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PD-07-109 Using Advanced Process Controls to Drive Regulatory Emissions Compliance

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ABSTRACT

Petroleum refining has been called "one of the most heavily regulated industries in the United States."[1] A recent EPA fact sheet cited that the EPA has settled enforcement actions with companies comprising over 30% of U. S. domestic refining capacity, and is currently engaged in settlement negotiations with companies comprising an additional 20%. The dominant environmental impacts from refinery operations currently involve air quality. About 75% of the Toxic Release Inventory poundage reported by refiners is released to the atmosphere.[2] Ever tightening environment restrictions which often limit unit capacity and/or conversion coupled with high refining margins, high fuel demand, and the need to maximize refinery capacity have created a "perfect storm" for refiners in managing operations.

Refiners are using existing IT infrastructure to support the deployment of real-time environmental data management systems to comply with air emissions monitoring and management.[3] These emissions management systems incorporate management processes, organizational changes, roles/responsibilities and tracking tools to achieve ongoing compliance with state and federal air regulations. Although several EMS systems provide real-time feedback needed for decision-making by operators, the current generation of EMS systems does not provide quantitative optimum guidance for operations to adjust process unit throughput and key operating conditions to meet air emissions rules and improve regulatory compliance.

Despite deployment of multivariable APC on most major refining processes, APC is often not utilized to work in conjunction with a refiner's EMS system to meet environmental constraints. Growing pressures are causing these two systems to converge and work together to support a refiner's ability to run to permitted emission limits. This paper explores a methodology for EMS and APC integration and provides an assessment for the potential benefits and technical challenges for success.

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1 George Birchfield, et al, "Technology Roadmap for the Petroleum Industry", February 2000, US Department of Energy, 07 May 07, www.eere.energy.gov/industry/petroleum_refining/pdfs/petroleumroadmap.pdf , p. 1.
2 Paul Chalmers, "Petroleum Refining: Impacts, Risks, and Regulations", Environmental Roadmapping Initiative, 11 Aug 04, National Center for Manufacturing Sciences, 07 May 07, ecm.ncms.org/ERI/new/IRRpetref.htm.
3 Kelly Coppola, et al, "Develop a 'Real-Time' Emissions Monitoring Strategy for Your Facility", Hydrocarbon Processing, December 2006, pg. 87-91.

