

# The Assay Simulator

Crude Assay Modeling based on Simple Whole Crude Properties

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*"Update Assays Based on Monitoring Data"*

Presentation to:  
The Crude Oil Quality Group

Jan 2003

# The Assay Simulator (Overview)

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## 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

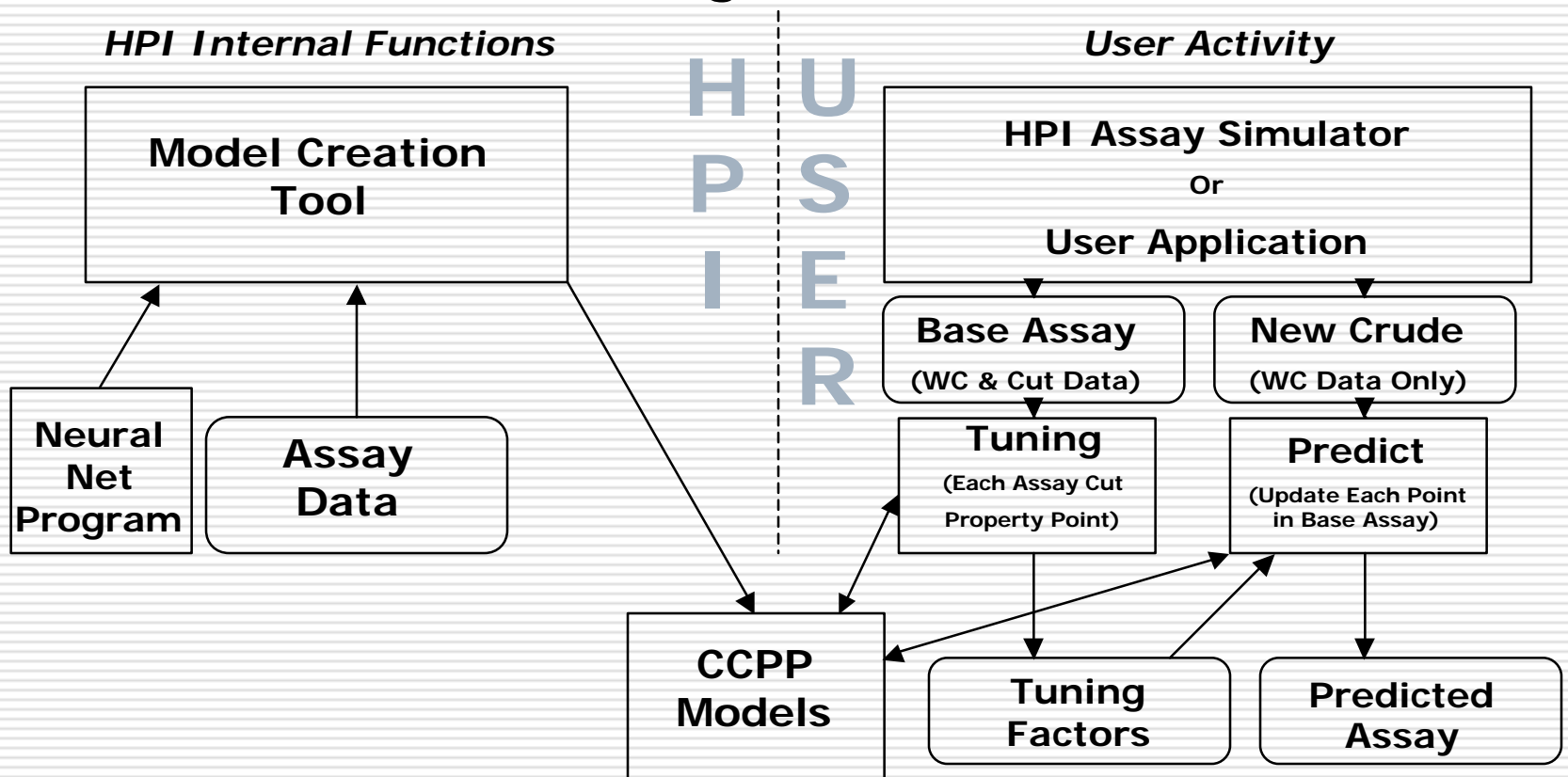
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## Questions to Answer:

