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Featured Article

Intrinsically Conducting Polymers (ICPs) in Energy Technology: Fundamentals, Applications, and Experimental Progress

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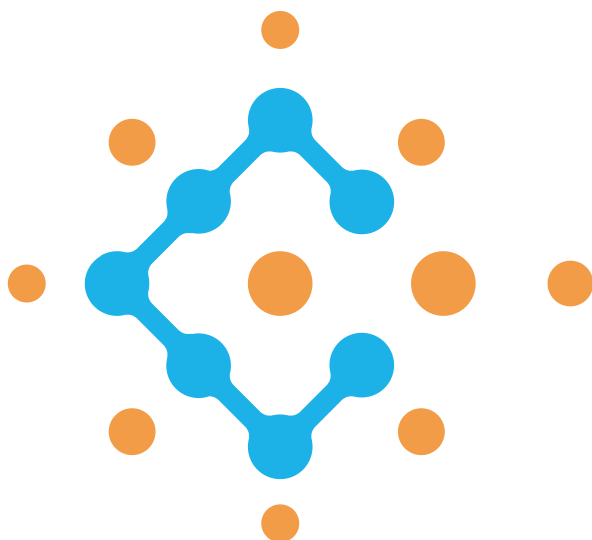




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Board Message

Dear Esteemed Readers,

It is with immense pride and excitement that we welcome you to the Third issue of volume 3 of our society's technical journal. Building on the foundation laid in our inaugural issue, this edition signifies our unwavering commitment to fostering innovation, sharing knowledge, and strengthening connections within our professional community.

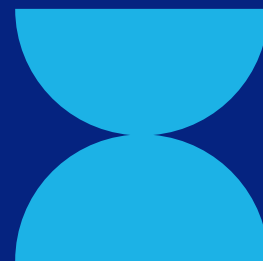
As our field continues to evolve, so too does the scope of ideas and challenges we face. This journal remains dedicated to providing a platform where groundbreaking research, practical insights, and diverse perspectives converge. It is our hope that these contributions spark dialogue, inspire action, and drive meaningful progress.

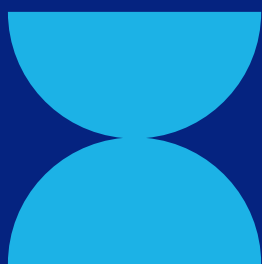
In this issue, you will find an enriched selection of articles that delve deeper into the complexities of our discipline. Each piece reflects the dedication and expertise of our contributors, as well as the collective vision of our society to lead and inspire. I encourage you to explore the content thoughtfully and consider how these insights might shape your work and broaden your understanding.

The success of this endeavor would not be possible without the support and collaboration of our authors, reviewers, and editorial team. Their hard work and passion have once again made this journal a testament to the vibrancy and depth of our community.

As we move forward, let us continue to celebrate the spirit of curiosity, innovation, and excellence that unites us. Thank you for your ongoing engagement and support. Together, we are shaping the future of our field.

Warm regards,





Letter From The Editor

Dear Colleagues,

Welcome to the Third issue of Volume 3 of the Journal of Chemicals Research and Innovation Society. As we embark on another year of scientific exploration and knowledge sharing, we are excited to continue our mission of fostering groundbreaking research and collaboration in the chemical sciences.

Building on the foundation laid in our previous volumes, this issue presents a diverse collection of studies that showcase innovative methodologies, novel discoveries, and practical advancements across various fields of chemistry. Each contribution reflects the dedication and expertise of our research community, and we are proud to provide a platform for such impactful work.

I extend my deepest gratitude to our authors, reviewers, and editorial team for their unwavering commitment to excellence. Your contributions ensure that this journal remains a trusted source of scientific progress and a hub for meaningful discourse.

As we move forward, I encourage you to actively engage with the journal, whether through submitting your research, participating in discussions, or sharing insights with your peers. Together, we can continue to drive innovation and push the boundaries of chemical research.

Thank you for your continued support, and I look forward to the discoveries and advancements that lie ahead.

Best regards,

Shakeel Ahmed, Ph.D.,

Editor-in-Chief

Journal of Chemicals Research and Innovation Society

Ambient-Stress Structural State and Intrinsic Texture of Hexagonal CaCO_3 Scale Deposits from Gas-Plant Equipment: A Rietveld Refinement Study

Noha S. Alshihri^{1*} and Husin Sitepu²

¹Research and Analytical Services Department (RASD), Saudi Aramco, P.O. Box 62, Dhahran 31311, Saudi Arabia

*Correspondence Author: noha.alshihri@aramco.com

²Retired from Saudi Aramco after more than 16 years of service in cutting-edge research

Abstract

Calcium carbonate (CaCO_3) scale formation presents persistent operational challenges in oil and gas processing facilities. Despite extensive investigations of carbonate rocks under stress, comparatively little attention has been devoted to defining their crystallographic characteristics under ambient conditions. In this work, hexagonal CaCO_3 scale deposits recovered from gas-plant equipment were investigated at ambient pressure (0 MPa) using powder X-ray diffraction (XRD) combined with full-profile Rietveld refinement. Structural analysis employed both a random orientation model and the March–Dollase preferred orientation correction to account for crystallographic texture effects. The diffraction data confirm a single-phase, well-crystallized hexagonal CaCO_3 structure. Incorporation of the March–Dollase model significantly improves refinement statistics, revealing measurable intrinsic texture within the scale deposits. The refined lattice parameters and atomic coordinates agree closely with established single-crystal data (Maslen et al., 1995) [1], confirming structural stability at ambient stress. These results establish a reliable ambient-stress structural reference for

CaCO_3 scale and provide insight into texture inheritance, anisotropic response, and compaction behavior relevant to carbonate reservoir systems.

Keywords: Calcium carbonate; Scale deposits; Rietveld refinement; March–Dollase model; Crystallographic texture; Carbonate reservoirs

Introduction

Carbonate minerals, particularly calcium carbonate (CaCO_3) [1], exert strong control over the mechanical and petrophysical properties of hydrocarbon reservoirs. Mechanical compaction, elastic anisotropy, permeability evolution, and fracture propagation in carbonate systems are closely linked to crystallographic structure and texture. Structural characterization using Rietveld refinement has proven especially valuable for investigating carbonate materials in geological and industrial contexts (Tzvetanova et al., 2020) [2].

While numerous studies have examined carbonate behavior under elevated pressure and temperature, less emphasis has been placed on defining a rigorous structural reference state at ambient stress. Scale

deposits formed during oil and gas production provide a unique opportunity to investigate carbonate crystallization under low mechanical loading. These deposits typically precipitate under near-ambient stress conditions ((Hill et al.,1993) [3]; (Post and Bish, 1989) [4]; (Snyder and Bish, 1989) [5]; (Dollase, 1989) [6]; (O'Connor et al., 1992) [7]; (Von Dreele, 1997) [8]; (Sitepu, 2002) [9]; (Sitepu, O'Connor and Li, 2005) [10]; (Sitepu, 2009) [11]; (Sitepu, AlYami and Zahrani, 2025) [12]), and therefore offer an appropriate baseline for evaluating subsequent pressure-induced structural modifications [13-20].

Powder X-ray diffraction combined with Rietveld refinement remains one of the most powerful techniques for extracting crystallographic parameters from polycrystalline materials. The method, originally introduced by Rietveld (1969) [21], enables simultaneous refinement of lattice constants, atomic coordinates, thermal displacement parameters, and profile functions through full-pattern fitting. However, carbonate materials often exhibit preferred orientation, which distorts diffraction intensities and may compromise structural reliability if uncorrected [21-25]. To address this, the March–Dollase correction model is widely applied to account for non-random crystallite alignment (Dollase, 1986) [6].

The present study investigates hexagonal CaCO_3 scale deposits collected from gas-plant equipment, focusing on their structural characteristics at 0 MPa. By integrating conventional Rietveld refinement (Rietveld, 1969) [21] with the March–Dollase preferred orientation correction (Dollase, 1986) [6], this work establishes a crystallographically robust ambient-stress reference state and

evaluates the presence of intrinsic texture within industrial carbonate scale.

Different healthcare centers adopt varying protocols for imaging frequency in order to strike a balance between treatment efficacy and accuracy. Incomplete

2. EXPERIMENTAL PROCEDURE

2.1 Sample Collection and Preparation

CaCO_3 scale deposits were mechanically removed from gas-plant equipment affected by carbonate precipitation. The collected material was cleaned to remove contaminants and finely ground using an agate mortar to obtain a homogeneous powder suitable for diffraction analysis (see a paper of Sitepu et al., 2025 [12] and the references therein [13-20] – for details).

2.2 X-ray Diffraction (XRD) Measurements

Powder X-ray diffraction (XRD) analysis was conducted at ambient pressure (0 MPa) using a Rigaku Ultima IV multipurpose X-ray diffractometer operated in Bragg–Brentano geometry. $\text{Cu K}\alpha$ radiation ($\lambda = 1.54060 \text{ \AA}$) was generated at 40 kV and 40 mA.

