

**White Paper on Technical Issues for Consideration in the Design and
Development of the Liquid Fuel Market Module (LFMM) of the
National Energy Modeling System**

Prepared For:
U.S. Energy Information Administration



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Introduction

The Energy Information Administration is currently reviewing and replacing or revising the NEMS liquid Fuel Market Model (LFMM) – a replacement for the current Petroleum Market Module. This white paper is one of four commissioned to explore design and implementation ideas and to address module requirements, scope, structure and methodology for the LFMM.

The current review was preceded by a survey of stakeholders on what issues questions and capabilities should a new LFMM be able to address in the context of a mid-term projection and analysis system. The top priority items included (but were not limited to):

- Provide fuel prices and margins by product and region,
- Analysis of carbon dioxide issues,
- Consider features for investment decisions,
- Include all non-petroleum sources of liquids,
- Capability to analyze renewable fuel standards and carbon policies

This white paper first discusses some of the limitations and concerns with the current PMM module, focusing on those for which suggestions/ideas are offered later on. The paper then highlights key market trends which will drive future refined product supply, refinery operations and product prices and margins, and which are critical for the development of a revised LFMM. Suggestions are then offered for the structure of LFMM and for concepts to be included in the design. Finally, the last section focuses on issues raised in EIA's white paper on the development of LFMM, other EIA correspondence, and discussions with DOE stakeholders.

Limitations and Concerns with Current PPM Module

The major limitations and concerns with the current PMM module are related to the costs and time required for maintaining and operating the module, the mismatch between analytic needs and PMM emphasis on liquid flows, overly complex refinery representation, outdated refinery model structure and overly simple linkage to the international liquids market. Difficulties have been encountered developing reasonable price differentials and margins, natural gas and still gas consumption, crude versus product imports and refinery expansions, retirements and new construction.

Some of the above limitations were addressed in a 2003 review of the PMM by Hart. The 2003 review noted that, as with any aggregate LP model, the NEMS refinery model is subject to over-optimization which will tend to result in overstatement of refinery processing capabilities and misrepresentation of relative product values and margins. Some inherent features of NEMS add to its potential for over-optimization. The model handles intermediate stream quality with linear combinations of streams of specified quality. This allows for optimal selection of intermediates for processing/blending, a capability not representative of actual situations. If a replacement refinery LP is selected for the LFMM, a property driven component model formulation is recommended. With the property driven approach, the model calculates actual intermediate qualities and processing yields are adjusted based in intermediate feed quality.

The current model is more complex than needed. Numerous processing options are available to the model to represent a wide range of processing options. Many of these options are not needed or used by the model for aggregate analyses and NEMS projections. As options, specifications, etc., were added over time, the model options required additional expansion for subsequent refinery processing. In the 2003 report an example is provided noting that the model included over 200 FCC gasoline streams, 5 options for further processing and about 20 quality parameters. Many of the options were not used or required in typical model runs.

In addition to adding complexity, this existing complex structure increased the potential for over-optimization. The more options that were available to the model, and in particular options for processing a specific high or low quality stream, the more opportunities were created for selective processing and over-optimization.

The property driven approach will eliminate the need for much of this model stream proliferation. In addition, the model can and should be streamlined to limit processing options to the minimum necessary to capture a reasonable simulation of average aggregate operations.

The current model does not provide for adequate technical detail for representation of emerging liquid fuel sources and the impact of non-petroleum liquids of refined product blending and associated refinery impacts.

Key Market Trends Driving Future Refining and Refined Product Supply, Pricing and Margins

Current refining and refined product markets are considerably different than those which were characteristic of the era when the existing PMM was developed. Refining and refined product markets will continue to change in view of issues such as growth of non-petroleum liquids, efficiency developments and declining demand in industrialized regions, and emphasis on climate change and fuel carbon. Some of the key market trends which will be critical for representing refining and refined product production, prices and margins are highlighted below.

Ethanol Role in Gasoline Market

The Renewable Fuel Standard will continue to force a greater share of the gasoline market to include ethanol. This will in turn decrease the portion of gasoline supplied by refinery/crude derived blend stock, impact refinery gasoline quality requirements, require adjustment in refining operations, costs and relative product values. From a refining perspective, one of the more significant impacts will be the result of higher ethanol blends. Although gasoline for non-flex vehicles is currently limited to 10% by volume, waiver requests for higher ethanol blend volumes are currently under review and eventually Hart believes higher blends (at least to 15%) will be allowed. The higher volume ethanol blends will have gasoline volume, volatility and octane implications and will indirectly impact refinery hydrogen production as well. All of these changes will impact gasoline production capability, costs and margins. (Note that the current AEO does not incorporate the higher blend volumes, but they are likely to be approved and marketed in the future).

