

# **SOUR GAS TREATING BREAKTHROUGH: UNIQUE MEDIA CONVERTS HYDROGEN SULFIDE TO RECOVERABLE SULFUR THROUGH NOVEL PROCESS CHEMISTRY**

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## **ABSTRACT**

A new and innovative process for quantitative removal of H<sub>2</sub>S from hydrocarbon vapor streams has been developed, patented, and is referred to as VOx by Vapor Point, LLC and its subsidiary, Strategic Materials Intellectual Technologies, LLC.

VOx is an activated lignite carbon-based product formulated through the incorporation of a novel oxo-inverse coordination iron complex to specific sites on the activated carbon media's conductive graphitic surface. The incorporation is accomplished such that the graphitic surface effectively becomes a ligand for one of the complex's three oxo-iron sites and related molecular orbitals.

The combination of the incorporated oxo-inverse coordination iron (III) complex's molecular orbitals and the conductive property of the graphitic lignite yield the novel electron density transfer pathway linking the oxo-inverse coordination iron (III) acetate complex ligand sites and the conductive graphitic pore surface. The incorporated oxo-inverse coordination iron (III) complex's hybridized orbital structure allows vapor-phase H<sub>2</sub>S to become a ligand to a non-surface bound oxo-iron of the complex thereby linking it to the conductive surface graphitic structure. The chemistry of this innovative product allows electrons from the H<sub>2</sub>S ligand to transfer through the oxo-inverse coordination hybridized molecular orbitals to a grounded graphitic electron sink yielding recoverable elemental sulfur. After H<sub>2</sub>S exposure, the base VOx material is reclassified to VOx-Sour, which contains sulfur as a ligand to the oxo-Fe site (in the form of a stable sulfur chain) as well as accumulated recoverable elemental sulfur. The overall reaction mechanism can be presented as  $[H_2S + VOx \rightarrow S_8 + H_2]$ . The underlying VOx chemistry does not require oxidants or chemical reagents and allows for total CO<sub>2</sub>-slip.

The paper will discuss the formulation and process chemistry of the VOx conversion of vapor-phase H<sub>2</sub>S to solid recoverable elemental sulfur compared to competitive technology. The product's capabilities have been validated for a range of real-world process conditions and applications for gas-phase treating utilizing a pilot test system. Predicted performance based on testing data from a variety of process conditions will be discussed.

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## **Introduction**

Hydrogen sulfide (H<sub>2</sub>S) control in vapor streams is commonly addressed with aqueous amine gas removal systems, liquid redox systems, fixed-bed systems, catalytic carbons, membranes, biological oxidation, or Claus/TGTU trains. Despite decades of optimization, these technologies impose costs and hazards: large footprints and CapEx/OpEx; oxidant handling and SO<sub>x</sub>-bearing side chemistry in two-stage redox systems; heat release and sulfate/thiosulfate risks during metal oxide use; strict cradle-to-grave practices for non-regenerative chemistries; permitting constraints when flaring off-spec gas; and the challenge of achieving consistent H<sub>2</sub>S treat below 1 ppm.<sup>1,2</sup>

VO<sub>x</sub> is a process medium that converts vapor-phase H<sub>2</sub>S to recoverable elemental sulfur to below detection limits (<1 ppm) in a purely vapor environment. The VO<sub>x</sub> chemistry requires no aqueous chemistries or oxidative reagents and allows for total CO<sub>2</sub>-slip: at a surface-incorporated oxo-inverse coordination iron (III) complex, H<sub>2</sub>S ligates and undergoes two-electron oxidation to neutral sulfur (S<sup>0</sup>) with electron density transferred into the conductive graphitic lattice. The oxo-Fe center remains Fe (III), and the carbon's redox potential disfavors back-reduction at the oxo-Fe site (in this instance and throughout the document, oxo-Fe refers to an iron atom of the oxo-inverse coordination complex bound to the μ<sub>3</sub>-O core of the complex). Consequently, sulfur oxidation states above S<sup>0</sup> are not within the oxidation potential of the VO<sub>x</sub> product and therefore SO<sub>2</sub>/SO<sub>3</sub> formation has not been observed in testing.

In this paper, VO<sub>x</sub> refers to the as-manufactured material prior to H<sub>2</sub>S exposure. After contact with H<sub>2</sub>S, when the bed contains both recoverable elemental sulfur (S<sub>8</sub>) and a bound sulfur ligand chain at the active oxo-Fe site, we refer to the material as VO<sub>x</sub>-Sour. This distinction clarifies reuse without an oxidant-based regeneration step and enables a separate post-exposure SDS and handling protocol, including cases where on-site solvent CIP (clean-in-place) cannot be performed and material must be transported offsite to remove accumulated sulfur and foulant carryover.