Diffraction data were collected over a 2θ range of 10° – 140° with a step size of 0.04° and a scanning rate of 1° min^{-1} . A position-sensitive detector was employed to ensure high counting efficiency and improved signal-to-noise ratio. Sample rotation was applied during measurement to minimize preferred orientation effects and enhance statistical representativeness [13-20].

All measurements were performed under ambient laboratory conditions corresponding to zero external mechanical stress (0 MPa). The instrumental parameters are summarized in Table 1.

Table 1. X-ray diffraction measurement conditions

Parameter	Description
Instrument	Rigaku Ultima IV multipurpose X-ray diffractometer
Radiation source	Cu anode, 40 kV, 40 mA
Wavelength	Cu K α_1 = 1.54060 Å
Geometry	Bragg–Brentano (480 mm measuring circle)
Slits	Divergence 0.67°, scattering 0.67°, receiving 0.3 mm
Specimen holder	Rectangular, 22 mm × 22 mm
Detector	Position-sensitive detector
Scan range	10°–140° (2 θ)
Step size	0.04°
Scan rate	1° min ⁻¹

2.3 Rietveld Refinement Strategy

Rietveld refinement was performed using full-profile least-squares fitting following the method of Rietveld (1969) [21]. Two structural models were evaluated:

1.Random orientation model (March parameter $r = 1.00$).

2.March–Dollase preferred orientation model allowing refinement of r (Dollase, 1986) [6].

Refinable parameters included scale factor, background, lattice parameters, atomic coordinates, isotropic displacement parameters, and peak-shape parameters [22–25]. Iterative refinement including preferred orientation (Dollase, 1986) [6] was continued until convergence was achieved with minimized residual factors [7,10,13].

3. RESULTS AND DISCUSSION

3.1 Phase Identification and Crystallinity

The diffraction patterns exhibit sharp, symmetric reflections characteristic of a highly crystalline carbonate phase. No secondary reflections or peak splitting were observed, confirming phase purity. The reflections are consistent with the hexagonal CaCO₃ structure. Similar structural identification of CaCO₃ scale in

gas-processing systems has been reported previously [7,10,12–20,22–25].

3.2 Lattice Parameters at Ambient Stress

The refined lattice parameters at 0 MPa, obtained using both the random orientation and March–Dollase models [6], are summarized in Table 2. For comparison, single-crystal X-ray diffraction data reported by Maslen et al. (1995) [1] are also included to evaluate structural consistency.

Table 2. Refined lattice parameters of CaCO₃ scale deposits at 0 MPa

Refinement Model	a = b (Å)	c (Å)	V (Å ³)
Random orientation	4.97612(5)	17.0893(10)	366.468(33)
March–Dollase [6]	4.97630(15)	17.0904(9)	366.520(31)
Single-crystal reference (Maslen et al., 1995) [1]	4.9882(2)	17.068(2)	367.8(3)

The equality of the a and b parameters confirms preservation of hexagonal symmetry at ambient stress. Differences between the random and March–Dollase [6] refinements are within experimental uncertainty, indicating that preferred orientation primarily influences peak intensities rather than intrinsic lattice geometry. The unit-cell volumes derived from both models are nearly identical and show excellent agreement with single-crystal values of Maslen et al. (1995) [1], demonstrating structural stability of the CaCO₃ scale under ambient conditions.

These results confirm that incorporation of the preferred orientation correction improves refinement reliability without altering fundamental crystallographic parameters, thereby validating the ambient-stress structural reference state established in this study.

Table 3. Atomic parameters and refinement statistics at 0 MPa

Parameter	Random orientation	March–Dollase	Single-crystal reference (Maslen et al., 1995) [1]
Ca Uiso (Å²)	0.0186(5)	0.0162(5)	0.00988(3)
C Uiso (Å²)	0.0109(16)	0.0110(16)	0.00834(9)
O x	0.2530(4)	0.2544(4)	0.2570(6)
O Uiso (Å²)	0.0264(10)	0.0247(9)	0.01129(7)
R _P (%)	10.23	9.75	—
R _{WP} (%)	13.99	13.30	—
R(F²) (%)	11.19	10.15	—
χ²	1.94	1.32	—
March parameter (r)	1.00	0.854(7)	—

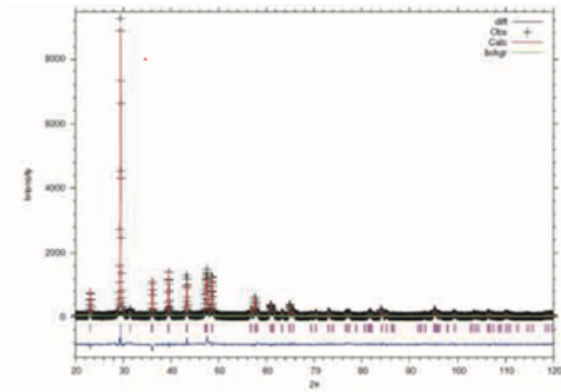


Figure 1. Rietveld refinement profile of hexagonal CaCO₃ scale deposits at 0 MPa using the random orientation model ($r = 1.00$). Observed intensities (symbols), calculated profile (solid line), Bragg reflection positions (tick marks), and the difference curve (bottom trace) are displayed. The refinement converges with $R_{WP} = 13.99\%$ and $\chi^2 = 1.94$.

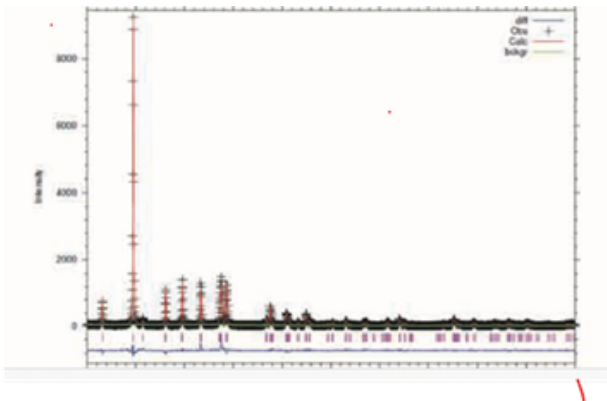


Figure 2. Rietveld refinement profile of hexagonal CaCO₃ scale deposits at 0 MPa incorporating the

March–Dollase preferred orientation correction. Symbols represent observed data, the solid line indicates the calculated profile, tick marks denote Bragg reflection positions, and the lower trace shows the difference curve. Incorporation of the preferred orientation model significantly improves the fit quality ($R_{WP} = 13.30\%$, $\chi^2 = 1.32$), confirming the presence of intrinsic crystallographic texture.

3.3 Atomic Parameters and Thermal Displacement

The refined atomic coordinates and isotropic displacement parameters (Uiso) at 0 MPa are presented in Table 3 and Figures 1 and 2, together with single-crystal reference data reported by Maslen et al. (1995) [1] for comparison.

The refined calcium and carbon atomic positions are consistent with the expected crystallographic sites of hexagonal CaCO₃ and closely match the single-crystal values reported by Maslen et al. (1995). The oxygen fractional coordinate (x) shows only minor deviation within experimental uncertainty, indicating preservation of the carbonate group geometry.

The isotropic displacement parameters for all atoms are slightly higher than single-crystal values, which is typical for polycrystalline materials due to microstructural effects such as residual strain, crystallite size variation, and minor lattice imperfections. Nevertheless, the magnitudes of isotropic temperature factor (Uiso) remain within physically reasonable limits, confirming structural stability and absence of significant disorder at ambient stress.

Incorporation of the March–Dollase preferred orientation correction leads to systematic improvement in refinement statistics (see Figures 1 and 2), as evidenced by reduced the crystallographic R-factors and goodness-of-fit-index (R_P , R_{WP} , $R(F^2)$, and χ^2) values. The refined March

parameter ($r = 0.854$) confirms measurable crystallographic texture within the scale deposits. Importantly, inclusion of preferred orientation refinement enhances model reliability without altering fundamental atomic positions, thereby strengthening the validity of the ambient-stress structural reference established in this study.

3.4 Intrinsic Texture and Preferred Orientation

The refined March parameter ($r = 0.854$) confirms measurable preferred orientation within the CaCO_3 scale deposits. Such non-random crystallite alignment likely developed during precipitation and growth within confined industrial environments. Similar observations of texture development in carbonate scale have been documented in previous Rietveld-based studies [3-11].

Crystallographic texture influences anisotropic mechanical response and compaction pathways in carbonate systems [3-11]. Establishing the magnitude of preferred orientation at ambient stress provides a baseline for interpreting texture evolution under elevated pressure conditions relevant to subsurface reservoirs.

