The Assay Simulator
Crude Assay Modeling based on Simple Whole Crude Properties

“Update Assays Based on Monitoring Data”

Presentation to:
The Crude Oil Quality Group
Jan 2003

HPI CONSULTANTS, INC.
The Assay Simulator (Overview)

Update Assays Based on Monitoring Data

- Update most cut properties – not just TBP
- Must add Light Ends to monitoring
- Make new assays and recut them
- Use to make better crude purchase decisions
- Use to update assays for Refinery LPs
The Assay Simulator

Questions to Answer:

- What is it?
- Why Does it Work?
- How is it Made?
- How is it Used?
- Where Will it be Used?
The Assay Simulator

The Big Picture

HPI Internal Functions

Model Creation Tool

Neural Net Program

Assay Data

CCPP Models

User Activity

HPI Assay Simulator

Or

User Application

Base Assay

(WC & Cut Data)

Tuning

(Each Assay Cut Property Point)

Predict

(Update Each Point in Base Assay)

New Crude

(WC Data Only)

Tuning Factors

Predicted Assay

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The Assay Simulator

Assay Updating Process – Data Flow

HPI Assay Simulator
Or
User Application

Base Assay
(WC & Cut Data)

New Crude
(WC Data Only)

Tuning
(Each Assay Cut Property Point)

Predict
(Update Each Point in Base Assay)

CCPP Models

Tuning Factors

Predicted Assay
The Assay Simulator

What is it?

- **Crude Cut Property Predictor (CCPP):** Models that predict assay cut properties based on simple WC input data.

- **Assay Simulator:** Program to use the models and to tune them using Base assay data.

```vba
Function World_VolPctC6(CutEnd, SG_WC6, Sulf_WC6, K_WC6)
    If CutEnd < CutMin Then GoTo Error
    If CutEnd > CutMax Then GoTo Error
    node(0) = CutEnd * 0.0014869888 - 1.2304832935
    node(1) = SG_WC6 * 8.0277585983 - 7.0734333992
    node(2) = Sulf_WC6 * 0.4172612428 - 1.0028541088
    node(3) = K_WC6 * 1.3204592466 - 15.613322258
    node(4) = 1.7402929068
    node(4) = node(4) + 0.4828311204 * node(0)
    node(4) = node(4) - 1.4768768549 * node(1)
    node(4) = node(4) + 0.3270048499 * node(2)
    node(4) = node(4) - 0.1032495275 * node(3)
    If node(4) > 7 Then
        node(4) = 7
    End If
    If node(4) < -7 Then
        node(4) = -7
    End If
    node(4) = Application.WorksheetFunction.Tanh(node(4) / 2)
    node(5) = 0.5535073876
    node(5) = node(5) + 3.5152971745 * node(0)
    node(5) = node(5) - 1.3423954248 * node(1)
    node(5) = node(5) + 0.6004559993 * node(2)
    node(5) = node(5) - 0.5151726603 * node(3)
    If node(5) > 7 Then
        node(5) = 7
    End If
End Function
```
The Assay Simulator

Why Does it Work?

- All Crudes are Related
  - They come from much the same organisms
  - have different histories of temperature, pressure and geology

- Crude property predictions work because:
  - Uses C6+ Whole Crude Properties (Remove Lt Ends)
  - Uses C6+ Characterization Factor (K) for Aromaticity
  - Uses a “Base” Crude to “Tune” model
The Assay Simulator

How Is the Model Built?

- Models made using a Neural Net
- Uses hundreds of old and new assays from many sources.
- HPI Application integrates Assay Data, Neural Net software and Statistical Data
  - User never sees it, only the resulting model
The Assay Simulator  (Make Model)

- Neural Net Structure

Result 1 = Tanh(Input A * cA-1 + Input B * cB-1 + Input C * cC-1)
Result 2 = Tanh(Input A * cA-2 + Input B * cB-2 + Input C * cC-2)
Answer = Tanh(Result 1 * cD1 + Result 2 * cD2)
The Assay Simulator (Make Model)

Making the Models -

- HPI Internal Application
  - Select variables & limit to Dist or Resid
  - Transform to linear forms
  - Create sub-set of data meeting requirements
  - Control Neural Net training
  - Monitor Outliers & Success of Models
  - Make VBA Functions
The Assay Simulator (Make Model)

Example: Viscosity Function

- Input to model is: Cut Viscosity, VisTemp, CutStart, CutEnd, C6+API, C6+Sulf, C6+K

- Convert Vis to Log(Log(Vis+1.5)), VisTemp to Log(VisTemp+460) and CutPoints to 1000/(CutPt+460)

- Separate Functions for Distillate and Resid cuts.