The LFMM gasoline blend approach presented later in this paper will provide for representation of higher blend volumes and capturing refining impacts.

Other Non-petroleum Liquid Sources

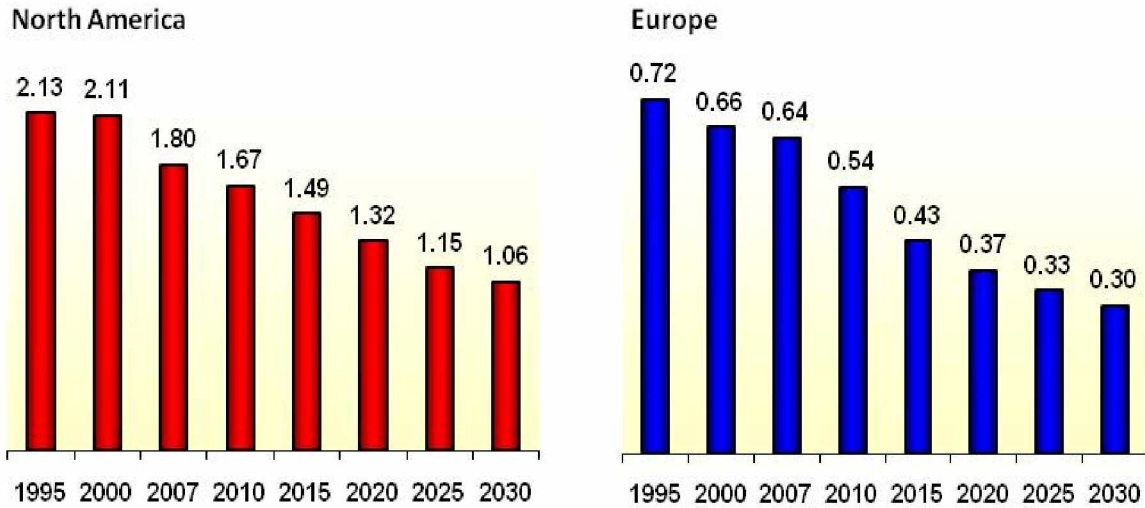
Likewise biodiesels, other fuel bio-components and GTL/CTL components will play a greater role in the future and their impacts need to be adequately represented in refining volumes, quality and costs.

Shift from Gasoline to Diesel

Anticipated market trends, fuel economy standards, fleet dieselization (primarily Europe), alternate fuels and biofuel penetration will dramatically impact refinery yield requirements for gasoline versus diesel. According to the AEO 2009, gasoline made up 46.3% of 2008 refined product demand and diesel fuel (including other distillates) made up 20.3%. By 2025, the product shares will be 45.2% gasoline and 23.6% diesel. When considering growth in ethanol and product imports, the yield shift for refinery production is considerably greater.

Figure 1 illustrates the impact of future yield shifts on the required ratio of refinery gasoline to distillate production for North America and Europe. Both regions (Europe less so) employ extensive FCC conversion capacity originally focused on gasoline production. The shift to diesel will place constraints on yield capability with impacts on gasoline-diesel price differentials. In Europe the required yield shift will exceed refinery capabilities and traditional FCC facilities will require replacement. The same may eventually be the case for the U.S. as well. In any case it is likely that the current refinery model structure does not adequately represent the capability and costs for required yield shifts.

Figure 1
North American and European Gasoline-to-Distillate Ratio (1995-2030)



Source: Hart Energy Consulting analysis and forecast (2008)

Reduction of Refinery Utilization/Capacity Requirements

U.S. refinery capacity requirements/utilization will decline over time while in the short term new complex capacity will come on line. According to the AEO 2009 refinery crude throughput will decline from 14.76 MMBPD in 2008 to 13.86 MMBPD in 2025. The same will be true in Europe, a primary source of U.S. imports. Surplus capacity will result in low margins. The model needs to recognize the decline in utilization and incorporate industry rationalization over time.

Rationalization can be handled with removal of capacity offline to maintain a range of utilization and/or margin or with model adjustments based on economics and/or utilization.

Incorporation of Low Carbon Fuel Standards/Carbon Intensity/Carbon Reduction

The elements of low carbon fuels and carbon intensity need to be incorporated to reflect emerging policies and future fuel production strategies. Carbon intensities and characteristics of various biofuel and non-refinery fuel components can be included in production modules for these components. For refinery components a carbon intensity factor is recommended for inclusion in the fuel component quality parameters.