4. CONCLUSIONS

This study establishes the ambient-stress crystallographic reference state of hexagonal CaCO_3 scale deposits recovered from gas-plant equipment. The material is confirmed to be single-phase, highly crystalline, and structurally consistent with established single-crystal data (Maslen et al., 1995) [1].

Application of the Rietveld method (Rietveld, 1969) [21] combined with the March–Dollase preferred orientation correction (Dollase, 1986) [6] significantly

improves refinement quality and reveals intrinsic crystallographic texture within the deposits. Although preferred orientation affects intensity distributions, it does not modify fundamental lattice geometry at 0 MPa.

These findings provide a structurally validated baseline for evaluating pressure-induced texture evolution, anisotropic mechanical response, and compaction behavior in carbonate reservoir systems.

5. OUTLOOK

Future investigations should extend this structural approach to elevated pressure and temperature conditions representative of deep carbonate reservoirs. Integration of diffraction-based texture analysis with elastic and petrophysical measurements will enable quantitative correlation between crystallographic texture and macroscopic anisotropy, supporting improved predictive models of carbonate reservoir behavior [11-20].

ACKNOWLEDGMENTS

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suggestions, which significantly enhanced the quality and clarity of this manuscript.

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Authors

Noha S. Al-Shihri is an Associate Scientist in the Research and Analytical Services Department at Saudi Aramco. She holds an M.Sc. in Chemistry from the Rochester Institute of Technology, Rochester, New York, USA. Her expertise focuses on advanced materials characterization, including Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and Raman spectroscopy, supporting research, process optimization, and failure analysis investigations. She has published and presented her work at international scientific conferences and is a co-inventor on several patents.

Dr. Husin Sitepu retired from Saudi Aramco after more than 16 years of service as a specialist in applied crystallography and diffraction science. His work centered on advanced structural characterization using XRF, XRD, synchrotron radiation, neutron powder diffraction, and the Rietveld refinement method. His contributions supported catalyst development, QA/QC of drilling additives and new chemical products, and complex failure analysis studies. Dr. Sitepu has authored over 70 peer-reviewed publications and contributed more than 80 CIFs to the ICDD PDF-5+ database. He holds a Ph.D. in Physics and remains active in professional organizations including the ICDD, IUCr, and NSSA.

Mesoporous Catalyst Design for Improved Hydrocracking of Heavy Oil Blends

Shakeel Ahmed

Interdisciplinary Research Center for Refining and Advanced Chemicals
King Fahd University of Petroleum & Minerals, Dhahran-31261, Saudi Arabi
Corresponding author: shakeel@kfupm.edu.sa

Abstract

Hydrocracking is a key refining process for upgrading heavy petroleum fractions into valuable lighter products. This study focuses on the development of Ni–Mo supported catalysts for hydroprocessing a vacuum gas oil (VGO) and de-metallized oil (DMO) blend (85:15), a relatively underexplored feedstock. Catalysts were prepared using different acidic supports, including USY, Beta zeolite, MCM-41, and amorphous silica–alumina (ASA), and evaluated for their physicochemical properties and catalytic performance.

Among the prepared catalysts, NiMo–MCM-41 exhibited the highest surface area and a favorable balance of acidity and mesoporosity. Catalytic testing was conducted in a batch reactor at 410 °C and 90 kg/cm² hydrogen pressure. The NiMo–MCM-41 catalyst demonstrated superior performance, achieving higher conversion (30%) compared to the commercial catalyst (27%), along with lower gas yield and higher diesel selectivity. All synthesized catalysts showed improved hydrodesulfurization activity (72–80%) relative to the commercial benchmark (56%). In addition, NiMo–MCM-41 displayed the highest hydrogenation activity, nearly twice that of the commercial catalyst.

The enhanced performance is attributed to its mesoporous structure and optimized acidity, which promote efficient diffusion

and conversion of bulky hydrocarbons. These findings highlight NiMo–MCM-41 as a promising catalyst for efficient hydrocracking of VGO/DMO blends.

Keywords: Hydrocracking; Mesoporous; MCM-41; VGO; Heavy oil

1. Introduction

Hydrocracking is a cornerstone conversion process in modern petroleum refining, offering exceptional flexibility for upgrading a wide range of feedstocks—from heavy residues to vacuum gas oil (VGO) and even lighter fractions—into high-value products such as naphtha, kerosene, middle distillates, lubricants, and petrochemical feedstocks. The continued growth of hydrocracking technology over recent decades is driven by increasing demand for cleaner fuels and stricter environmental regulations, necessitating efficient removal of sulfur, nitrogen, and metals from increasingly heavier and more complex feedstocks [1,2].

Industrial hydrocracking processes are typically configured as single-stage or two-stage systems, depending on feed characteristics and desired product distribution. Central to these processes is the use of bifunctional catalysts, which combine hydrogenation–dehydrogenation functionality with acidic cracking sites. The hydrogenation function is usually provided

by noble metals (e.g., Pt, Pd) or sulfided base metals such as Ni–Mo or Co–Mo, while the acidic function is supplied by supports including zeolites (e.g., USY, Beta), amorphous silica–alumina (ASA), and emerging mesoporous materials [1,3]. The catalytic performance strongly depends on the balance between these two functionalities, which governs activity, selectivity, and resistance to deactivation via coke formation [4].

Recent advances in catalyst design have focused on improving accessibility to active sites through the development of hierarchical and mesoporous materials, such as MCM-41, which facilitate the diffusion of bulky polyaromatic hydrocarbons present in heavy feedstocks [5,6]. These materials offer tunable acidity and large pore structures, making them promising candidates for enhancing hydrocracking efficiency [7-11].

Despite extensive research on VGO hydrocracking, studies involving blends of VGO with de-metallized oil (DMO) remain limited, primarily due to the restricted availability of DMO streams. DMO, typically produced in specialized refineries such as the Riyadh Refinery in Saudi Arabia, contains higher levels of metals and polyaromatics, posing additional challenges for catalyst stability and performance. Therefore, there is a need to develop robust catalyst systems capable of efficiently processing VGO/DMO blends.

In this study, a series of Ni–Mo supported catalysts were prepared using different acidic supports, including USY, Beta zeolite, MCM-41, and amorphous silica–alumina. The catalysts were evaluated for the hydrocracking of a VGO/DMO (85:15) blend. Particular emphasis was placed on

understanding the role of support structure and acidity. Among the catalysts investigated, the MCM-41-supported system exhibited superior performance in terms of conversion, selectivity, and hydrogenation activity compared to conventional and commercial catalysts.

2. Experimental

2.1. Catalyst Preparation

A series of Ni–Mo supported on USY-, Beta-zeolite, MCM-41, and ASA (amorphous silica alumina) was prepared by the incipient wetness impregnation method. MCM-41 with Si/Al molar ratio of 10 was prepared in the laboratory following the method of Kim et. al., using cetyl trimethyl ammonium bromide as a templating agent ³. The extrudates of 1/16" were prepared by mixing 70 weight % of alumina binder (Cataloid AP-1) and one of the acidic components to form support. The extrudates were calcined in a muffle furnace at 500 °C for 6 hours. The calcined support was impregnated with a solution of nickel nitrate and ammonium heptamolybdate to provide a catalyst with a final loading of these metals as 2.0 wt % Ni and 8.0 wt% Mo.

2.2. Catalyst Characterization

Prepared MCM-41 samples were characterized by XRD using Jeol JDX-3530 using Cu broad focus tube at 40 Kv and 30 mA. The diffraction pattern was generated by a 2-theta/theta scanning diffractometer. Prepared hydrocracking catalysts were characterized by N₂ sorption analyzer supplied by Quanta Chrome (Model NOVA-1200) at 77 K. Temperature programmed reduction (TPR) experiments were carried out using a system supplied by Ohkura Riken, Japan (Model TP-2000).

2.2.Catalyst Evaluation

Five catalysts, including one commercial reference catalyst, were evaluated for hydrocracking activity test in a batch autoclave reactor of 300 ml capacity. An amount of 100 grams of feed (VGO-DMO blend 85-15%) and 3 grams of presulfided catalyst were loaded into the vessel housed in an electric furnace. The vessel was purged with N₂ and pressurized with H₂, and a leak was checked by an H₂ detector. The reaction was carried out at 410 °C and at an initial H₂ pressure of 90 kg/cm² for 1 hour. The system was allowed to cool down to room temperature, and then it was purged with N₂ after removing the product gas sample for GC analysis. The liquid product is analyzed by the simulated distillation technique. Properties of the feedstock are given in Table 1.

Table 1. Feedstock Properties.

