

REINHOLD ENVIRONMENTAL[®]



2023 Reinhold/PCUG Round Table Presentation

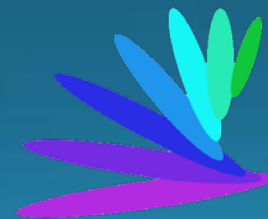
Cohosted by Duke Energy and Vistra in The Westin Hotel,
Cincinnati, OH on June 26-27, 2023

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2023 REINHOLD/PCUG CONFERENCE
Chaired by Duke Energy and Vistra / Hosted by
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SCR Catalysts

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Research and Consulting Engineers

Overview

1. Fundamental Design

- *How a catalyst works*
- *Definitions*

2. Catalyst Management

- *Initial Potential*
- *Deactivation*
- *Plugging*

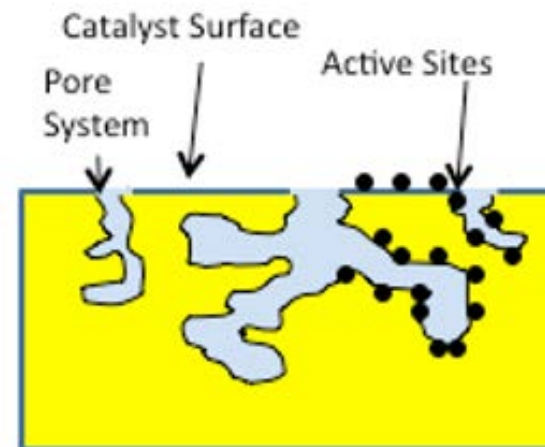
3. SCR Catalyst Types and Designs

- *Plate*
- *Corrugated*
- *Honeycomb/Extruded*

FUNDAMENTAL DESIGN

Many factors affect catalyst performance

- Physical Geometry
- Internal Pore Structure (porosity, tortuosity, etc.)
- Formulation (chemical make-up including substrate material, primary catalytic species, and “promoters” and other supporting chemical species)



PERFORMANCE CONSIDERATIONS

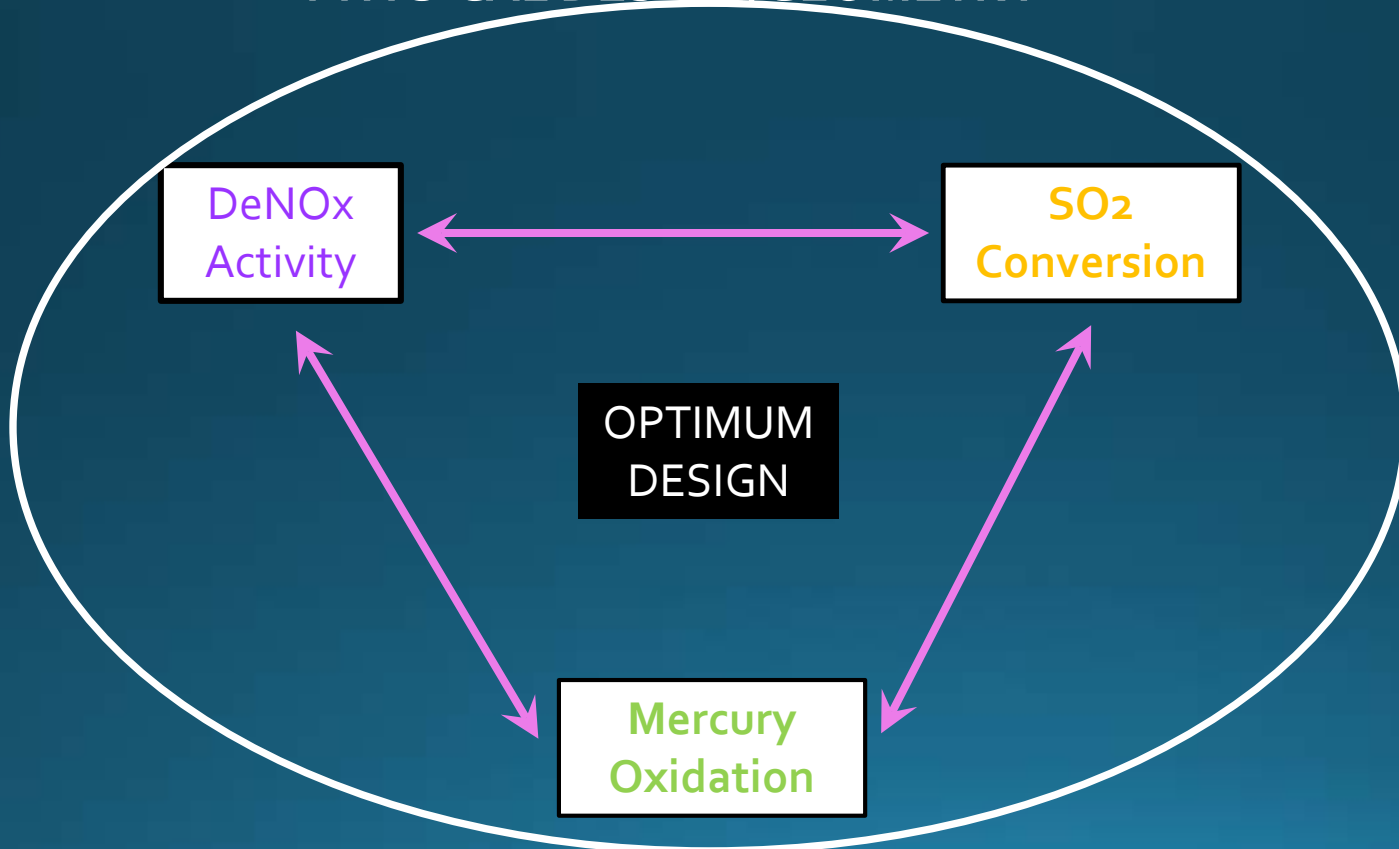
Primary function is to promote the reaction of NO_x with ammonia.

SCR Catalysts also promote SO₂ conversion and mercury oxidation.

Design must balance performance parameters.

ASK FOR OPTIONS WHEN BIDDING CATALYSTS!

PHYSICAL DESIGN/GEOMETRY



Fundamental Equations: DeNOx

EXCELLENT RESOURCE - EPRI.com

[Laboratory Testing Protocol for Coal-Fired SCR Catalyst: 3rd Edition](#)

Product ID:3002013048 Pages:132 Published: November 15, 2018 Type:

Technical ResultsLevel:Membership

DeNOx

The fundamental purpose of SCR technology is to remove NOx from the flue gas. The amount of removal is usually expressed as the “deNOx rate,” or simply “deNOx.” DeNOx is expressed according to the following equation. Different units can be utilized as long as both the inlet and outlet are on the same unit basis; this includes; lb/MMBtu, ppmv (at consistent O₂ and wet/dry basis), and lb/hr.

$$\text{DeNOx Rate (\%)}: \frac{(\text{NO}_{\text{xin}} - \text{NO}_{\text{xout}})}{\text{NO}_{\text{xin}}} \times 100\%$$

Where; NO_{xin} = NOx into the reactor
NO_{xout} = NOx out of the reactor

Fundamental Equations: Area Velocity, AV

Area Velocity

Area velocity (AV) is defined as the flue gas flow rate divided by the total geometric surface area of the installed catalyst. Area velocity is typically specific to a particular layer of catalyst, such that reactors with multiple layers of catalyst will have an applicable area velocity for each catalyst layer. If layers are identical in terms of catalyst volume and specific surface area, then they will have the same area velocity.²¹ High area velocities indicate that a layer has a high flue gas throughput compared to the geometric surface area, while low area velocities indicate a low throughput. Area velocity is calculated according the following equation, and uses flow expressed at standard temperature (0 °C).

$$AV = \text{Area Velocity (m/hr)} = \frac{F}{SSA * V}$$

Where; F = flue gas flow rate (m³/hr at 0 °C, actual O₂ and moisture)
SSA = catalyst specific surface area of layer (m²/m³)
V = catalyst volume of layer (m³)

Fundamental Equations:

DeNOx Activity, K (lab measurement)



CAUTION: This equation is not a reactor design equation – cannot be used to determine minimum potential for a field unit!