An example of a refinery fuel carbon intensity factor is provided in the following example for calculating refined product CO₂ emission factors:

$$\text{CO}_2 \text{ (Tons/Ton fuel)} = \text{CF} * (44/12)$$

Where CF is the fraction of fuel carbon in Ton C/Ton fuel
(44/12) is the tons CO₂ combustion product per ton fuel carbon.

For components specifically identified in gasoline blends (butane, benzene, etc) carbon factors can be specified based on chemical composition. For other gasoline components gasoline can be specified based on aromatics, olefin and other. The gasoline carbon fraction for this portion of the gasoline can be determined as:

$$\text{CF} = \text{A} * .907 + \text{O} * .857 + \text{P} * .85$$

Where A is the fraction of aromatics assumed to have an average carbon fraction of .905, O is the fraction of olefin assumed to have an average carbon fraction of .857, P is the fraction of paraffin, cycloparaffin and other compounds assumed to have an average carbon fraction of .85. Aromatics and olefin are traditional gasoline quality parameters and paraffin makes up the remainder.

For diesel fuels either of two methods is suggested:

$$\text{CF (Diesel)} = .864 + (\text{A} - \text{Ab}) * (\text{ACF} - .864)$$

Where A is the diesel aromatic content and AFC is the appropriate carbon factor for incremental diesel aromatic species.

Or

$$\text{CF (Diesel)} = .864 + (\text{LC} - \text{LCb}) * (\text{LCCF} - .864)$$

Where LC is the fraction of light cycle distillate component blended in the base and supplemental case, and LCCF is the appropriate carbon factor for light cycle oil.

Incorporation of CO₂ Emission Factors for Refinery Processing and Other Liquid Fuel Production

The LFMM will likely need to incorporate GHG emission factors for consideration of emerging climate policies. These will largely be associated with fuel consumption. For refinery operations, the emissions need to include FCC coke burning operations and hydrogen production. As policies emerge, consideration may be needed for allocation of emissions for refinery electricity (between refining and utilities).

Impact of Bunker Fuel Reformulation

MARPOL regulations will require reduction in bunker fuel sulfur. This will initially result in a shift from residual to diesel demand but eventually may involve refinery production and markets for low sulfur residual fuel. As the LFMM is developed the likely bunker fuel outcome should be evaluated.

Canadian Oil Sand Processing

Increased Canadian oil sand processing will require special refinery processing capability, primarily coking capacity. The balance between bottom processing capacity and processing requirements will be the primary driver of crude differentials and light heavy product differentials. Canadian crude processing and capacities need to be adequately adjusted/incorporated into the LFMM.

Structure of LFMM and Concepts to be Included in Design

General Module Representation

Hart recommends that EIA continue to employ the refinery LP model as the core of the LFMM. The LP provides the best option for incorporating interactive technology relationships, considering crude and product qualities and representing economic factors that will establish refinery level crude quality differentials and refined product prices and margins. The refinery LP also provides a wide range of flexibility for adapting to changing environments and technology developments. Although a simplified module approach is desired, this latter flexibility is required to keep pace with changing markets.

The current LP model structure can be revised and updated for the LFMM, but this option is not recommended for a number of reasons. First, given the proliferation of model activities over the years and its current complexity, it is doubtful that significant savings and efficiency could be gained by keeping the existing refinery module. Second, as pointed out previously, the use of linear combinations of various quality intermediate streams adds to complexity and over-optimization and will lead to further excessive model size proliferation as model updates are required. A property driven model approach offers a far superior option. Third, the current model structure does not easily represent multiple quality parameters in intermediate streams, an option which becomes more critical with increasing stringency of specifications and greater blending interactions with non-petroleum liquids (primarily ethanol).

Regional Representation

It is probably best to maintain the current regional representations in the model (with the possible exception of the East Coast change discussed later). The PADD regions provide a good representation of key regional trade and refining differences in the U.S. and are well documented

and familiar to the agencies. The separate East Coast region distinguishes the primary import district, PADD 3 represents the marginal U.S. supplier and the primary petrochemical processor, PADDs 2 and 4 represent the major Canadian Oil Sands processors, and PADD 5 includes California which is characterized by unique product specs, refinery configurations and the region of initial low carbon initiatives. The required conversions to regions of other NEMS modules are already established. If further simplification of the model is desired, PADDs 2 and 4 can be combined without significant impact.

Processing and Blending Representation

A replacement generic refinery LP model with component properties (recursion) will overcome most of the shortcomings of the current model structure. With advances in refinery LP techniques and software, a replacement model will most likely be less complex in terms of incorporating the module into EIA forecasting systems. Some of the factors that were driving over-optimization in the existing model will be eliminated, but no LP, and in particular global LP, will be immune to over-optimization tendencies. These must be addressed with careful design of the model structure, constraints, and data and an understanding of the goals of the simulation and drivers in the industry.