Feedstock Properties	VGO	DMO	VGO/DMO 85% / 15%
Specific Gravity	0.92-0.93	0.96-0.97	0.93-0.94
Nitrogen, wt ppm	700-900	1300-2100	1100-1200
Sulfur, wt%	2-3	3-3.5	2.6-2.8
ASTM Distillation, D2887			
5%, °C	279	402	
50%, max °C	472	596	495
90%, max °C	543	678	615
Ni + V wt. ppm	< 1	8.0-13.5	2-3

3. Results and discussion

Physical properties of the prepared catalysts are given in Table 2. The highest surface area was observed in the case of the MCM-41-based catalyst, whereas ASA-based catalysts showed the lowest surface area as well as acidity. The acidity measurement showed that zeolitic catalysts have total acidity in a close range of about 0.5 mmol/g. Pore volume and average pore diameter measured from the N₂ sorption analyzer are in close range; however, the ASA-based catalyst showed the largest pore diameter among all the catalysts prepared in this study.

TABLE 2. Textural characteristics of the prepared catalysts.

Catalysts	BET Surface Area (m ² /g)	Pore Volume (cm ³ /g)	Pore Diameter avg. (Å)	Acidity (mmol/g)
NiMo-ASA	186	0.33	36	0.33 (264)*
NiMo-MCM-41	324	0.40	25	0.50 (252)
NiMo-β	313	0.41	26	0.56 (233)
NiMo-USY	300	0.35	23	0.59 (238)

* Peak temperature (°C) from TPD of NH₃.

Catalyst evaluation results indicate relative lower amount of gaseous product in the case of the NiMo-MCM-41 catalyst as compared with other prepared catalysts. The commercial catalyst produced the lowest amount of gaseous products (Table 3). The gas make was correlated with the acidity of the prepared catalysts (Figure 1).

TABLE 3. Product gas analysis.

Gas HCs (Vol%)	NiMo-ASA	NiMo-MCM-41	NiMo-Beta	NiMo-USY	Com. Cat.
CH ₄	0.97	0.24	1.56	1.31	0.07
C ₂	0.59	0.12	0.00	0.00	0.00
C ₂ =	0.63	0.00	0.65	0.49	0.05
C ₃	0.00	0.11	0.00	0.00	0.00
C ₃ =	0.00	0.00	0.00	0.00	0.00
C ₄ s	0.05	0.06	0.00	0.00	0.00
C ₅ s	0.04	0.00	0.00	0.00	0.00
Total	2.28	0.53	2.22	1.81	0.12

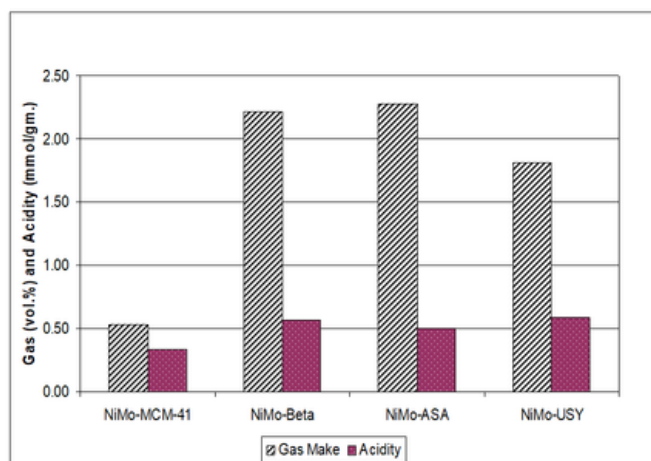


Figure 1. Relationship of acidity and gas make.

Figure 2 shows the hydrocracking product selectivity of the catalysts evaluated in this study. It is evident that all prepared catalysts have yielded almost the same naphtha yield and more diesel yield than the commercial catalyst. However, NiMo-MCM-

41 catalyst has produced the highest diesel yield and the lowest gas make amongst all tested catalysts. This can be attributed to the main feature of this catalyst being mesoporous and having lower acidity. This result makes the NiMo-MCM-41 catalyst very attractive to be considered as a hydrocracking catalyst for VGO/DMO blend feed. On the other hand, all tested catalysts, including the commercial catalyst, have the tendency to produce more diesel than naphtha. The lower residue yield was also observed with the NiMo-MCM-41 catalyst compared to the commercial and other prepared catalysts. The other three prepared catalysts, namely NiMo-ASA, NiMo-b, , and NiMo-USY, had almost similar residue to the commercial catalyst. Therefore, all of the tested catalysts can be tagged as a diesel selective catalyst or a diesel mode catalyst.

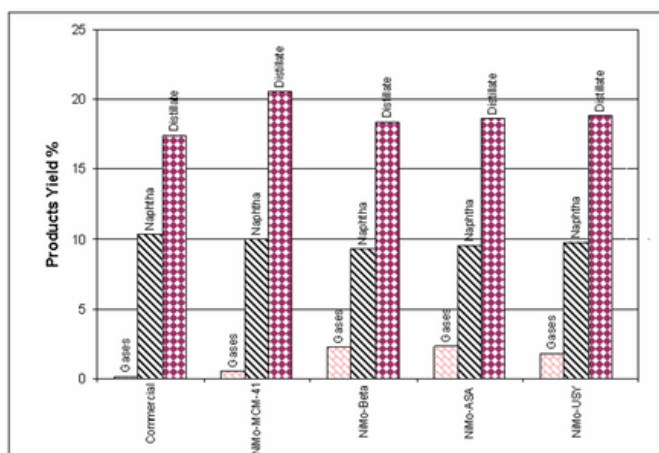


Figure 2. Catalysts' selectivity for hydrocracking activity.

Figure 3 shows that NiMo-MCM-41 was able to convert hydrocarbons contained in the 800 °F – 900 °F cut better than the commercial and the other prepared catalysts. However, in the heavier cut (900 °F – 1050 °F), all tested catalysts had relatively similar conversion. It is imperative to mention that the heavier cut was easier to crack and convert than the lighter cut.

Thus, this is one of the advantages of NiMo-MCM-41, being able to accommodate both cuts and achieve relatively higher conversion in both of them, unlike other tested catalysts.

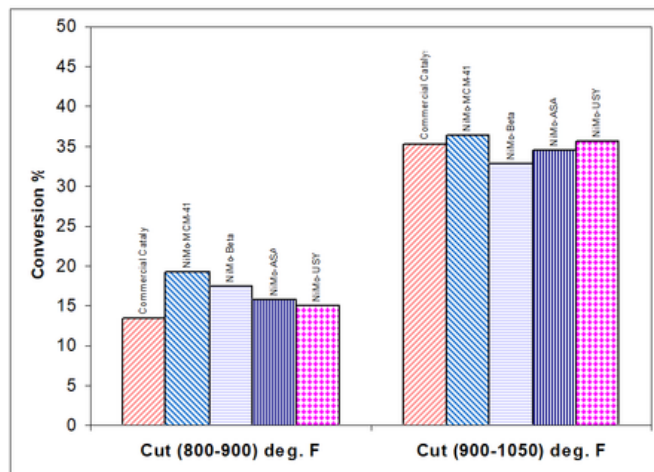


Figure 3. Catalyst conversions for 800-900 °F cut and 900-1050 °F cut.

Figure 4 shows the HDS activity of the prepared catalysts as compared with the commercial catalyst. It is obvious that all of the prepared catalysts offered much better HDS activity than the commercial catalyst. The HDS activity of the prepared catalysts ranges between 72 % ~ 80 %, as compared to 56 % HDS activity obtained by the commercial catalyst. In addition, the blank run did not achieve any sulfur reduction, which is expected since no catalyst was present to enhance the HDS reactions.

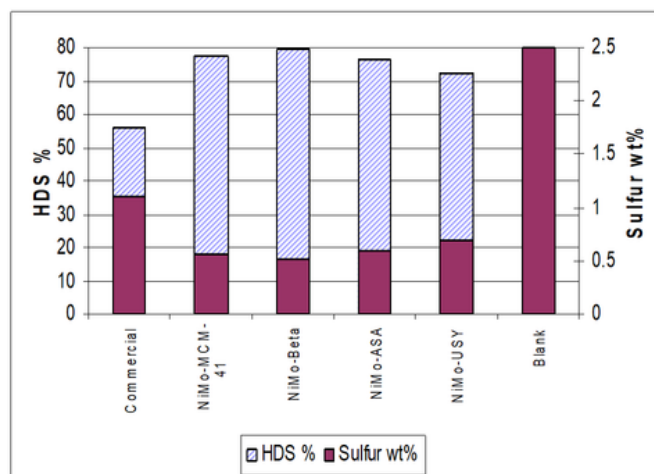


Figure 4. HDS activity of the tested catalysts.