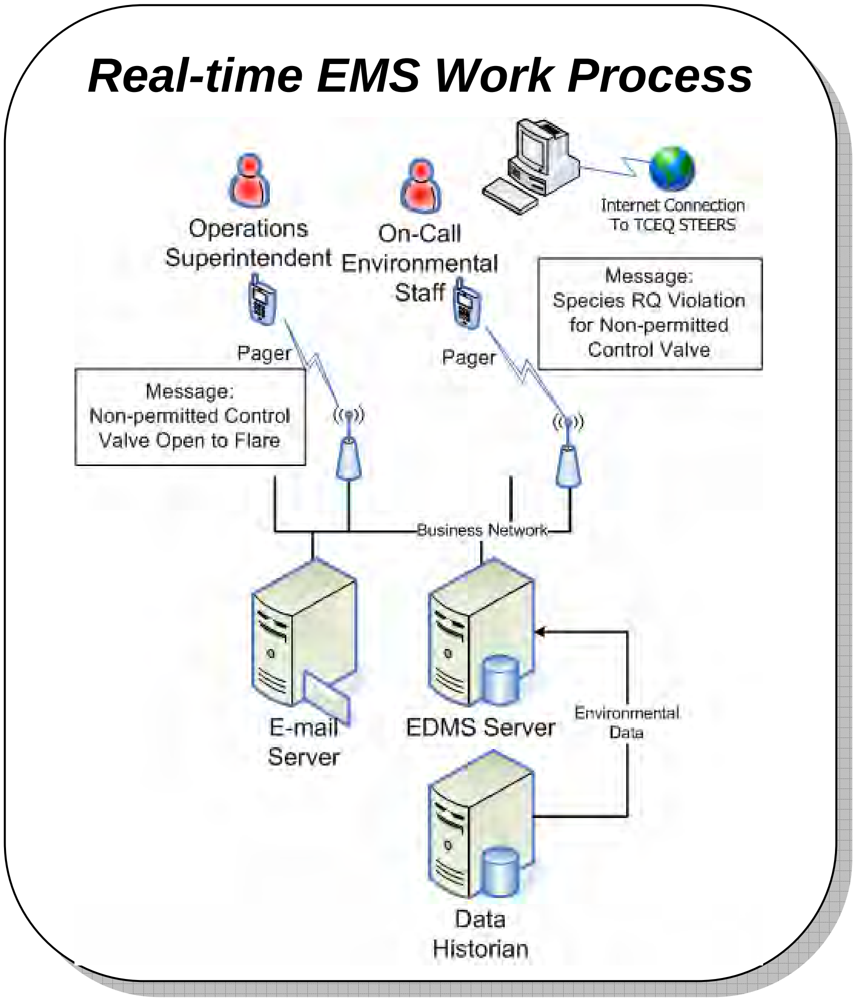
INTRODUCTION

The public has demanded that state and federal governments place restrictions on contaminants that refineries and chemical plants release. These restrictions such as the Highly Reactive Volatile Organic Compound (HRVOC) rule from the Texas Commission on Environmental Quality (TCEQ) set requirements to bring areas like the Houston/Galveston area into attainment for ozone per the Clean Air Act.[4] The dominant environmental impacts from refinery operations currently involve air quality. About 75% of the Toxic Release Inventory poundage reported by refiners is released to the atmosphere.[2] These ever tightening environment restrictions which often limit unit capacity and/or conversion coupled with high refining margins, high fuel demand, and the pressure to maximize refinery capacity have created a "perfect storm" for refiners to manage and optimize operations.

To comply with regulatory emissions requirements, refiners and chemical plants have employed the use of existing IT (Information Technology) infrastructure to support the deployment of real-time environmental data management systems in order to comply with air emissions monitoring and reporting.[3] These emissions management systems (EMS) incorporate management processes, organizational changes, roles/responsibilities and tracking tools to achieve ongoing compliance with state and federal air regulations. Although several EMS systems provide real-time feedback needed for decision-making by operators, the current generation of EMS systems provide notification (Figure 1) but do not provide quantitative guidance for operations to adjust plant operations such as process unit throughput and other key operating conditions to run to permit limits while maintaining regulatory compliance.

[4] Kelly Coppola, et al, "Implementation of a Real-Time Environmental Data Management System to Ensure HRVOC Program Compliance", NPRA 2006 Environmental Conference, ENV-06-158.

Figure 1 - Example of a Real-time EMS Work Process[5]



Despite deployment of multivariable Advanced Process Control (APC) on most major refining processes, APC is often not utilized to work in conjunction with a refiner's EMS system to meet environmental constraints. Using this information as operating constraints in a process unit multivariable control is a logical extension of the control solution given the availability of reliable real-time emission and compliance information. Growing pressures are causing these two systems to converge and work together to support a refiner's ability to run to permitted emission limits and future even more demanding environmental operating constraints. This paper explores a methodology and challenges for EMS and APC integration and provides an assessment for the potential benefits and technical challenges for success.

5 Paul Glaves, et al, "Enhanced Air Emissions Monitoring Using a Real-Time EDMS", 2007 A&WMA Annual Conference, Paper 372.

EMS/APC Integration Requirements

Integration of real-time air emission calculations with a close-loop APC application demand stringent requirements of both the EMS and APC system in order to be effective. The EMS must be designed and implemented to provide an accurate source for air emissions data and information. This system is commonly used for short term compliance monitoring by plant personnel (Health Safety & Environmental and Operations), long term compliance monitoring and reporting and data archiving as required by regulations. The following additional requirements are needed for this information to be used directly in APC calculations:

- Be available in the Distributed Control System environment
- Have a high degree of accuracy and reliability which is essential for real-time control
- Comply with accepted regulatory agency calculation guidelines

Estimating Air Emissions

Accurately estimating air emissions requires a balance of an understanding of complex environmental regulations and applying sound chemical engineering principles. In certain cases the regulatory methods are difficult to interpret or may not be the most accurate method of estimating the emissions but the regulatory methods must be followed. Any variation of specific regulatory-required calculations must be specifically approved in writing by the governing regulatory body.

An example of requirements for calculation of air emissions under TCEQ are as follows:

> *TCEQ regulations require emissions to be calculated using the following methods, in order of preference:*
>
> 1. *Continuous Emissions Monitoring Systems (CEMS)*
> 2. *Valid stack sampling that represents average or typical operating conditions,*
> 3. *Vendor supplied emissions factors based on stack samples,*
> 4. *AP-42[6] and other EPA approved factors including EPA software programs*
> 5. *Material balance based on an accounting of actual material usage, and*
> 6. *Estimated based on best available process operating data.*

[6] "Emission Factors & AP 42", US Environmental Protection Agency, 02 Sep 07, http://www.epa.gov/ttn/chief/ap42/index.html.