DeNOx Activity

The deNOx activity, or simply the catalyst activity (K-value), is defined according to an industry-standard measurement methodology which provides a convenient metric.¹³ The equation below shows the basic formula for calculating this activity metric. *Note that this formula is only valid under laboratory test conditions, where the NH₃/NOx ratio is at or just above 1.0. This equation cannot be used to directly predict field performance or to directly determine minimum potential.* The use of this K-value in SCR modeling to determine expected field performance and minimum potential is discussed in the “Catalyst Management” chapter.

$$K = -AV \cdot \ln(1 - \%deNOx)$$

(Note: only valid for NH₃/NOx = 1.0-1.02)

Where; K = deNOx activity (m/hr)

AV = area velocity (m/hr)

%deNOx = NOx removal efficiency expressed as a fraction

Fundamental Equations: deNOx Potential, P

Individual Layer DeNOx Potential

The deNOx potential of a layer changes with operational hours as a function of deactivation, indicated by the applicable deNOx activity (K-value) at those hours. Therefore, the potential at any operational time t is simply the K-value at time t divided by the AV. The following equation describes the calculation of deNOx potential. DeNOx potential is a dimensionless parameter.

$$P_t = \text{deNOx Potential} = \frac{K_t}{AV}$$

Where; P_t = layer potential at t operational hours

K_t = catalyst activity at corresponding t operational hours (m/hr)

AV = area velocity (m/hr)

The fresh catalyst deNOx potential (P_0) is a commonly used parameter and represents the potential of a layer prior to any flue gas exposure. P_0 is calculated according to the following equation, where the applicable activity is the fresh activity (K_0).

$$P_0 = \text{initial (or fresh) deNOx potential} = \frac{K_0}{AV}$$

Where; P_0 = layer potential at time 0 (fresh catalyst)

K_0 = catalyst activity at time 0 (fresh catalyst, m/hr)

AV = area velocity (m/hr)

Fundamental Equations:

Total reactor deNOx potential, P_{rxr}

Reactor Potential

The reactor potential is simply the sum of the potential of each individual layer. The reactor potential at any time t corresponds to the sum of the potentials for each layer at time t . Reactor potential is calculated according to the following equation.

$$P_{RXR} = P_1 + P_2 + P_3 \dots$$

Where; $P_{1,2,3\dots}$ = potential of individual layers

Minimum Reactor Potential

The minimum reactor potential is defined as the minimum potential that is required to meet a certain set of performance specifications. For reactors as a whole, the required deNOx, inlet NOx, allowable ammonia slip, and distributions in NH₃/NOx, flow, and temperature will all affect the minimum potential for the application. Minimum potential is determined using SCR models which take these factors into account. Minimum potential is a fundamental parameter used in catalyst management and will be discussed in more detail in the “Catalyst Management” chapter. Minimum potential typically refers to the minimum required potential for the reactor as a whole. However, during catalyst management efforts, a minimum potential required for specific layers may be determined for catalyst specification purposes.

Fundamental Equations: Actual potential including plugging

Actual versus Theoretical DeNOx Potential – Effect of Channel Plugging

The potential calculations described above are based on laboratory-measured K-values, and do not include the effect of plugging, since the K-values represent clean catalyst values. In practice, when catalyst channels become plugged, the AV for the layer increases since the geometric surface area available for reaction is reduced. The actual potential, which includes the effects of plugging, can be calculated according to the following equation. This actual potential represents the actual deNOx capability of the catalyst as it present in the field reactor.

$$P_{\text{actual}} = P * (1-\% \text{Plugging})$$

Where; P = potential calculated using laboratory K-values
%Plugging = plugging for the layer expressed as fraction

Minimum DeNOx Potential (Pmin)

This represents the minimum deNOx potential that must be maintained in the reactor to accomplish the required deNOx, within slip limits.

- Must be determined using an SCR model.
- Inputs include inlet NOx, deNOx, slip
- Inputs also include assumed distributions for NH₃/NOx, flow, and temperature



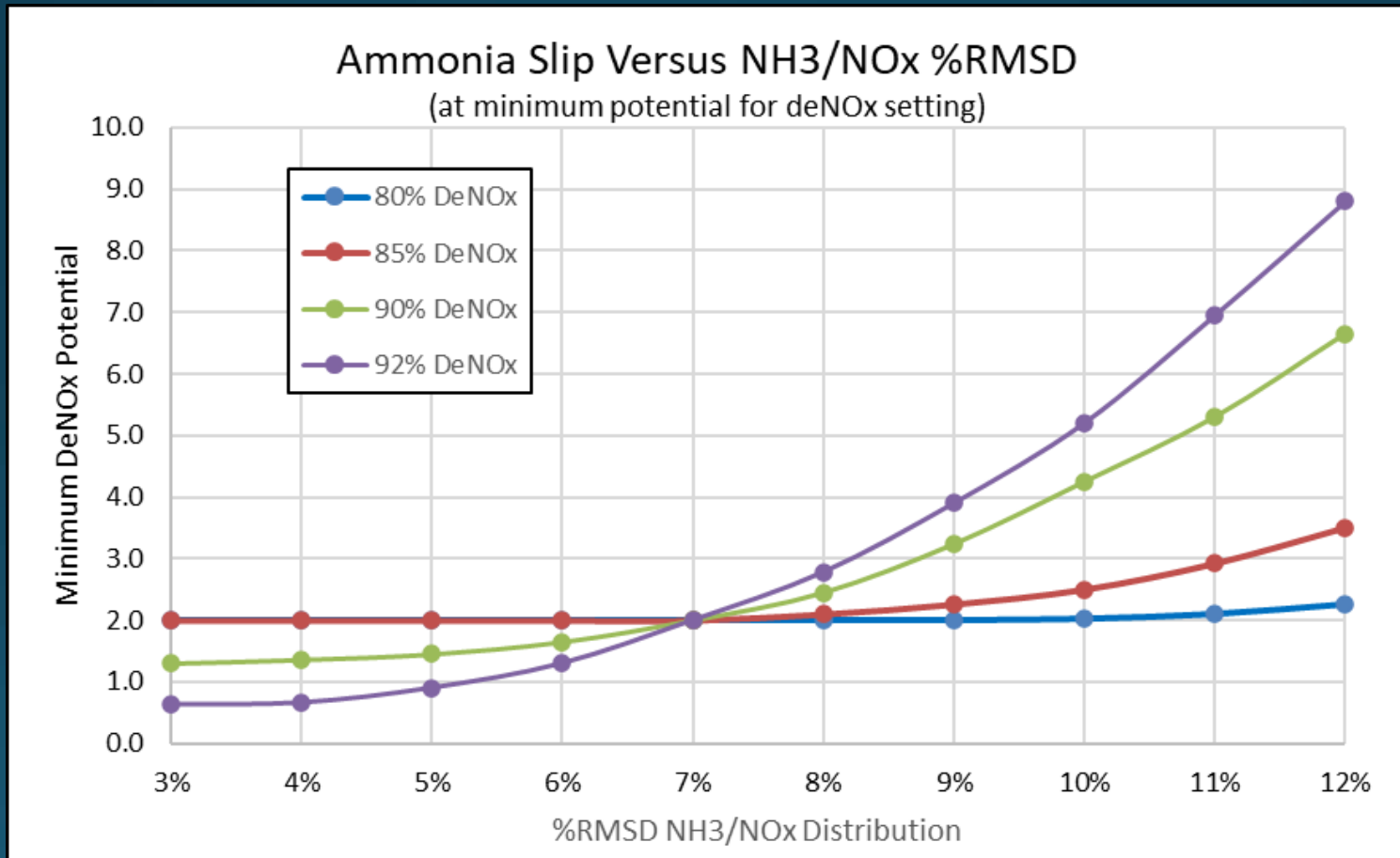
Pmin cannot be calculated using the laboratory equation for K.



$$K = -AV \cdot \ln(1 - \%deNOx)$$

Example Effect of NH₃/NO_x Distribution on Minimum Potential

(350 ppm inlet NO_x, 2 ppm NH₃ slip)



