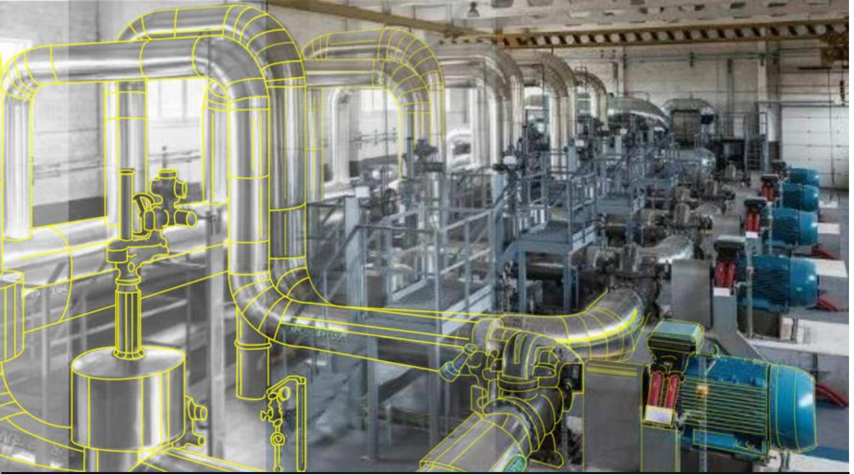
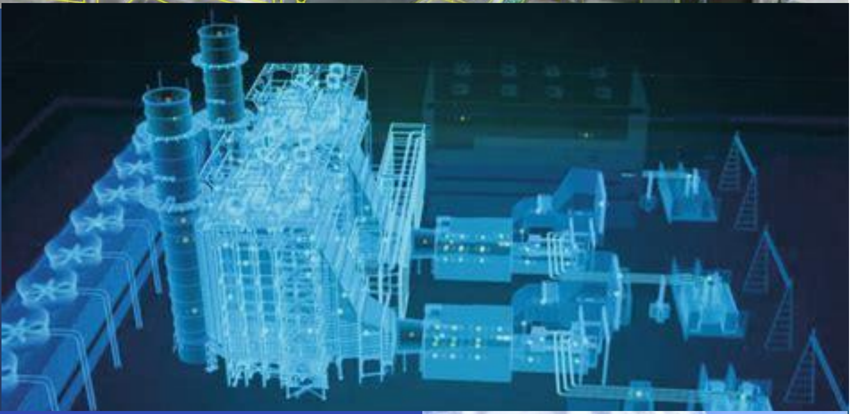
Process Digital Twins for Optimal Plant Operations

Presented by Bill Poe
South Texas Section AIChE
November 2, 2023





- **Digital Twins**
- **Engineering Digital Twins**
- **Process Digital Twins**
- **Online Process Digital Twins**
- **Closed Loop Optimization**
- **Processes and Typical Benefits**
- **What’s Next**

What is a Digital Twin?

Digital Twins integrate internet of things, artificial intelligence, machine learning and software analytics with spatial network graphs to create living digital simulation models that update and change as their physical counterparts change.

© Microsoft – Azure Digital Twin

"A Digital Twin is a virtual representation of a real object. Digital Twins are designed to optimize the operation of assets or business decisions about them, including improved maintenance, upgrades, repairs and operation of the actual object. Digital Twins include the model, data, a one-to-one association to the object and the ability to monitor it."

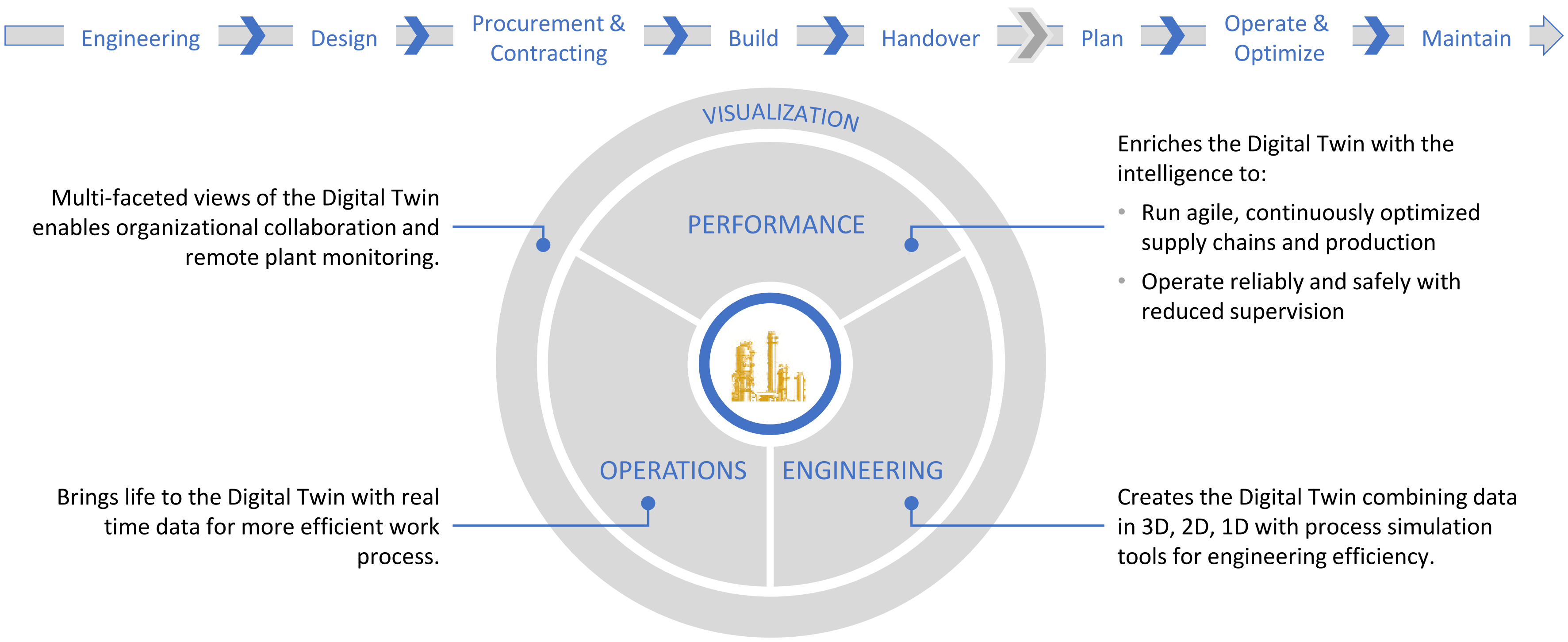
© Gartner – Adopt a Data Governance Strategy for Long-Term Digital Twin Success (Published 20th Dec. 2018, ID: G00377062)

A digital twin is a digital representation of a physical object, person, or process, contextualized in a digital version of its environment. Digital twins can help an organization simulate real situations and their outcomes, ultimately allowing it to make better decisions.