Operationally, H<sub>2</sub>S slip can impose disproportionate risk, cost, or emissions. VO<sub>x</sub> is optimally suited for vapor-phase streams at ≤500 ppm H<sub>2</sub>S with integrated deep polish to meet specification. For vapor-phase streams with H<sub>2</sub>S levels ≥500 ppm, the product can be utilized by varying the oxo-inverse coordination complex loading or utilizing product already exposed to H<sub>2</sub>S containing a sulfur chain referred to as VO<sub>x</sub>-Sour. Additionally, a lead/lag-bed configuration with scheduled solvent washes can be considered to remove accumulated elemental sulfur if the rate of formation blinds off the carbon pore surface and prevents diffusion of H<sub>2</sub>S to the oxo-inverse coordination complex. Examples at the ≤500 ppm H<sub>2</sub>S level include primary removal and polish downstream of amine gas treating (AGRU) when slip pushes H<sub>2</sub>S above spec; flare-avoidance service during

temporary exceedances; LNG feed-gas service before liquefaction to keep H<sub>2</sub>S below detectable levels (<1 ppm) into cryogenics; and final spec-trim at custody-transfer/pipeline points.

This paper presents: the design logic and synthesis of VO<sub>x</sub> from its two starting materials, scalability, the mechanism for oxidizing H<sub>2</sub>S to recoverable elemental sulfur without an oxidant or chemical reagents, current testing and experimental methods, comparative context versus ferric(hydr)oxide (i.e. Iron Sponge) beds, and operational and field-deployment considerations.

## VO<sub>x</sub> Design Logic

The underlying chemistry of VO<sub>x</sub> design utilizes a member of the family of transition metal complexes with a “reverse topology” as the metal is not the center of coordination or molecular orbital structure but has a more electro-negative atom as its coordination center (Figure 1, A).<sup>3</sup> In this structure, the μ<sub>3</sub>-oxo core is linked to three iron atoms, forming an [Fe<sub>3</sub>(μ<sub>3</sub>-O)] framework stabilized by acetate bridging ligands. The hybridized molecular orbitals of the framework delocalize electron density across the three iron centers, allowing the terminal orbitals of each Fe to communicate (Figure 1, B). Building on reports that similar oxo-inverse coordination complexes can accept electron density into these hybridized orbitals without decomposing, the design rationale was: if a material had ligand sites that the oxo-Fe site can bind to and function as an electron sink, then oxidation occurring at another oxo-Fe can transfer electrons through the [Fe<sub>3</sub>(μ<sub>3</sub>-O)] framework into that sink resulting in an oxidation reaction without the use of a oxidant.

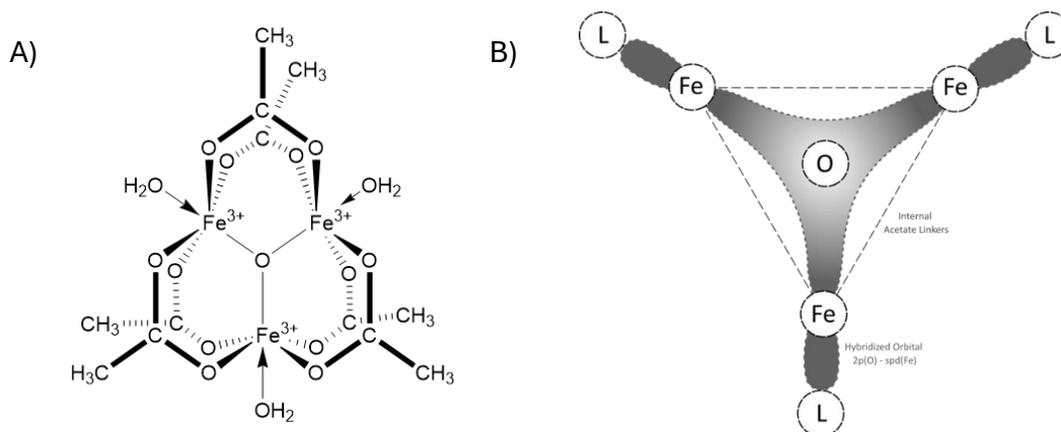


Figure 1 – (A) Oxo-inverse coordination basic iron (III) acetate inverse complex; (B) Illustrative representation of the metal-oxo-metal hybridized orbitals of [Fe<sub>3</sub>(μ<sub>3</sub>-O)] framework and neutral terminal ligands “L”

To provide true ligand character, the material must present appropriate surface olefinic structures that the oxo-Fe site can bind to. The VO<sub>x</sub> development team has intensive knowledge of activated carbon and is well-versed in the ability of activated carbon to act as a potential electron-sink ligand due to intrinsic conductive properties.<sup>4</sup> Moreover, certain activated carbon production processes yield surfaces containing embedded olefinic defects that can function as ligands for the oxo-Fe site.<sup>5</sup> Conventional two-step activation (pyrolysis followed by high-temperature chemical activation) tends to minimize defects, producing pristine graphene-like surfaces (Figure 2, A). In contrast, single-step, syngas production processes that yield activated lignite containing a conductive graphitic network that retains a higher population of suitable embedded olefinic binding sites (Figure 2, B). For example, a known binding site would be a cyclopentadiene-like

structure, analogous to known ferrocene-type complex bonds, which provides the necessary electron pathway.<sup>6</sup> Aligning the complex's terminal oxo-Fe ligand orbital with these embedded olefinic defects creates a hybridized orbital between the oxo-Fe and the graphitic surface, bridged by the  $[\text{Fe}_3(\mu_3\text{-O})]$  framework. Conceptually, the product is an oxo-inverse coordination iron (III) acetate complex incorporated into the graphitic pore surface with an established continuous inner-sphere electron transfer pathway from a terminal oxo-Fe ligand orbital to the conductive graphene content of the activated lignite.