In keeping with the objective of developing a simple, low maintenance representation of liquid fuel production providing reasonable supply and economic relationships, Hart would recommend that LFMM processing and blending representations be structured to provide simple, low complexity processing schemes where possible in combination with more detail for those technologies that will be the primary drivers of marginal production capability, investment requirements, refinery economics, price differentials and margins.

The first step in simplifying the representation is to minimize processing options through the use of average aggregate operations. The idea is to simulate refinery operations, capacity utilization, blending for a major portion of each region with minimal complexity and for which actual historic data can be used to set a portion of refined product production. For example, the aggregate operations would specify average crude quality and production of miscellaneous, low volume products. Secondary refinery processes or those which will have little impact on incremental supply, process and margins should be represented by a single or few processing options. For example, light oil processing operations such as alkylation, polymerization and dimerization may be combined and only one or two operating modes included. The options for other major processes should be limited, where possible, to only a few options and a limited range of operations. For example existing hydrocracking operations can be characterized by one or two feed options and one or two yield structures.

Figure 2 provides an example of a refinery LP processing model representation incorporating simple low complexity processing and more detailed critical marginal operations. The simple model representations would include all existing refinery processing capacity and technologies but with simple limited representations/options (as indicated on the first page of Figure 2). Supplementing the simplified refinery processing representations would be a set of detailed

Figure 2
 Simple Low Complexity Refinery Representation with
 Detailed Marginal Processing
 (Simple Aggregate Refining Representation)

