

**MODELING IMPACTS  
OF  
REFORMULATED DIESEL FUEL**

**ORNL Sub-Contract 80X-SY527V  
Modification No. 6**

**2006 Cases**

**Draft Report  
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## MODELING IMPACTS OF REFORMULATED DIESEL FUEL

### Introduction

In June, EnSys undertook a first pass analysis of the effects of sulfur reduction in gasoline, on-road and off-road diesel. This interim report summarizes the approach to and results of a second series of cases undertaken with modifications based on feedback and commentary on the first run set. A final report will follow.

The interim report discusses:

1. The RYM model changes made for the second pass runs
2. The results from the cases for 100% ULSD conversion to ultra-low sulfur
3. The results from the cases for phased introduction of ULSD at 10 ppm sulfur.

Readers are reminded that EnSys' "mandate" was to assess the costs of refinery ULSD production at reliable levels of supply, i.e. our base assignment was to take a relatively conservative approach rather than one relying entirely on prospective technologies. Results are presented and discussed primarily for the Base scenario. However, the cost effects of a possible Optimistic scenario are also presented.

The analysis was built on a calibration of the latest RYM model against 1994 PADD3 actuals, adjusted forward to 1996 and thence to 2006. The development of the 2006 Base Case is described in the Appendix. It embodied 1996 product qualities, including on-road diesel at 360 ppm and off-road at 2450 ppm. Gasoline sulfurs (CG and RFG) were then reduced to 30 ppm and the total investments related to this and to shifts in moving to 2006 were locked in to create a forward base case with gasoline at the new properties and distillates still at 1996 qualities. Results for ULSD sulfur reduction thus reflected the situation where refiners would have decided first on investments for gasoline sulfur and would later/separately decide on those for diesel sulfur. The analysis did not study opportunities for integration (optimization) of gasoline and ULSD sulfur reduction but focussed solely on the latter.

### Model Changes for Second Pass Cases

Based on feedback received and on further technology assessment work, EnSys made the following modifications to the RYM model:

- \$ the capital costs for deep HDT units HD1 and HD2 were modified by (a) eliminating a 30% contingency factor that had been present and (b) raising the base size for investment to a more typical 25,000 bpsd. These changes brought the capital costs into the range of costs provided by vendors and other third parties.
- \$ a redundancy factor of 15% was retained on all the deep HDT processes in view

\$ of the critical duty of these units and uncertainties over service factor. This same 15% factor had been applied to FCC gasoline desulfurization processes refiner and vendor data and industry feedback were employed to further differentiate the distillate deep HDT processes in the model. The June version contained conventional distillate desulfurization (DDS), SynSat type desulfurization to around 300 ppm (SYD), first stage deep desulfurization to 30-20 ppm using proven technology (HD1) and second stage UOP Unisar proven deep desulfurization to sub 10 ppm with very substantial (90%) de-aromatization. These latter two units were reworked into 4 “notional” units:

- HL1 - first stage processing (to 30-20 ppm) of low sulfur straight run and low sulfur low conversion LCO only
- HD1 - first stage processing (to 30-20 ppm) of high sulfur straight run streams and medium plus high sulfur and high conversion LCO streams
- HS2 - second stage processing of all first stage products to sub 10 ppm except the most difficult cracked stocks (coker gas oil and high sulfur high conversion LCO)
- HD2 - second stage processing of to sub 10 ppm of the most difficult cracked stocks (coker gas oil and high sulfur high conversion LCO)

\$ the purpose of this was to enable a more accurate representation of costs, especially of the costs of processing easy versus difficult streams and of moving below 20-30 ppm sulfur, which is indicated as a critical break-point for more difficult streams

\$ capital costs for these units were developed directly from industry and vendor data

\$ hydrogen consumptions were constructed as a function of feedstock type, degree of sulfur removal and degree of de-aromatization

\$ the representations reflect latest available technologies but are tied to actual industry data notably on the difficult stocks.

- The HS2 unit reflects latest developments of second stage catalysts that will desulfurize to sub 10 ppm with limited (30%) de-aromatization - but which were judged unlikely to be able to handle the most difficult feedstocks as described above. The selected level of 30% de-aromatization was based on vendor advice of an expected range of 30-40%.
- The HD2 unit still reflects proven technology, yet relative to the HS2 unit has a more active catalyst (which could be base or noble metal depending on the specific technology) with higher de-aromatization levels. Costs are based on industry actuals with de-aromatization levels at 70% (not the extreme 90% for the first pass HD2), versus 30% for HS2. 70% (relative) reduction in aromatics was considered a reasonable conservative basis for severe stocks,

based in part on industry data indicating a 45% relative de-aromatization associated with reaching 50-100 ppm. It is known that further desulfurization to sub 10 ppm levels requires appreciable further de-aromatization – based on current catalyst technology.

- HS2 handles all but the most refractory stocks which are reserved for the HD2 unit. Both capital costs and hydrogen consumptions were lower on the revised HD2 unit than that used for the first pass cases.
- Offsites capital costs as a percentage of onsites were reduced to 40% from 50% in the first pass cases; this based on industry data and reflecting the fact that all new or revamped HDS capacity in the US will be built in existing refineries
- Based on industry data and vendor feedback, the average cost reduction achieved by revamping an existing unit - or by integrating a new unit into existing facilities rather than building standalone - was set at 40% for the onsite capital cost. A further allowance was made for the fact that, with revamps, related offsite costs tend to be lower than the 40% allowed for new units. Consequently, the overall onsite+offsite cost reduction factor used for revamps/integration was 50%.
- Other changes were also made to the model:
  - the capital cost size bases for the CDTech and OCTGAIN units were made consistent. This resulted in the model selecting both processes in the base cases.
  - based on feedback from EPA and review of model data, the capital cost of the reformat splitter was reduced. (It was high relative to e.g. the FCC gasoline fractionator.)
  - catalytic reformer hydrogen yields were reviewed and selected yields reduced
  - in addition steps were taken to control cat reformer operating modes in order to reduce scope for over-optimization of octane and hydrogen production. (The first pass cases had shown too little need to add incremental hydrogen capacity. With the above adjustments, the second pass subject cases all added hydrogen capacity.)