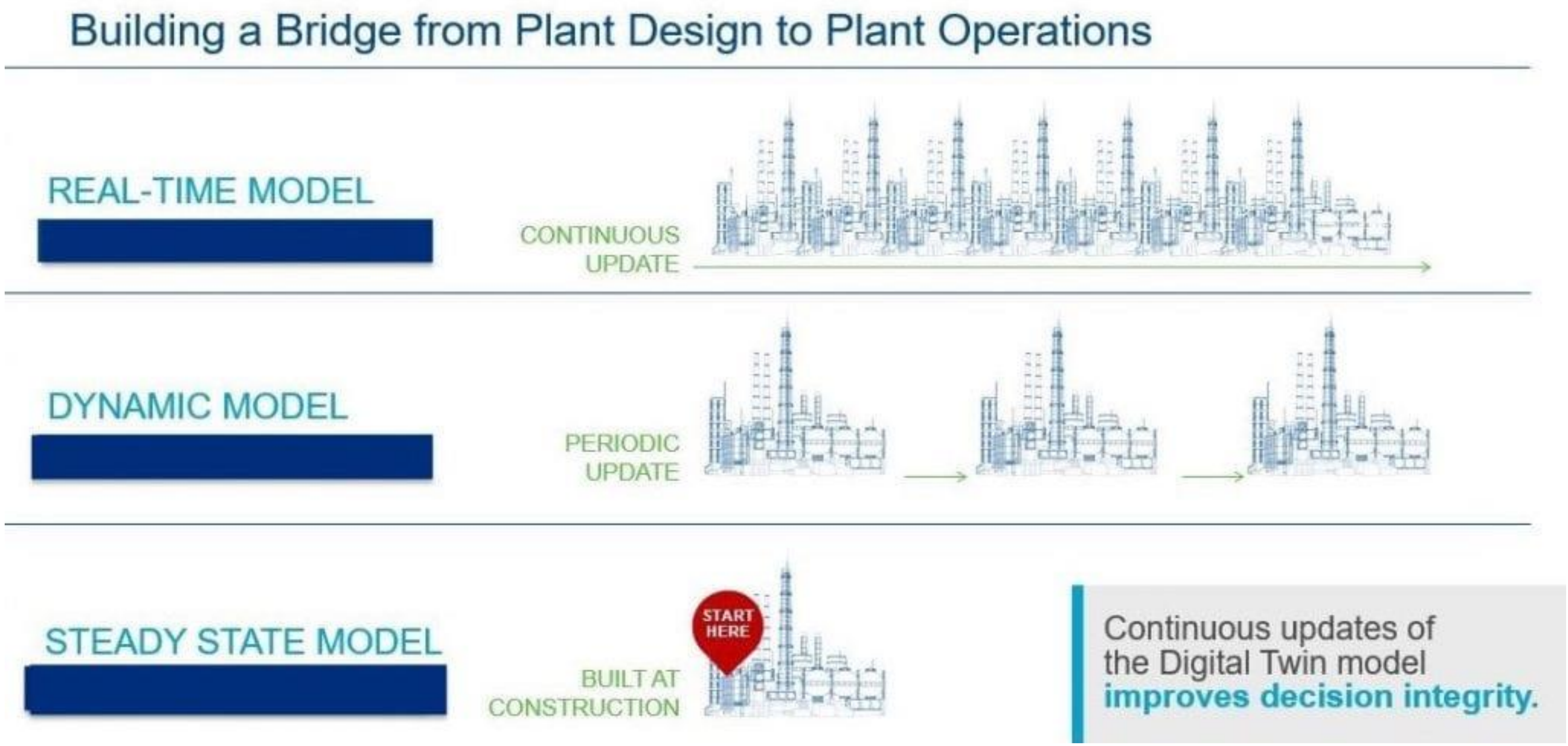
McKinsey -What is digital-twin technology? July 12, 2023 | Article

Types of Engineering Digital Twins

- Physical
  - External Structures
  - Piping
  - Instruments Equipment
  - etc.
- Electrical
  - Transmission
  - Distribution
- Equipment
  - Asset Performance
- Production
  - Supply Chain
- **Process**
  - **Steady State**
    - **Design, Debottleneck**
  - **Dynamic (Behavior)**
    - **Mechanical Studies**
    - **Operations, Control**
  - **Real-time Model**