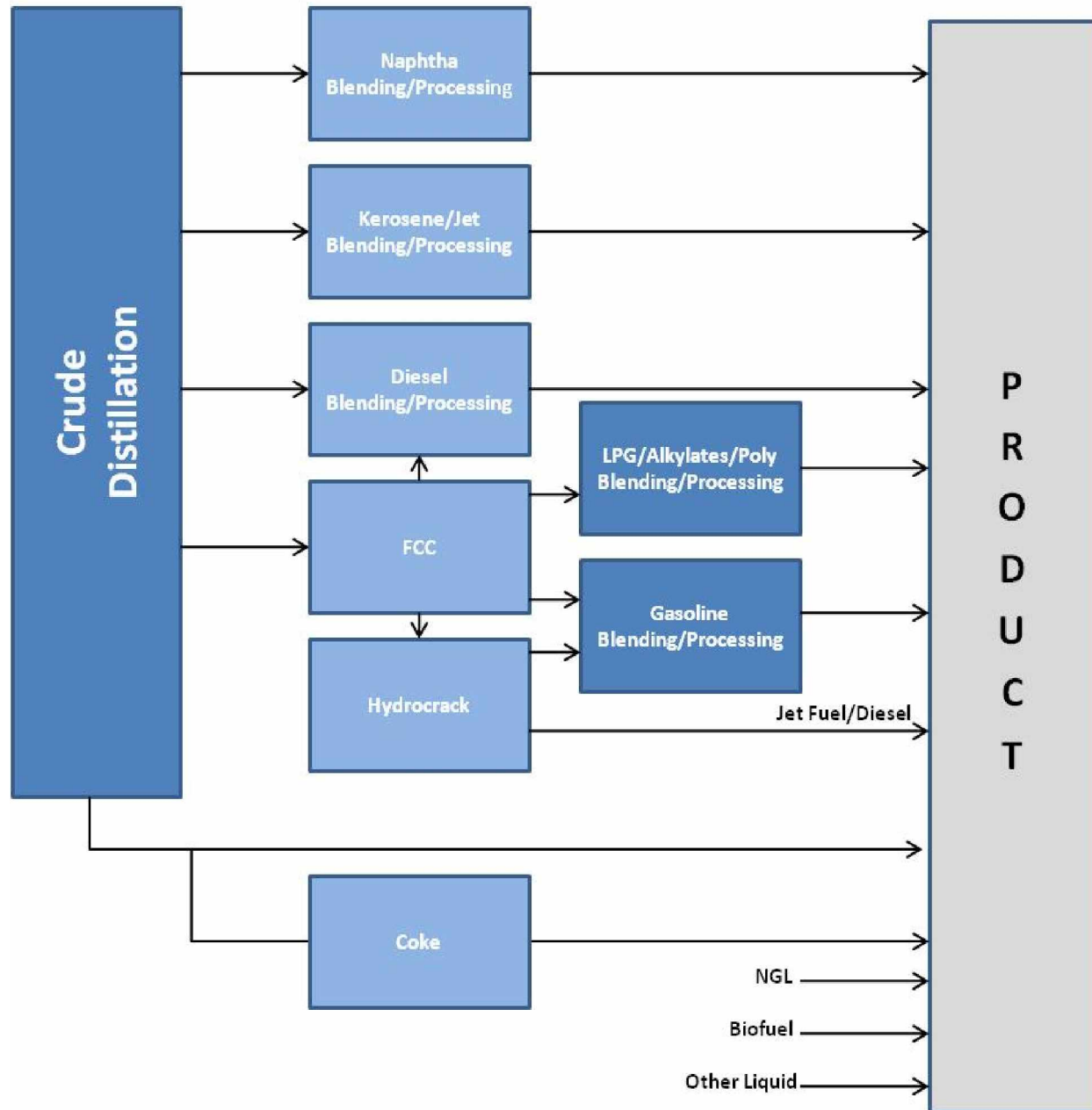
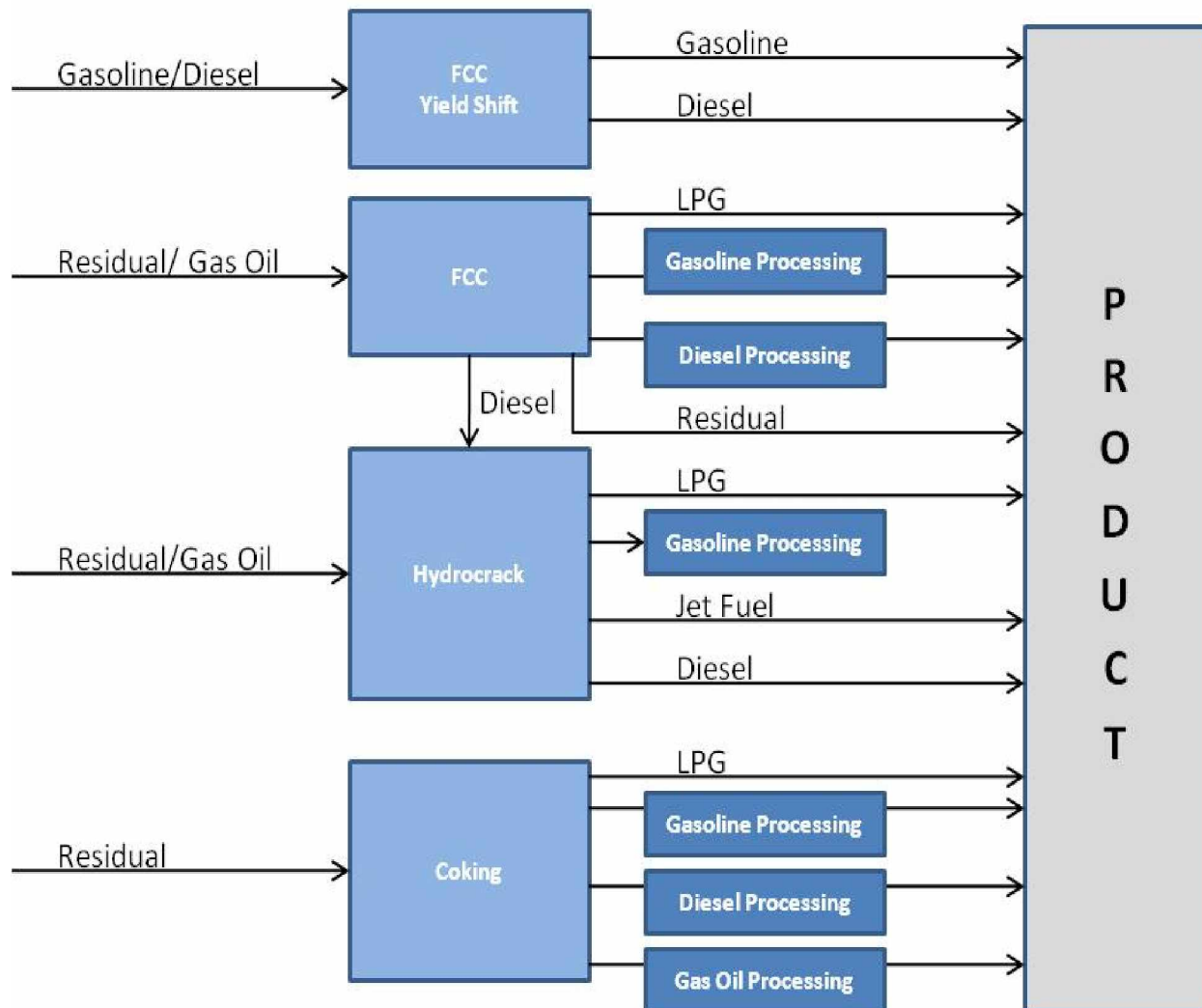


Figure 2 continued...