- Result is Vis Prediction within 10-30% over the full CutPoint and VisTemp range for distillate cuts.
The Assay Simulator  (Make Models)

Two types of models
- Detailed “Family” models
  - More Precise
  - Cost more to develop
  - Must know Family members
  - Give good representation without “Base” assay, but still improved (slightly) by Base
- “World” model
  - Must use a “Base” assay
  - Not quite as accurate as Detailed models
  - Model is tuned during update to match “Base” assay data.
The Assay Simulator (Make Model)

Predicted versus Actual Graph is Used

- Blue dots are individual yield points
- Red Triangles are points for one crude
- Light Blue lines represent 2 Std Deviation limits
- Can see outliers
- Can see slight modeling problem above 80% Actual

Yields (all Crudes), SD=3.17
The Assay Simulator

Model Accuracy

- **World Model** (Before tuning with Base assay)

<table>
<thead>
<tr>
<th>Property</th>
<th>Avg Error</th>
<th>Count</th>
<th>% Variance Removed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yields, Vol%</td>
<td>3.09</td>
<td>6754</td>
<td>79</td>
</tr>
<tr>
<td>Freeze, F</td>
<td>10.9</td>
<td>905</td>
<td>53</td>
</tr>
<tr>
<td>Smoke, mm</td>
<td>2.1</td>
<td>1126</td>
<td>50</td>
</tr>
<tr>
<td>Aniline Pt, F</td>
<td>6.1</td>
<td>3063</td>
<td>71</td>
</tr>
</tbody>
</table>

The input to model is: \( C_6+\text{SpGr}, \ C_6+\text{Sulfur}, \) and Avg K of Dist Cuts

Accuracy after tuning with Base assay data is much more better than this.
The Assay Simulator (Make Model)

Accuracy Data for Cloud Point

<table>
<thead>
<tr>
<th></th>
<th>Total</th>
<th>365</th>
<th>448</th>
<th>546</th>
<th>573</th>
<th>612</th>
<th>674</th>
</tr>
</thead>
<tbody>
<tr>
<td>Avg Prediction Error (Abs)</td>
<td>10.9</td>
<td>12.3</td>
<td>11.9</td>
<td>8.8</td>
<td>13.8</td>
<td>11.2</td>
<td>11.7</td>
</tr>
<tr>
<td>Avg Offset (Abs)</td>
<td>1.5</td>
<td>2.6</td>
<td>5.1</td>
<td>0.6</td>
<td>-0.4</td>
<td>1.9</td>
<td>-0.5</td>
</tr>
<tr>
<td>SD Target (Abs)</td>
<td>23.0</td>
<td>19.9</td>
<td>23.2</td>
<td>20.3</td>
<td>23.8</td>
<td>26.0</td>
<td>24.4</td>
</tr>
<tr>
<td>Avg Target (Abs)</td>
<td>32.5</td>
<td>-75.7</td>
<td>-48.5</td>
<td>3.1</td>
<td>12.8</td>
<td>20.4</td>
<td>55.9</td>
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<tr>
<td>Count</td>
<td>1054</td>
<td>45</td>
<td>170</td>
<td>313</td>
<td>55</td>
<td>152</td>
<td>319</td>
</tr>
<tr>
<td>% Data Variance Removed by Model</td>
<td>52.5</td>
<td>38.2</td>
<td>48.7</td>
<td>56.7</td>
<td>42.0</td>
<td>56.9</td>
<td>52.0</td>
</tr>
</tbody>
</table>

Average Prediction Error
Compare to Test Accuracy
(about 5 degrees F)

% Data Variance Removed by Model
100 = Perfect Model,
0 = No improvement over average value.

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The Assay Simulator (Use Models)

Implementation of the CCPP Models

**Excel Functions:**
- Function Name = Model Name + Property Name
- Standard Parameters: Cut Points and Whole Crude properties
- Code tells function what result to return
- Additional parameters for tuning, etc.