**First Series HDT/HDA Unit Parameters**

	HD1	HD2
capital cost – onsites, \$ per bbl per SD	3000	1900
Stream day factor	0.85	0.85
Effective calendar day availability	0.95	0.95
feed sulfur range ppm	1500 – 20000	20 - 30
Product sulfur range ppm	20 – 30	5 - 7
HD1 revamp total capital cost at 60% of onsite cost, 0% of offsite HD2 new unit total capital cost at 100% of onsite, 0% of offsite		

<b>Revised HDT Unit Capital Costs For Second Series Cases</b>				<b>INVUNT Cap Cost New Unit</b>	<b>CAP factor</b>	<b>Effective Cap Costs New/revamp- integrated</b>
Unit	Feed S	Prod S	Duty	DsIB feed \$mmISBL	<b>Tables HL1 etc.</b>	\$mmISBL
	Redundancy/contingency factor:			1.15		
	Revamp/integration factor:					60%
HL1	0.2	30	LS kero		<b>0.8</b>	980/590
			LS hkero		<b>0.9</b>	1110/670
	0.2	30	LS DsIb	<b>1230</b>	<b>1.0</b>	1230/740
HD1	1	30	HS kero		<b>0.8</b>	1570/940
			HS hkero		<b>0.9</b>	1760/1060
	2	30	HS DsIB	<b>1960</b>	<b>1.0</b>	1960/1180
	2+	30	LCO (5)		<b>1.3</b>	2550/1530
		30	LC6/CGO		<b>1.5</b>	2940/1760
HS2 30% HAD	30	7	SR kero		<b>0.8</b>	920/550
			SR Hkero		<b>0.9</b>	1040/620
	30	7	SR DsIB	<b>1150</b>	<b>1.0</b>	1150/690
	30	7	LCO (5) No LC6		<b>1.3</b>	1500/900
	30	7	SR kero		<b>0.8</b>	1100/660
			SR hkero		<b>0.9</b>	1240/740
HD2 70% HAD	30	7	SR DsIB	<b>1380</b>	<b>1.0</b>	1380/830
	30	7	LCO (5)		<b>1.3</b>	1790/1070
	30	7	LC6/CGO		<b>1.5</b>	2070/1240

Offsites factor 0.4 versus previous 0.5

## Cases Run

The second pass cases run were per EnSys' Mod 6 Statement of Work:

Case 1: 2006 PADDIII case at 1996 product qualities

Case 2 series: 100% of on-road diesel at sulfurs from 20 - 8 ppm. (Cases were actually run at 50, 30, 20, 10 and 8 ppm.) Off-road at 2450 ppm.

Case 3: Effect of converting all off-road diesel and heating oil to 500 ppm nominal (360 ppm actual) with 100% of on-road diesel at 10 ppm

Case 4: Phased introduction of 10 ppm on-road diesel (from 360 ppm) with all off-road already at 360 ppm actual. Cases were run at 0%, 25%, 50%, 75% and 100% on-road at 10 ppm.

Cases were undertaken with the uncomposed modified RYM model:

- a. because the process modifications to the Composite RYM had not been completed but
- b. more important, to allow the analysis to fully differentiate between deep hydrotreating of easy versus difficult streams.

Result details are available in an attached spreadsheet.

## Summary of 100% ULSD Results

The LP model results obtained corresponded to EnSys' Base scenario, i.e. to costs consistent with (technologies for) low risk, high reliability supply of ULSD. Post optimal calculations were undertaken to present a Optimistic scenario, i.e. costs that would result if all PADD3 refineries were to be able to implement ULSD under the most favorable cost and technology conditions that it is estimated could obtain pre 2006. Specifically, for the Optimistic scenario to apply, a 30% reduction in capital costs versus the base would be required – corresponding to some of the more aggressive current vendor cost estimates – and catalyst breakthroughs that would enable sulfur removal from cracked stocks with reduced hydrogen consumptions versus those in the Base scenario.

- Figure 1 below summarizes the cost results obtained. Each c/gal cost represents the additional cost versus the Base Case B2 (on-road at 360 ppm) not versus the next sulfur level
- All results show a relatively flat progression from 50 ppm to 20 ppm but thereafter costs rising more steeply down to 8 ppm. For the Base scenario, the costs at 50 ppm are 4.1 c/gal at no revamp/integration, and 3.3 c/gal at 100% revamp/integration, 5.7/4.5 c/gal at 20 ppm rising to 8.0/6.3 c/gal at 10 ppm and 8.5/6.7 c/gal at 8 ppm
- Figure 2 illustrates this effect more sharply by showing the incremental cost of moving from 360 to 50 ppm and so on down to 8 ppm expressed as c/gal per 10 ppm sulfur reduction
- *The all revamp/integration cost level thus represents those refiners who have sufficient suitable distillate HDS equipment already in place to be able to convert to ULSD entirely by revamping this into new facilities and/or fully integrating new facilities into the existing units*
- *The nil revamp/integration cost level is representative of*
  - (a) *refineries that have no suitable existing facilities that can be used as the basis for revamp, e.g. "challenged" refineries and*
  - (b) *the new facilities needed to meet growth in demand (although growth again might be met in part by revamping/de-bottlenecking)*
- *All capital costs assumed new/revamped units in existing refineries*
- We believe this cost progression is realistic since it reflects the added difficulty of achieving sulfur levels below 20-30 ppm, especially on the difficult stocks (LCO and coker gas oil) since these stocks require a higher degree of ring saturation (de-aromatization) in order to remove sulfur at low levels. In other words, this quantitative finding is consistent with the feedback obtained from third parties, including industry and vendor representatives. To process LCO and CGO to below 30 ppm, it is still necessary to undertake high cost deep HDT/HAD which is not required with the easier streams.
- The uncomposited RYM model processed low and high sulfur straight run streams and low, medium and high sulfur cracked stocks, the latter each at low and high conversion/aromatics levels. The model preferentially selected the lower cost HL1 first stage unit over HD1, the first stage unit for high sulfur feeds. It could be argued that, because of its prototypical stream structure, the RYM model was over-optimizing in this respect (had too much low sulfur material available). EnSys assessed this effect by estimating the incremental capital cost and c/gal cost if, in reality, 50% of the selected HL1 capacity should be the higher cost HD1. This adds 0.35/0.21 c/gal at 50 ppm, rising to 0.58/0.35 c/gal at 8 ppm with 0%/100% revamp/integration. These adjustments were included in all the results presented.