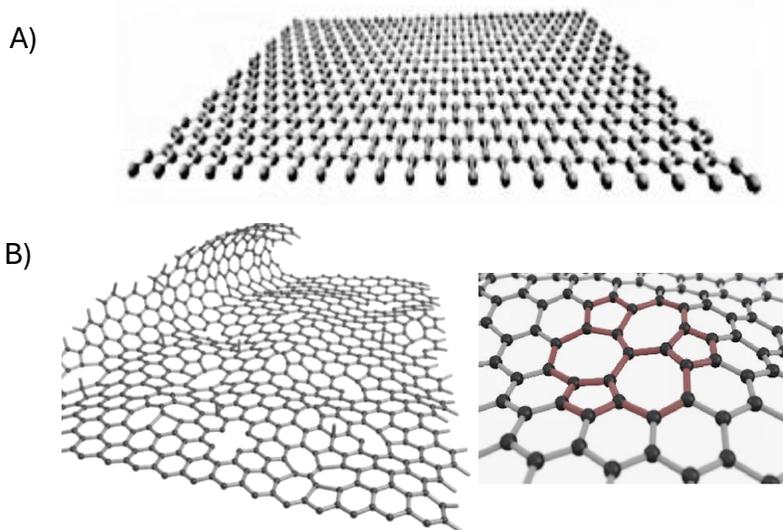


Figure 2 – Illustrative representation of graphitic surface of pristine activated carbon (A) and activation of lignite with surface defects (B)

### *Mechanistic Consequence Of Design*

When one of the oxo-inverse coordination complex's neutral Fe ligands are chemically incorporated into a graphite/graphene surface, the oxo-centered molecular orbitals provide a pathway for electron density transfer from the other complex's neutral ligands. Thus, the underlying VOx chemistry that converts sulfide ( $\text{S}^{-2}$ ) to atomic neutral sulfur ( $\text{S}^0$ ) bound as a Fe-S<sup>0</sup> ligand results from the choice of our specific  $[\text{Fe}_3(\mu_3\text{-O})]$  complex framework and the carbon surface with conductive embedded structures capable of forming ligands that incorporate the oxo-inverse complex's molecular orbitals. Once the oxo-inverse complex is incorporated to the surface, the overall structure provides an electron potential pathway for electron density to transfer from the  $\text{S}^{-2}$  ligand to the graphitic pore surface yielding an oxo-Fe-S<sup>0</sup> ligand. No oxidation or chemical reagents are required for VOx oxidation chemistry, and the conductive property of the graphitic carbon transfers the electrons from ligated sulfur oxidation to ground. Moreover, the oxidation chemistry of VOx affords total CO<sub>2</sub>-slip as CO<sub>2</sub> is unable to ligate at the oxo-Fe site.

### *Synthesis Of VOx*

VOx is formulated from two commercially available starting materials: the cationic oxo-inverse coordination iron (III) acetate complex and granular activated lignite with a sufficient density of cyclopentadiene-like sites embedded in the graphitic surface. An aqueous acidic Reagent Liquor

(RL) formulated to containing the cationic complex, represented as  $[\text{Fe}_3(\mu_3\text{-O})(\text{CH}_3\text{CO}_2)_6(\text{H}_2\text{O})_3]^+[\text{NO}_3]^-$ , is used to deliver the oxo-inverse coordination onto activated carbon pore surfaces at application-specific concentrations followed by uniform distribution using a wetting solvent such as ethanol. The bulk wetted activated lignite carbon is then subjected to a stepwise, controlled heating process configured to produce VOx in a continuous process. The heating process is designed to first remove the excess solvents and related acid anions present in the RL, then distribute and align the oxo-inverse coordination complex to the activated lignite surface at targeted reaction sites, and, as a last step, form hybridized molecular orbitals that incorporate the complex into the pore surface without its decomposition.

Although the oxo-inverse coordination complex is formally cationic in solution, surface incorporation via a cyclopentadiene-type ligand yields a novel surface-incorporated species  $[\text{Fe}_3(\mu_3\text{-O})(\text{CH}_3\text{CO}_2)_6(\text{H}_2\text{O})_2(\eta^5\text{-C}_5)]$  (Figure 3). The combination of this incorporated neutral complex and the conductive activated lignite forming the novel electron density transfer pathway linking the iron (III) complex ligand orbitals and the conductive graphitic pore surface.

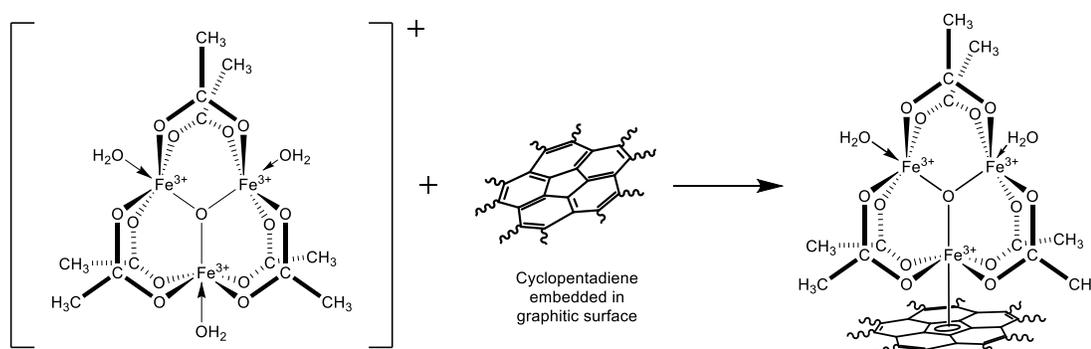


Figure 3 - Synthesis of VOx using the cationic oxo-inverse coordination basic iron (III) acetate and cyclopentadiene surface defect embedded in the graphitic surface.