Simple Low Complexity Refinery Representation with Detailed Marginal Processing (Marginal Processing Representation)



representations for specific key processing technologies as indicated on the second page of Figure 2. The detailed marginal processes represented would be those which represent the primary drivers of supply, price, etc. These processes will also incorporate the option to invest in capacity expansions and/or include new technologies. The detailed marginal representations would include separate sub models for the primary processes with a full range of processing options, intermediate product quality, etc as required to capture refining requirements and economics.

Both the simplified and detailed representations in Figure 2 and discussed above would be included in the same model. One crude unit in the model would be provided for the simple base representation and an average regional crude mix and volume would be available to the activity. It would in turn generate average quality intermediates that would be available to the first set of FCC capacity, reforming, etc. A second (or more than one additional) crude process would have the option of processing incremental low, high or other marginal crude oils available to the region. The intermediates from these crudes would be sent to the set of FCC, hydrocracking, etc. with more detailed representations of available technologies and operating severities.

The final processing streams for blending from both the base operation and the detailed incremental operations would be made available for final product blending. Figure 3 is another flow diagram for the combined simple base level operations and the marginal detailed representations, also showing the integration of the final product blending.

Again, the model includes a base level of operations characteristic of a region and representative of typical regional operations close to historic regional operations. The base crude oil distillation operates on average (or close to average) crude quality and crude and other non crude throughput is limited to approximately 80 to 85 percent of recent actual.

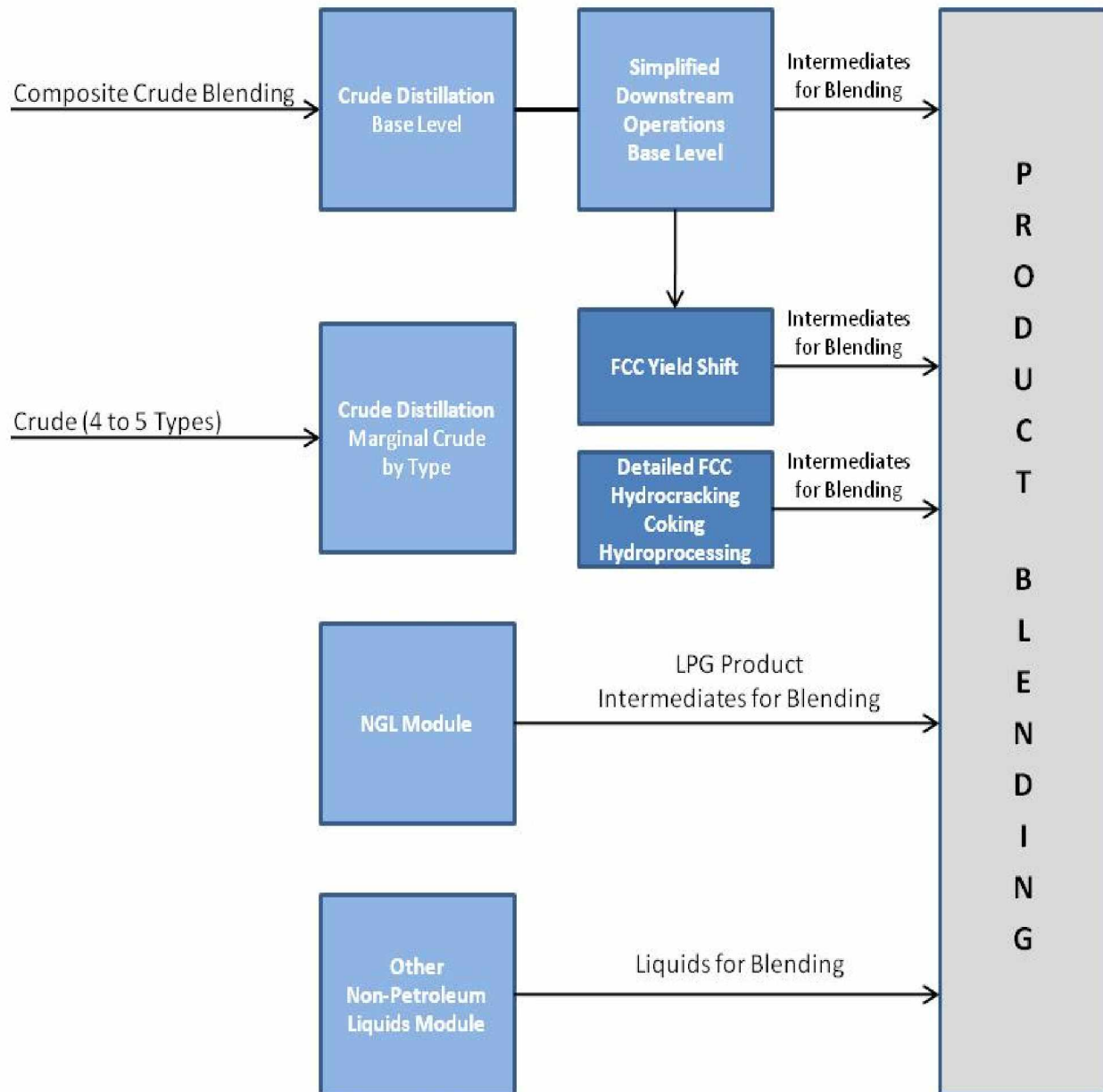
Downstream processes are limited in processing flexibility and all miscellaneous secondary processes which have limited impact on incremental supply and operations are included in the base operations. The base operations produce most of the miscellaneous product for the region.