CEMS data must be used for emissions calculations if valid and available. CEMS that are not operated according to EPA/TCEQ-approved methods are not considered valid.

Valid stack testing data is the next preferred method of estimating emissions. Hand-held analyzers or other unofficial tests are not considered valid stack tests since they were not obtained using TCEQ/EPA-approved methods.

If no valid stack test results are available, then a vendor-supplied stack test can be used.

"AP-42" Emission factors published by the USEPA are the next preferable method. Emission factors for various source types are provided in the AP-42 documents.

Material balances can be used if there are no AP-42 factors available. One exception is for sulfur dioxide emissions from hydrogen sulfide or total sulfur compositions. When good data of sulfur compounds is available and a valid CEMS is not available for a combustion source, a material balance is the preferred estimation method.

Refiners will fall under different regulatory requirements dependant on their geographic location and State and locate environment.

EMS Calculations in a Real-Time Environment

Calculations for the EMS require a underlying system that incorporates associated management processes, organizational changes, roles/responsibilities and tracking tools to ensure calculation accuracy and reliability and ongoing compliance with state and federal air regulations. EMS systems have been implemented to provide a single, accurate, transparent source for air emissions data and information.[4] Specific functional requirements for the EMS system include:

- provide a common and reliable "book of record" for emissions data and calculations
- support compliance to emission regulations via timely emissions calculations
- provide proactive notification of performance with respect to emission limits to both HSE and Operations
- facilitate creation of long term compliance reports (e.g. Title V Deviation Reporting)
- provide emission values and targets for the APC application.

An overview of a typical EMS system is illustrated in Figure 2.