Lab and pilot-plant production of VOx is validated with an in-house QA/QC program that quantifies oxo-inverse coordination complex concentration in the RL, complete incorporation of said complex to the activated lignite carbon and confirms absence of volatile RL solvents and acid anions. Routine analyses ensure batch-to-batch reproducibility and will provide traceable specifications from pilot-plant materials through the production process. We have produced lab-scale batches and operated continuous pilot-plant configurations under representative compositions and duty cycles dependent on providing expected quantities for targeted applications as discussed later in the paper. Pilot-plant production at commercial scale will be housed in a 50,000-ft<sup>2</sup> facility designed for producing up to 100 super sacks per day with integrated curing, classification, and packaging using commercially available equipment.

## Oxidation Of H<sub>2</sub>S To Recoverable Elemental Sulfur

Prior to exposure of H<sub>2</sub>S, the neutral oxo-inverse coordination iron (III) acetate complex initially has a neutral water ligand at an iron which is linked to the oxo-center, linking the oxo-Fe-OH<sub>2</sub> to the graphitic surface to a surface-incorporated oxo-Fe (Figure 4, A). Upon inelastic collision with H<sub>2</sub>S, substitution proceeds by an S<sub>n</sub>2-like mechanism: weakening of oxo-Fe-OH<sub>2</sub> and release of the water ligand via formation of an oxo-Fe-SH<sub>2</sub> ligand (Figure 4, B). This ligand exchange aligns with classical kinetics that distinguish dissociative, associative, and interchange limits and with

analogous water-exchange behavior in transition-metal complexes.  $\text{H}_2\text{S}$  is thermodynamically and kinetically favored over  $\text{H}_2\text{O}$  as the entering ligand because sulfur's lone electron pair is more polarizable, favoring oxo-Fe-S bonding.

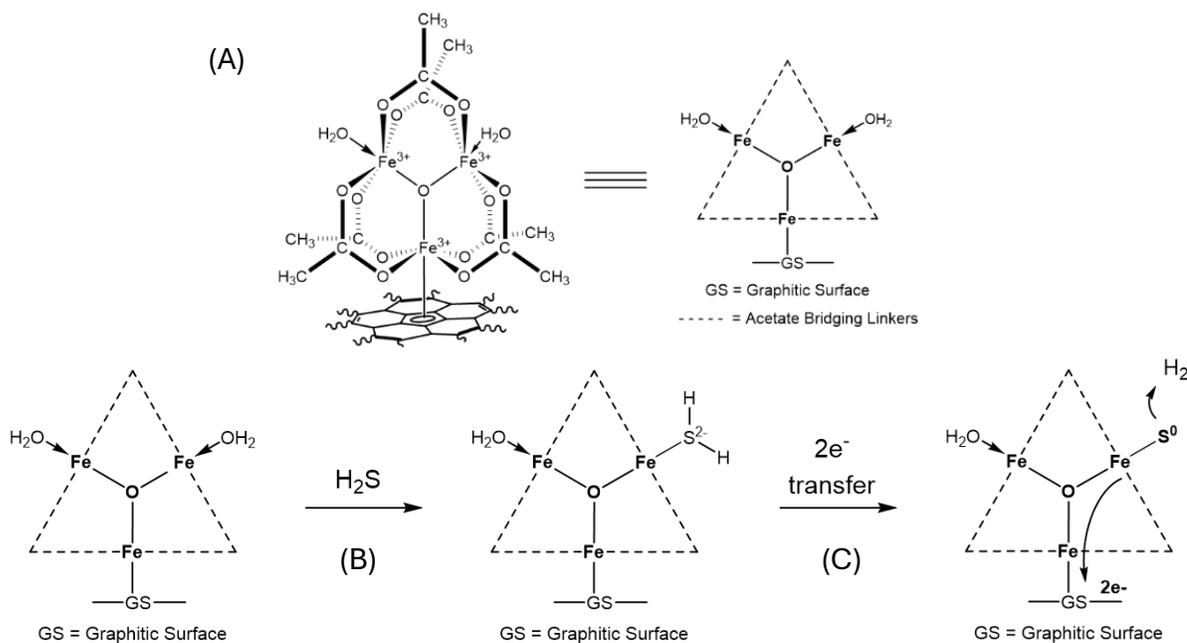


Figure 4 – (A) Simplified model of surface incorporated oxo-inverse coordination complex; (B) Water/ $\text{H}_2\text{S}$  ligand exchange followed by (C) two electron transfer forming the oxo- $\text{Fe-S}^0_{n=1}$  complex and hydrogen gas