CATALYST MANAGEMENT

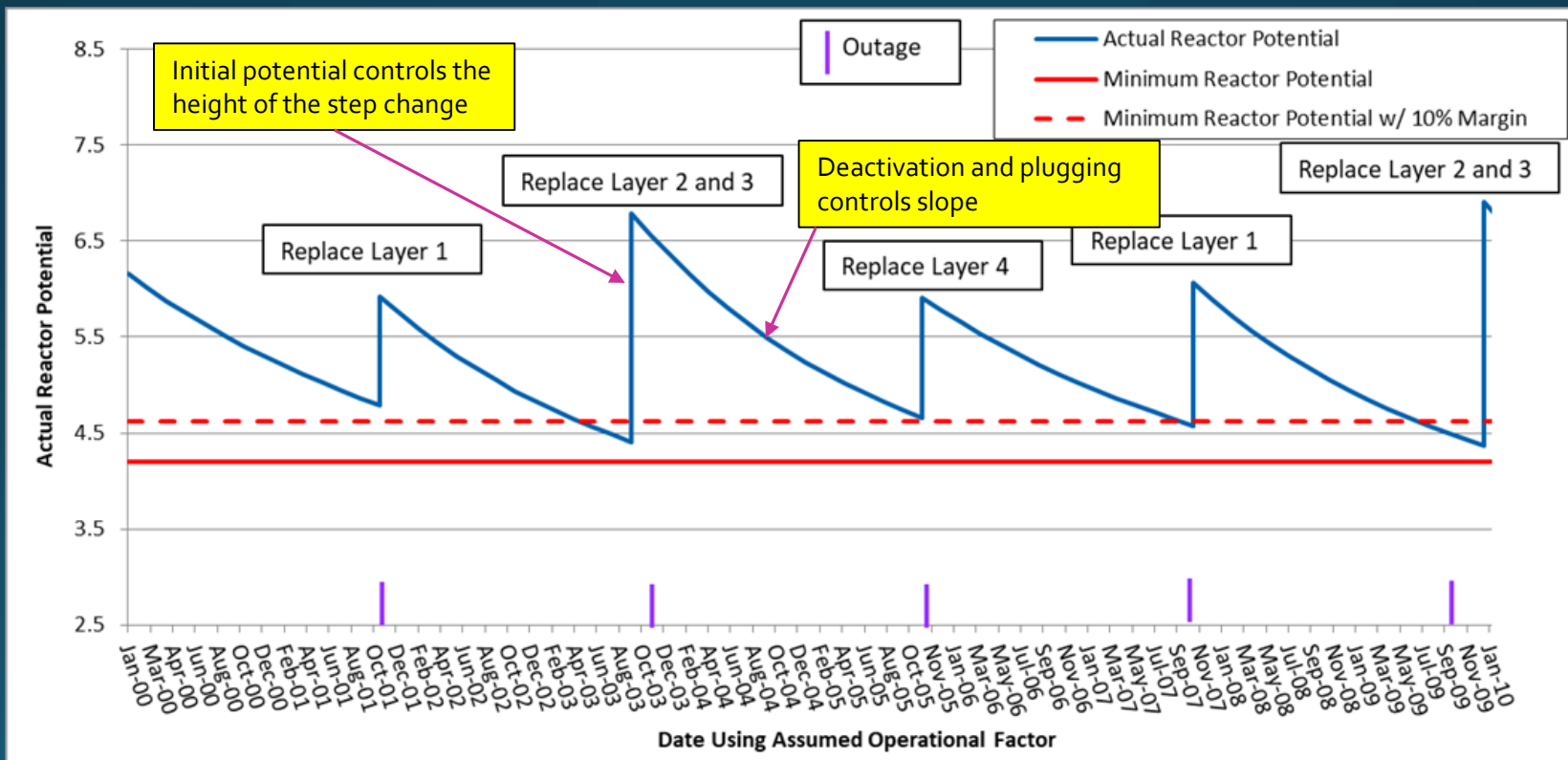
THE BIG 3

1. Initial Potential
2. Deactivation
3. Plugging

CATALYST MANAGEMENT PLANS

Blue Line: Represents actual reactor potential as a function of time. This line depends on the catalyst initial potential (volume, specific surface area, and activity), and declines as a function of deactivation and plugging.

Red Line: Represents minimum potential required for the system, which is a function of inlet NO_x, outlet NO_x (deNO_x), and distributions of NH₃/NO_x, flow, and temperature (typically as %RMS).



Initial Potential

$$P_0 = \frac{K_0 * SSA * V_{cat}}{F}$$

$$P_0 = \text{initial (or fresh) deNOx potential} = \frac{K_0}{AV}$$

$$AV = \text{Area Velocity (m/hr)} = \frac{F}{SSA * V}$$

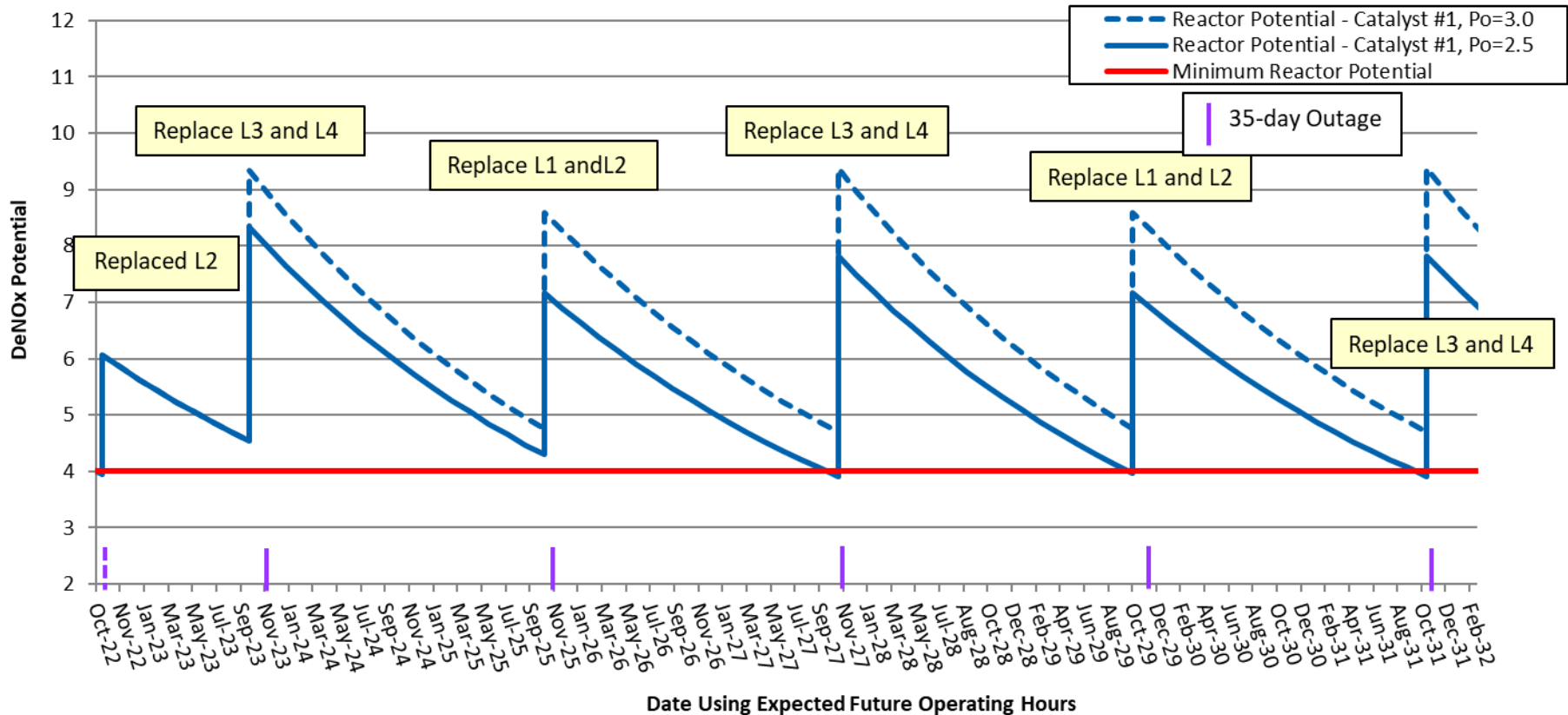
Where: F = flue gas flow rate (m³/hr at 0 °C, actual O₂ and moisture)
 SSA = catalyst specific surface area of layer (m²/m³)
 V = catalyst volume of layer (m³)

Example Catalyst Offering Comparison Table

Supplier							
Offering	Base	Option 1	Option 2	Option 3	Option 4	Option 5	Option 6
Catalyst							
Length (mm)	1,000	1,000	1,000	1,060	1,060	1,060	1,060
Pitch (mm)	7	5.7	5.7	7	5.7	5.7	7
SSA (m ² /m ³)							
Number of RXRs							
Cat. Vol. Per RXR (m ³)							
Total Cat. Vol. (m ³)							
Total SA (m ²)							
Ko (m/hr)							
SO2 Conversion (%)							
Hg Conv.(%)							
Life Guarantee (hrs)	24,000	24,000	24,000	24,000	24,000	24,000	24,000
AV	20.8	17.0	17.0	19.6	16.1	16.1	19.6
Total Po	2.31	2.87	2.64	2.39	2.98	2.74	2.24