- The Optimistic scenario leads to costs 0.8/0.4 c/gal below the Base at 50 ppm growing to 2.3/1.4 c/gal below the Base at 8 ppm. Again, these are considered by EnSys as representing a prospective rather than certain outlook and one that cannot today assure high reliability of supply. Even if such cost and catalyst improvements did become commercially available, it is unlikely the whole PADDIII refinery pool would follow this lower cost route. Refiners that invested early would tend to follow the Base scenario and costs.
- All the costs presented here are based on EIA's 2000 AEO Reference Case outlook for 2006 industrial user natural gas price at \$3.24/MMBtu (with crude at \$20.59/bbl - US refiners' acquisition cost). A reduction of natural gas price to \$2.50/MMBtu would lower ULSD sulfur costs by around 0.75 c/gal
- Cetane index values reported by RYM were high especially on Base Case blends. Cross-checks indicated that EnSys' values for the highly reformulated streams and blends appear correct but those for more conventional streams and blends are high by approximately 6 numbers. This should be borne in mind in reviewing the detailed results in the spreadsheet. This calibration error in the RYM model did not affect the ULSD cost results.

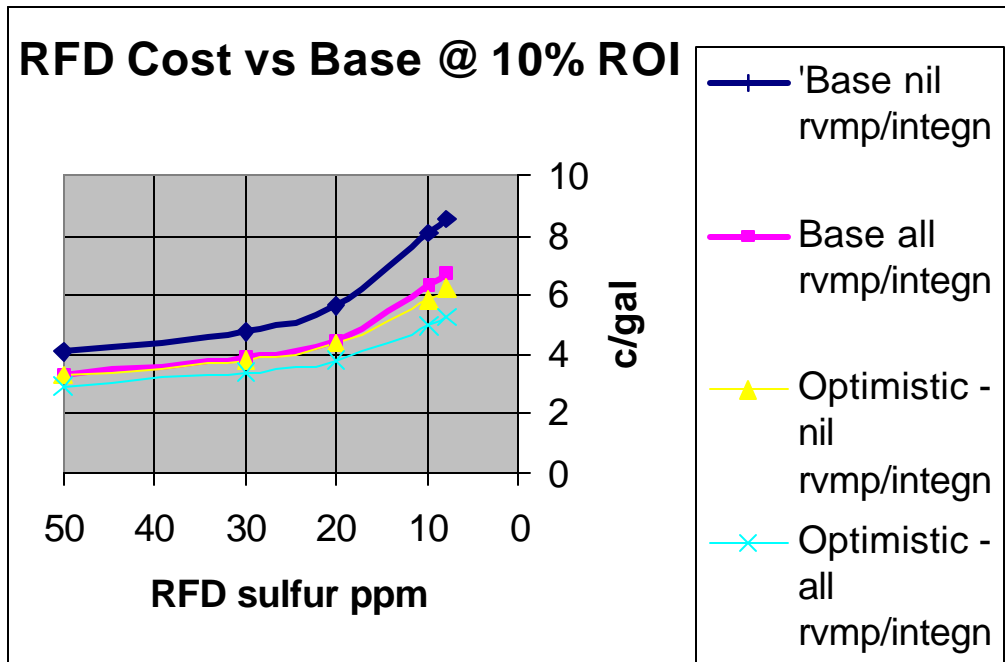


Figure 1

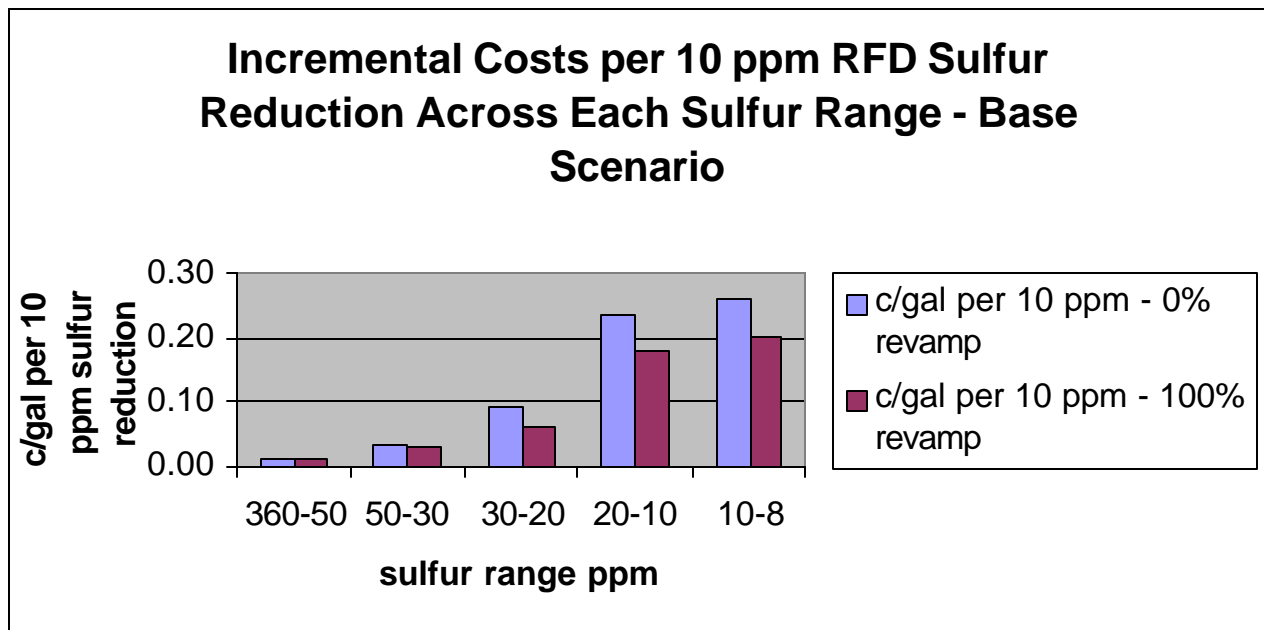


Figure 2

## Summary of Off-Road Distillate Results

The cost was assessed in two ways for converting all off-road diesel - including No2 heating oil and exports - from “traditional” 2450 ppm sulfur to 500 ppm nominal, 360 ppm actual.