A second set of processes in Figure 3 represent the key marginal operations. For marginal operations, flexibility is provided to process 4 to 5 crudes representative of available and/or typical marginal crude available to a region. Special crude and downstream options would be included to adequately represent processing Canadian oil sands crude. The crudes would include a high level of yield and quality detail to adequately capture marginal impacts on downstream operations, final product blending and economics.

The downstream processing in the represented detailed processing options would include a full range of operating modes and capability to process ranges of intermediate feeds considered typical or a potential for the region. The marginal operations also include process options for adjusting yields for base operations or for further processing output from base operations. For example the marginal operations would include yield representations and limits to shift from gasoline to diesel in the FCC and would include capability for additional conversion of residual fuel or hydrotreatment of gasoline/diesel components. Additional technology requirements would be included in the marginal capacities such as technology options to produce a low sulfur bunker fuel.

The base case operation process capacities plus first level of marginal capacity for a process would be limited to the total regional capacity for the process. Additional marginal capacity can be added subject to a per barrel capital charge. The sum of all of a process capacity activity would be correlated to regional capacity constraints and expansions, i.e.:

Figure 3
Recommended LFMM Processing and Blending Representation



Regional Capacity – Base capacity use – Marginal capacity use = 0

With this base-marginal operations approach, the use of the base case operation, specified based on actual historic operation, will simplify the regional simulation and provide an available basis (historic data) for the simulation. The marginal operations will provide required and desired (economically driven) product production and marginal costs.

The process scheme in Figure 3 also includes an NGL module and the non-petroleum liquid module. The NGL module would distinguish LPG and other NGL products for blending, processing or final product disposition. For the non-petroleum module, individual process modules or process options would be provided for each non-petroleum liquid available. The individual modules would include feed stock and costs, processing yields, fuel and utility consumption, operating costs, qualities and carbon intensities. Subsidies, tax exemptions could as well be included.

The final element of the above modeling approach is the product blending. All refinery gasoline, jet fuel and distillate (diesel) intermediates from both the base and marginal processing are made available to final product blending with associated quality parameters. In addition, the non-petroleum liquids are provided to blending, also with associated quality parameters. Therefore final product blending considers the impact of non-petroleum liquids on product blend volumes and qualities and as well provides for simulation of the impact of these liquids on refinery operations. The blending will also include carbon intensities or equivalent for refinery and non-petroleum liquids.

The blending operations of Figure 3 provide the option of producing conventional blends (i.e., gasoline or gasoline-10% ethanol blends) or alternate fuels/blends (i.e., E85 or gasoline-15% ethanol blends). Inclusion of the non-petroleum liquids in the LP blending allows for better representation of their impact on product price differentials and product margins.

Representing Domestic and International Markets

One of the greatest challenges for LFMM will be in the representation of international markets and their relationship to domestic markets. Imports, primarily of gasoline, will be a significant determinant of domestic supply, product prices and price differentials. One option for handling international operations would be to incorporate international regions into LFMM. However, this would add to model complexity and more importantly to resource requirements to specify international demand, transportation linkages and costs, international subsidies, etc. Furthermore, with the complexity of international trade flow, the validity of the international representation would be questionable.

Another option would incorporate portions of the international market into LFMM, minimizing the interaction and impacts of the remaining markets. Two options are suggested: specify levels and types of imports from Canada and Puerto Rico/USVI and incorporate Eastern Canada and Puerto Rico/VI into the PADD 1 model.