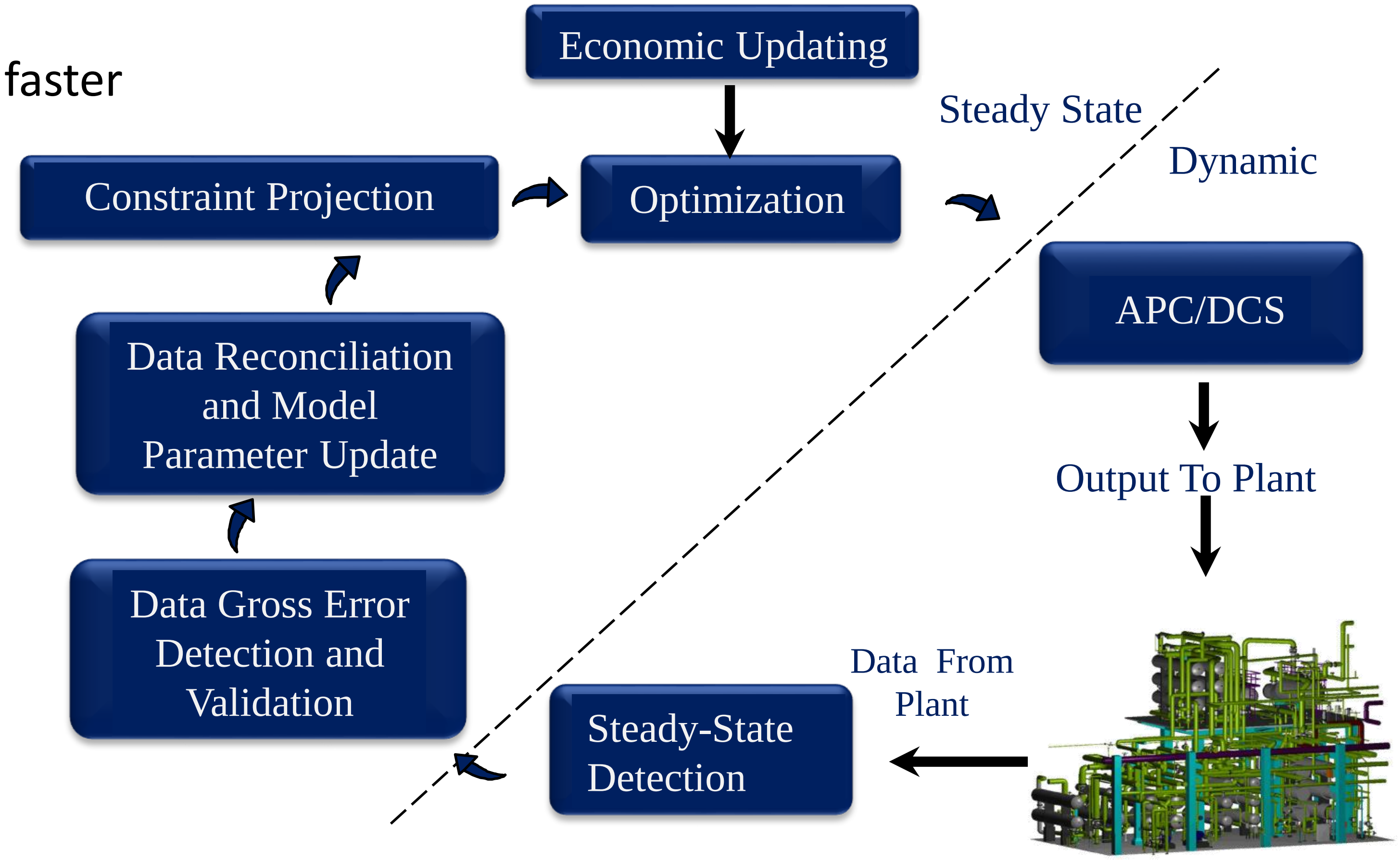


Process Digital Twins

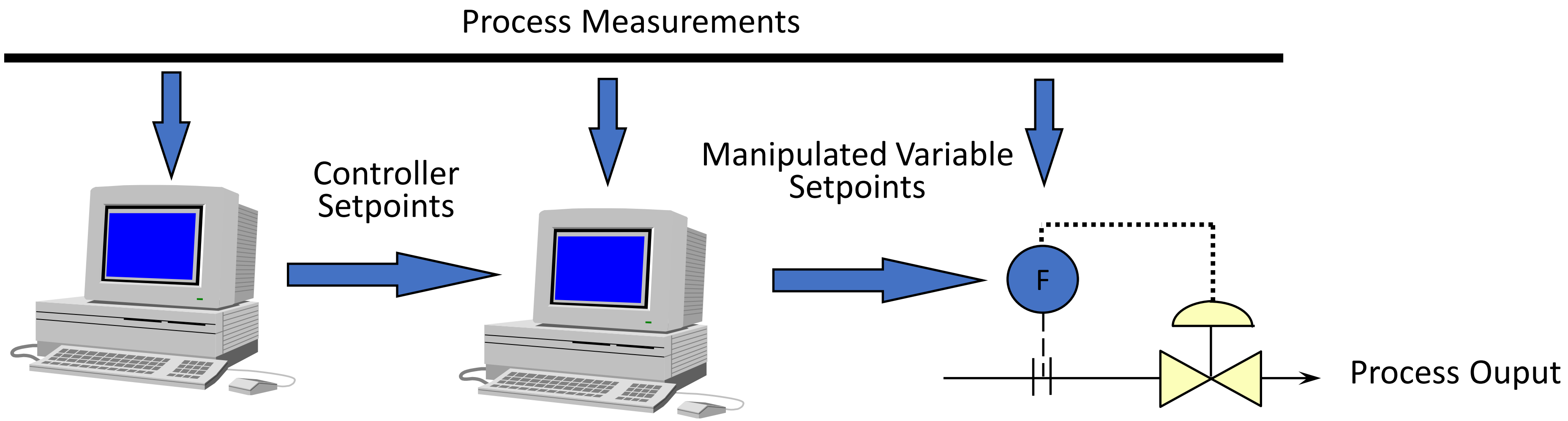


Keys to Closed Loop Online Optimization

- Reactor Models
- Equation Oriented Models – converge faster
- Real Time Sequencer
  - Steady State Detection
  - Data Reconciliation
  - Model Parameter Update
  - Constraint Projection
  - Solve Objective Function
  - Send Optimization Targets
- Nonlinear Solver
- Closed Loop



Control Perspective



On-line Optimization:
- Maximize Economics
- Steady-state operation
- Operating constraints

Updates: 4-8 hours

Adv. Process Control:
- Dynamic operation
- Constraint handling
- Disturbance rejection
- Multivariable

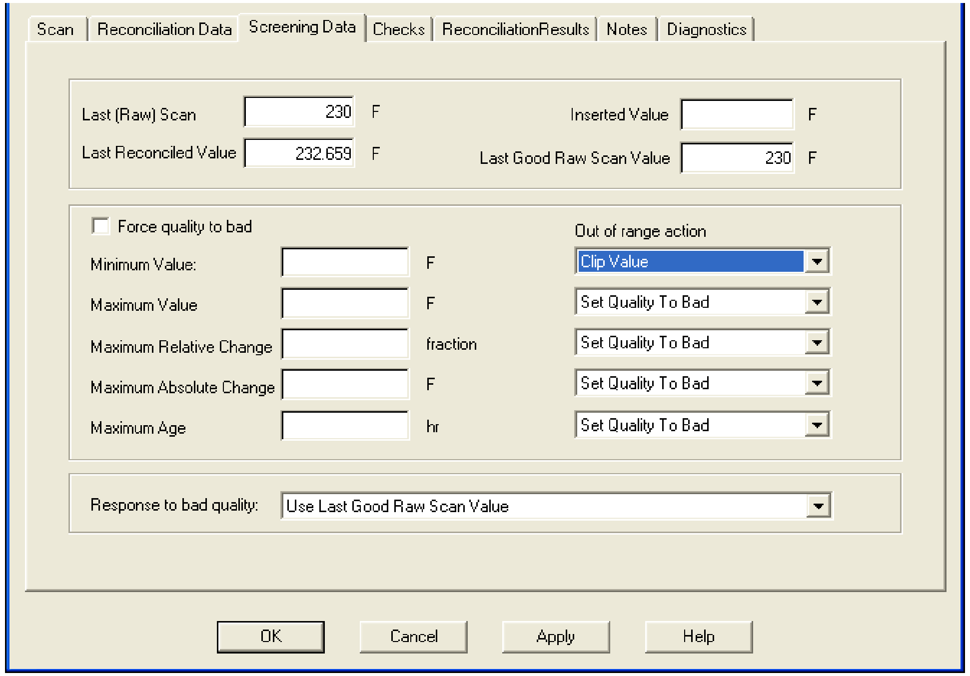
Updates: ~ 1 min.

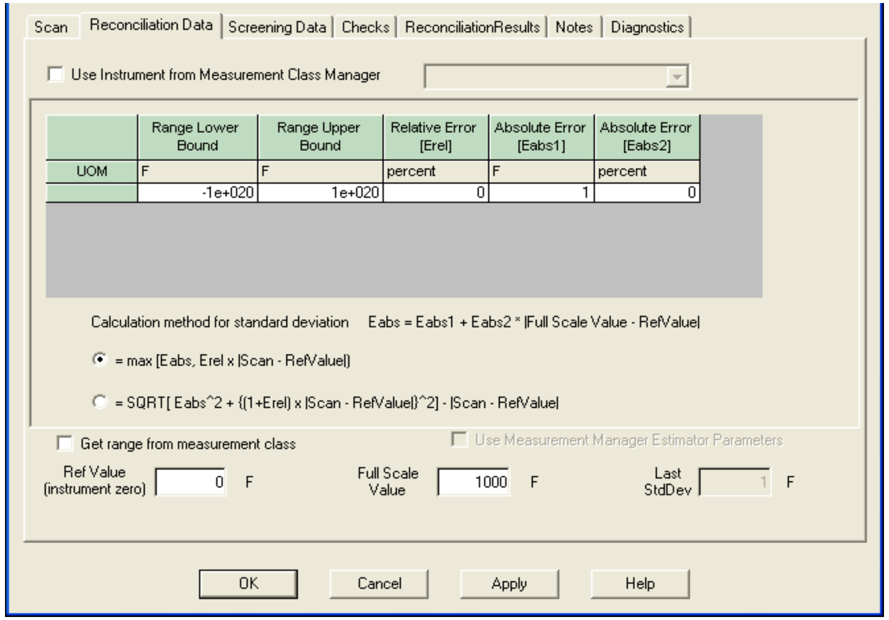
Basic Control:
- Regulatory
- SISO or MISO systems

Updates: ~ 1 sec.

