For example, the model would go infeasible if the constraint is to produce high-quality ULSD when there is no ULSD in the configuration.

Crude production by type will generally have less certainty compared to the **movement** of crude production by type. Most data characterizes the movements as “crude,” not by Light Sweet or Medium Sour. Some of this uncertainty will be driven by the final decisions of crude characterizations. If crude types are differentiated, to a large extent, the model will determine these movements during the optimization process. For example, if a country runs 100 MBPD of Saudi crude, and the model has both Saudi Light and Saudi Heavy, the model can group the two types to a 100 MBPD limit, but the model will calculate the volume ratio of Light and Heavy. The model will have limited use to determine the cost of specific country program. For example, using the World Model to estimate the program cost of a 30 ppm regulation in Country “X” is inappropriate. This analysis is best completed by de-coupling the country from the World Model and performing an independent analysis.

Analysts must have the capability to analyze World Model results. Thorough analysis is another mitigating effort for uncertainty. The ability to analyze is a direct function of a central theme of this model's design: Balance. Too much detail can be chaotic for development, running, and analysis of the model, and too little detail can be catastrophic. Comprehensive output from a multi-refinery model will likely exceed a thousand pages, so in addition to standardized reports, the model developers need to create specialized output reports for analytical reports, including but not limited to:

- Single-page input/output material balance for each Refinery Block
- Single-page input/output for each Terminal Block
- Summary unit operations for all refinery blocks, including marginal values for increase capacity incentives, and throughputs as a percent of stated capacity
- Key operating parameters in the Refining Block

  - FCC conversion
  - HYK conversion
  - Reforming Severity
  - Refinery hydrogen balance
- Key summary of blending constraints (marginal values) for key products
  - Gasoline: Octane, RVP
  - Diesel: Cold Flow, Density, Cetane
  - Residual Fuel: Density, Viscosity
- Summary of swing cut movements

The World Model will be used in conjunction with other external models for analytical purposes. This step will also mitigate uncertainty. Checking, vetting, and validating the World Refining output with other quantitative and qualitative analytical methods is critical.

12. Conclusions and Recommendations

The development and design of the Global Hydrocarbon Supply Model is challenging and ambitious, but represents an extraordinary opportunity to create an energy modeling system for today's complex energy analysis while setting the foundation for future analytical platforms and systems.

Some objectives of the model are a function of the analytical platform chosen for the modeling system, whether linear programming, commercial based, or otherwise. These objectives include: model stability, solving time, and flexibility to name a few. The model platform expertise of the author is linear programming, which is the recognized standard in the refining industry.

The recommendation is to evaluate and purchase a commercially-based software system for the refining sub-module. The focus of the EIA should be on model development and model operations. The EIA should not be tasked with developing, maintaining, and supporting a new modeling platform.

With this recommendation, some stated objectives can readily be achieved with a commercially-based LP platform:

- Flexibility to develop multiple, aggregate regions
- Ability to operate on a stand-alone basis
- Break-out aggregate regions into smaller, country models
- Switch to different periods (summer, winter, average)
- Quickly add new products, mapping, and specifications
- Transfer data to and from the refining model
- Include Terminals and Transportation (logistics) within the model
- Process sub-model operations spanning a wide range of sophistication
- Stream pooling, index methods, and pseudo-definitions
- Coupling of assay data to model, quick addition of new assays
- Training methods and courses for users

The emphasis throughout the CDR is balance. The balance objectives discussed included crude, refining, logistics, products, and the regional aggregation of these blocks. While the CDR focus is Refining and Transformation, there are other sub-models that will influence the "balance" requirements, such as Upstream, Gas and NGL, and biofuels which ultimately will be considered in context with the Refining model, and vice-versa. Some of the specific blocks discussed include:

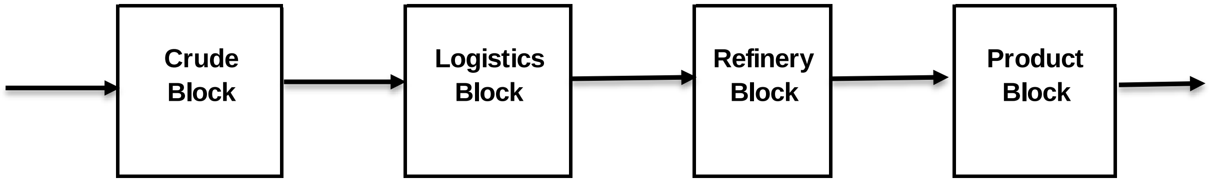

Figure 22. Block Method

A balanced design considers many elements in the model:

- Number of regions
- Number of crudes
- Number of products
- Transportation modes
- Number and types of product specifications
- Complexity of refinery sub-models
- Availability and maintenance of data

It is unlikely that the model design will be limited by technical constraints. Some commercial platforms can be developed with up to 99 separate refinery/terminal locations. The constraint will be on the human element; the ability to develop, implement, and maintain data is significant. Equally important is the ability to run and analyze the results. It would be a significant model failure if the model can provide "the answer," but the analysts cannot explain "why." A fifty region model can be developed within technical constraints, but would be overwhelming to operate.