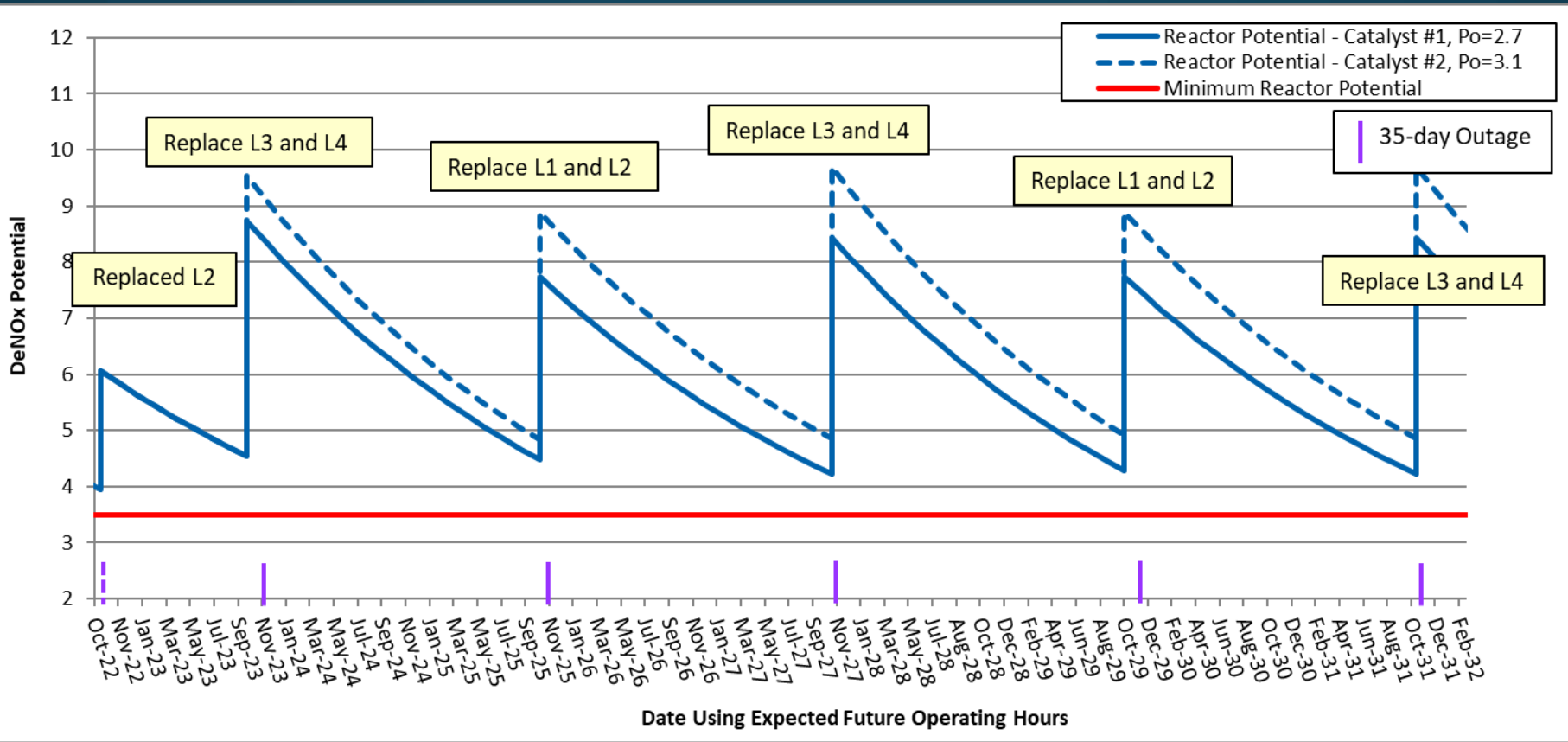
Example Catalyst Management Plan Comparing Two Catalysts

In this case, catalyst selection is very important in generating margin.



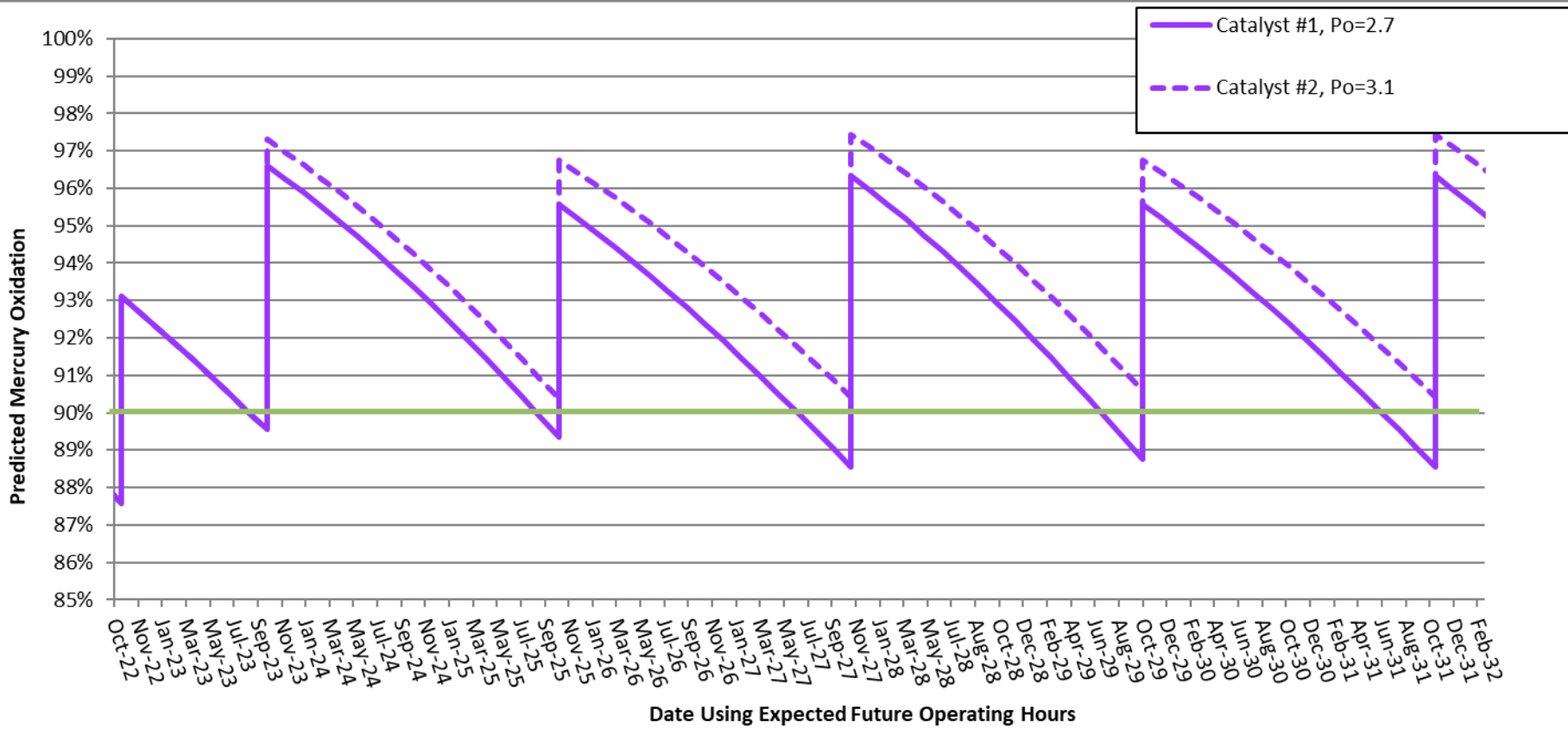
Example Catalyst Management Plan Comparing Two Catalysts

In this case, there is plenty of margin with both catalysts, thus more freedom for selection.



Mercury oxidation prediction for previous example.

In this case, if 90% mercury oxidation is the target, then mercury oxidation trumps deNOx potential, and which then influences selection.

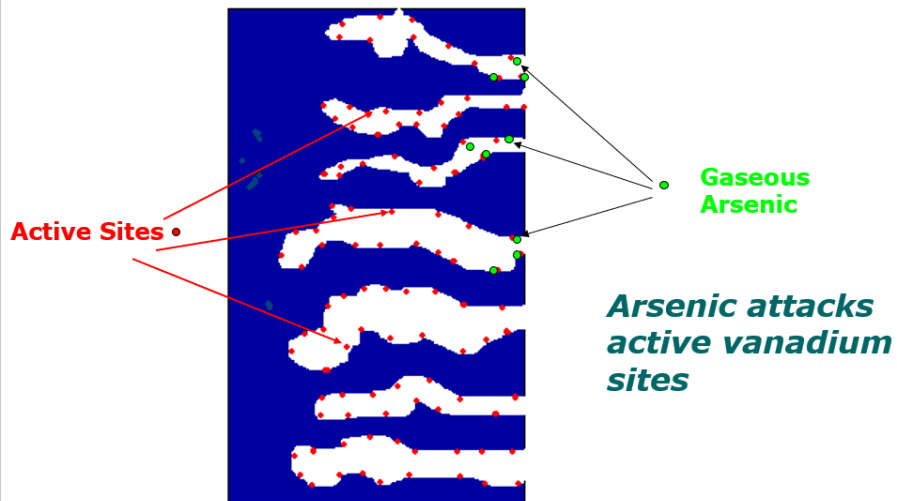


Deactivation

Two primary types

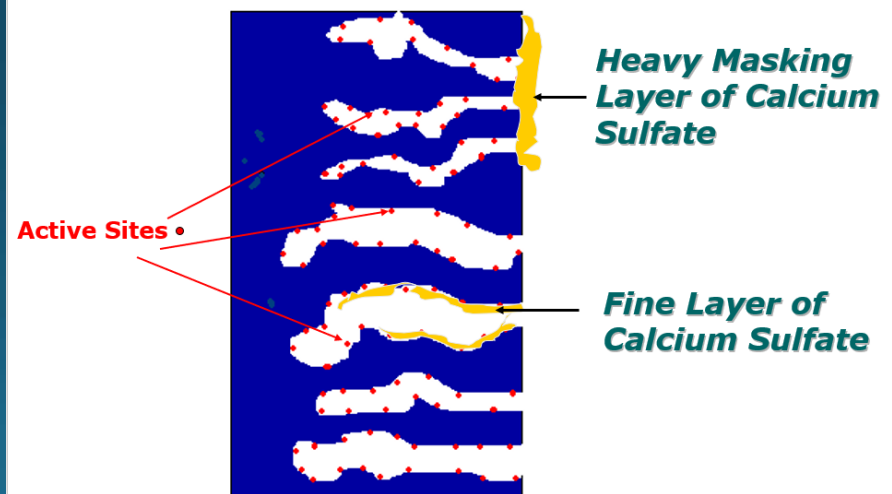
Arsenic Poisoning

Generally associated with Eastern Bituminous Fuels. Chemical poisoning where arsenic binds with vanadium active sites, rendering them incapable of catalyzing the deNO_x reaction.