After coordination of  $\text{H}_2\text{S}$  as a ligand, two electrons are transferred from the sulfide of the ligated  $\text{H}_2\text{S}$ , delocalized into the graphitic matrix, and generating an oxo- $\text{Fe-S}^0_{n=1}$  species with a neutral atomic sulfur ligand (Figure 4, C). Formation of this formal atomic neutral sulfur ligand on an iron (III) atom has not been reported for traditional or oxo-inverse coordination complexes. The site-level hydrogens undergo inner-sphere H-H coupling to produce hydrogen gas. Stabilization of oxo- $\text{Fe-S}^0_{n=1}$  arises from intrinsic properties of the oxo-inverse coordination complex: the terminal ligand site is filled by an electron density pair donated from the neutral atomic sulfur molecule so that the surface-incorporated oxo-inverse coordination complex does not change its formal charge. Moreover, the oxidation potential between the graphitic surface and the incorporated oxo-Fe site prevents the ligated neutral sulfur being oxidized past a neutral sulfur atom ( $\text{S}^0$ ). If the neutral complex were to undergo a similar reaction mechanism analogous to an iron oxide bed, oxo-Fe oxidation from (III) to (II) to form the iron-sulfide ( $\text{FeS}$ ,  $\text{FeS}_2$ ), the neutral complex cannot internally hold and stabilize the additional electron. This would lead to the oxo-inverse coordination complex having a negative formal charge and decomposing to iron oxide, which has never been observed during testing.

Successive  $\text{H}_2\text{S}$  oxidations at the oxo- $\text{Fe-S}^0_{n=1}$  site repeats the  $\text{H}_2\text{S}$  ligation followed by two-electron transfer and  $\text{H}_2$  evolution mechanism to extend the sulfur ligand into a growing sulfur linear chain (Figure 5, D.). All literature centered around the study of sulfur allotropes details the fundamental chemistry of larger allotropes grow via chain-growth characteristics up to the most stable cyclic  $\text{S}_8$  species.<sup>7,8</sup> The sulfur allotrope chain continues to grow to a length suitable for intramolecular disproportionation and yielding recoverable elemental sulfur ( $\text{S}_8$ ) and the very

stable oxo-Fe-S<sub>n=4</sub><sup>0</sup> ligand anchor (Figure 5, E). Through statistically reproducible experiments, established analytical techniques, and in-house methodologies to measure Fe:S molar ratio on any carbon product post H<sub>2</sub>S exposure, we confirm and validate the formation of a stable tetrasulfur ligand chain after solvent-assisted removal of formed elemental sulfur.

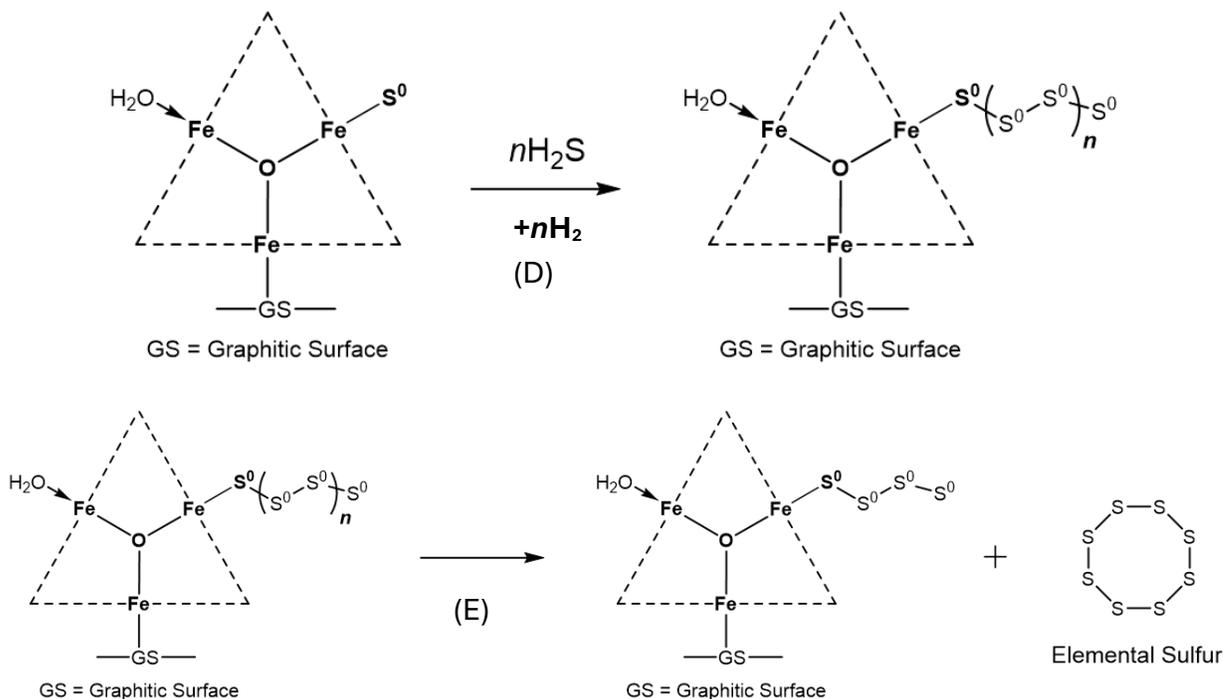


Figure 5 – Chain growth of the sulfur ligand chain from H<sub>2</sub>S ligation/oxidation reactions (D) followed by disproportionation of the growing sulfur chain to afford elemental sulfur (S<sub>8</sub>) and oxo-Fe-S<sub>n=4</sub><sup>0</sup> (E). Where  $n \geq 2$