The CDR provided an example of 22 base regions, which could be coupled with additional stakeholder "preferences." A World Model represented with approximately 30 regions is reasonable. The CDR further recommends regional crudes by types — either characterized by an actual crude, or a blend — versus World Blends of Heavy Sour, Light Sweet for example. Using approximately 15 – 20 crudes should reasonably capture the regional World crude types. This will be a function of the Upstream model data inputs. Combining the World crudes into broad aggregate blends (e.g., Hvy Sour, Med Sour, Med Swt) is overly simplistic, which can have negative consequences to achieving stated goals.

The CDR recommends using a High-Quality and Low-Quality product as a guideline for model development. Each country can have a unique specification system (e.g., US gasoline specifications can be different from Western Europe). Some countries will have a single quality, others will have both qualities, and others can combine to create an average product. The use of primary and secondary sets of specifications can be beneficial to model development and operations. These specifications can be invoked with a switch. Higher-quality products require more processing, and consume more energy, which impacts emissions and energy efficiency; this is the basis for recommending more than a single grade product.

Intermediates balancing will be challenging. Intermediates can include naphthas, intermediate distillates, VGO, resids, and slurry. Data in the United States are fairly robust but are difficult to obtain in the rest of the World. Balancing aromatics and petrochemicals supply/demand will also be challenging. Aromatics can be produced and sold at a refinery block, but no attempt should be made for a World supply/demand balance during this prototype.

The World Model will transport products to satisfy import, export, and consumption demands. This will be done with the use of a single quality of product that will satisfy any regional demand, to greatly simplify all the potential grade movements. The developers can change protocol and create a unique export material if the volume or quality warrants a unique distinction (e.g., US export gasoline to Mexico).

The process sub-modeling system should be reasonably consistent with the recommendations of the CDR. Process sub-models will have different modes and feed quality adjusters, and while not as advanced as process simulations, the technology will be sufficient to reasonably distinguish yields and operations for the multiple crude quality types defined. Moreover, reasonable technology must be employed for modeling goals of energy and emissions balances.

Developers should not let the “number” of regions, crudes, products, or specifications be the defining criteria for the model. These are flexible, and deviations can be expected. One of the fundamental objectives that must be accomplished is a World weight and material balance, which will be done through accurate representations of inputs, operations, and outputs. This is the defining criteria, not the number of countries, crudes, or products.

Logistics, transportation, and terminals can be implemented inside the refining sub-model. Terminals will be the balance point for all country (or aggregate) balances. Crude terminals can be used as independent blocks to “collect” the specific crudes from the Upstream model. Terminals will receive imports and ship exports. The refinery will move product to the terminal to represent the production. A product sale represents a consumption. Ultimately, for every product the terminal will represent the balance point for production, imports, exports, and consumption.

Transportation vectors can be defined to move products by type, origin, destination, and mode (e.g., VLCC, pipeline). All transportation vectors can have individual transportation costs. Vectors can be combined and grouped to represent aggregate limits.

With the abundant data requirements and operational decisions, one philosophical development strategy is design the model with the lowest common data denominator in mind. Broadly speaking, data include crude production, the refining model, and the World regional logistics. The “lowest common data denominator” is a notional concept, but emphasizes examples that 50 crudes do not align with 25 regions, or 6 grades of gasoline are not needed to balance a region's gasoline demand. Examine areas of low data resolution or least confidence to form a basis to bridge to the other blocks. This strategy can be the force to allocate additional resources to shore up the gaps, with the goal that all the blocks reasonably align in data strategies, sophistication, fidelity, and protocols. This model will be designed for strategic analysis and insight. The level of detail is not intended for refinery-specific analysis, for which separate models can be developed.

The model will be designed with data bounds to reflect reasonable tolerances on known operational points. Most modeling platforms will “move the World around to save a penny.” The World Model — at least in an LP platform — will optimize margin across all the World operations, but in reality, the industry does not operate “optimally.” These facts require some mitigating code: if a regional crude run is 100 MPBD, add a minimum and maximum of 90 and 110 MPBD, respectively, as an example.

And finally, this CDR initiated with the following: “The primary objective of the Petroleum Refining Component sub-module is to provide a reasonable representation of the World refining industry. However, the definition of 'reasonable' is wide, depending on an individual stakeholder’s needs.” Defining reasonableness will require deliberate efforts of stakeholders. This model design should incorporate numerous strategic, “whiteboard” sessions, led by an industry facilitator before, during, and after prototype development. These sessions will bridge the gaps, and provide alignment, between numerous components: tools, methods, goals, platforms, knowledge base, integration, and personnel. Maintaining a balance of reasonableness with sophistication will form the foundation for a word-class global refining model.

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