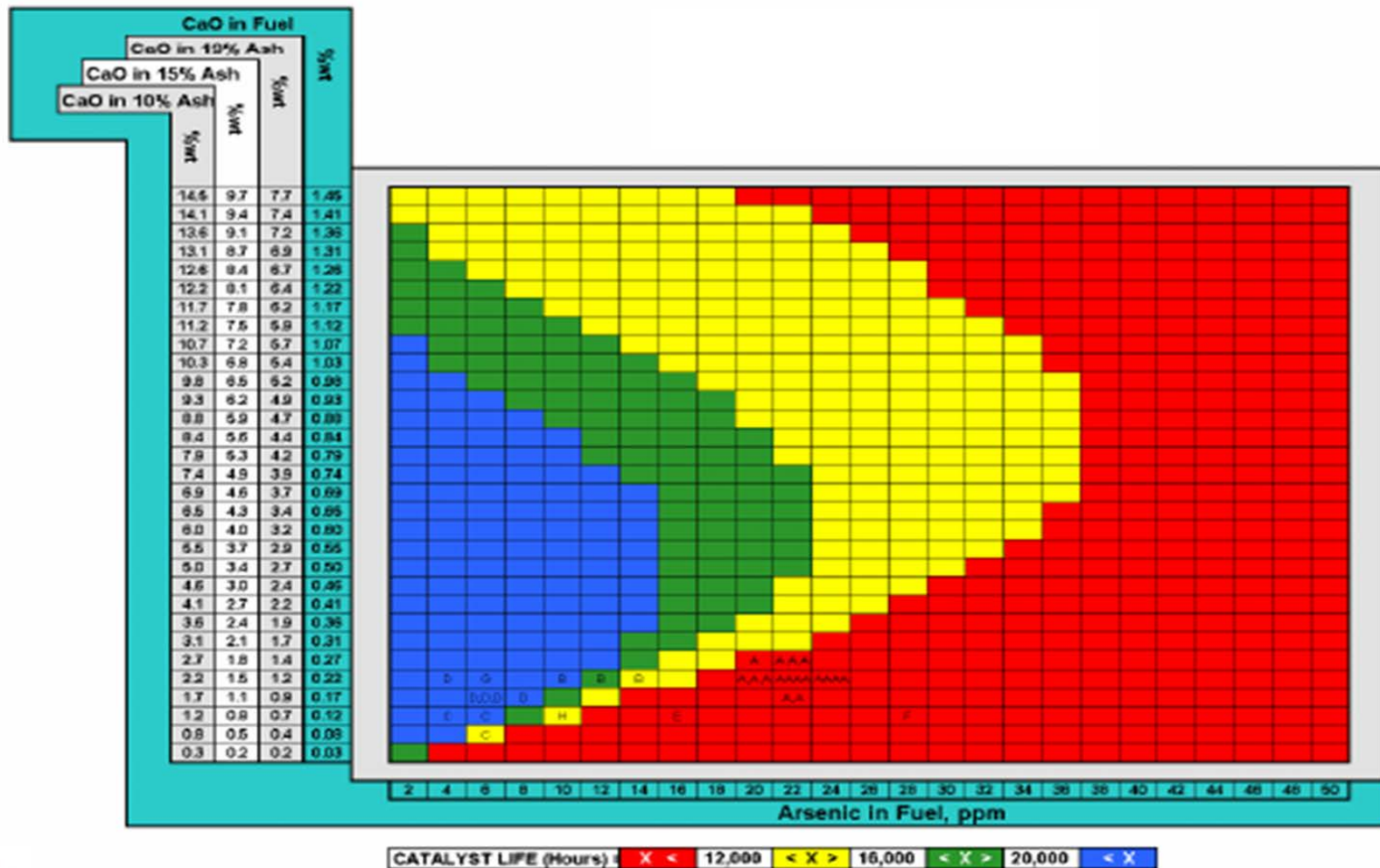
Calcium Sulfate Masking

Often called “PRB” poisoning, associated with high-calcium fuels, where calcium and calcium compounds (calcium sulfate) mask or “blind” surfaces preventing reactants from reaching the active sites.

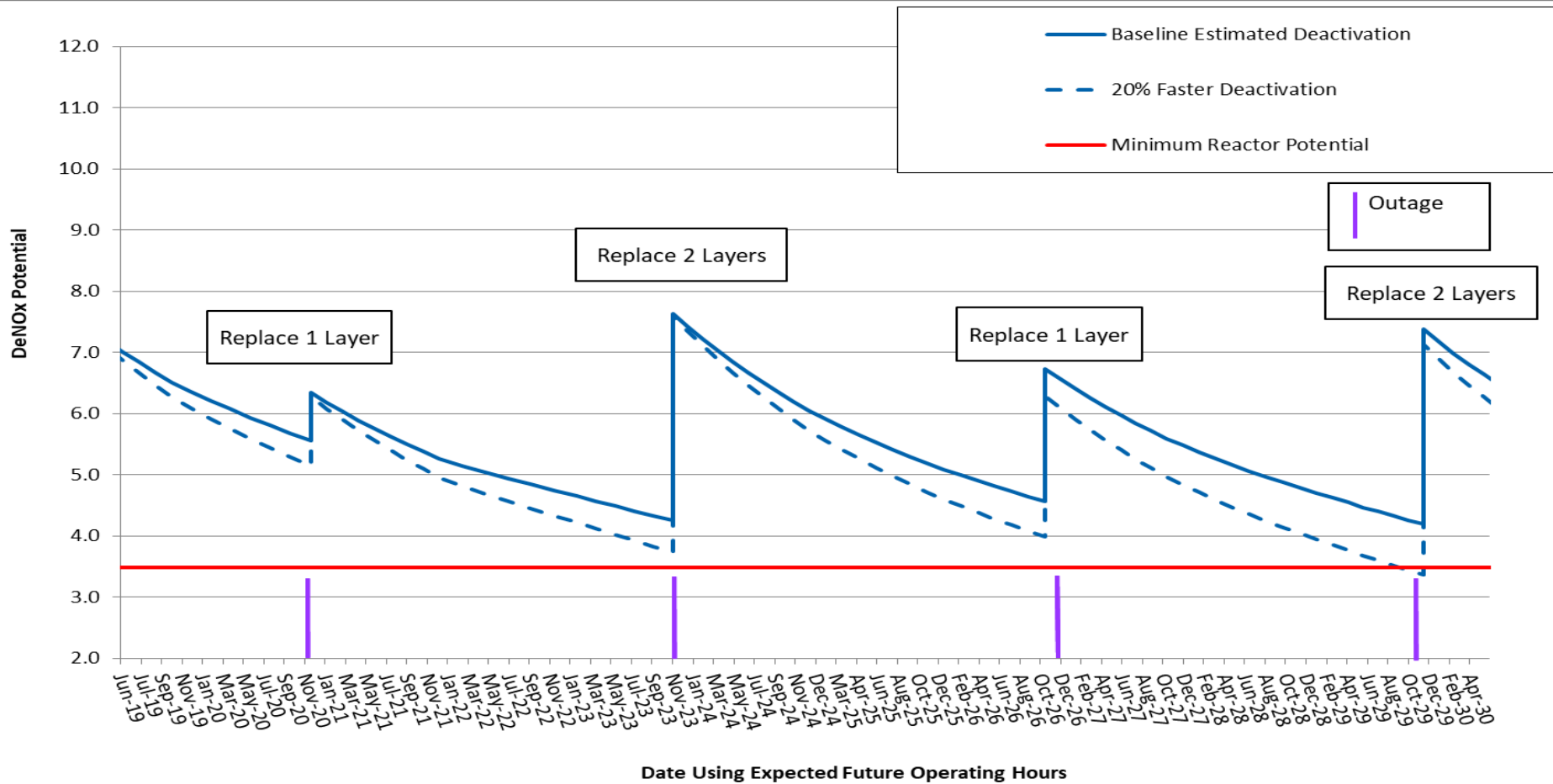


Arsenic Poisoning: Interrelationship between calcium and arsenic in coal

Moderate levels of calcium can help to mitigate arsenic poisoning. This is the underlying phenomenon for limestone addition for arsenic mitigation.