It is clear from Figure 5 that NiMo-MCM-41, NiMo- β , and NiMo-USY catalysts, which are nickel-promoted, had higher hydrogenation activity as compared to the commercial catalyst. However, NiMo-ASA, which has the lowest surface area, had lower hydrogenation activity than the commercial catalyst. This indicates that the prepared zeolitic catalysts, including NiMo-MCM-41, have better metal dispersion than the amorphous catalysts (Commercial and NiMo-ASA), which resulted in better hydrogenation activity. However, NiMo-MCM-41 catalyst showed the best hydrogenation activity, which is almost double the activity of the commercial catalyst. It seems that NiMo-MCM-41 has a very good tendency to utilize hydrogen in saturating the unsaturated hydrocarbons resulting from cracking reactions. On the other hand, no hydrogenation took place in the case of the blank run.

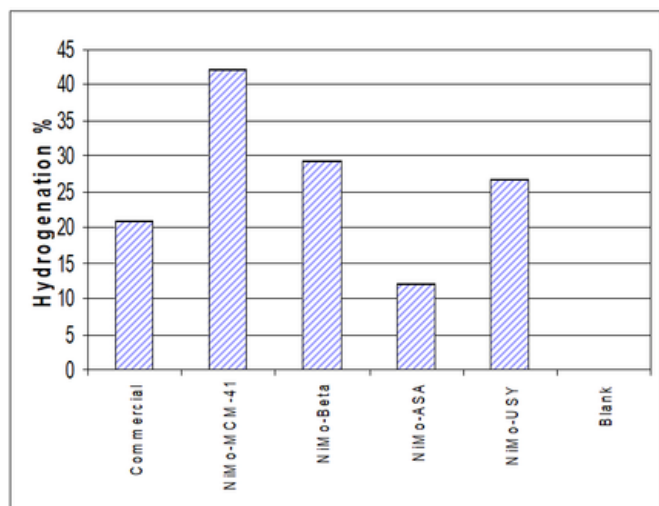


Figure 5. Hydrogenation activity of the tested catalysts.

It is evident from Figure 6 that zeolitic catalysts, represented by NiMo-MCM-41, NiMo- β , and NiMo-USY, produced more carbon deposits than the amorphous catalysts (Commercial and NiMo-ASA). This is due to the fact that zeolitic catalysts are more acidic and have more surface area for

reactants to over-crack. Coke formation has a direct effect on the catalyst stability; however, this cannot be measured by means of a batch reactor. It can rather be measured by a flow reactor, which can be run for a longer period of time to quantify the catalyst lifetime.

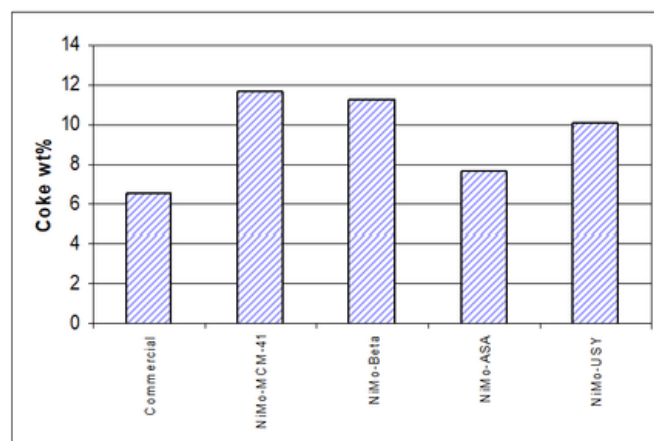


Figure 6. Coke deposited on the spent catalysts.

CONCLUSIONS

All prepared catalysts showed better hydrodesulfurization activity than the commercial catalyst. NiMo-MCM-41 showed the highest hydrogenation activity amongst all tested catalysts. It had almost double the hydrogenation activity of the commercial catalyst. The prepared catalysts had relatively similar hydrocracking activity to the commercial catalyst. However, the NiMo-MCM-41 catalyst performed better by achieving 30% overall conversion as compared to 27% achieved by the commercial catalyst. All tested catalysts were diesel selective catalysts with slight variations. The tested catalysts produced similar naphtha yield. However, in the case of diesel, the prepared catalysts produced more diesel than the commercial catalyst, especially NiMo-MCM-41, which yielded 21% diesel as compared to 17% diesel yield produced by the commercial catalyst.

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Authors

Dr. Shakeel Ahmed is a Senior Research Scientist at the IRC for Refining & Advanced Chemicals at King Fahd University of Petroleum & Minerals. His primary areas of expertise include industrial catalysis, inorganic synthesis, and instrumental analysis. With more than 200 publications and over 80 co-invented patents, Dr. Ahmed has made significant contributions to his field. He has received numerous national and international awards and is recognized among the top 2% of scientists worldwide.

Evaluation of Corrosion Inhibitor Batch Treatment Using a Downhole Monitoring Tool in Sour Gas Wells

Tao Chen; Feng Liang; Qiwei Wang, Jairo Leal

Saudi Aramco's Research & Development Center, Dhahran, Saudi Arabia

Corresponding author email: tao.chen@aramco.com

Abstract

Iron sulfide scale formation is a corrosion-induced problem in sour gas wells. Batch corrosion inhibitor (CI) treatment is widely used where continuous injection is unavailable, yet its performance under real downhole conditions is difficult to quantify. This study applies a newly developed Downhole Corrosion and Scale Monitoring (DCSM) tool to evaluate CI batch treatment in a sour gas well. Two field trials were conducted in the same well: a baseline without CI treatment and a trial with CI batch treatment. Coupons matching tubing metallurgy were deployed and analyzed using SEM/EDS, XRD, weight change, and surface profilometry. Thin iron sulfide layers formed in both cases. While weight change did not differentiate performance, post-analysis showed reduced general and pitting corrosion rates with CI. CI also altered iron sulfide mineralogy, promoting pyrite formation. The DCSM enables direct downhole assessment of corrosion and scale mechanisms and supports optimization of CI strategies.

Introduction

Sour corrosion and iron sulfide deposition are major integrity and flow-assurance challenges in sour gas wells, particularly at depth where temperature and pressure are high. Iron sulfide deposition is

corrosion-induced and can exacerbate under-deposit corrosion, leading to metal loss, pitting, and operational issues. Batch CI treatment is commonly applied where downhole injection lines are absent, but performance evaluation remains challenging. Conventional monitoring tools have limitations under high-temperature, high-pressure (HTHP) sour conditions. This paper presents application of a DCSM tool to directly monitor corrosion and scale under real downhole conditions and evaluate CI batch treatment effectiveness.

Methodology

DCSM Tool and Deployment

The DCSM consists of a gauge hanger and coupon holders exposing metal coupons to production flow, simulating tubing internal conditions. Coupons are isolated to ensure exposure only on the outer surface. Multiple coupons can be deployed simultaneously.¹ The DCSM arrangement is shown in **Fig. 1**.

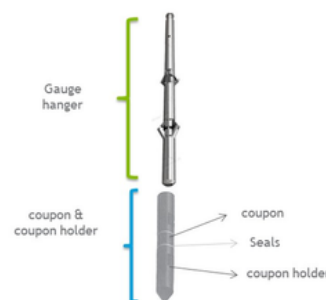


Fig. 1—Downhole corrosion and scale monitoring (DCSM) tool.¹

Field Evaluation

A sour gas well (~5% H₂S, ~3% CO₂; ~125 °C; ~5000 psi) was selected. Coupons were T-95 carbon steel, matching tubing metallurgy. Two trials were performed at same depth in downhole:

- **Baseline:** Without CI.
- **CI Treatment:** With 2000 gal treatment fluid containing 200 gal fatty-acid/pyridinium CI; 24-h shut-in.

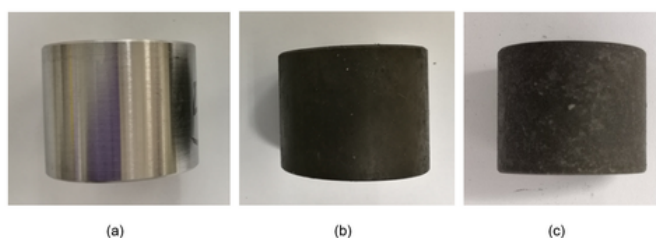
Post-Exposure Analysis

The test DCSM and coupons were retrieved after 3-5 months deployment. Retrieved coupons were analyzed by SEM/EDS for morphology and elemental composition, XRD for mineralogy, and surface profilometry for general and pitting corrosion after controlled deposit removal. Weight change was recorded but interpreted cautiously due to competing effects of corrosion loss and scale gain.

Results and Discussion

Surface Deposition and Weight Change

Fig. 2 shows the images of test coupons before field trial, after exposure in the field in the absence of corrosion inhibitor treatment, and after exposure in the field in the presence of corrosion inhibitor treatment respectively. Thin dark deposits formed in both trials (Fig. 2b/Fig. 2c). The dark deposition could be the iron sulfide formed on the surface of test coupon due to the sour corrosion reaction shown in Equation (1).



ig. 2— Images of test coupons. a) Before trial test; b) After exposure without corrosion inhibitor treatment; c) After exposure with corrosion inhibitor treatment.