The reaction mechanism for converting a steady feed of H<sub>2</sub>S to elemental sulfur results in formation of the oxo-Fe-S<sub>n=4</sub><sup>0</sup> sulfur ligand chain, confirming the chain-growth mechanism of sulfur allotropes building up as a ligand at the oxo-Fe site, since H<sub>2</sub>S can only react at the oxo-Fe site one molecule at a time. The sulfur tetramer ligand chain is indefinitely stable on exposure to oxygen and water and retains its ability to treat H<sub>2</sub>S unless the complex is thermally decomposed at temperatures  $\geq 270$  °F in the presence of an oxidant.

The product bearing the oxo-Fe sulfur chain ligand and residual elemental sulfur, prior and post solvent extraction, is reclassified as “VOx-Sour.” Lab and pilot-scale testing have confirmed that exposing VOx-Sour to H<sub>2</sub>S will resume the sulfur allotrope chain growth and subsequently produce recoverable elemental sulfur without a decrease in product performance compared to VOx.

### VOx/VOx-Sour Vs. Iron Sponge Beds

Building on the design logic and the reaction mechanism, this section contrasts VOx and VOx-Sour with Iron Sponge fixed beds along four practical dimensions: redox pathway, operating window and safety, waste outcome, and economics.

### *Redox Mechanism*

VOx performs conversion of sulfide to neutral sulfur ( $S^0$ ) at an oxo-Fe site where the complex oxo-Fe center maintains Fe (III), with electron density transfer into the conductive graphitic lattice. No oxidant is required, and sulfur oxidation states above  $S^0$  are not accessed. In contrast, Iron Sponge beds proceed through iron sulfide formation (e.g., FeS), reducing Fe (III) to Fe (II) during  $H_2S$  uptake;  $O_2$ -based regeneration then re-oxidizes iron and oxidizes sulfur species, generating heat, elemental sulfur, and  $SO_2/SO_3$ .

### *Operating Window and Product Handling*

Iron Sponge fixed beds exhibit a narrow humidity/oxygen window and can present pyrophoric change-out risks when the reduced dry FeS is exposed to air during handling or  $O_2$ -based regeneration. VOx broadens the operating window by eliminating oxidant streams and aqueous contacting. Both VOx and VOx-Sour are non-hazardous, non-toxic, and non-pyrophoric, and retains typical activated-carbon handling policies (conventional vessels, loading/unloading, shipment in supersacks, toxicity characteristic leaching procedure “TCLP,” etc.). VOx-Sour will be supported by a dedicated post-exposure SDS to reflect the presence of elemental sulfur and bound sulfur ligands, including cases where on-site solvent washes are not performed prior to shipment.

### *Waste Management*

Iron Sponge systems involve labor-intensive fused beds changeouts, pyrophoric iron sulfides, and  $SO_x$  during operation, regeneration, and bed changeouts requiring strict cradle-to-grave policies. Waste implications for VOx are limited to vapor-phase elemental sulfur management. VOx-Sour does not require oxidant-based regeneration after exposure to  $H_2S$ ; treating capability is restored by periodically removing accumulated  $S_8$  (e.g., solvent cleaning in place or transport off-site). After  $H_2S$  exposure, VOx-Sour is classified as activated carbon containing sulfur (non-hazardous); where any vapor-phase elemental sulfur is transported out of the bed and captured on a solid medium or in a liquid-gas scrubber, the sulfur is reclaimable and saleable, the scrubbing liquid can be reused, and the solid capture medium is disposed and classified as non-hazardous. This contrasts with iron sponge change-outs that manage FeS-bearing solids and  $O_2$ -regeneration byproducts with associated pyrophoric risk and  $SO_x$  formation.

### *Product Economics*

Typical and ideal VOx application characteristics provide for semi-continuous operation through the combination of recoverable sulfur sublimation and sulfur bed accumulation, not single use reaction pathways, as is the case with typical Iron Sponges. Capacities of Iron Sponges typically observe approximately 15% wt. capacity resulting in a one-time use and disposal, whereas VOx does not require an oxidative regeneration step to produce a “reactivated product” after solvent removal of accumulated elemental sulfur. The solvent washed product, VOx-Sour containing the oxo-Fe sulfur ligand chain and residual elemental sulfur, is immediately capable of converting  $H_2S$  to elemental sulfur. Because the iron remains Fe (III) and there is no FeS formation, no  $SO_x$  side chemistry, and no oxidant ingress, the material follows a no-decomposition pathway, only  $S_8$  accumulation, so service life is significantly longer than iron sponge beds that cycle through FeS and  $O_2$ -based regeneration. While iron Sponges are advantageous to most competitive systems

from a CapEx standpoint, they are more OpEx intensive. VOx is competitive to Iron Sponge CapEx cost considerations, including the additional CapEx required for sulfur recovery step, and OpEx cost is an order or magnitude lower for VOx. The compact, zero-oxidant configuration also reduces footprint and lifecycle cost compared to liquid loops and metal oxide beds.