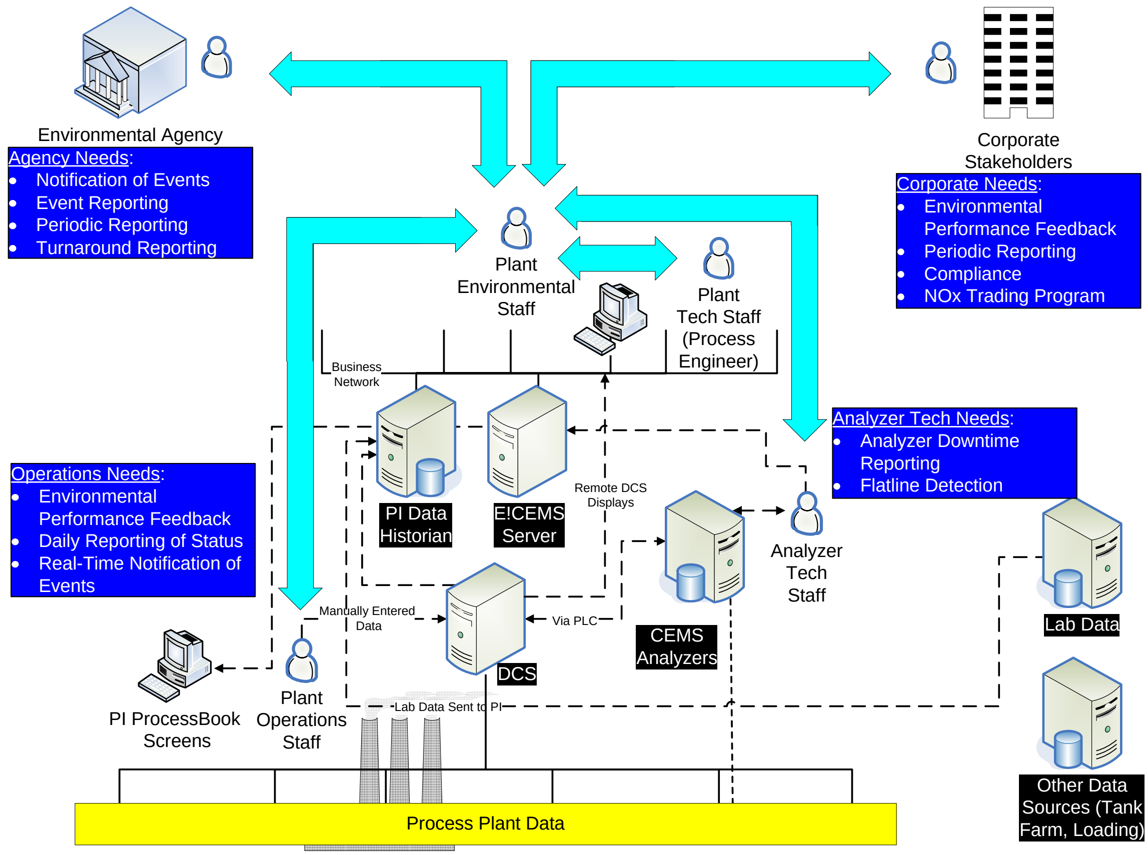


Figure 2: Overview of EMS Work Process

Permit Compliance Targets

Permitted Fluid Catalytic Cracking Unit (FCCU) emissions compliance targets are typically based on weekly and yearly rolling averages based on rolled-up and validated CEMS data. These targets must be calculated with CEMS data management practices in 40 CFR Part 60 Subparts A and J, or Alternative Monitoring Protocols approved by EPA for the refiners site.

An example method for determining rolling averages are provided below:

<u>*7-Day Rolling Average (7-DRA):*</u>

- *Compute the rolling average as an average of all "valid hours" of CEMS data for 7 consecutive days (a day is a 24-hour period from midnight to* *midnight); the "valid hours" for each day may be used to calculate weighted daily average emission concentrations, and the 7-DRA can be based on 7 weighted daily averages;*

- *A "valid hour" of CEMS data is determined in accordance with §60.13 and Appendix F;*

- *Any hour during the 7-day period that does not have "valid" CEMS data would be excluded from **both** the denominator **and** the numerator in that day's daily average that is used in computing the 7-DRA;*

- *Any "valid hour" of CEMS data during periods of unit outages "will be included in computing the 7-DRA; an explanation of any unusual averages resulting from inclusion of the data will be provided in the next quarterly report;*

- *Any "valid hour" of CEMS data during periods of "startup, shutdown, or malfunction (SSM)" will be included in computing the 7-DRA; an explanation the of events associated with the SSM event will be provided in the next quarterly report.*