Example effect of accelerated deactivation (20%) - *sensitivity analysis*



Plugging

Plugging is the parameter for which operations have the greatest control.

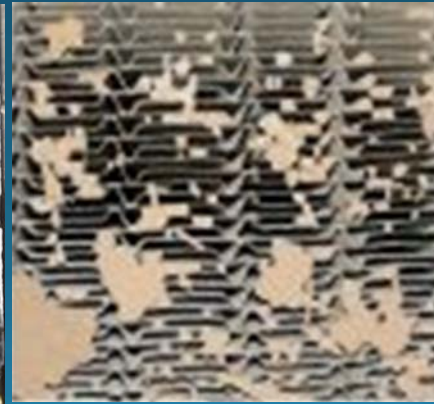
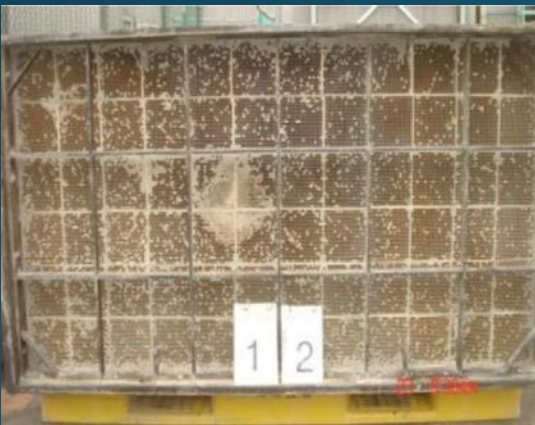
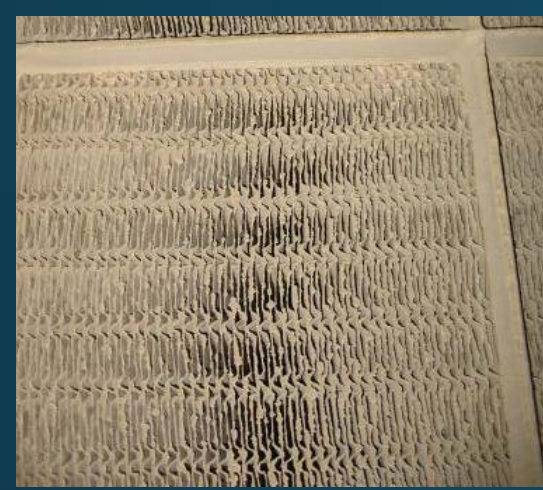
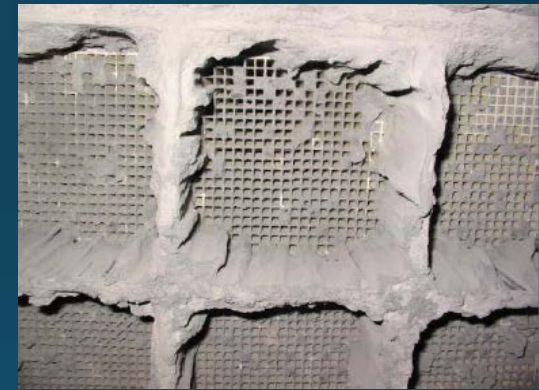
Plugging is a function of:

- Fuel, combustion, milling, etc.
- SCR and ductwork design (flow and particulate distributions, etc.)
- Sootblowing/cleaning design and maintenance
- Catalyst Design

Many issues manifest as catalyst plugging. The type/nature of plugging indicates the appropriate solution.

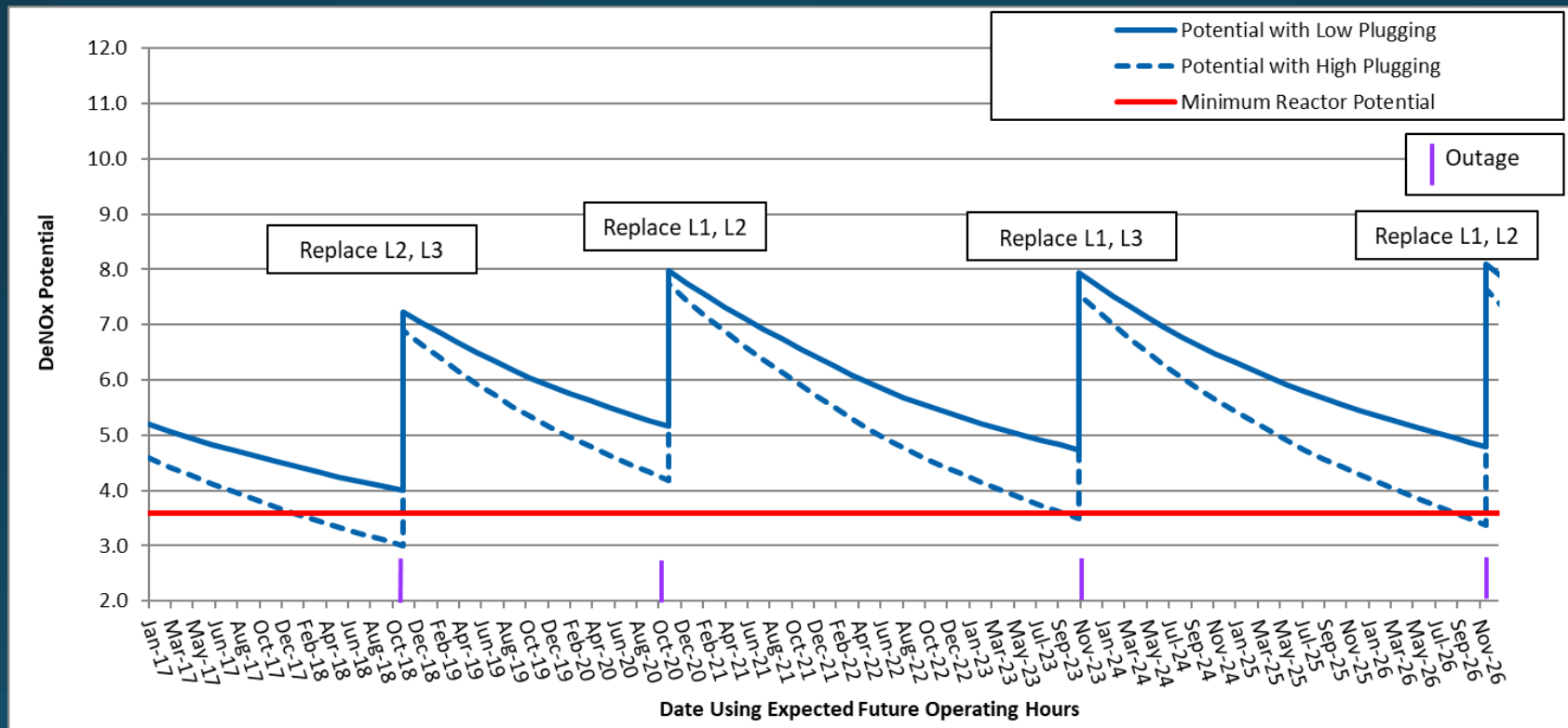
Too often the catalyst design is the entire focus, when in reality other issues are at the root of the problem

A correct "diagnosis" is key to finding the right "medicine."