1. Versus the Base Case with On-road at 360 ppm and off-road at 2450 ppm, the cost of converting both on-road to 10 ppm and off-road to 360 ppm (Case DNF) was compared with the cost of converting on-road only to 10 ppm (Case D10). The difference between DNF and D10 showed the incremental cost of off-road conversion undertaken integrated with on-road conversion. This cost was 2.1 c/gal at 0% revamp. Cost at 100% revamp was not calculated but would be approximately 1.6 c/gal. Conservative assumptions on HL1 versus HD1 investment would add 0.57/0.34 c/gal.
2. The cost of converting all off-road to 360 ppm was calculated as a stand-alone cost (Case P00) versus the Base Case (B2). These costs were 3.43/2.86 c/gal.

## Summary of ULSD Phase-in Results

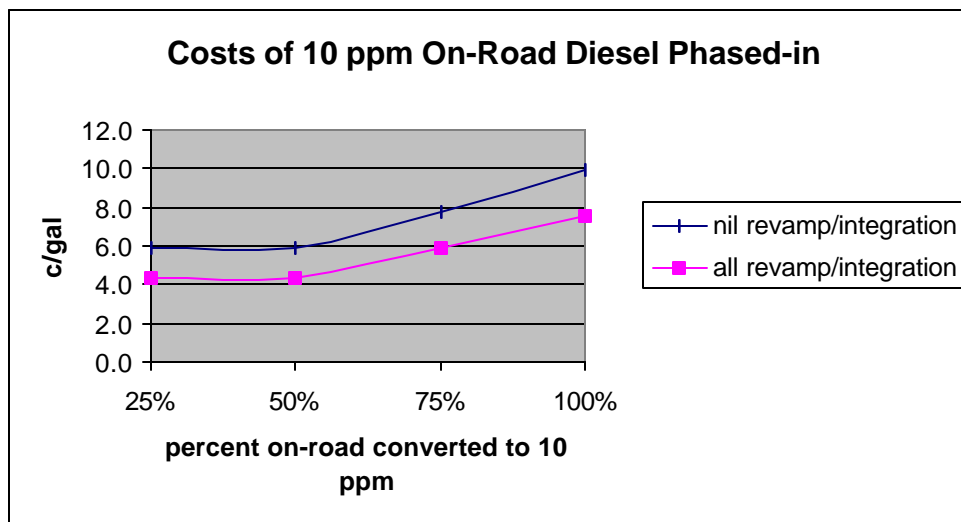
The costs of ULSD “phase-in” at 10 ppm were analyzed against a base case (P00) which had all off-road at 360 ppm. In the cases P25 through P100, the proportion of the on road pool converted from 360 to 10 ppm was raised in steps from 25 to 100%. The cost of converting off-road to 360 ppm was not locked in but was re-optimized (integrated) in each phase-in case. The 100% ULSD conversion case P100 was thus the previously run 100% ULSD case DNF.

This “phase-in” analysis can be interpreted in two ways:

1. As the refining costs of chronologically phasing in 10 ppm ULSD over time and
2. As the incremental costs of converting each successive quartile of the on-road pool from 360 to 10 ppm.

Figure 3 shows the incremental (differential) costs of the first 25% versus 0% ULSD at 10 ppm, the second 25% versus the first 25% and so on across the four quartiles.

Figure 3



- The results show an essentially flat cost of around 5.9/4.3 c/gal for the first 50% converted to 10 ppm.
- The average cost across each quartile then rises significantly, 7.8/5.9 c/gal average across the third quartile and 9.9/7.5 c/gal average across the fourth.
- Note, these cost increases occurred with tight controls in the model on sulfur. All off-road was at 360 ppm, all distillate and resid products were at max sulfur and Sox scrubber capacity was required to process any increase in FCC Sox emissions versus the Base Case (B2).
- Recognizing these controls in place, the results reflect the logical expectation that the refining system would select the easiest streams for conversion first (while keeping all remaining products on spec) and leave the most difficult streams to the last
- These results appear consistent with refiner feedback that the costs of converting the last most difficult streams (higher sulfur, highly refractory LCO and CGO) to sub 10 ppm would be of the order of 10-15 c/gal (representing the “tail end” of the last quartile)

## Commentary on Results

The “100%” and “phase-in” results raise questions over how the refining sector will actually react to a mandate for on-road ULSD, especially at or below 10 ppm sulfur ex-refinery, as modeled here.

- The phase-in results obtained may have understated the steepness of the cost curve in moving from 0 to 100% ULSD at 10 ppm. This is because the modeling was done effectively simulating a single aggregate refinery whereas, in reality, a refinery processing sweet crude could convert its “easy” streams without any impact on the quality of distillate pools in other refineries. In the model, the withdrawal of “easy” streams from the on-road pool required a compensating change to keep the balance of the on-road pool in spec on sulfur
- The costs of the last quartile are sufficiently high that – barring appreciable degradation of the quality of heating oil or further technology advances to deal at low cost with cracked stocks– it is questionable whether refiners would invest to convert the more difficult stocks (at 9+ c/gal) to sub 10 ppm
- Clearly, product commitments can be met to some degree by inter-refinery exchanges
- However, this question leads in turn to the questions of who will invest and how this proposed regulation can lead to a balanced market that is a “win win”
- It could arguably be most efficient for the global supply system as a whole to have refiners outside the US, with laxer local standards, process their “easier” streams to sub 10 ppm and export those to the US. (Foreign refiners generally have a lower proportion of cracked stocks in their distillate pools.)
- For this to happen though, it would require an investment and therefore long term supply commitment from the foreign refiners, e.g. in the Greater Caribbean. Arguably refiners with low cost natural gas, hence hydrogen, would be logical suppliers. A balanced market could result but the US would then be in a position of increased dependency on foreign refiners for supplies of a premium fuel
- US and foreign refiners *in toto* are likely to either over or under invest, especially against a single date for 100% on-road conversion.
- Under-investment would raise prices and tighten supply in the US to the point where either US and/or foreign refiners would eventually invest to meet demand. Recent evidence indicates though that the road to such a balance may be peppered with supply and price issues.
- Over-investment, e.g. defensively by US refiners, looks as though it would lead to some high cost units to process difficult stocks and to the prospect of an inadequate return on investment (as has happened with RFG).