Defense against Bad Data

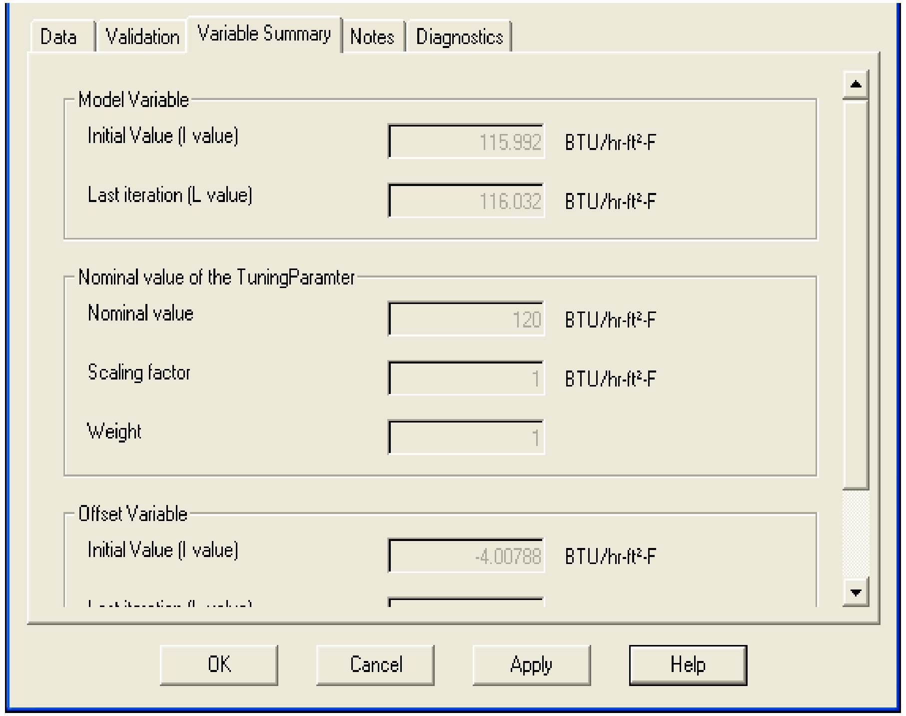
- **Data Screening, Flexible Consequences**
  - Use Last Good Scan
  - Use Last Reconciled Value
  - Substitute Curve Fit Value
  - Stop solution
- **Simplified Material Balance & Reconciliation**

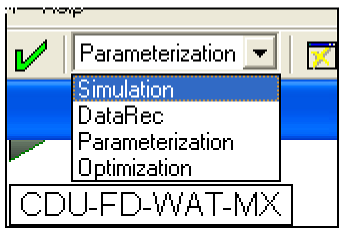




Data Reconciliation and Performance Calculation

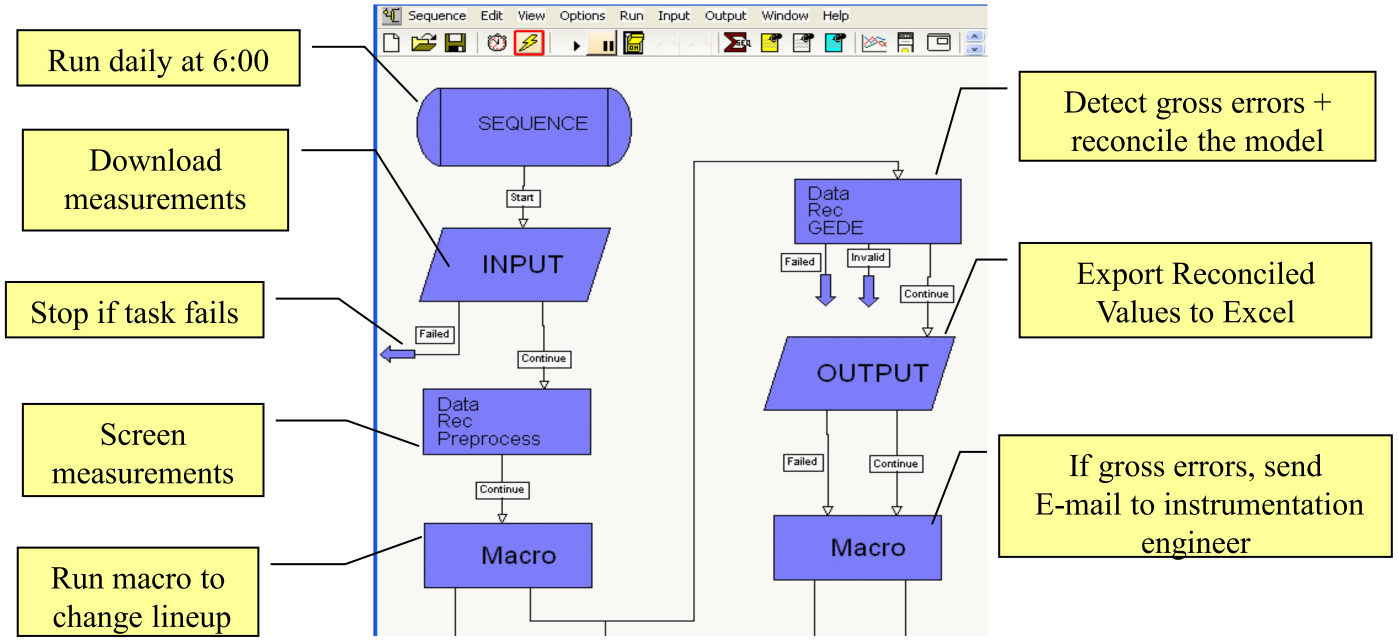
- Integrated Data Reconciliation
  - Reconcile inconsistent process data
  - Rigorous Soft Sensor for process parameters
  - Provide a continuously self tuning model of the process
- Performance Calculations
  - Calculate equipment performance parameters
  - Identify performance deterioration

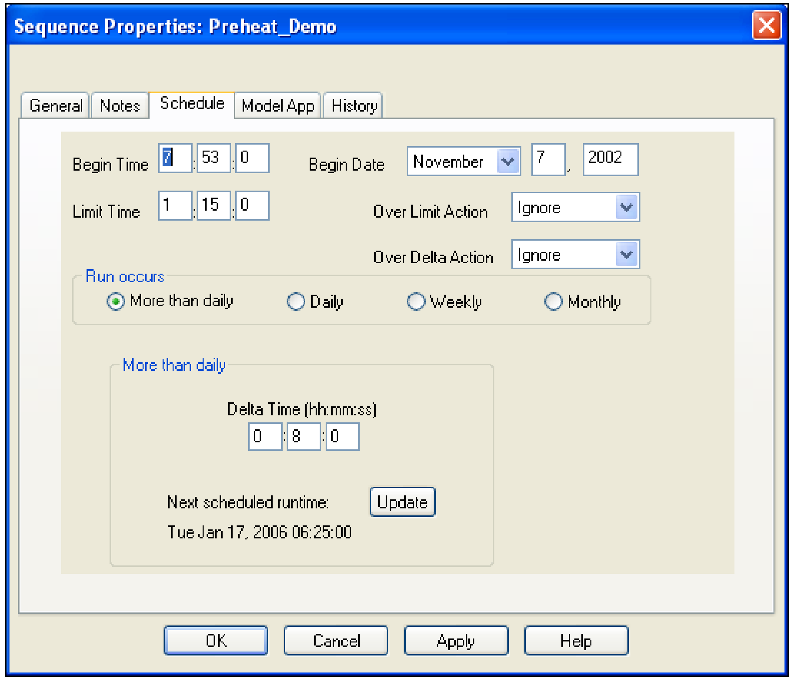




Automate Performance Monitoring

- Real Time System (RTS)
- Graphical environment for scheduling and sequencing real-time activities
  - Monitor online sequence