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

# The Assay Simulator

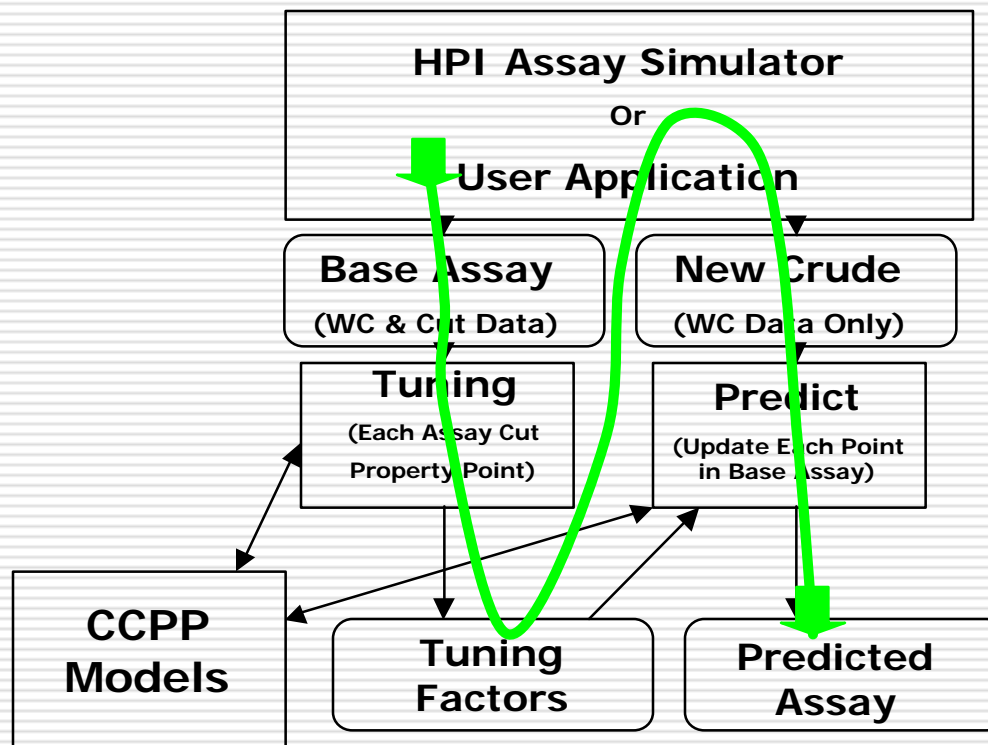
## The Big Picture



# The Assay Simulator

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## Assay Updating Process – Data Flow



# The Assay Simulator

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## 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.

```
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
```

# The Assay Simulator

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## 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

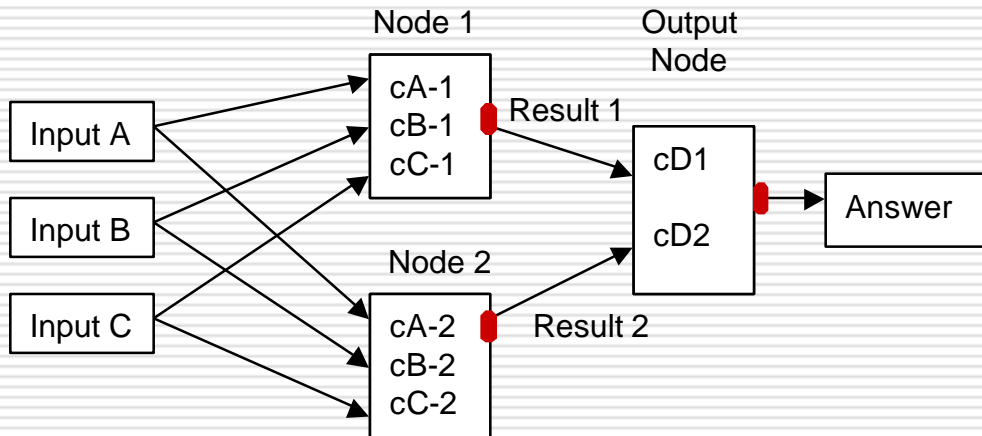
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## How Is the Model Built?