- Some of the supply issues look like they would be mitigated if the diesel standard were set in the 20-50 ppm sulfur range.

In conclusion, EnSys believes this second pass analysis has provided deeper and more realistic understanding of the cost impacts of ULSD introduction but has raised questions regarding how this can be made a successful and economically efficient regulation.

## **Appendix A: 2006 Base Case Development**

### **INTRODUCTION**

This report summarizes the development by EnSys of its PADD3 RYM/RYM<sub>c</sub> model 2006 Base Case starting from 1998 and earlier base data and based on the 1994 Calibration Case as described in a separate Report.

This first part of this report describes the development of 2006 premises and comments on associated issues. The second part reviews the base case results.

### **2006 PREMISES**

#### **Crude Volumes & Quality**

- Domestic crude inputs to PADD3 were based on 1998 PSA volumes (Table 14) for PADD 3 production plus PSA Table 32 for inter PADD crude movements. There were only minor movements of PADD3-produced crude out of PADD3 (approx 2,000 bpd to PADD2) and essentially nil movements of Alaskan crude into PADD3 in 1998. Movements from PADDs 1, 2, 4 and 5 (California) were allocated to RYM crude types based on history and prior ICF and NPC work.
  
- Domestic crude refinery input volumes were projected based on ratio of 1998 to 2006 crude production consistent with 2000 AEO Table 80 as below

<b>Domestic Regional Crude Production Growth Rates 1998-2006 Source: 2000 AEO Table 80</b>			
<b>region</b>	<b>production million bpd</b>		<b>average annual growth rate</b>
	<b>1998</b>	<b>2006</b>	
<b>Lower 48 Onshore</b>			
Gulf Coast	0.85	0.59	-5.00%
Mid Continent	0.37	0.31	0.8%
South West	1.11	1.08	1.0%
Rocky Mountain	0.45	0.39	0.3%
West Coast	0.72	0.59	-0.6%
<b>Lower 48 Offshore</b>			
Gulf Coast	1.29	1.26	0.30%

- total PADD3 refinery crude input was taken from PSA 1998 Table 9 and escalated at the annual growth rate for US total crude usage from AEO 2000 Table A11 (0.6%), an increase of 340,000 bpd by 2006

#### Foreign Crude Inputs

PADD3 refineries are projected to take in an additional 50,000 bpd Venezuelan syncrude from Hamaca joint venture production. Actual figures could be higher depending on the new Venezuela energy policy

Projected coker capacity additions and start-ups in PADD3 (totaling approximately 275,000 bpd) are expected to take in typical heavy, sour “coking” crudes of approximately Mayan quality. With a vacuum resid yield on crude of the order of 45%, this additional coking capacity running generally full will bring in approximately 600,000 bpd of associated heavy sour crude (barring any further coker expansions by 2006). Note, PADD3 coker capacity has risen from 643,000 bpcd in January 1995 to

903,000 in January 2000 with a further 275,000 bpcd under construction. Delayed coking represents the main construction activity in PADD3.

- Total foreign crude intake to PADD3 was then used as the balancing measure to reach a total crude input for 2006 of 7,289,000 bpd. Note, severe discrepancies exist on crude imports and movements in the 1998 PSA between Tables 9, 23, 24 and 32. The make-up of foreign crudes remaining in PADD3 rather than passing on to PADD2 therefore had to be estimated
- The resulting crude slate for 2006 is heavier than that for 1998, continuing the decline in PADD3 that has persisted for several years. Sulfur content remains fairly constant.

<b>PADD3 Crude Slate Quality</b>			
	<b>1994 PSA</b>	<b>1998 PSA</b>	<b>2006 projection</b>
domestic crude		3427	2900
foreign crude		3530	4398
total crude Mbpd		6957	7298
API	32.21	31.49	30.83
Sulfur	1.18	1.45	1.42

### **Non-Crudes Volumes & Quality**

NGL's/Natural Gasoline refinery inputs escalated from 1998 PSA Table 16 based on 2000 AEO Reference Case Table A-11, Petroleum Supply & Disposition Balance

Other Inputs escalated as per NGLs except:

- merchant MTBE input allowed to float at a price 1.3\*(CG/RFG average) but MTBE use controlled by max 3% ether spec on all

- gasolines
  - based on guidance from ORNL in turn based on un published ORNL work “Ethanol/MTBE Transitions”, ethanol input was set at zero, the 3% MTBE policy keeping ethanol use in Winter gasoline only.

Natural Gas input allowed to float as marginal source of hydrogen plant feedstock and refinery fuel.

- other refinery fuel inputs held constant at 1998 levels per 1998 Table 47
- zero H2S allowed to refinery fuel

Unfinished Oils inputs escalated as per other Inputs

## Product Volumes

- Refinery Production Volumes based on 1998 PSA Table17 escalated to 2006 using the growth rate for crude consumption increase from 2000 AEO Table A-11 except:
  - S residual fuel to be escalated at overall -0.6% p.a. rate per 2000 AEO Table A11 for residual fuel demand growth
  - S on-road versus offroad/high sulfur diesel/distillate splits were developed from PSA Table 17, PMA Table 46 and API/NPRA 1996 PADD3 data, plus 1995 earlier EnSys/ICF work on PADD3
  - S all major product volumes were fixed, but energy content was checked and adjusted for across the subject cases on gasolines and diesel
  - S minor products, notably: NC4, residual (N6H 1-2%), coke (high and low sulfur), elemental sulfur were priced and allowed to float
  - S specialty products: lubes, asphalt, naphthas, aromatics were fixed