The weight of test coupons before and after field application were measured and recorded in **Table 1**. The weight change of for the sour corrosion is composed of two major factors, the wight loss due to the general sour corrosion and the weight gain due to the iron sulfide surface deposition. The total weight change is reflected by the combined effects of the weight loss due to corrosion and the weight gain due to surface deposition. The average monthly weight change of two trials was measured and calculated to be 0.011 g/month and 0.012 g/month, respectively. Weight change showed slight gains in both cases, indicating limited sensitivity for sour corrosion assessment.

Table 1— Weight measurement of coupons before and after field exposure.

	Weight before (g)	Weight after (g)	Average weight change (g/month)
No corrosion inhibitor treatment	118.647	118.680	0.011
Corrosion inhibitor treatment	117.821	117.880	0.012

The test coupons were cut and made the cross-section available for further analysis. High-resolution SEM and EDS analysis were carried out at the cross-section of test coupons to analyse the thickness and the composition of the surface deposition (**Fig. 3**).

Thin layers of deposit of ~10 mm and ~20 mm in thickness were observed on the coupon surface over field application in the absence of corrosion inhibitor treatment and in the presence of corrosion inhibitor treatment (Fig. 3). The deposits were mainly composed of Fe (Fig. 3b) and S (Fig. 3c). This indicated that the deposited layer was

mainly composed of iron sulfide.

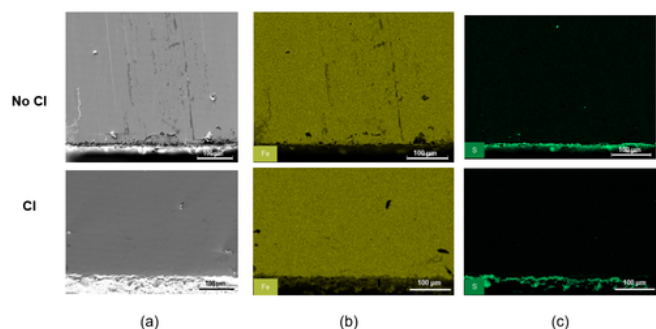


Fig. 3—SEM images and EDS analysis of cross-section of test coupons. a) SEM image; b) EDS analysis of Fe; c) EDS analysis of S.

The colour of sulfur distribution shown in Figure 3c was darker at the interface of metal surface and lighter at the out layer of iron sulfide deposition, which indicated that denser iron sulfide deposited at the interface of metal surface than out layer. The initial general corrosion at the interface of metal surface was higher and caused denser iron sulfide deposition at the interface. The iron sulfide surface deposition could work as a protective layer to reduce the further interactions between the metal tubulars and the produced gas/fluid media.^{2,3} The further corrosion could be reduced and further reduce the iron sulfide surface deposition. This observation agreed with Zheng's study that the corrosion induced iron surface deposition is somewhat protective, as the final steady-state corrosion rates were much lower than the initial general corrosion.⁴

Many types of iron sulfide with different ratio of iron and sulfur can form in the oil and gas industry, such as amorphous ferrous sulfide (FeS), mackinawite (Fe_{1+x}S), cubic ferrous sulfide (FeS), troilite (FeS), pyrrhotite (Fe_{1-x}S or FeS_{1+x}), smythite ($\text{Fe}_{3+x}\text{S}_4$), greigite (Fe_3S_4), and pyrite (FeS_2). The different type of iron sulfide has different physical or chemical properties, for example, conductivity, acid solubility,

etc.⁵

Iron Sulfide Mineralogy

XRD was performed to further analyze the crystallization of the iron sulfide formed in both cases. The results are shown in Fig. 4, where Figure 4a is in the absence of corrosion inhibitor treatment and Figure 4b is in the presence of corrosion inhibitor treatment. XRD revealed different mineral assemblages. Without CI, deposits comprised mainly pyrrhotite, troilite, magnetite, and minor marcasite. With CI, pyrrhotite dominated with significant pyrite formation. CI thus influenced iron sulfide mineralogy, which has implications for mitigation and scale removal strategies.

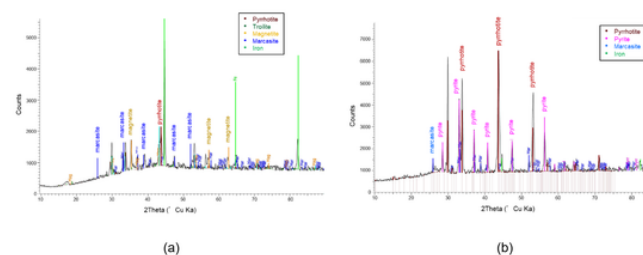


Fig. 4—XRD composition analysis of surface deposition after field application.

Corrosion Rates

Surface profilometry showed reduced corrosion with CI. Average general corrosion decreased from ~ 1.7 – $3.3\mu\text{m}/\text{month}$ (no CI) to ~ 0.6 – $1.6\mu\text{m}/\text{month}$ (with CI). Average pitting depth decreased from ~ 6.7 – $8.3\mu\text{m}/\text{month}$ to $\sim 2.6\mu\text{m}/\text{month}$. It showed that CI mitigated both general and localized corrosion despite similar deposit quantities.

Implications

Iron sulfide layers were denser at the metal interface, suggesting initially higher corrosion followed by partial protection. CI reduced corrosion severity and altered deposit characteristics. Weight-loss methods alone are insufficient for sour

environments; integrated downhole monitoring and post-analysis are required.

Conclusions

1. The DCSM tool enables direct monitoring of corrosion and scale under real downhole sour conditions.
2. CI batch treatment reduced general and pitting corrosion rates but did not significantly change deposit quantity.
3. CI altered iron sulfide mineralogy, promoting pyrite formation.
4. Weight change alone is inadequate to evaluate sour corrosion performance.
5. Integrated downhole monitoring supports optimized corrosion and scale management strategies.

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Authors

Dr. Tao Chen is a Petroleum Engineering Consultant at Saudi Aramco, based in Dhahran, Saudi Arabia. With over 25 years of experience in oilfield scale and corrosion management, he is a Fellow of AMPP and the Fellow Royal Society of Chemistry. He holds a Ph.D. in chemical engineering from Heriot-Watt University and an MBA from Warwick University.

Dr. Qiwei Wang works in Saudi Aramco's Research & Development Center as a Senior Research Science Consultant in oil field scale mitigation. He has over 25 years of R&D and technical support experience in oil field production chemistry, scale management, and water treatment.

Dr. Feng Liang is currently Production Technology Leader at the Aramco Services Company, Aramco Research Center, Houston, TX. She received her Ph.D. degree in Organic Chemistry from Rice University, Houston, TX. Her research interests are the new materials and product development in fracturing fluid, advanced fluid additives, waterless fracturing technologies, biodegradable diversion materials, sand control products, cement additives, and nanomaterial reinforced elastomers.

Dr. Qiwei Wang is an active member of the Society of Petroleum Engineers (SPE) and National Association of Corrosion Engineers (NACE). He has organized workshops, served on technical committees and chaired several conferences for both organizations. Qiwei received his Ph.D. degree in Oceanography from Texas A&M University, College Station, TX.

Jairo Leal was a Petroleum Engineering Consultant at Saudi Aramco, based in Dhahran, Saudi Arabia. He retired from Saudi Aramco in 2026, with over 30 years of experience in production technical support in oil and gas industry.

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Impact of Wind Speed and Temperature on the Performance and Energy Yield of Thin-Film Photovoltaic Modules

Imtiaz UL Hasan^{1*} and Qamar Abbas^{2**}

¹Department of Chemical Engineering, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

²Department of Mechanical Engineering, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia.

*Corresponding author: Email: g202315990@kfupm.edu.sa

**Co-Corresponding author: Email: g202315910@kfupm.edu.sa

Abstract

The performance of photovoltaic (PV) modules is directly influenced by environmental conditions, including ambient temperature and wind speed. High module temperatures reduce efficiency, affecting the overall energy output. Wind, as a passive cooling mechanism, enhances convective heat transfer and helps regulate the module temperature. This study analyzes the impact of wind speed and temperature on the performance of a Copper Indium Gallium Selenide (CIGS) PV module installed in Khuzdar, Baluchistan, Pakistan (27.8165° N, 66.6057° E). The hourly meteorological data was first validated through quality checks to ensure accuracy. The temperature of the PV module was then estimated considering convective cooling due to wind and its effect on efficiency and energy generation. The results indicate that each degree rise in module temperature leads to a 0.45% reduction in energy generation, while the convective cooling effect of wind lowers the module temperature, improving efficiency. The annual energy generation, capacity factor, and performance ratio were evaluated, showing an increase in the capacity factor from 25.70% to 26.58%

when wind effects were considered. The Levelized Cost of Electricity (LCOE) and tariff calculations were also performed using available data from the National Electric Power Regulatory Authority (NEPRA). The study highlights the significance of incorporating wind effects in PV system performance modeling to achieve higher efficiency and economic feasibility in hot and dry regions.