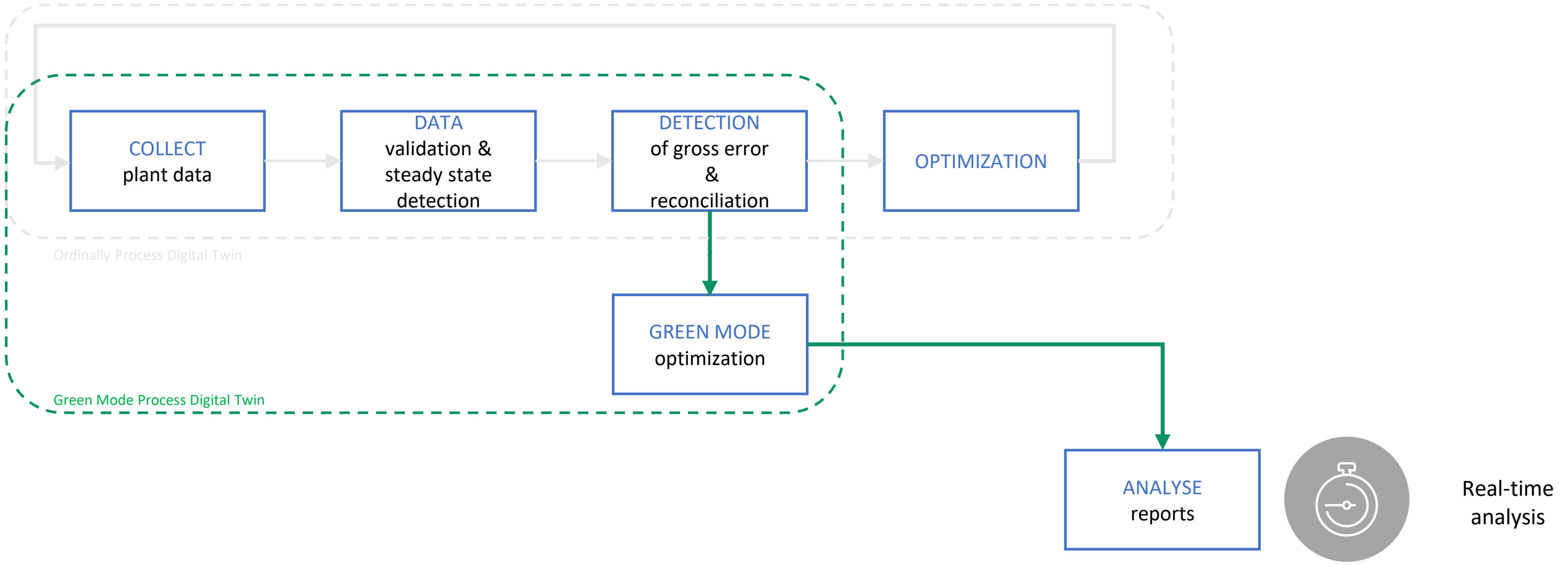


Other Online Optimizer Features

- Communication with Plant Historian and other Databases
- Interactive Modeling Environment
- Open for Third Party Components
  - Reactor Technologies
  - User Added Models
- Model Reparameterization
  - Heat Exchanger Fouling Factors
  - Equipment Efficiencies
    - Rotating Equipment
    - Fired Equipment
  - Catalyst Activity
- Expose Sensitivities – partial derivatives
- Reporting

Other Online Process Digital Twin Uses

- Material Balance – Material and Volume Balances Only – Find meter errors
- Process and Equipment Performance Monitoring
- LP Vector Updating for Planning Systems
- Utilities Optimization – Requires Mixed Integer Linear Programming (MINLP)
- Plant Wide Optimization
- Green Optimization



Stepwise Approach to Optimization

Material Balance	Heat & Material Reconciliation	Rigorous Data Reconcilation	Performance Monitoring	Optimization Online or Advisory
Mass & Volume Balance	**Mass & Heat Balance**	**Mass, Heat & Equilibrium**	**Reconciliation & Simulation**	**OPTIMIZATION**

Incremental Value

• Daily Material Balance • No Thermo required • Monitor Meter accuracy • Gross Error Detection	• Material & Heat Reconciliation • No separation prediction	• KPI Evaluation • Inferential sensors • Separation efficiencies	• KPI Evaluation • Unit/Equipment Monitoring • What-if Case Studies	• Closed loop 24x7 optimization • Automated Setpoints • Integrated with APC

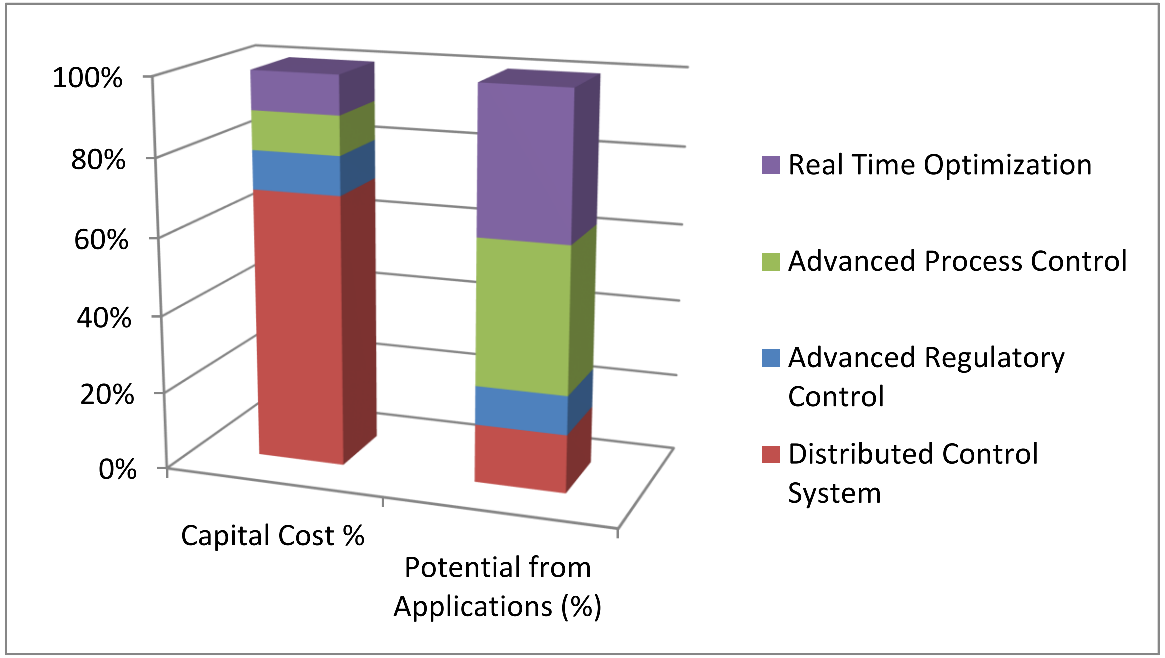
Increasing Model Fidelity →

Increasing Benefits →

Typical Processes and Benefits

- Refining
- Olefins
- Natural Gas Processing
- Utilities
  - Cogeneration Plants
  - Electrical Import/Export
  - Hydrogen Management

Unit	Typical Benefits	Typical Capacity	Typical Annual Benefits
Crude / Vacuum	10 cpb	135 kbpd	$4,455,000
FCC	18 cpb	60 kbpd	$3,564,000
Hydrocracker	18 cpd	30 kbpd	$1,782,000
Ethylene	$5 per mt	500 ktpa	$2,500,000
LNG	$1.50 per mt	1000 ktpa	$1,500,000
NGL Recovery / Fractionation	$15/MMSCFD	200 MMSCFD	$1,100,000
Utilities			$500,000 - $2,000,000