## **Configuration And Handling**

Both the VOx (pre-exposure) and VOx-Sour (post-exposure) products are not hazardous, toxic, or pyrophoric and conform to typical activated carbon handling practices within plants and refineries, including conventional vessel dimensions, loading/unloading, and shipment in supersacks. VOx-Sour will carry a dedicated post-exposure SDS to account for the presence of recoverable elemental sulfur and bound sulfur ligands and material is transported offsite. After curing, testing utilizing ISO 17025/17034 certified methane/H<sub>2</sub>S blends confirm the process be capable of being configured to achieve H<sub>2</sub>S treatment below detection limits (less than 1 ppm). The product and hardware are configurable: oxo-inverse coordination complex surface incorporation and activated lignite carbon matrix are selected according to the H<sub>2</sub>S level, temperature window, and impurity profile, and VOx vessels are arranged (lead/lag, parallel trains, isothermal jackets) to align with the conversion chemistry and sulfur-capture strategy.

If fouling occurs despite the front-end maintenance system, VOx treating beds can be cleaned-in-place as post-H<sub>2</sub>S exposed VOx-Sour is stable relative to typical solvents such as toluene or alcohol. When necessary, the overall application configuration will include standard up-stream hardware systems that would manage feed stream impurities known to impact the VOx treating bed performance such as man-made chemicals.

## **Testing And Experimental Methods**

The pilot-plant testing system can simulate process conditions and expose the formulated VOx product to conditions that are representative to potential field applications. Adjustable process variables that can be investigated are inlet H<sub>2</sub>S concentration (50 to 5000 ppm), total flow (1 to 50 SLPM), temperature (60 to 180 °F; 15 to 82 °C), and pressure (ambient to 120 psi) while monitoring performance in real time (Figure 6). Pilot-plant testing rigs with contacting vessels, isothermal jackets, and mass-flow control ensure controlled residence times (10 to 120 seconds). In-line galvanic H<sub>2</sub>S analyzers at the inlet and outlet provide breakthrough curves and removal efficiencies at second-to-minute intervals. Automated data logging synchronizes gas analytics, temperature profiles, and flow to produce full material balance and run-history traceability.

Systematic bed autopsy post-run maps the mass-transfer front and correlates Fe:S molar ratios with conversion, linking kinetics to gas molecule transport into the porous activated lignite carbon. These tests provide the evidence base to translate bench and pilot results into design rules for field units. QA/QC combines microwave-assisted acid digestion and ICP-OES for total iron, ASTM D4239A for total-sulfur, and rapid liquid-phase soluble elemental sulfur extraction using a Petra liquid sulfur analyzer. This integrated verification and QA/QC framework connects real-time

treating performance with compositional analytics, ensuring that each production lot performs predictably under the targeted process conditions.



Figure 6 – Pilot-Plant Scale testing rig for simulating field process conditions with in-line Galvanic H<sub>2</sub>S analyzers

We are continuing to value-engineer the VO<sub>x</sub> formulation variables by varying oxo-inverse coordination complex loading utilizing the basic manufacturing procedure and evaluating them with respect to H<sub>2</sub>S treating levels to in potential commercial applications. Our pilot-scale test systems allow us to assess a range of H<sub>2</sub>S concentrations in the feed while monitoring H<sub>2</sub>S slip in real time with in-house analytical systems to mass balance produced elemental sulfur and characterization of VO<sub>x</sub>-Sour bed material composition.

## Operational Use Cases

This section summarizes where VO<sub>x</sub> provides the most leverage in vapor-phase service for  $\leq 500$  ppm inlets: acting as a deep H<sub>2</sub>S polish. The driver across these applications is reliable attainment of H<sub>2</sub>S below detection limits ( $< 1$  ppm) without oxidative reagent handling and with total CO<sub>2</sub>-slip. At H<sub>2</sub>S concentrations  $\geq 500$  ppm, VO<sub>x</sub> or VO<sub>x</sub>-Sour at varying oxo-inverse coordination complex loading can be assessed through testing and experimentation, which may include batch or lead/lag configurations and scheduled solvent washes for S<sub>8</sub> removal as detailed in a prior patent.<sup>9</sup>

### *AGRU Slip And Fuel-Gas Networks*

In plants with amine acid gas treating, elevate H<sub>2</sub>S in treated fuel-gas can result from transient slip during turndown, load swings, or solvent variability. In the  $\leq 500$  ppm regime, VO<sub>x</sub> functions as the polish stage: trimming to specification without changing amine circulation or regenerator severity, stabilizing heater/boiler/turbine feeds, and limiting SO<sub>2</sub> in stack gas and downstream corrosion/sulfation. As an AGRU polish stage the potential exists for the increase in throughput capacities, while lowering of OpEx associated with the liquid recirculation circuit.

### *LNG Pre-Liquefaction Polishing*

For LNG pretreatment, H<sub>2</sub>S entering the cryogenic section risks freeze-out/plugging, corrosion and equipment reliability, and product-quality deviations. VOx applied upstream of chilling provides deep polish for vapor-phase feeds ≤500 ppm, driving H<sub>2</sub>S to below detection limits (<1 ppm) at the plant boundary condition. This reduces operational sensitivity to short-duration upsets while preserving a compact equipment footprint.