- *If a process is shutdown for 7 or more consecutive calendar days (such as a TAR), then the start of the 7-DRA period will be **reset**; the first day of the new 7-DRA will be the day in which the first "valid hour" of CEMS data is collected after startup of the process;*

365-Day Rolling Average (365-DRA):

- *Compute the rolling average as an average of all "valid hours" of CEMS data for 365 consecutive days (a day is a 24-hour period from midnight to midnight); the "valid hours" for each day may be used to calculate weighted daily average concentrations , and the 365-DRA can be based on 365 weighted daily averages;*

- *A "valid hour" of CEMS data is determined in accordance with §60.13 and Appendix F;*

- *Any hour during the 365-day period that does not have "valid" CEMS data would be excluded from **both** the denominator **and** the numerator in that day's daily average that is used in computing the 365-DRA;*

- *Any "valid hour" of CEMS data during periods of unit outages will be included in computing the 365-day average; an explanation of any unusual averages resulting from inclusion of the data will be provided in the next quarterly report;*

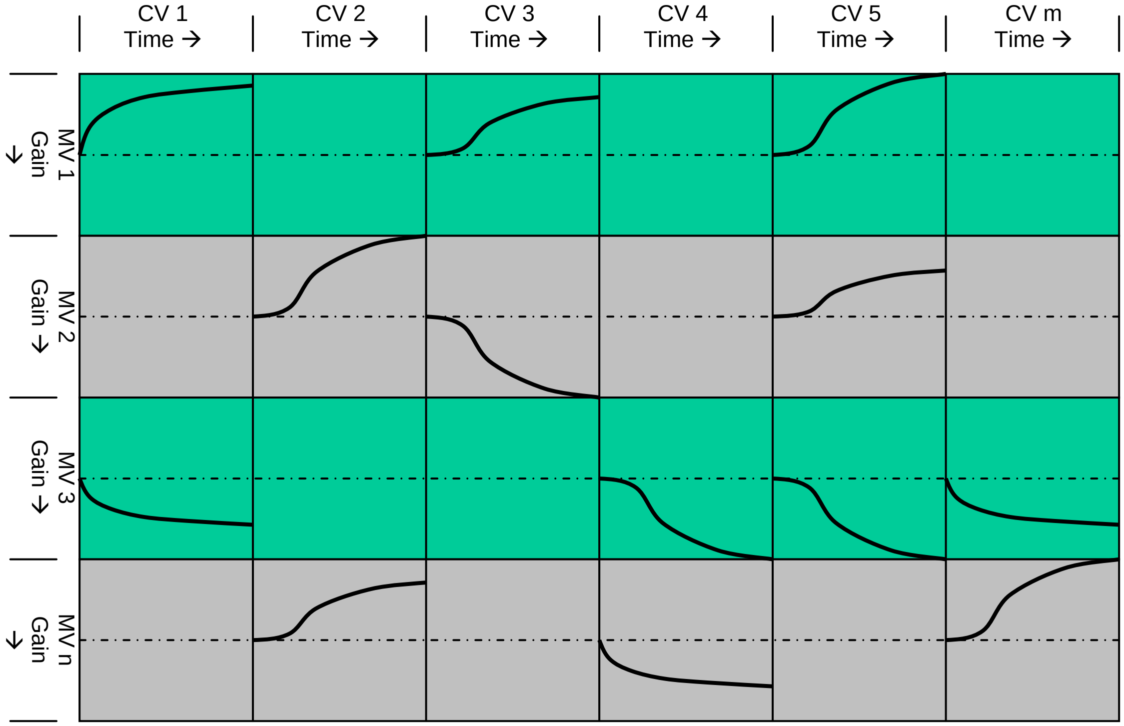
- *Any "valid hour" of CEMS data during periods of "startup, shutdown, or malfunction (SSM)" will be included in computing the 7-DRA; an explanation the of events associated with the SSM event will be provided in the next quarterly report.*