Material Balance Case Study

<u>Problem</u>

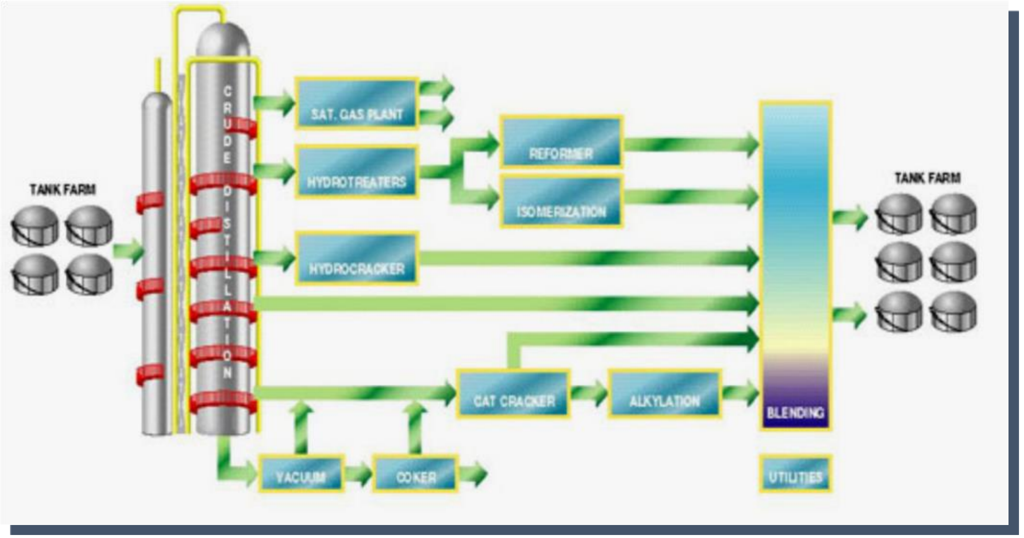
- Meter inaccuracy hindering decision making in planning, maintenance, process engineering and optimization
- Current refinery-wide planning tool could not match refinery operations

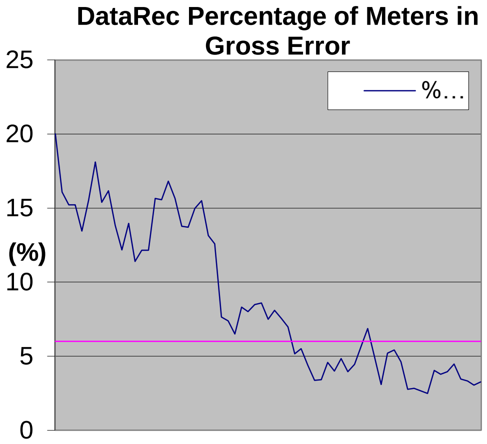
<u>Objectives</u>

- Daily material balance around each major unit & plant
- Identify bad meters
- Pinpoint material loss location
- Simplified mass balance of the entire refinery including intermediate tanks

<u>Benefits</u>

- Reduced Meter errors from 20% to less than 5%
- Found meter error in Hydrocracker Feed and Reformer overhead liquid flow
- Prevent emissions & improved yields

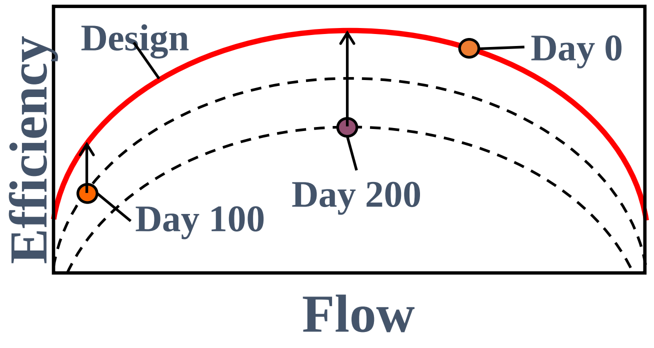




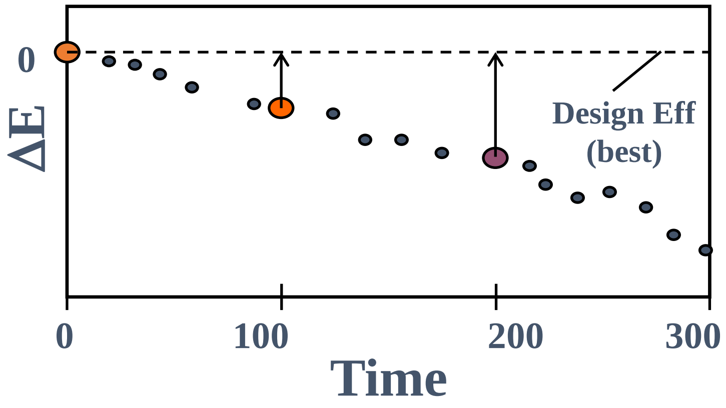
Process Equipment Performance Monitoring

- Problem
  - Compressor and heat exchanger performance degrades over time
  - Operations don't know impact of performance degradation
  - How is the compressor operating currently vs. how it is supposed to operate
  - How is exchanger fouling impacting process performance
- Solution
  - Model based performance monitoring
  - Track Design vs. Actual efficiency for compressors
  - Track impact of clean versus actual heat exchanger performance on energy usage and throughput
- Benefits
  - Know when it is economical to service compressors and clean heat exchangers
  - Prevent damage to valuable and costly machinery