**Example:** Aniline Point using the “World” Model

\[ =\text{World\_AnilPt}(\text{CutStart}, \text{CutEnd}, \text{SpGr\_WC6}, \text{Sulf\_WC6}, \text{K\_WC6},'V') \]

where “_WC6” means Whole Crude C6+ basis
and “V” can be replaced by “A” for accuracy, “T” for tuning, etc
The Assay Simulator (cut Models)

Spin-Off: Property Models of Cuts

- Model of property from Cut data
  - Uses Cut Points and Cut Density
  - Accuracy Prediction available for each Property Prediction
  - Accuracy Prediction is by average Cut Pt
  - Can use to check lab results
  - Will be separate product from Assay Simulator and CCPP

<table>
<thead>
<tr>
<th>Statistical Property</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>Avg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mid Cut pt</td>
<td>363</td>
<td>507.6</td>
<td>649.3</td>
<td>815</td>
<td>966.5</td>
<td>689.5</td>
</tr>
<tr>
<td>Avg Prediction Error</td>
<td>0.09</td>
<td>0.08</td>
<td>0.10</td>
<td>0.15</td>
<td>0.20</td>
<td>0.11</td>
</tr>
<tr>
<td>SD Target</td>
<td>0.24</td>
<td>1.03</td>
<td>7.68</td>
<td>89.67</td>
<td>561.86</td>
<td>108.72</td>
</tr>
<tr>
<td>Avg Target</td>
<td>1.00</td>
<td>2.11</td>
<td>6.54</td>
<td>23.84</td>
<td>159.10</td>
<td>31.57</td>
</tr>
<tr>
<td>Count</td>
<td>452</td>
<td>1052</td>
<td>1373</td>
<td>1529</td>
<td>731</td>
<td>5137</td>
</tr>
<tr>
<td>% Err Removed by Model</td>
<td>62.50</td>
<td>92.23</td>
<td>98.70</td>
<td>99.83</td>
<td>99.96</td>
<td>99.90</td>
</tr>
</tbody>
</table>

Example:
Viscosity of Distillate Cuts - From Cut Points, Visc Temp & Cut SpGr
The Assay Simulator (Uses)

CCPP Models Will Impact Many Groups

- Laboratory
- Crude Assay “Keepers”
- Crude Supply and Trading
- Refinery Planners
The Assay Simulator

Laboratories

☐ They never like modeling (they think it means less assays)

☐ They should get a lot more requests for Lt Ends analysis

☐ Labs might make deals on test costs

☐ Users will be more fussy about results
The Assay Simulator (Uses)

Crude Assay “Keepers”

- Assay Simulator can provide a good reference crude (what values to expect)
- Can make Assay from limited data (and have estimate of how good or bad the assay is)
- Recut more accurately – Based on model of crude oil, not curve-fitting technique
The Assay Simulator (Uses)

Crude Supply Departments
- They catch delivery samples
- Get limited data now, just to check contract
- Only use for LP users: Need New Assay?
- Add the Light Ends and it is more useful to Refiners
- Crude Monitoring database will become common ground.
- Sales people: not technical, Need simple tools
The Assay Simulator (Uses)

Crude Trading Departments

- Similar to Crude Supply
- Trying to get true value of crude
- Some connect refinery model to assay and add finished product prices
- Typically not computer savy
The Assay Simulator (Uses)

Major Use: LP Models

- Need accurate Assay data - else garbage in = garbage out
- Users will not be Assay experts
- Needs simple process
- Will need access to monitoring data
- Updated Assay purpose changes:
  - Was part of Assay Making process
  - Now part of LP Modeling process
The Assay Simulator (Uses)

Assay Usage is Changing

Make Assay
Flash Assay Cut Assays
Assay Library

Make Assay
Assay Library

Updated Assay
Re-Cut or Fractionate Assays

Current
Refinery LP

Future
Refinery LP
The Assay Simulator (Uses)

Simple Fractionated Cuts
- Models Continuous- can do 20 F Cuts
- Can do simple Fractionation as:
  \[ \text{Vapor} = (\frac{\text{VaporPress}}{\text{Total Press}})^{\# \text{Trays}} \]
- Can use plant data to get \# \text{Trays}
- \#\text{Trays} can be different for Stipping and Rectifying section
- Simple Solution will make you a Hero with Refiners (usually overkill due to Vendors)