- *The 365-DRA is **not reset** following any shutdowns, including TARs.*

Incorporating Compliance Targets with APC

Model predictive APC has been implemented throughout refining and petrochemical industry to improve the performance of refining process units by improving the control of key process and equipment constraint and product qualities while driving the process to true economic constraints.[7] Dynamic models like the example illustrated in Figure 3 are developed from plant test data and/or dynamic simulation.

[7] Paul Robinson & Dennis Cima, "Advanced Process Control," Chapter 22 of Practical Advances in Petroleum Processing, Springer: New York, 2006, (ISBN-10: 0-387-25811-6).



Dynamic models represent interactions between any number of manipulated variables and any number of controlled variables over the specified time horizon

Figure 3: Multivariable Control Dynamic Model Example

These models relate manipulated variables (MVs) to the dynamic, time dependant response of controlled variables (CVs) over a fixed time horizon know as the time to steady-state (TSS). A history of past movement in MVs together is used to predict the future behavior of dynamic behavior of CV to both control and optimize the movement of MV's in order to reduce process variability and drive the process to an economic optimum as illustrated in Figures 4 and 5.

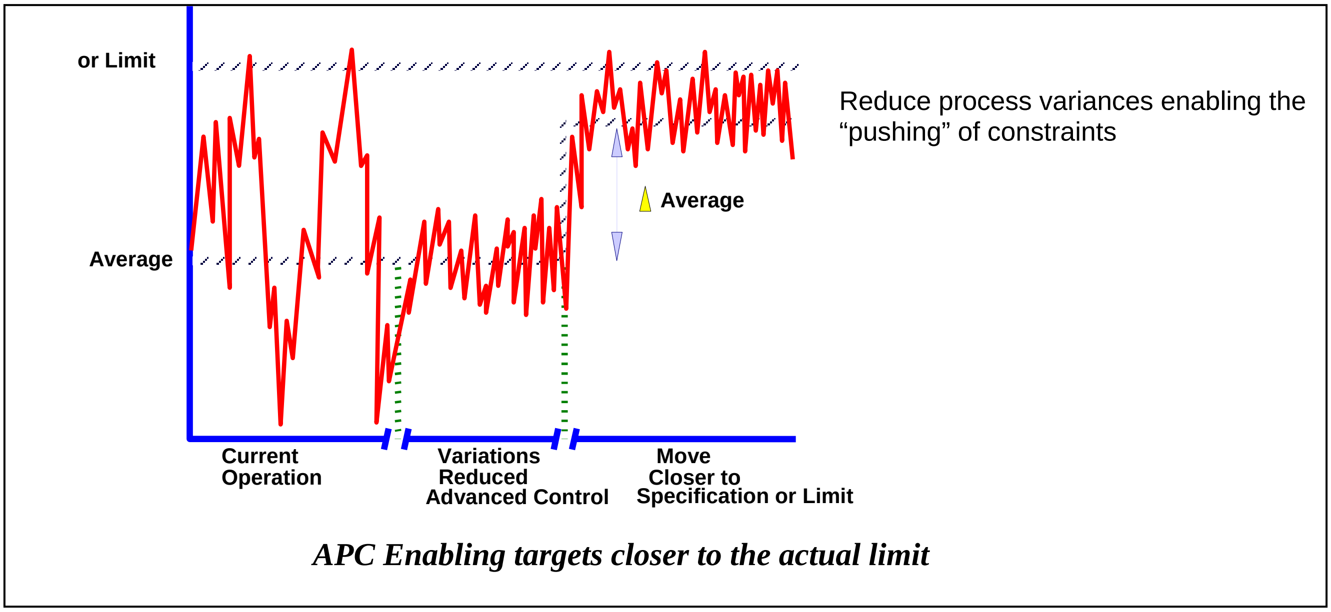


Figure 4: Improved Control Through Reduced Variability

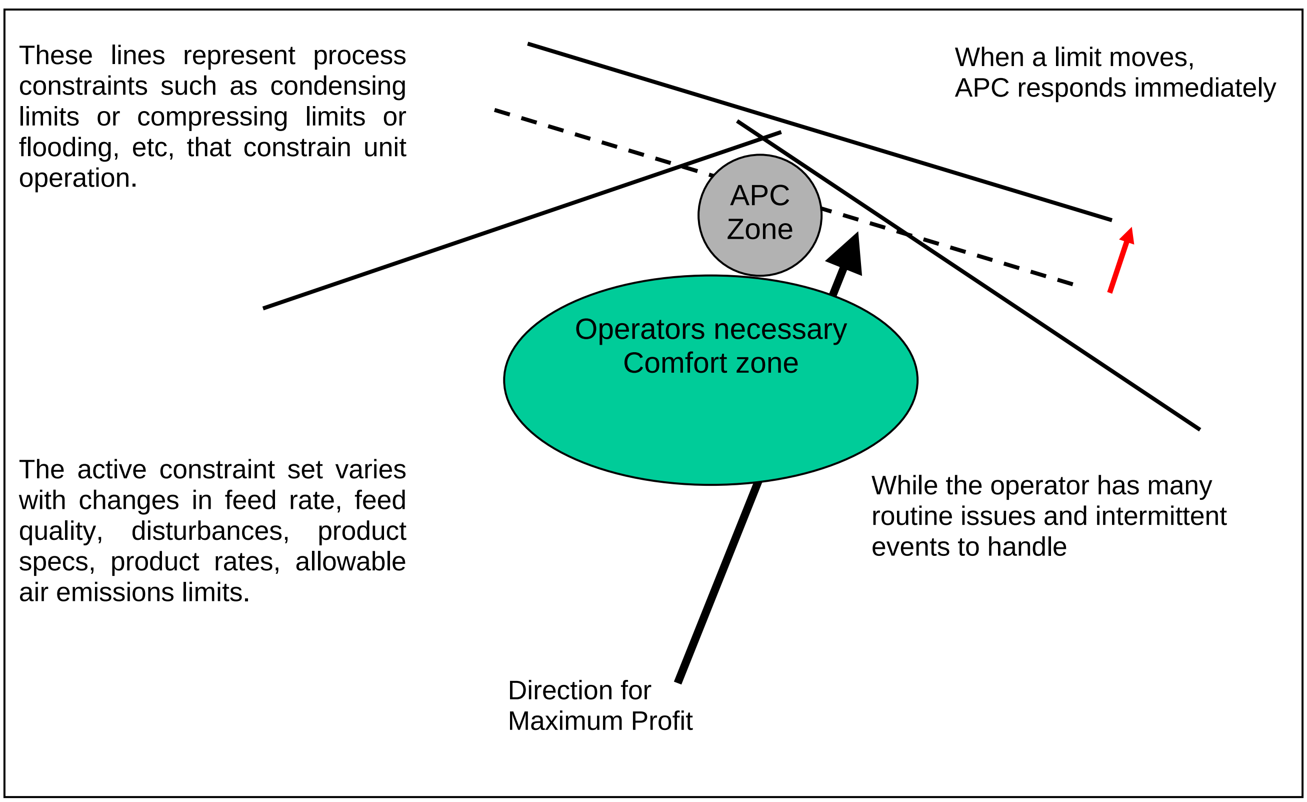


Figure 5: APC Constraint "Pushing" and Optimization

Emission Target Constraints

Emissions constraints that are likely candidates for the integration of into existing or planned APC applications are listed in Table 2 below.

Emission Sources – Daily – Hourly Avg.