Keywords: Photovoltaic; Temperature; Wind; Performance; Efficiency

1. Introduction

Conventional methods for power generation, such as the use of fossil fuels, pollute the environment. Gas emissions during power generation cause global warming and many other environmental issues [1-3]. The world energy demand is increasing exponentially, and fossil fuels are depleting. These are the major reasons people transition from fossil fuels to renewable energy resources. Solar energy is the major green energy resource being researched and utilized. Solar energy has great potential for power production because of its unlimited energy resource,

i.e., the sun. The energy obtained from solar irradiance is almost 10,000 times higher than the world's annual energy demand [4]. Solar energy is an asset as it is environmentally friendly and sustainable. Photovoltaic cells are used for the direct conversion of solar irradiance into electricity. However, their efficiency is the major drawback of using photovoltaic cells (PV). Even the best efficiency copper indium gallium arsenide solar cells convert 14-23.4% of solar irradiance into electricity, and the rest is dissipated as heat [5]. Researchers are working on improving the efficiency of PV cells so that they can be used for industrial and domestic purposes on a larger scale.

The performance of solar cells directly depends upon ambient conditions like wind speed, ambient temperature, and irradiance. When the irradiance falling on the PV panel increases, the number of charge carriers generated in the PV cell increases, and hence, the output power of the cell increases, but at the same time, this leads to a rise in the temperature of the PV cell [6, 7]. When the ambient temperature of a location is higher, it also tends to enhance the temperature of the PV cell [8]. The efficiency of PV cells decreases with the increase in temperature, and the high temperature reduces the life span of a solar cell [7]. The efficiency of crystalline photovoltaic cells decreases to about 0.42% with each degree rise in the temperature of the solar cell [9]. The effect of irradiance and temperature on the performance of the PV module is presented in [10]. The results of [10] depict that the performance ratio of PV cells decreases with latitude because of the high temperature. The regions with higher latitudes have a higher performance ratio because of the low temperature. Regions

like Antarctica, the Himalayas, and the southern Andes have the highest PV cell performance. The PV cells that are less temperature-sensitive are preferred in the areas where the ambient temperature is higher, and the more temperature-sensitive PV cells are chosen for the regions of low ambient temperature [11].

The effect of temperature on the electrical output of PV cells with proper relations is explained in [12]. The variation in the output power of PV cells with the ambient temperature, the location's latitude, and wind speed is simulated in [13]. Different active or passive thermal management techniques are being utilized to reduce the temperature of PV cells. The effect of phase change material on the reduction of the temperature of the PV cell and then that reduction in temperature on the electrical output of the module is available in [14]. The wind is used as a passive cooling technique for PV cells. In certain cases, it acts as an active cooling technique when the fan is used. The efficiency of the PV module strongly depends upon the wind speed, shading, material of the cell, and dust accumulation [15]. To analyze the effect of the wind speed on the PV module performance either by natural or forced convection, experiments were performed, and the results showed that the efficiency of the PV module increased by 8.6% and 12.6%, respectively [16]. The effect of the direction of the wind on the performance of the PV module is studied from the data of Hadley Solar Farm [17]. An increase in energy production by PV cells by 5.7% and a performance ratio of 3.4% has been observed in [18].

The effect of temperature and wind speed on the performance of photovoltaic modules has been extensively studied in the literature. Previous studies confirm that as

the temperature of a PV module increases, its efficiency decreases, leading to a reduction in power output. Research has also shown that wind plays a crucial role in cooling PV modules by enhancing convective heat transfer, which helps maintain a lower operating temperature and improves efficiency. However, most existing studies are based on controlled experimental conditions, where wind speeds are fixed, and do not fully account for the variability in real-world meteorological data. Additionally, while some studies focus on the technical performance of PV modules, limited work has been done to assess the economic implications, such as the Levelized Cost of Energy (LCOE) and tariff estimations, which are essential for evaluating the feasibility of solar energy projects.

Another key limitation in prior research is the use of Global Horizontal Irradiance (GHI) instead of Plane of Array Irradiance (POA-Irradiance), which is required by IEC TS 61724-2:2016 for accurate PV thermal modeling. In this study, a comprehensive analysis is conducted to assess the combined effects of wind speed and temperature on the performance of PV modules using actual meteorological data from Khuzdar, Pakistan. The study evaluates both the technical and economic aspects of PV performance, incorporating POA-Irradiance to ensure compliance with IEC standards. The findings provide a detailed assessment of how wind cooling impacts the overall efficiency, capacity factor, and energy generation of PV modules while also examining the economic benefits of improved performance. This research contributes to the optimization of PV system design in hot and dry regions where wind conditions can significantly

influence system performance and financial viability.

2. Methodology

2.1 Selection of Manufacturer

Table 1 tabulates the location, PV module, and its assigned rated power.

Table 1. Assigned Parameters

Location	Khuzdar
PV Module	Copper Indium Gallium Selenide
Rated Power	305W
Capacity	50kW

Table 2 lists the manufacturers of Copper Indium Gallium Selenide (CIGS), a thin-film photovoltaic technology, with rated power as assigned. The PV module is selected based on its highest efficiency and minimum power coefficient. Thin-film solar panels behave differently than crystalline silicon panels, especially in terms of efficiency, temperature dependence, and degradation. They typically have a lower temperature coefficient compared to crystalline silicon PV cells. The chosen manufacturer is highlighted in Table 2.

Table 2. Selection of Manufacturer.

Manufacturers	Efficiency (%)	Normal Operating	Temperature
		Conditions of Temperature (NOCT) (°C)	Coefficient of Powers (%/K)
Run Tech China	17	40	-0.45
Solar Tech Power	13.2	42	-0.43
Ji'nan Linquan Industry	14	41-43	-0.45
Global Solar	13.5	45	-0.43
SINOLTECH	17	45	-0.40

The bar chart is also plotted to determine the optimum manufacturer, i.e., the PV cell with the lowest power coefficient and highest efficiency. The plot is depicted in Figure 1.

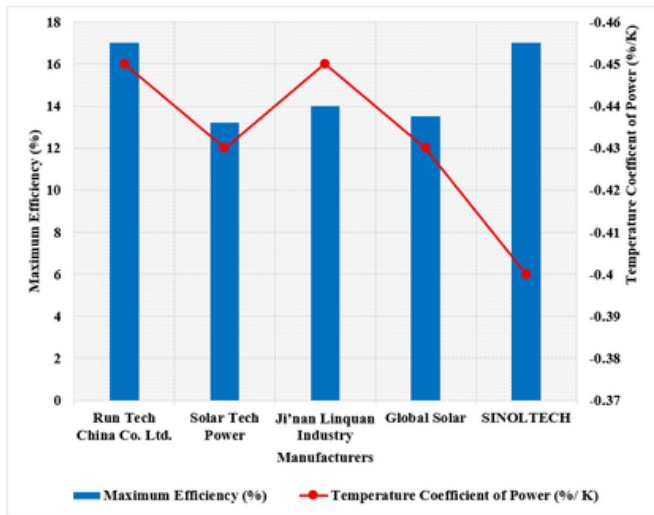


Figure 1. Selection of Manufacturer.

The weather data provided is not uniform, i.e., the values have been missing for some years. We must select the data that has all the hourly measured values. We measured the values for each year and found out which of the year's data was complete. The following quality checks, based on [19-22], were applied to the hourly data to ensure accuracy and consistency.

1. $0.03GHI_{toa} < GHI < \min(1.2I_o, 1.5I_o \cos(SZA)^{1.2} + 100)$
2. $2.0 < BNI < I_o$
3. $-90 < Temp < +60$
4. Maximum steps for two consecutive temperature values should be less than $8^{\circ}C$
5. $5.0 < Hum < 100$
6. Maximum steps for two consecutive relative humidity values should be less than 30%.
7. Maximum steps for two consecutive wind speeds should be less than $15ms^{-1}$.
8. Consistency Check i.e. for $GHI > 20Wm^{-2}$, $GHI/(BHI + DHI) = 0.15$ and this test is not possible if $GHI < 20Wm^{-2}$.

Where,

GHI_{toa} = Horizontal irradiance at the top of the atmosphere

BHI = Beam horizontal irradiance

I_o = Normal irradiance at the top of the atmosphere

SZA = Solar zenith angle (rad)

The data given is used to assess the quality of the above criteria. The data for the year 2016 fulfils the requirements, so it is utilized in the calculations.

2.2 Mathematical Modeling

For the mathematical modeling of the system, instead of GHI, the plane of array irradiance (POA) is used, which covers the slope of the PV panel. The slope PV panel is considered the same as the latitude. Detailed modeling is described below. To calculate the plate temperature without considering wind effects, equation 1 is used [23].