- Models made using a Neural Net
- Uses hundreds of old and new assays from many sources.
  - HPI has issued Assay Libraries in 1981, 1987, and 1995. Each with hundreds of assays, from dozens of 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



$$\text{Result 1} = \text{Tanh}(\text{Input A} * cA-1 + \text{Input B} * cB-1 + \text{Input C} * cC-1)$$

$$\text{Result 2} = \text{Tanh}(\text{Input A} * cA-2 + \text{Input B} * cB-2 + \text{Input C} * cC-2)$$

$$\text{Answer} = \text{Tanh}(\text{Result 1} * cD1 + \text{Result 2} * cD2)$$

# The Assay Simulator (Make Model)

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## 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)

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## Example: Viscosity Function

- ❑ Input to model is: Cut Viscosity, VisTemp, CutStart, CutEnd, C6+API, C6+Sulf, C6+K
- ❑ Convert Vis to  $\text{Log}(\text{Log}(\text{Vis}+1.5))$ , VisTemp to  $\text{Log}(\text{VisTemp}+460)$  and CutPoints to  $1000/(\text{CutPt}+460)$
- ❑ 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)

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## 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

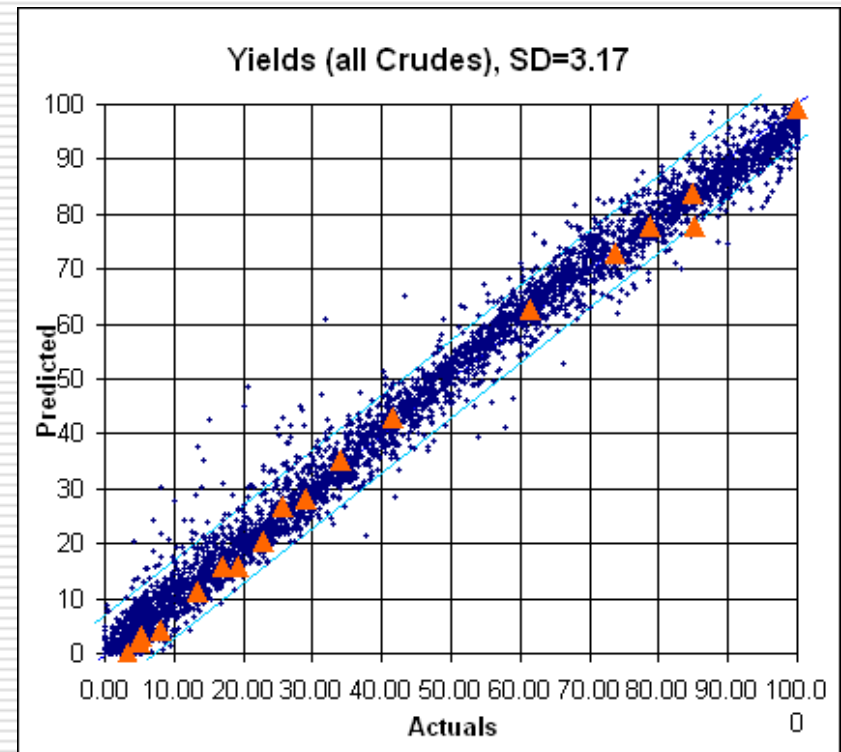
Blue dots are individual yield points

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



# The Assay Simulator

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## Model Accuracy

### ■ World Model (Before tuning with Base assay)

Property	Avg Error	Count	% Variance Removed
Yields, Vol%	3.09	6754	79
Freeze, F	10.9	905	53
Smoke, mm	2.1	1126	50
Aniline Pt, F	6.1	3063	71

Average Prediction Error  
*Compare to Test Accuracy*

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

The input to model is: C6+SpGr, C6+Sulfur, and Avg K of Dist Cuts

Accuracy after tuning with Base assay data is much more better than this.