## Summer Season

- All the above data were developed based on annual averages. Summer seasonal factors were applied per NPC Table A-25 to adjust PADD3 refinery crude intake and production. Note:
  - S all the seasonal swing on crude (1.013) was taken on foreign crude

- S inputs with domestic crude inputs left unchanged
- S all the seasonal swing on distillate was taken on domestic No2 heating oil production
- S summer gasoline split was based on PSA 1998 monthly data, yielding 17.15% RFG in total gasoline refinery production. By comparison the 1993 NPC study class split was close at 17.85% RFG

### Finished Product Quality

product qualities were based on API/NPRA Summer 1996 (Tables 1 and 2A), NPC and on prior EnSys/ICF PADD3 calibration for 1994 as for 1998 calibration case except

- diesel cetane numbers were from API/NPRA Summer 1996 Table 2B. Note the numbers given there are clear cetanes. Ignition improver concentrations were also given but did not need to be applied since RYM operates on a clear cetane basis
- analysis of PADD3 1996 Summer CG and RFG quality from API/NPRA showed emissions qualities within Phase II Summer Region B and C standards on both fuel types with the exception of a (Phase II) 3.0% overage on CG Nox. Altering the blend sulfurs to the projected 30 ppm level lowered all three emissions significantly on both CG and RFG and brings all emissions within RFG Phase II standards. See tables below.
- given this situation, the EPA Complex Model was used to test the flexibility that existed in the 1996 blends adjusted to 2006 by lowering sulfur to 30 ppm and oxygen so that RFG contained 0.545 wt% from MTBE (equivalent to 3 vol% MTBE in the blend) with zero oxygen from ethanol, i.e a reduction in oxygen content from 1996 for RFG and a potential increase for CG. In practical terms, refiners have only four Complex Model variables with any flexibility: aromatics, olefins, E200 and E300. For each RFG Region and for CG, adjusted as above, each of these four qualities was relaxed from 1996 levels in turn until an emission (total VOCs, toxics or Nox) hit the 1996 level. Recognizing that these qualities act in

pairs, with aromatics and olefins primarily affecting toxics and E200 and E300 primarily VOCs, the identified individual flexibilities were at least halved. The resulting conservative flexibilities were then applied to arrive at final specifications for 2006 that, taking account of the switch to 30 ppm sulfur and to 3% MTBE, would ensure no emissions back-sliding versus 1996. Given the focus in this study on diesel not gasoline, the approach was taken that this representation of gasoline emissions would be satisfactory. Emissions calculations can thus be limited to post optimal cross-checking of blends via the Complex Model to double check there has been no back-sliding versus 1996. E200 and E300 specs are available in RYM but these and the conventional percents off at 212, 257 and 356 degF were all converted to a TBP equivalent basis and then graphed to “lock” the percent off specs to act to further control E200 and E300 at their 1996 levels within tight limits.

- CG and RFG oxygen contents were allowed to float subject to a max limit on RFG and CG of 0.545% max limit, from max 3% MTBE. Summer 1996 CG actual oxygen content was 0.09%. RFG oxygen content reduction would affect mainly toxics. Total oxygen elimination of the projected 30 ppm 2006 RFG would increase toxics by 4%; reduction to 0.545% oxygen by 3%. To prevent toxics quality back-sliding through oxygen reduction, first base case olefins and aromatics upward flexibilities versus 1996 Summer actuals were set very tight.
- in general, product qualities were set within narrow rather than wide tolerances to prevent significant scope for deviation from actuals.

<b>PADD III Summer 1996 RFG and CG Qualities</b> Source: API/NPRA Table 1		
	<b>RFG</b>	<b>CG</b>
Octane (R+M)/2	89.14	88.57
RVP	7.25	8.14
Oxygen vol %	1.94	0.09
Sulfur ppm	302.8	356.3
Olefins vol %	12.0	13.31
Aromatics vol %	23.39	32.42
Benzene vol %	0.66	0.91
E200	48.97	43.66
E300	81.94	79.55
API gravity	57.79	57.75

<b>PADD3 Summer 1996 CG Emissions Performance</b> (Versus Phase 2)				
region	B	B at 30 ppm S	C	C at 30 ppm S
VOCs	-7.6%	-11.3%	-6.8%	-10.8%
Toxics	-10.5%	-18.9%	-10.2%	-18.6%
NOx	3.0%	-9.2%	3.0%	-9.2%

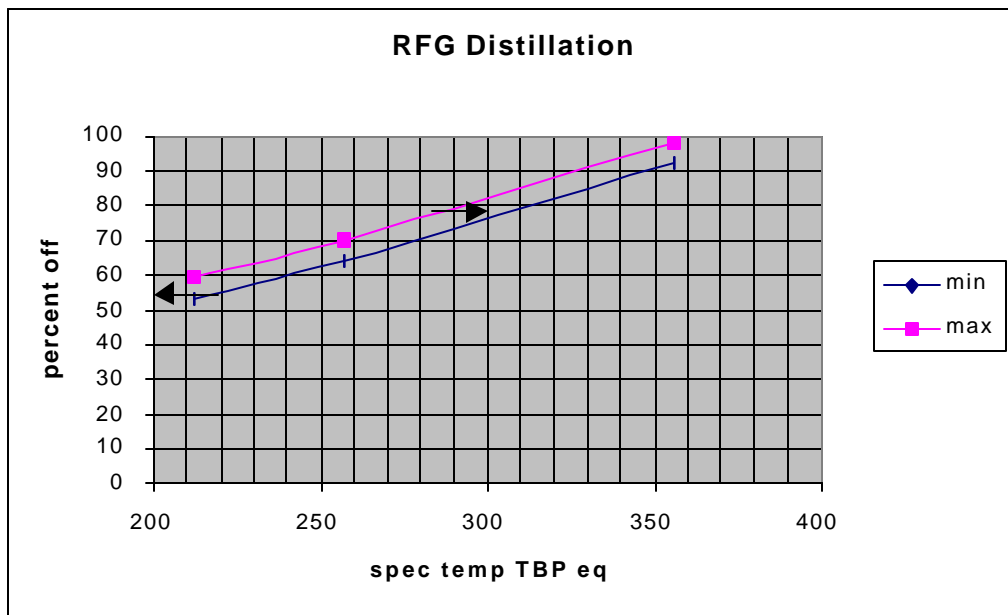
<b>PADD3 Summer 1996 RFG Emissions Performance (Versus Phase 2)</b>				
Region	B	B at 30 ppm S	C	C at 30 ppm S
VOCs	-24.6%	-27.7%	-14.9%	-16.1%
Toxics	-27.5%	-33.5%	-28.5%	-30.8%
Nox	-0.02%	-11.4%	-7.4%	-12.52%