Compressor monitoring

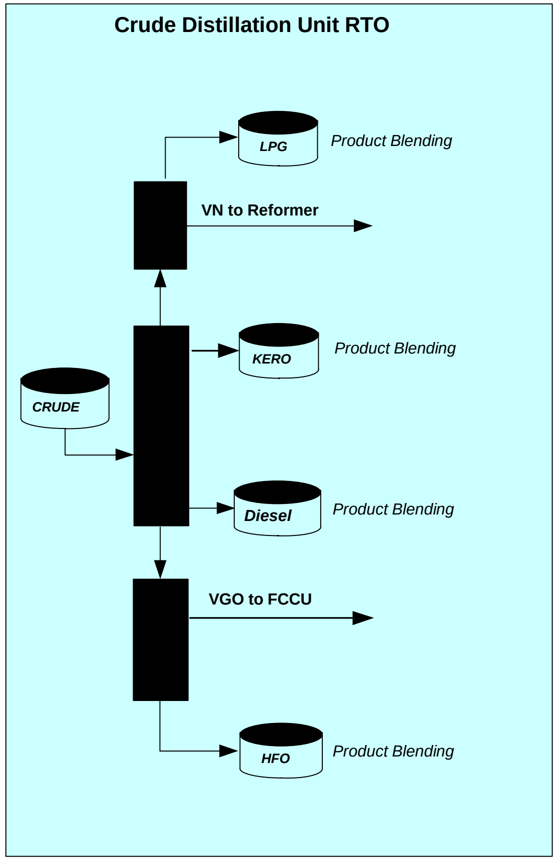


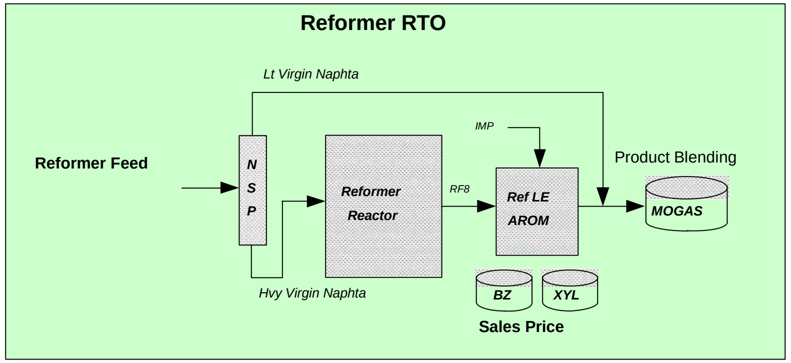
Heat Exchanger Monitoring

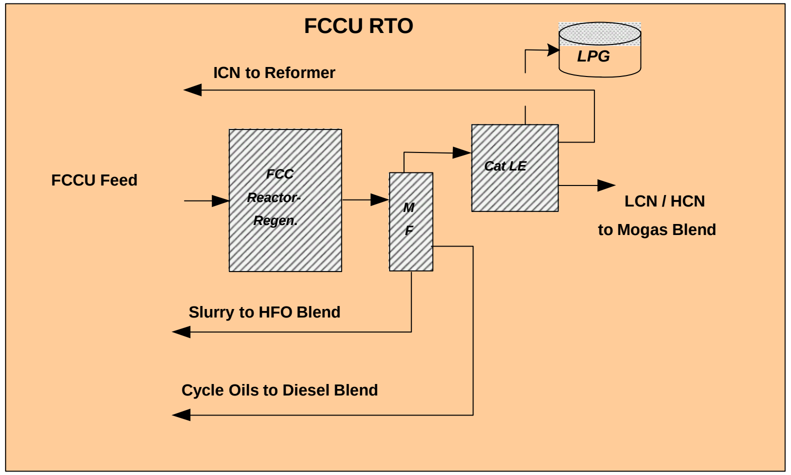


Stand-alone Real-time Optimization (RTO) Implementations

- Independent Unit RTOs
  - CDU/VDU products characterize the feed of the units downstream
  - Many refineries and chemical sites have installed RTOs for one or more processing units
    - Crude distillation units, reformers, FCCU, energy systems, H_2 systems, etc.
  - A number of these sites have RTO systems on all major process units

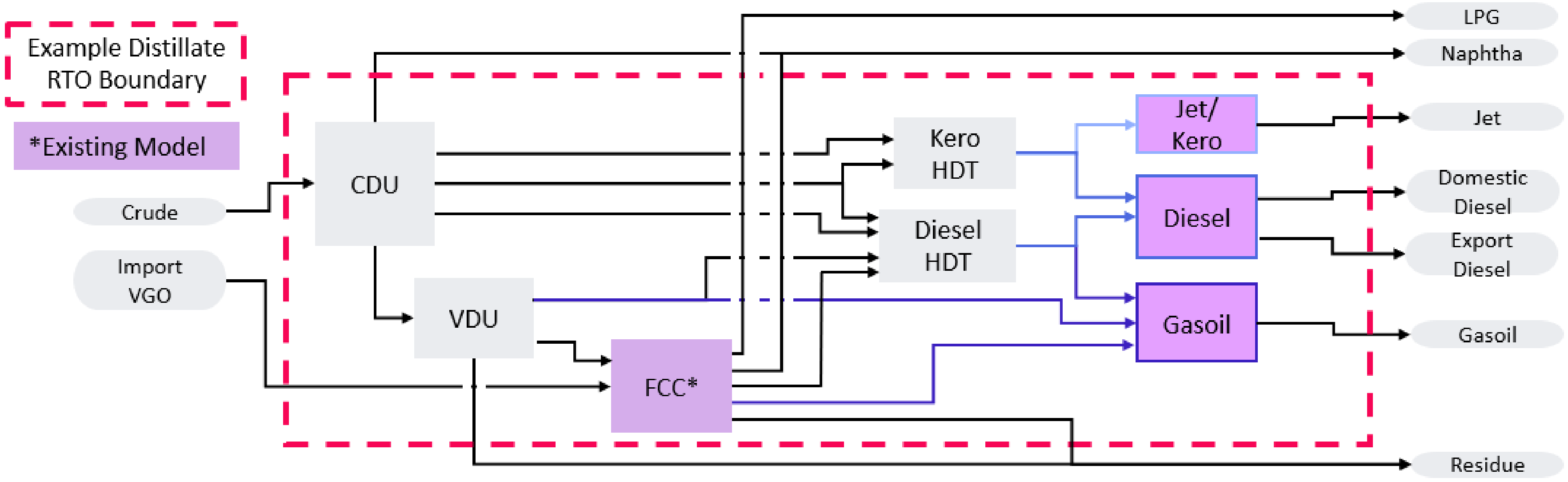




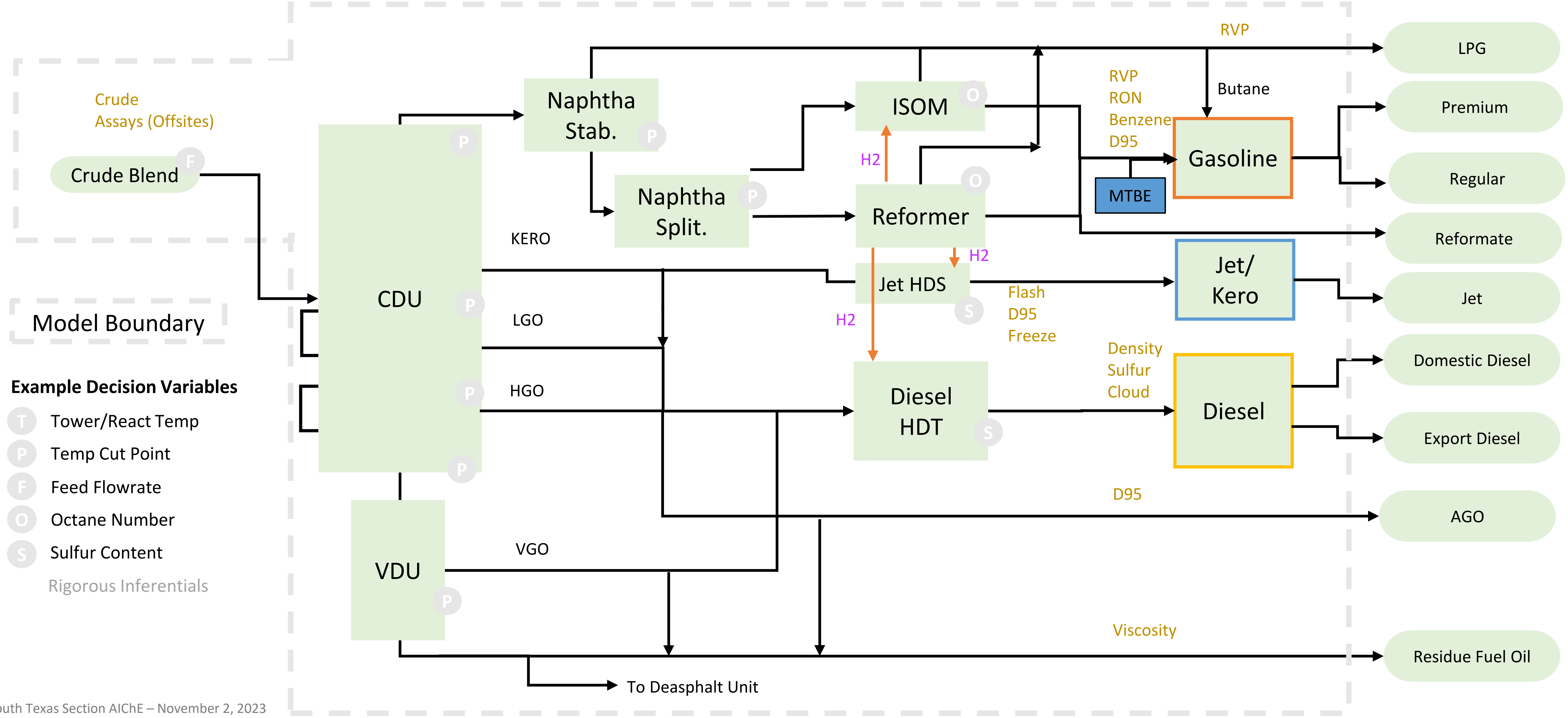


Multi-Unit / Refinery-wide Product Complex

- **Optimizes a whole process complex**
  - e.g. Naphtha Complex, Distillate Complex
- **Scope includes finished product blending**
  - Product specifications, demand/supply drive the optimization of upstream processes
  - Economics driven by feed and finished product prices – few / no intermediate product prices
- **Scheduler specifies daily feed and product supply / demand needs directly in the RTO/APC**
- **Flexible to respond to different product demand / supply and operating situations**
  - Maximizes profit, or when logistics constraints, minimizes loss