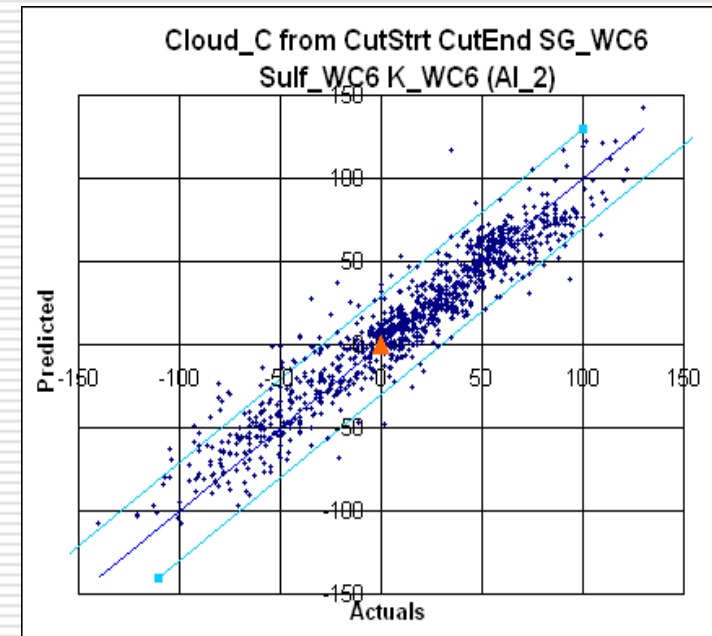
# The Assay Simulator (Make Model)

## Accuracy Data for Cloud Point

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

**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.



# The Assay Simulator (Use Models)

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## Implementation of the C CPP 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

=World\_AnilPt(CutStart, CutEnd, SpGr\_WC6, Sulf\_WC6, K\_WC6, "V")

where "\_WC6" means Whole Crude C6+ basis

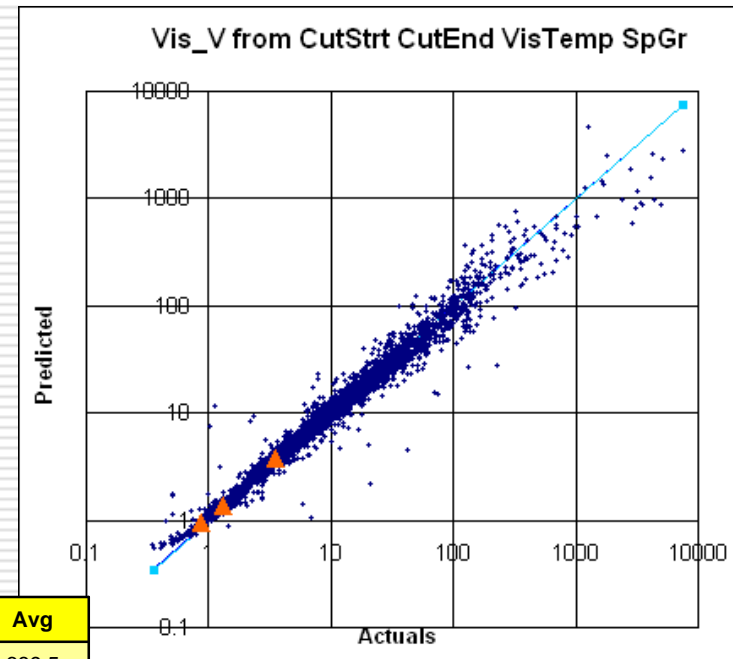
and "V" can be replaced by "A" for accuracy, "T" for tuning, etc

# 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 CCP

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



**Example:**  
**Viscosity of Distillate Cuts -**  
**From Cut Points, Visc Temp**  
**& Cut SpGr**

# The Assay Simulator (Uses)

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## CCPP Models Will Impact Many Groups

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

# The Assay Simulator (Uses)

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## 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)