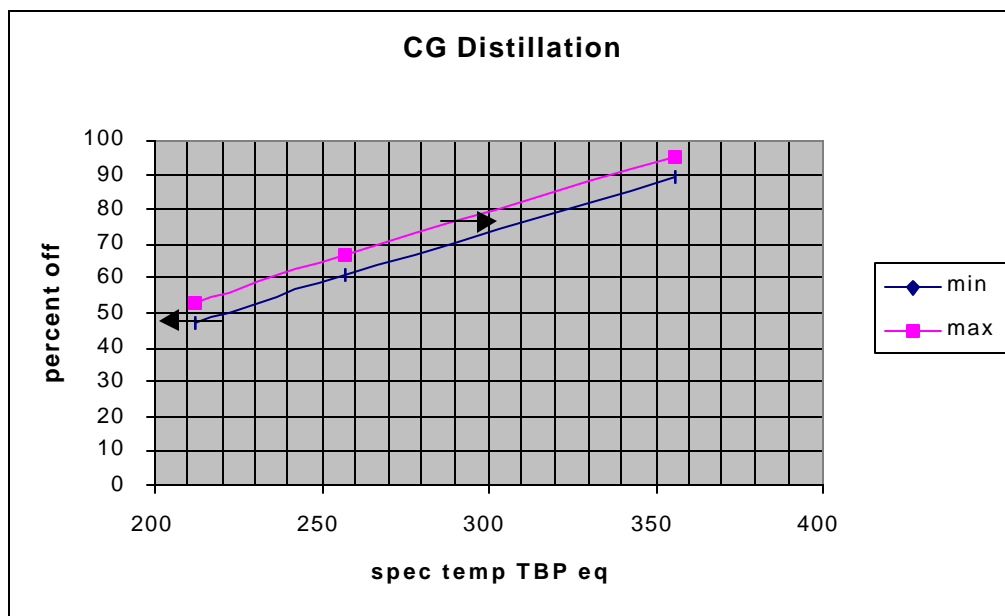
<b>PADD III Summer 2006 RFG and CG Qualities Derived from 1996 with sulfur and MTBE adjustments and with limited flexibility within limits that prevent emissions degradation vs 1996</b>						
	<b>RFG</b>			<b>CG</b>		
	base	flex	final specs	base	flex	final specs
Octane (R+M)/2	89.14	-	89.14	88.57	-	88.57
RVP	7.25	-	7.25	8.14	-	8.14
Oxygen vol %	1.94	-	1.94 <sup>(1)</sup>	0.09	+0.46	0.55 <sup>(2)</sup>
Sulfur ppm	302.8	n.a.	30	356.3	n.a.	30
Olefins vol %	12.0	+2	14.0	13.31	+2	15.31
Aromatics vol %	23.39	+1	24.39	32.42	+1	33.42
Benzene vol %	0.66	-	0.66	0.91	-	0.91
E200	48.97	-3	45.97	43.66	-3	40.66
E300	81.94	-1	80.94	79.55	-1	78.55

(1) oxygen from MTBE limited to 0.55 wt%, balance from ethanol  
 (2) MTBE up to 3% vol, leading to 0.55 wt% oxygen assumed allowed

Final RFG and CG Distillation Specs to Match E200/300 all Specs on TBP Equivalent Basis					
	212	257	356	E200	E300
RFG min	53	64	92	54.0	79.0
RFG max	59	70	98		
CG min	46	61	89	48.6	76.5
CG max	52	67	95		

See graphs. 212, 257 and 356 specs were set with +/- 3 (total range of 6)





## Raw Material and Product Prices

Prices and Costs were maintained in 1998 constant dollars but were AEO Reference Case projections for 2006, notably driven by growth in world oil price. Key prices affecting analytical results are those for: marginal crude, natural gas, methanol, ethanol. Prices associated with fixed quantities of purchased or output streams have nil impact on the results and diesel costs

Crude Oil Price for swing crude (Saudi Medium) was taken as the AEO 2006 "world oil price" (Table 1, \$20.59) representing US refiners' average acquisition cost of imported crude. (Saudi Medium quality is similar to that for average import crude.)

Natural gas price was taken from AEO Table 14 for gas delivered to industrial users (\$3.24/MMBTU). Note, this represents a real increase bringing natural gas price essentially equal to crude price on a Btu basis, in turn affecting the economics of hydrogen production, raising the cost of hydro-desulfurization

Purchased methanol price was taken as approximately 45 c/gal based on research of first quarter 2000 actual prices

Similarly, low and high sulfur coke prices were based on research of first quarter 2000 prices

Purchased MTBE price was taken as 1.3 times the average of RFG and CG price

Purchased electricity price was taken from AEO Table A8 (4.1 c/kwh)

## Refinery Capacity

### Capacity Additions

Final base case 2006 projected capacity was arrived at as the net of the following:

1. Jan 1, 2000 base operating capacities **plus**
2. firm capacity additions and start-ups undertaken or announced through 1<sup>st</sup> quarter 2000 **plus**
3. capacity “creep” debottlenecking to 2006 **plus**
4. plant capacity additions made in the initial 2006 base case run (and subsequently locked in to form total base 2006 capacity).

The following were key to the above:

- Jan 1, 2000 capacities were taken from Oil & Gas Journal and cross checked against EIA data from the 1998 PSA for Jan 1, 1999
- Actual plus firm capacity additions were arrived at by reviewing the April 2000 construction survey published in the Oil & Gas Journal (OGJ April 24<sup>th</sup> 2000, page 60)

- projects listed as under engineering or construction were included
- projects listed as “planned” were excluded
- the total PADD 3 new capacity construction and start-ups thus arrived at are summarized in the table below. They comprise major projects at 16 refineries in PADD3.