EMISSION SOURCES	#	SPECIES CALCULATED
Heaters – NOx/CO CEMS	15	NO2, NO, CO, VOC, PM, SO2
Heater – Non-CEMS	63	NOx, CO, VOC, PM, SO2
Sulfur Recovery Units	4	NOx, CO, PM, VOC, SO2, H2S
FCC/HOC	2	NOx, CO, PM, PMSO4, VOC, SO2, H2SO4
Engines / Turbines	7	NOx, CO, VOC, PM, SO2

Table 1: Typical Refinery Emission Sources[5]

Large process heater such as atmospheric crude and vacuum tower heaters and Fluid Catalytic Cracking Unit flue gas stack emissions such as NOx, SOx, and CO are likely candidates for the integration into existing or planned APC applications.

FCCU NOx Example

Calculation of FCCU flue gas concentration is quite complex and can be described as follows:

The TCEQ NOx 117 regulations require the installation of exhaust stack flow meters. The flow meters are currently being installed. Instrumentation in the exhaust stack measures the following parameters:

- *Actual velocity (ft/sec)*
- *Actual temperature (R)*
- *Actual pressure (psia)*
- *Actual moisture (volume percent water vapor)*

It is desirable to perform all of the calculations for the exhaust flow rate within the EMS software environment. This will allow for data substitution rules and averaging rules to be consistent and compliant with regulatory requirements. The EMS software should also allow for enhanced detection of failures of raw data inputs.

First, the actual stack exhaust flow rate is calculated based on the actual measured velocity (ua) and stack cross-sectional area (A) of the exhaust stack:

$$Q_a = (u_a)(A)$$

The ideal gas equation is used to convert the actual volumetric flow rate to standard conditions:

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}\text{, so}\quad V_2 = \frac{P_1 V_1 T_2}{P_2 T_1}$$

where:

V1 = actual volume

V2 = volume at standard conditions

P1 = actual pressure in exhaust stack near the velocity meter, psia

P2 = standard pressure (14.7 psia)

T1 = Actual temperature near exhaust velocity meter (R)

T2 = standard temperature (68F = 528 R)

The volumetric flow rate at standard conditions must be corrected for moisture so that the flow rate is on the same moisture basis as the pollutant concentrations. Moisture correction is necessary since the stack pollutant analyzers measure concentration on a dry basis. A separate instrument will provide the stack moisture content, in units of volume fraction water vapor in the exhaust stack (s). The final form of the equation is shown below:

$$NOx\,(lb/hr) = \left(u_a\,\frac{ft}{\sec}\right)\left(3{,}600\,\frac{\sec}{hr}\right)\left(A\ ft^2\right)\left(\frac{P_1 V_1 T_2}{P_2 T_1}\right)x$$
$$\left(\frac{ppmvd\ NOx}{1{,}000{,}000\ SCF}\right)\left(\frac{46\ lb\ NOx}{385.2\ SCF\ NOx}\right)(1-s)$$

where:

ua	*= actual measured velocity in the exhaust stack (ft/sec)*
A	*= cross-sectional area in exhaust stack near the velocity meter (ft2)*
ppmvd NOx	*= parts per million NOx by volume, dry basis, uncorrected for oxygen, from stack analyzer*
s	*= volume fraction of water vapor in exhaust stack (dimensionless)*

Mass emission rates for other CEMS-measured pollutants are calculated by substituting the correct molecular weight in the equation.

Multivariable Control Inputs

For the FCCU NOx example, the current calculated NOx emissions value and rolling DRA value would be used as CVs in the FCCU multivariable controller design. NOx and DRA NOx data is collected along with other MV and CV variables during an APC plant response test. During this test, FCCU MVs are stepped by operations or with the aid of automated step testing tools and the response of the CVs are collected. Dynamic models are developed with commercially available multivariable regression software to build, simulate and validate MV vs. CV relationships. NOx CV models are then incorporated into the overall FCCU APC dynamic model. Real-time updates of emissions calculations from the EMS system provide feedback from the process for the APC system.

Determining APC Targets to Run to Permit Limits

APC multivariable control a number of either CV limits, external targets, and ideal resting values to provide emission targets that represent permit limits. Setting these targets requires knowledge of both peak air emission limits and an acceptable compliance margin which provides a “cushion” to insure unplanned or unmeasured upsets do not cause permit violations.

Anticipated Benefits

Benefits are expected from both the prevention of permit violation and the ability to operate refining units closer to permit constraints. A recent EPA fact sheet stated that the EPA has settled enforcement actions with companies comprising over 30% of U. S. domestic refining capacity, and is currently engaged in settlement negotiations with companies comprising an additional 20%.

Summary

Refiners and chemical plants have an opportunity to both improve regulatory compliance while running units closure to permit capacities by integrating existing EMS systems with APC multivariable controllers. The technical challenges lie in providing robust and accurate EMS emission calculations and successfully integrating them in to the multivariable control environment. Refiners should benefit from the successful integration and deployment of these technologies. Mustang Engineering is in discussion with several refiners to implement this solution.