Example Effect of Plugging Rate

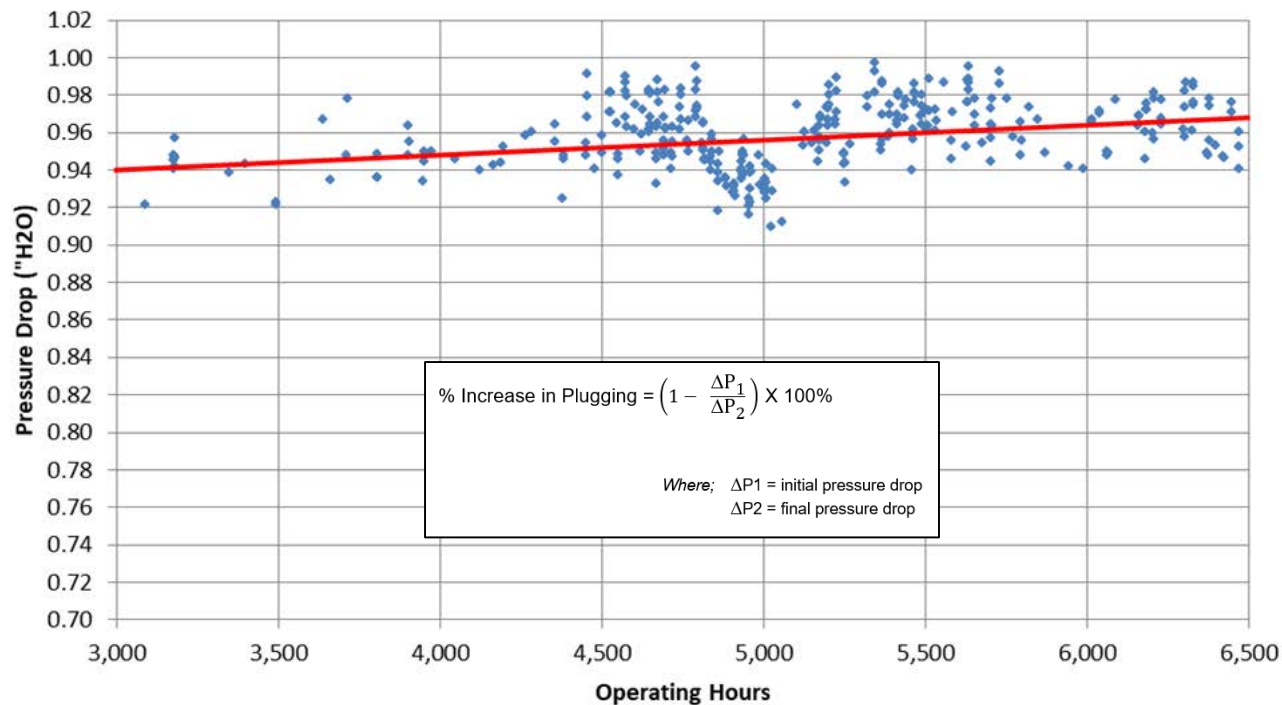
Important parameter for catalyst management purposes, usually expressed as %pugging/8K hrs, etc.



Estimating Plugging

1.) Physical Inspections

2.) Pressure Drop Tracking



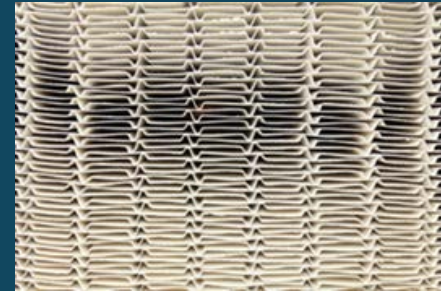
Honorable Mention: EROSION



SCR CATALYST TYPES AND DESIGNS

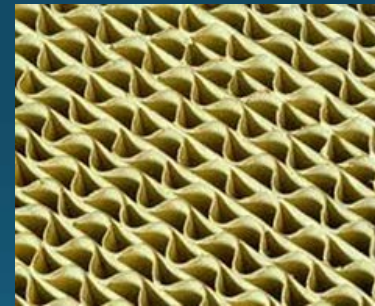
Plate

Mitsubishi Power Systems Americas, Inc. (MPSA)
CERAM USA, Inc.
Others



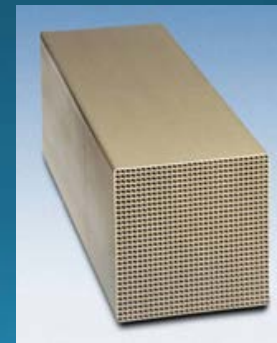
Corrugated/Hybrid

Umicore Catalyst USA, LLC

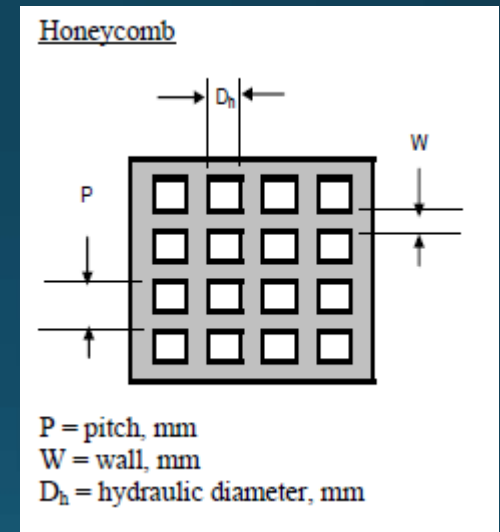
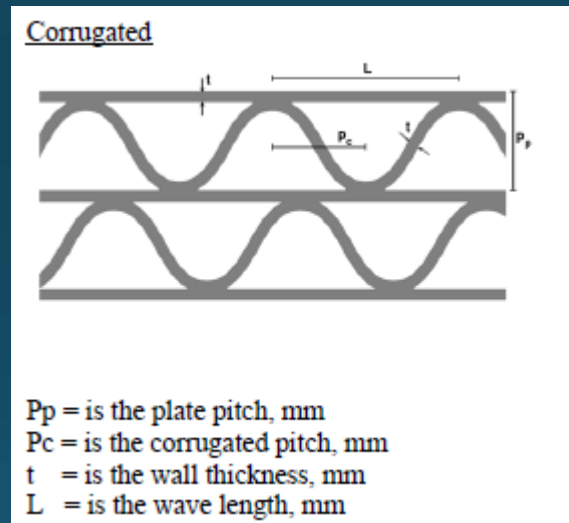
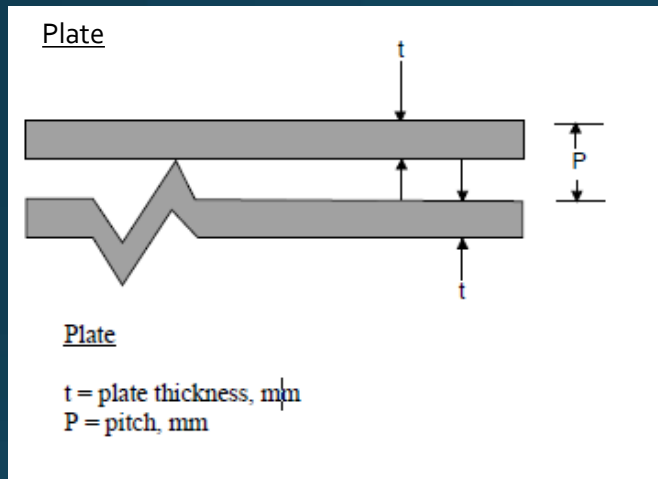


Honeycomb

Cormetech, Inc.
CERAM USA, Inc.



Pitch Definitions



EXCELLENT RESOURCE - EPRI.com

[Laboratory Testing Protocol for Coal-Fired SCR Catalyst: 3rd Edition](#)
 SO₂ conversion Test protocol v ... 2 See "Protocol for Laboratory Testing of
 SCR Catalyst: 2nd Edition, EPRI, Palo Alto CA, December 21, ... Prior
 editions of this protocol were also utilized.

Product ID:3002013048 Pages:132 Published: November 15, 2018 Type:
 Technical ResultsLevel:Membership

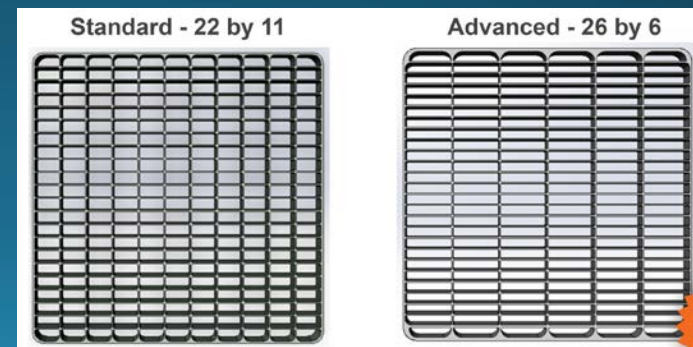


Plate Catalysts (MPSA, CERAM)

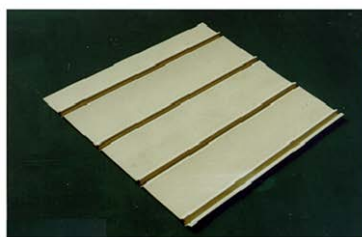
Distinguished by separate plates which are "stacked" to form a box/block. Roughly 60-90 plates per box/block depending on pitch.

Samples by removing pairs of plates from various locations.

For 4-notch plates (5.7 pitch) need 14 plates, or 16 if XRF included.

For 3-notch plates (~7.4 pitch) need 12 plates, or 14 if XRF included.

Sample 16 plates to cover all bases.