<b>PADD3 Firm Capacity Additions</b>	
<b>unit</b>	<b>additional capacity bpd</b>
crude distillation	160,000
vacuum distillation	350,000
fluid cat cracking	26,000
delayed coker	270,500
FCC/VGO hydrofiner	101,500
Resid hydrofiner	0
Catalytic reforming	0

refinery closures were taken as nil since there were no recent announcements of closures in PADD3.

capacity “creep” was estimated at 0.2% per annum across all process units based on based on historical trends.

Revamps

Revamping was assumed between 2000 and 2006 for the following units:

**FCC**

- to full ZSM and ZSM high light olefin modes with increase in potential severity to 78% from 75%

- increase in resid cracking capability (low sulfur feeds only) to 20% (from 8% in 1990/1995).

### **Catalytic Reforming**

- continuation of limited activity in revamping high pressure units to low pressure continuous such that, by 2006, a further 100,000 bpd of the 2000 high pressure capacity has been converted to low pressure.

### **Distillate Desulfurization**

- conservatively, no revamping was allowed to deep desulfurization or dearomatization relative to capacity in place in 2000; this on the basis that the 2006 Base Case has no change in distillate sulfur specifications versus 2000, therefore no rationale for refiners to install deep HDT units. The low sulfur diesel subject cases do allow both revamping and new investment. See later

### **Capacity Utilization Rates**

- Maximum unit utilization rates were derived from NPC Table A-7 for PADD3, API/NPRA Survey 1996 and EIA PSA 1998 for 1997 data. Since capacity data are generally now published on a calendar day (CD) basis and since RYM is run on a CD basis, process capacity data were entered into Table CAP on a CD basis. THE “STF” modifier was therefore used to reflect effective unit availabilities as a percent of CD capacity.
  - distillate HDS/HDA rates were set at 90% of CD to more closely reflect historical utilization rates and the effects of seasonality on limiting utilization
  - a sulfur recovery plant utilization rate of 75% of CD was used (consistent with NPC at 68% of SD) to reflect historically lower rates on these units because of the need for back-up capacity
  - hydrogen plant utilization rates were set at 90% of CD to reflect levels closer to historical and future potential need for spare hydrogen capacity to avoid major refinery throughput reductions in

the event of an unscheduled hydrogen plant or catalytic reformer shutdown

- utilization rates on residuum desulfurization, visbreaking and polymerization were set at reduced levels to reflect lower historical utilization rates.
  
- note that process unit standard stream day factors are applied in the model to capital (and fixed operating) costs. Also the effective availability (STF) in Table CAP is applied so that each unit of nameplate CD investment generates the cost per effective bpd of capacity added

### **Capital and Operating Costs**

- Capital Recovery Factor of 24.2% was employed in the LP to correspond to a 15% DCF ROI hurdle rate to reflect the threshold for new investment. In the case reports, this factor was adjusted back to 17.2%, corresponding to 10% ROI typical return.
  
- Total Annualized Investment and Fixed Operating Costs were built-up in industry-standard fashion employing the factors in the table below:

<b>Annualized Investment &amp; Fixed Operating Cost Factors</b>		
	<b>Annual</b>	<b>Initial</b>
offsites investments as % of onsites		50%
		altered to 40% for second pass
land as % of onsites + offsites		0.2%
Buildings as % of onsites+offsites		3.0%
Catalyst, chemicals, spares as % onsites		1.0%
Environmental as % of onsite		7.0%
Engineering & start-up as % total investment		10.0%

	<b>Annual</b>	<b>Initial</b>
offsites investments as % of onsites		50%
		altered to 40% for second pass
onsite maintenance as % investment*	4.0%	
offsite maintenance as % investment*	2.0%	
taxes, insurance & overhead as % total inv.	2.1%	
Supervisory labor as % direct labor	55%	
admin. Labor as % total labor*	90%	
payroll burden as % total labor*	39%	

	Annual	Initial
offsites investments as % of onsites		50%
		altered to 40% for second pass
Operating supplies as % total labor	10%	
capital charge (recovery factor)	24.2%/17.2%	
Corresponding capital rate of return	15%/10%	
*Consistent with / based on NPC Table A-6		

**Cost Escalation and Location Factors**

- Capital and fixed operating costs in the RYM model had been adjusted to a January 2000 basis using Nelson indices for investment labor cost, labor productivity and refinery operating cost.
- Given the capital costs update, a capital cost location factor of 1.0 was used.

## Process Unit Operating Modes

Major operating constraints were set as follows:

<b><u>FCC</u></b>	<b>2006</b>	<b>1990/95 NPC</b>
max. low sulfur resid in feed	20%	7.9%
max. high sulfur resid in feed	0%	0%
max. ultra low sulfur operation	100%	
max. high light olefin mode	100%	
max. low olefin mode	100%	
max. distillate feed	10%	5.7%
max. ZSM catalyst operation	100%	
max. severity	78%	73.8/74.7

### **Catalytic Reformers**

max. sustained severity (RONC)	
- high pressure	97.2
- medium pressure	97.9
- low pressure continuous	98.7
max. ultra-low pressure & benzene mode	
- low pressure continuous	100%

## Process Technologies & Economics

A separate EnSys report under this contract describes the work undertaken to review latest RFG and ULSD technologies and to bring the RYM model fully up to date; also to undertake other model improvements. For RFG and ULSD, RYM as used here embodies the latest versions - as of first quarter 2000 - of key processes:

- FCC gasoline desulfurization (CDTech, OCTGAIN and others),
- distillate deep hydro-treating/hydro-dearomatization (SynSat and generic two stage deep HDT/HDA)
- FCC feed pre-treatment VGO hydro-cracking including the MAK process and mild hydro-cracking.

In addition, up-to-date representations of bio-desulfurization and GTL processes were

implemented. The GTL representations are based on Shell and SASOL technologies. These are effectively “mini-refineries” with multiple processes and consequently have very high investment costs (approximately \$20,000 per bbl/day). Certain processes with potential but not yet commercialized, such as Phillips S Zorb or Black & Veatch IRVAD, were not implemented but are anticipated to be reviewed in any future update.