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## 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)

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## 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)

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## 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 savvy

# The Assay Simulator (Uses)

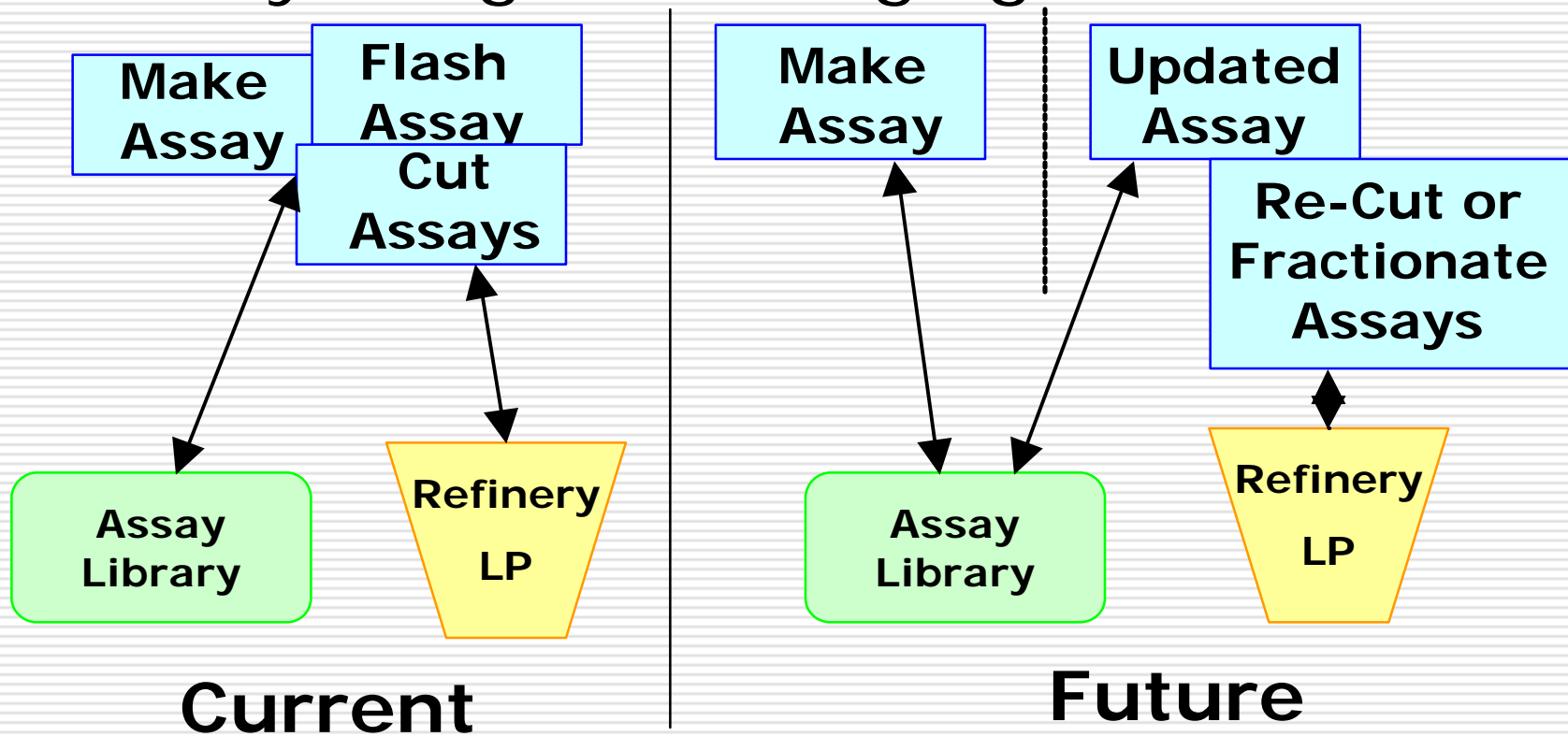
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## Major Use: LP Models

- ❑ 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



# The Assay Simulator (Uses)

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## Simple Fractionated Cuts

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