### *Cryogenic NGL Recovery And Dehydration Trains*

Glycol-based and molecular-sieve dehydration units are susceptible to H<sub>2</sub>S-related freeze-out, adsorbent fouling, solvent degradation, FeS formation, foaming, and corrosion. Operating as a polish bed in the ≤500 ppm inlet range, VOx lowers H<sub>2</sub>S to concentrations below detection limits (<1 ppm), protecting cryogenic hardware and adsorbents/solvents without introducing an oxidant loop or liquid contacting.

### *Pipeline/Specification Compliance, Custody-Transfer, And Hydrogen Networks*

At custody-transfer points or pipeline spec gates, variability upstream can create intermittent non-compliance in the low ppm range. VOx serves as a final trim to the contractual limit. The same applies to sulfur-sensitive units (reformers, PSA, or membrane H<sub>2</sub> recovery), where a guard bed delivering deep polish protects process catalysts.

### *Flare Avoidance, VRUs, Tank Vents, And Compressor Seal Vents*

During upsets or maintenance conditions, streams otherwise routed to flare can carry ≤500 ppm H<sub>2</sub>S. Treating these vapor-phase streams with VOx as a final polish reduces SO<sub>2</sub> formation and visible-emission risk. Analogously, VRUs, tank vents, wastewater off-gas, and compressor-seal vents benefit from the same approach to reach concentrations below detection limits (<1 ppm) prior to discharge, incineration, or thermal oxidation.

## **Operational And Field-Deployment Considerations**

Our pilot-plant data and mechanistic understanding drive application-specific VOx system designs. Each potential application and installation will be evaluated based on our pilot-plant data. If our system is shown to be technically and cost effective, an application specific VOx configuration will be tailored to the desired application. Designs begin with a verified treating basis, then progress to vessel geometry, thermal management, and sulfur-handling selections that preserve product performance and run length. Standard pretreatment filtration manages the two predominant contaminants: free water and man-made additives such as drag reducers and surfactants using off-the-shelf units sized to the feed: knock-out pots for free liquids, coalescers for aerosols, and carbon guard beds for surface-active organics. The recommended pretreatment configurations will be based on testing data and field experience and will be custom designed to manage site specific VOx bed fouling and minimize system maintenance washes.

Our pilot plant system has been designed to facilitate understanding and evaluate differing process conditions and the subsequent capture of elemental sulfur that is transported out of the VOx treating vessel to prevent fouling and corrosion of the pipeline. This can be achieved by leveraging

the physical properties of elemental sulfur. Vapor-phase S<sub>8</sub> management is managed downstream of the reaction and can be configured from commercially available technology selected based on site utilities and constraints, including temperature controlled solid-media capture and gas-liquid contacting methods.

Where extremely low concentrations of H<sub>2</sub>S are observed (i.e., LNG polish) system configuration could allow for the sulfur capture within the VOx treating bed, eliminating the need for transport of elemental sulfur, where through solvent wash elemental sulfur is recovered, following standard facility maintenance protocols.

## Conclusion

This paper presented the design logic, generalized synthesis, reaction mechanism, comparative context, configuration/handling, testing methods, and use cases for VOx, a process stable engineered material that has been designed and tested to convert vapor-phase H<sub>2</sub>S to recoverable elemental sulfur with total CO<sub>2</sub>-slip without oxidative or chemical reagents by electron density transfer into a conductive graphitic lattice at an incorporated oxo-inverse iron (III) complex.

The design deliberately leverages an [Fe<sub>3</sub>(μ<sub>3</sub>-O)] framework with hybridized molecular orbitals and a defect-rich, conductive activated carbon surface ligand to establish a continuous inner-sphere electron density transfer pathway. The generalized synthesis, delivering the oxo-inverse coordination complex with a Reagent Liquor at application-specific concentrations and using a wetting solvent to uniformly distribute across the carbon pore surface, followed by controlled curing, produces a surface-incorporated species that maintains Fe (III) oxidation state at the oxo-Fe site during conversion of sulfide to neutral sulfur (S<sup>0</sup>).

Mechanistically, H<sub>2</sub>S ligates at oxo-Fe and undergoes a two-electron oxidation to S<sup>0</sup> with electrons conducted into the graphitic lattice; H<sub>2</sub> forms by inner-sphere hydrogen recombination; sequential exposure yields oxo-Fe-S<sup>0</sup><sub>n</sub> chain growth with disproportionation to S<sub>8</sub>. In testing, SO<sub>2</sub>/SO<sub>3</sub> formation has not been observed. Configuration and handling remain aligned with typical activated carbon practice, and testing with ISO-certified methane/H<sub>2</sub>S blends demonstrates capability to configure treatment below detection limits (<1 ppm).

Compared with Iron Sponge fixed beds, VOx avoids Fe (III) to Fe (II) cycling and associated FeS intermediates, broadens the operating window, shifts the waste outcome from inherent handling issues inherent with iron oxide beds and SO<sub>x</sub> to recoverable elemental sulfur, and achieves high H<sub>2</sub>S conversion capacity with an order-of-magnitude lower complex loading at competitive CapEx/OpEx.

Ongoing work includes scale-up and field configurations optimized to H<sub>2</sub>S feed levels, QA/QC for manufacturing reproducibility, sulfur recovery/handling practices, and extended testing across humidity and oxygen excursions to further map operating boundaries while retaining the electron density transfer pathway central to the mechanism.

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