Appendix – Example Rolling Average Calculations

Table A-1
7-Day Rolling Average Calculation Example

	CEMS Data		7-Day Rolling Ave (7-DRA) Data			
Day	No. of "Valid Hours"	Weighted ppm of all "Valid Hours"	Weighting Factor	7-Day Rolling Average (ppm)	Days Included	Comments
1	22	27	594	--	--	
2	24	29	696	--	--	
3	21	33	693	--	--	
4	12	32	384	--	--	
5	24	30	720	--	--	
6	24	28	672	--	--	
7	24	29	696	30	1-7	1
8	24	27	648	29	2-8	
9	21	23	483	29	3-9	
10	CEMS Down		--	28	4-10	2
11	22	32	704	28	5-11	
12	24	77	1848	36	6-12	3
13	Source Shutdown		--	--	--	
14	Source Shutdown		--	--	--	
15	Source Shutdown		--	--	--	
16	Source Shutdown		--	--	--	
17	16	44	704	53	11-17	4
18	24	36	864	53	12-18	
19	24	18	432	31	13-19	
20	Source Shutdown		--	--	--	
21	Source Shutdown		--	--	--	
22	Source Shutdown		--	--	--	
23	Source Shutdown		--	--	--	
24	Source Shutdown		--	--	--	
25	Source Shutdown		--	--	--	
26	Source Shutdown		--	--	--	
27	6	88	528	--	--	5
28	24	65	1560	--	--	
29	24	26	624	--	--	
30	CEMS Down		--	--	--	
31	CEMS Down		--	--	--	
32	16	28	448	--	--	
33	24	33	792	42	27-33	6
34	24	55	1320	42	28-34	7
35	24	68	1632	43	29-35	7
36	24	38	912	46	30-36	

Comment

1. Day 7; the 7-DRA is the weighted average of all valid 1-hour CEMS data for days 1 thru 7.

2. Day 10; the CEMS is down the entire day; therefore, there is no valid data for Day 10 and it is excluded from both the numerator and denominator for Days 10, 11, and 12. Day 10; the CEMS is down the entire day; therefore, there is no valid data for Day 10 and it is excluded from both the numerator and denominator for Days 10, 11, and 12.

3. Day 12; A malfunction occurs in the process that causes high emission levels. The malfunction is documented; the data for the period of the malfunction is "valid" data, it is included in the 7-DRA calculation; an explanation the of events associated with the SSM event will be provided in the next quarterly report, including a calculation of the rolling average without the CEMS data during the SSM event.

4. Day 17 thru 19; The 7-DRA for these 3 days are based on small number of valid 1 hour averages, since the process was shutdown for a few days. When such instances occur, they should be identified in quarterly reports, since the average may be skewed by data that represents periods of time that may be significantly less than 7 days.

5. Days 27 & 28; During startup of the process high emission occur. The startup is documented; the data for the period of the startup are "valid" data, it is included in the 7-DRA calculation; an explanation the of events associated with the SSM event will be provided in the next quarterly report, including a calculation of the rolling average without the CEMS data during the SSM event.

6. Day 33; After a process shutdown, such as a TAR, that lasts for 7 days or more, the start day for the 7-DRA is reset. The first day of the new 7-DRA will occur during the day in which the first "valid hour" of CEMS data is collected after startup o the process. Thus, Day 27 starts the 7-DRA.

7. Days 34 & 35; a unit outage occurred which caused unusually high CEMS data; the data is included in the 7-DRA and it is explained in the quarterly report. However, for the FCCU a special provision applies. The report will include a calculation of the rolling average without the CEMS data during the unit outage, as long as the unit outage plan is complied with.

Table A-2

Example Hourly Data for 24 Hour Period

	CEMS Data		24 Hr Avg	
Hour	"Valid Hour"	Average ppm of "Valid Hour"	Weighted ppm of all "Valid Hours"	Footnote
1	1	23		
2	1	22		
3	1	24		
4	1	29		
5	1	33		
6	1	32		
7	1	30		
8	1	28		
9	1	33		
10	1	27		
11	1	24		
12	1	26		
13	1	28		
14	--	--		1
15	--	--		1
16	1	25		
17	1	27		
18	1	26		
19	1	25		
20	1	23		
21	1	27		
22	1	24		
23	1	28		
24	1	30		
	22	594	**27**	

Footnote:

1 Data not valid due to CEMS maintenance