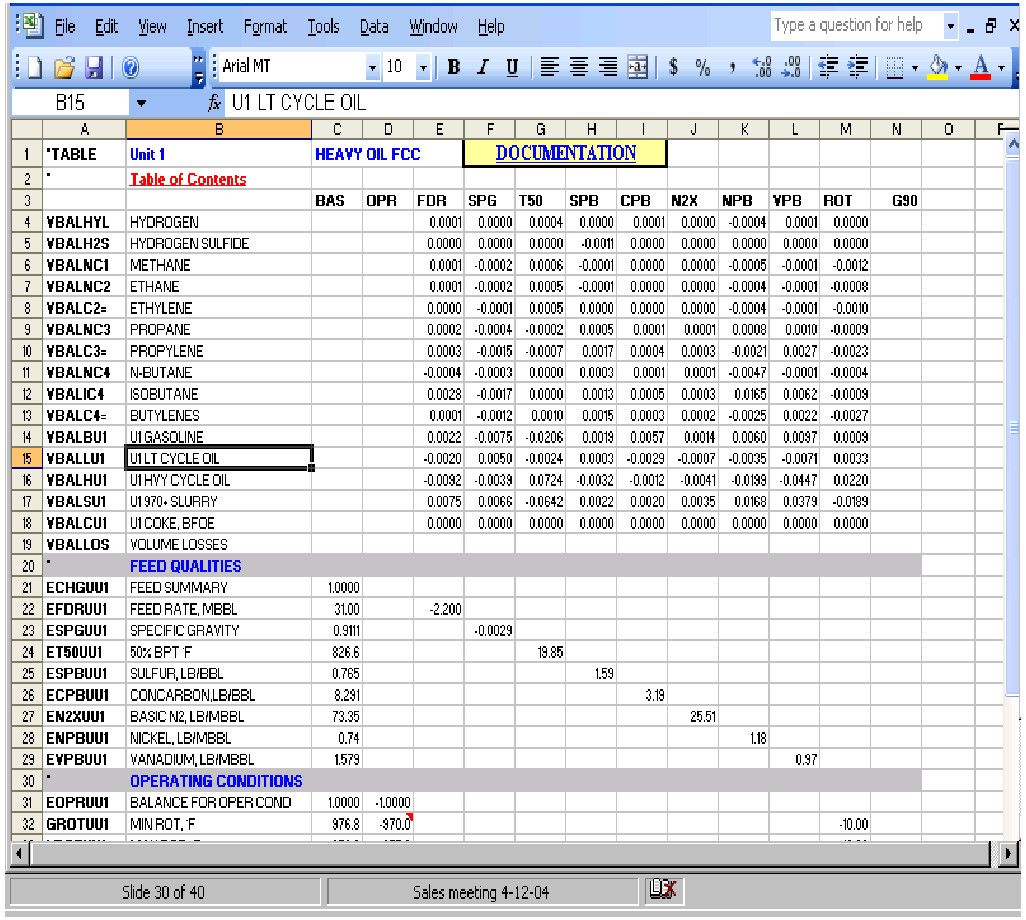


Refinery-wide Optimization



Long Term Planning

- Planning and Decision Support
  - Nonlinear
  - Turnaround scheduling
  - Evaluate feedstock
  - Evaluate cost of constraints
  - Update LP vectors On a More Frequent Basis



B15 U1 LT CYCLE OIL

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	*TABLE	Unit 1	HEAVY OIL FCC			DOCUMENTATION								
2	*	Table of Contents												
3			BAS	OPR	FDR	SPG	T50	SPB	CPB	N2X	NPB	VPB	ROT	G90
4	VBALHYL	HYDROGEN			0.0001	0.0000	0.0004	0.0000	0.0001	0.0000	-0.0004	0.0001	0.0000	
5	VBALH2S	HYDROGEN SULFIDE			0.0000	0.0000	0.0000	-0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	
6	VBALNC1	METHANE			0.0001	-0.0002	0.0006	-0.0001	0.0000	0.0000	-0.0005	-0.0001	-0.0012	
7	VBALNC2	ETHANE			0.0001	-0.0002	0.0005	-0.0001	0.0000	0.0000	-0.0004	-0.0001	-0.0008	
8	VBALC2=	ETHYLENE			0.0000	-0.0001	0.0005	0.0000	0.0000	0.0000	-0.0004	-0.0001	-0.0010	
9	VBALNC3	PROPANE			0.0002	-0.0004	-0.0002	0.0005	0.0001	0.0001	0.0008	0.0010	-0.0009	
10	VBALC3=	PROPYLENE			0.0003	-0.0015	-0.0007	0.0017	0.0004	0.0003	-0.0021	0.0027	-0.0023	
11	VBALNC4	N-BUTANE			-0.0004	-0.0003	0.0000	0.0003	0.0001	0.0001	-0.0047	-0.0001	-0.0004	
12	VBALIC4	ISOBUTANE			0.0028	-0.0017	0.0000	0.0013	0.0005	0.0003	0.0165	0.0062	-0.0009	
13	VBALC4=	BUTYLENES			0.0001	-0.0012	0.0010	0.0015	0.0003	0.0002	-0.0025	0.0022	-0.0027	
14	VBALBU1	U1 GASOLINE			0.0022	-0.0075	-0.0206	0.0019	0.0057	0.0014	0.0060	0.0097	0.0009	
15	VBALLU1	U1 LT CYCLE OIL			-0.0020	0.0050	-0.0024	0.0003	-0.0029	-0.0007	-0.0035	-0.0071	0.0033	
16	VBALHU1	U1 HVY CYCLE OIL			-0.0092	-0.0039	0.0724	-0.0032	-0.0012	-0.0041	-0.0199	-0.0447	0.0220	
17	VBALSU1	U1 970+ SLURRY			0.0075	0.0066	-0.0642	0.0022	0.0020	0.0035	0.0168	0.0379	-0.0189	
18	VBALCU1	U1 COKE, BFOE			0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
19	VBALLOS	VOLUME LOSSES												
20	*	FEED QUALITIES												
21	ECHGUU1	FEED SUMMARY	1.0000											
22	EFDRUU1	FEED RATE, MBBL	31.00		-2.200									
23	ESPGUU1	SPECIFIC GRAVITY	0.9111			-0.0029								
24	ET50UU1	50% BPT °F	826.6				19.85							
25	ESPBUU1	SULFUR, LB/BBL	0.765					1.59						
26	ECPBUU1	CONCARBON,LB/BBL	8.291						3.19					
27	EN2XUU1	BASIC N2, LB/MBBL	73.35							25.51				
28	ENPBUU1	NICKEL, LB/MBBL	0.74								1.18			
29	EVPBUU1	VANADIUM, LB/MBBL	1.579									0.97		
30	*	OPERATING CONDITIONS												
31	EOPRUU1	BALANCE FOR OPER COND	1.0000	-1.0000										
32	GROTUU1	MIN ROT, °F	976.8	-970.0									-10.00	

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Artificial Intelligence and Machine Learning versus First Principles Modeling

- Some digital twins are not based on exact physical models
    - only use experimental datasets and machine learning algorithms
- AI does have some advantages
- For example, build a model using a deep neural net to capture the true dynamics of the data
- However, generalizing this model to other objects requires a large number of samples in order to obtain a reliable general model.
- Also, are Mass, Energy and Equilibrium balances assured?
- When working with physical models we require less data to obtain an accurate general model.

Thank You!

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