CATALYST ELEMENT/PLATE



CATALYST UNIT



CATALYST MODULE
(AS IMPORTED)



Laboratory Sample

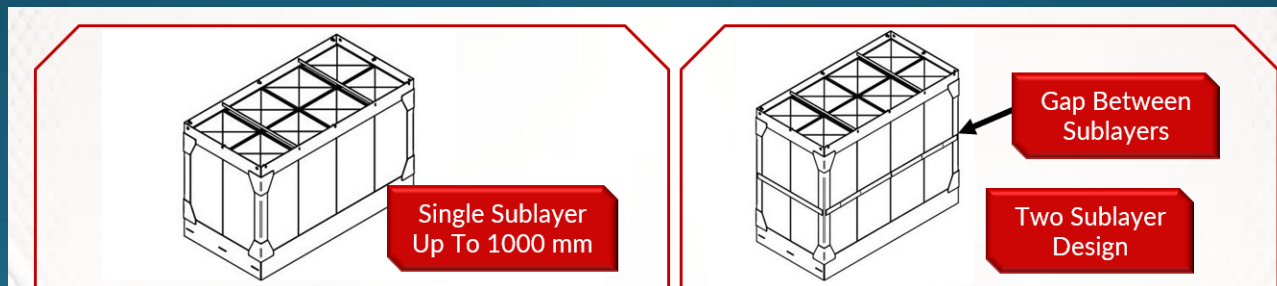
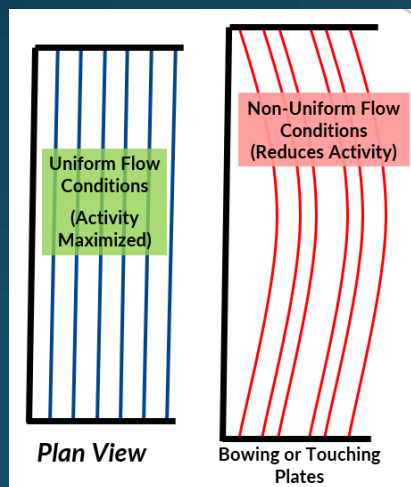
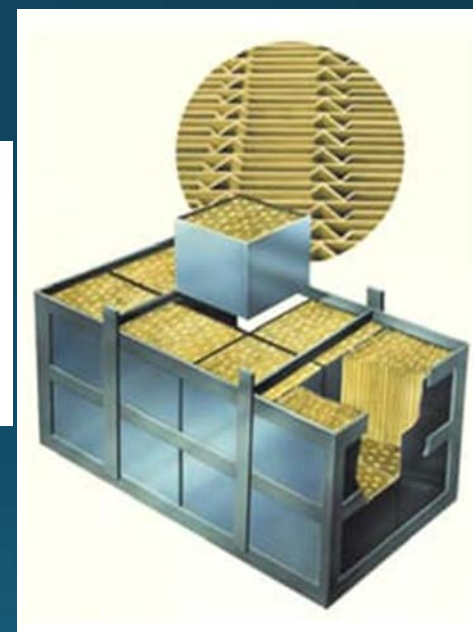
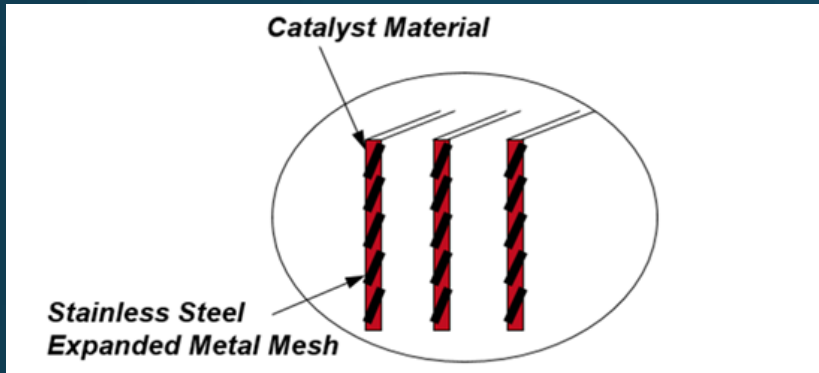


Plate catalyst are supported on expanded metal screen.



Hybrid/Corrugated Catalysts (Umicore)

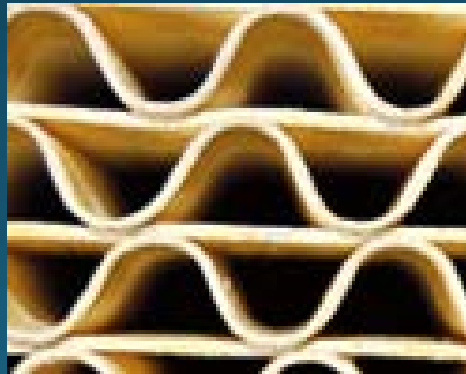
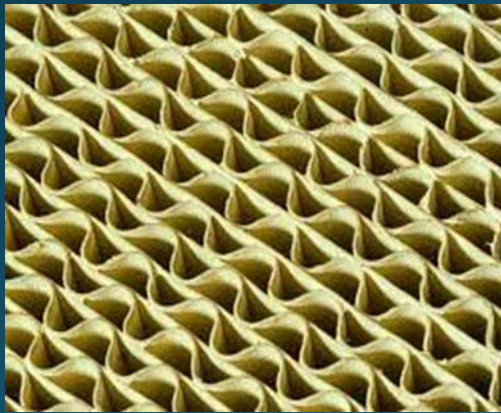
Has properties common to both plate and honeycomb catalysts.

Manufactured using separate plates/layers, but final product is a monolith, with “plates” that are bonded.

“Fiber reinforced” construction where catalytic material is bonded onto non-woven fibrous “mat”. Considered homogenous in that fibers and catalyst are distributed evenly throughout.

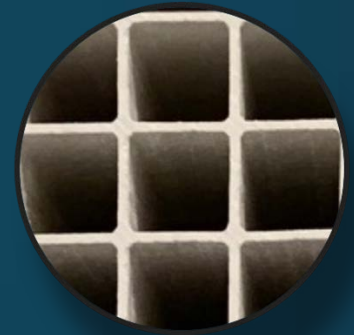
Modules/blocks similar to plate, with two sub-layers often used.

Sampled using pre-fab sample section, similar in size to honeycomb element, can be cored.



Honeycomb Catalysts (Cormetech, CERAM)

Extruded manufacture, considered “homogeneous” because the catalytic material is constant throughout the cross section of each wall.



Comprised of individual extruded “elements” of roughly 6”x6” cross-section, giving typical 6x12 element arrangement in module.

Sampled by removing entire elements of full length, usually facilitated by sleeved, easily removable, sample elements.



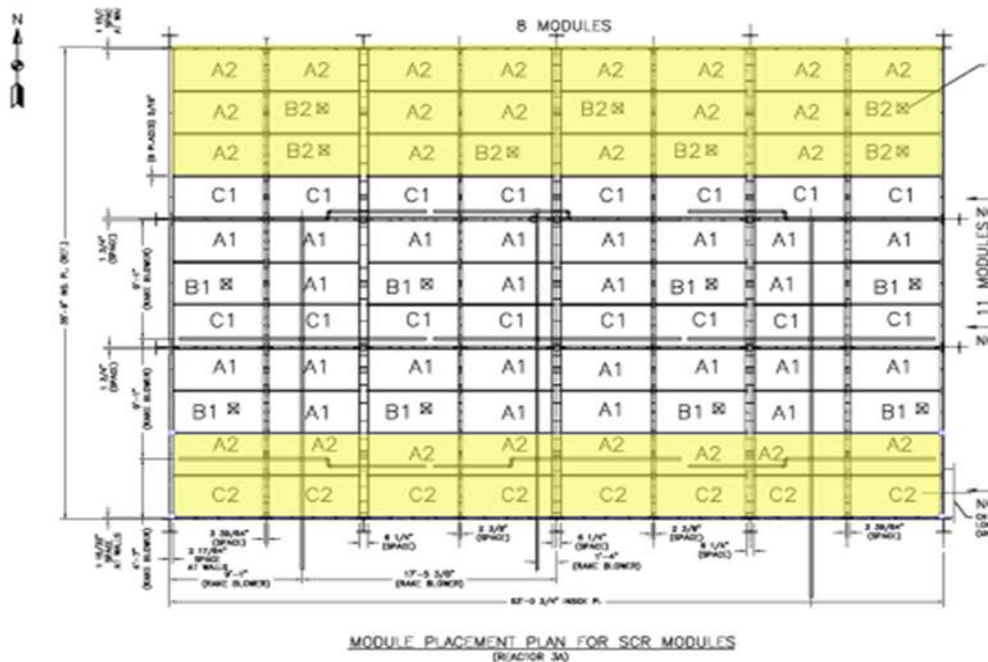
Hybrid Configurations

Involves matching the catalyst design to differing areas in the reactor with respect to plugging, velocities, etc.

Most experience with Dustbuster combined with traditional honeycomb, but potentially applicable to all catalyst types



Hybrid Arrangement



- **Yellow highlighted rows**
 - Areas identified with heaviest plugging during Fall 2021 inspection
 - Installed 26X6 DustBuster™ in Spring 2022
- **Non-highlighted rows**
 - Installed regenerated 8.2 mm pitch standard honeycomb in Spring 2022
- **All modules installed with CatFlow™ module screens**

MISCELLANEOUS THOUGHTS

- Ozone season operation – SCR by-pass
- SCR on oil/gas units
- NOx credits/overcompliance
- OEM/EPC design is not necessarily the best long-term design.

Questions?