Canada and Puerto Rico/VI represent a major share of U.S. product imports. Refineries in these regions are dedicated to the U.S. East Coast market and provide a stable level of East Coast imports. Imports from these sources could be held constant or adjusted slightly (to account for growth in indigenous demand).

The second option would be to include Eastern Canada and Puerto Rico/VI into the East Coast model. A separate product demand set could be specified for Canada and Puerto Rico/VI to maintain US supply demand balances. For Hart's World Refining and Fuel Service international refining simulations, Eastern Canada and Puerto Rico/VI are combined with PADD 1.

For exports, a specified level of product export from PADD 3 to Mexico should be specified. This could be varied over time based on anticipated Mexican demand and refinery capacity expansion schedule.

For imports excluding Canada and Puerto Rico/VI, Europe provides the major source. The current procedure could be continued, with an estimated supply curve limited to Europe. Alternatively, a simple model of European operations could be run off line with supply curves representing incremental diesel supply to Europe from CIS and Middle East. The model output would supply an estimated utilization for Europe and volumes/prices of gasoline surplus available to the U.S. market. A supply curve could be developed from the simulation. The simple European model can use the same LFMM refinery LP system.

Imports from other regions are small and can be ignored, particularly in view of the declining utilization rates in the U.S.

Other Issues

Special Analysis Models

Models designed to support the forecasting activity will not necessarily be appropriate for special studies of fuel, refining or other policies. However, improvements in LFMM specified for forecasting will most like have broader application for special analysis.

For the recommended model approach in Figure 2/3, the detail provided for marginal operations and blending will significantly enhance NEMS capabilities for policy analyses. The base processing operations can be expanded to further improve the model's analytic capability if desired for specific policy analyses. The recommended model processing attributes are/would also be constructed to address the major anticipated market trends/policies identified in the key market trends section.

The forecast model formulation will not adequately address all analytic requirements. For these cases versions of the model used for the LFMM can be maintained on a separate platform.

The closer the basic structure is to the LFMM version, the easier it will be able to be modified by in-house modelers.

Product Detail

Refined product detail should include the following:

Gasoline – conventional and reformulated, 10% ethanol and other ethanol blends depending on the status of waivers,

E85

Kerosene jet fuel

Distillate fuel – heating oil, 15 ppm diesel, 500 ppm diesel, 1000 ppm bunker diesel, kerosene,

Residual fuel – 5000 ppm low sulfur, high sulfur, low sulfur bunker fuel

LPG

Petrochemicals – naphtha, gas oil, propylene, aromatics

Other – lubes, wax, asphalt, aviation gasoline, special naphtha, still gas and coke.

EIA has noted past difficulty in producing reasonable projections natural gas and still gas. An initial still gas volume should be benchmarked against actual data as a starting point. To achieve closure with the actual still gas volume, adjustments may be required with LPG in the still gas pool. Once this is established, there should be no difficulty arriving at a reasonable projection.

Likewise, the model should be calibrated to provide historic refinery fuel consumption. With residual fuel consumption held constant, natural gas will provide incremental fuel and reasonable projections should not be an issue. There will be a tradeoff between incremental electricity supplied by the refinery versus purchased from utilities which will impact refinery natural gas projections. Offline analysis of refinery utility sources should allow for reasonable electricity and natural gas projections.

Capacity Investments and Planning

Capacity investments are made considering a multi-period outlook while the recommended forecast structure includes the ability to invest in desired capacity (increase capacity utilization incurring a per barrel capital charge) based on individual annual solutions. Hart does not believe that the multi-year consideration is necessary and investment projections based on annual operations are adequate. In the near term there will be surplus capacity and little need for investment. Longer term investment requirements are not anticipated to be cyclical or required in a manner that the gradual increase generated under the annual investment basis will not be representative.

Investments currently underway should be specified in the model, by year of anticipated completion. No other capacity expansions should be allowed until 5 years after the first year of analysis.

Foreign Unfinished Oil Supply

Foreign unfinished oil supplies represent about 4 to 5% of total refinery input. Unfinished volumes have increased over the past few years, but the increase (over the past 4 years) represents only about 1 to 2 % of refinery input. Foreign unfinished oil inputs should be characterized based on the most recent historic data (volume and type of unfinished input). This figure should be held constant for future years, unless a know user is scheduled to shutdown. The unfinished oils are an economically attractive substitute for crude oil for specific refining situations. In the absence of these volumes, refiners would make up the volume with crude purchases. Therefore, not capturing any change in these volumes will not lead to unreasonable forecasts.