T_p , T_a , and T_{NOCT} are the panel ambient and normal operating cell temperatures, respectively, and POA is the plane of array irradiance. The temperature of the PV module considering the wind flowing at the speed of " v " ms^{-1} can be calculated from equation 2 [24].

The actual efficiency of the PV module having the reference efficiency η_r at STC and power coefficient β can be calculated from equation 3 obtained from [13]. The reference efficiency and the power coefficient are taken from the manufacturer's datasheet.

The energy generation without considering the wind effects can be calculated from Equation 4 [25].

The performance ratio (PR) can be calculated using Equation 5 [26].

Where E_{STC} is the energy obtained from the PV cell at STC.

The annual energy gain (AEG) can be obtained from equation 6 [25].

3. Results

3.1 Metrological Data

The hourly weather data for Khuzdar, Pakistan, is taken from the National Solar Radiation Database [27]. First, that data is converted into daily data by taking the average for the whole day. The irradiance data, ambient temperature, wind speed, and relative humidity are also plotted and given in Figures 3, 4, and 5, respectively. The plots show the data for each day of the year 2016.

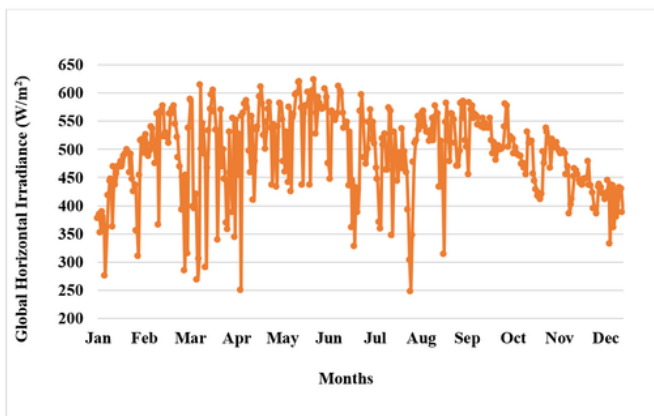


Figure 2. Global Horizontal Irradiance.

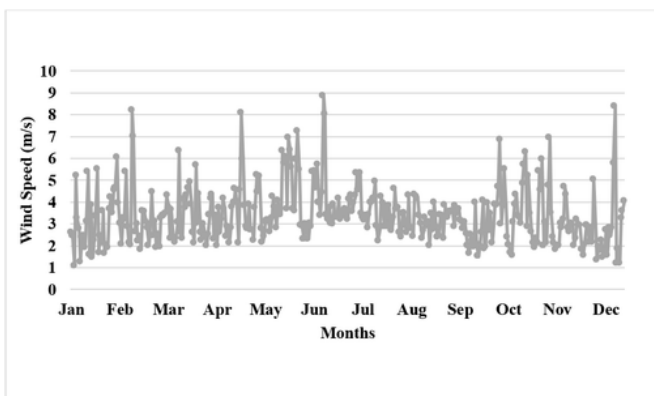


Figure 3. Wind Speed.

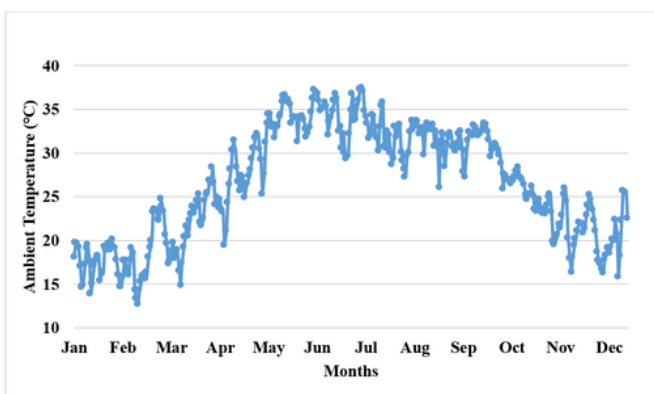


Figure 4. Ambient Temperature.

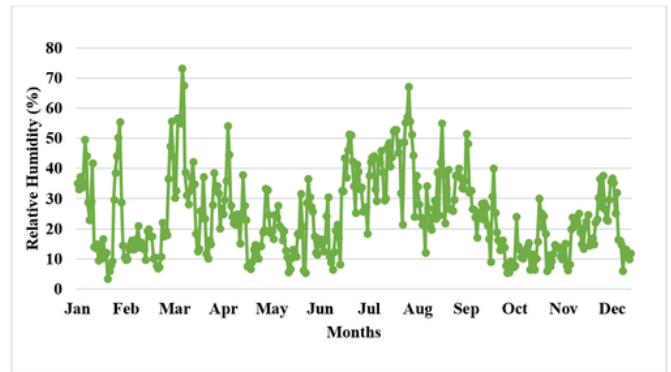


Figure 5. Relative Humidity.

3.2 PV Panel's Performance Analysis

The PV module temperature was calculated using hourly weather data for the entire year. Figure 6 compares the module temperature with and without wind effects, showing that the temperature is consistently lower when wind is considered. This happens because wind increases heat loss through convection, helping to cool the module. Since the convective heat transfer coefficient depends on wind speed, higher wind speeds lead to more efficient cooling. As a result, the module loses heat faster, keeping its temperature lower and improving overall performance.

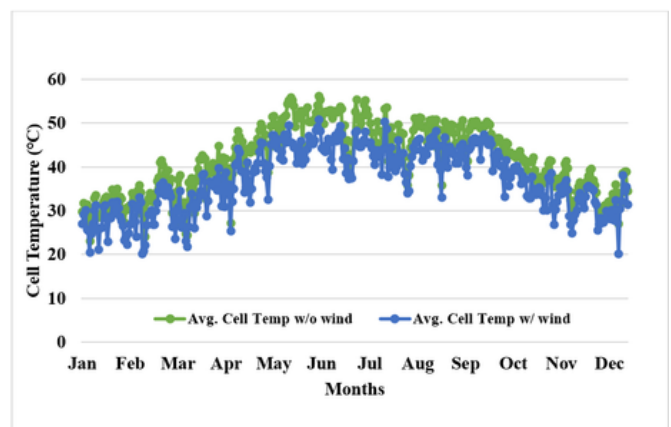


Figure 6. Average cell temperature without (w/o) and with (w/) wind effects.

The impact of module temperature on solar cell efficiency was analyzed, and the results for the entire year are shown in Figure 7. The graph clearly illustrates that as temperature increases, efficiency decreases, which is consistent with

previous studies. To understand the role of wind, Figure 8 compares efficiency with and without wind effects. The results show that wind helps improve efficiency by cooling the PV module, reducing its operating temperature. This cooling effect minimizes heat-related efficiency losses, leading to better overall performance throughout the year.

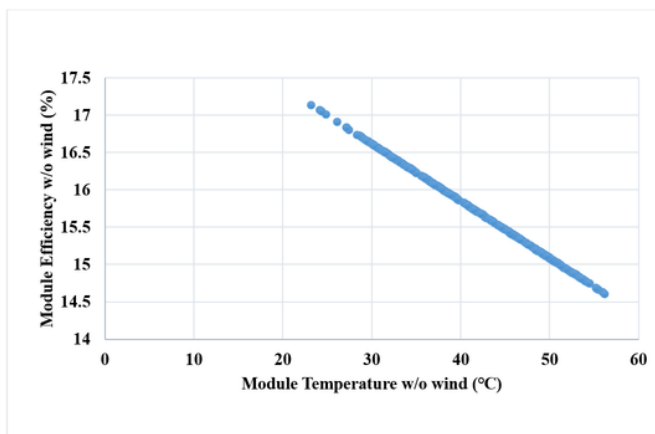


Figure 7. Effect of module temperature on module efficiency without (w/o) wind effect.

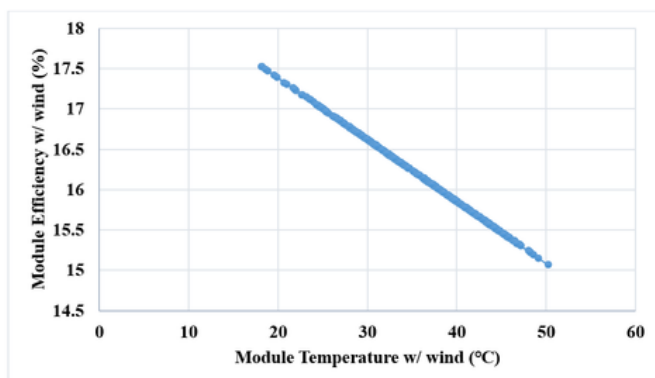


Figure 8. Effect of module temperature on module efficiency with (w/) wind effect.

To understand how wind speed affects solar cell efficiency, Figure 9 compares PV efficiency throughout the year with and without wind effects. The results show that efficiency drops between April and October, which corresponds to the hot summer months in Khuzdar, Baluchistan, Pakistan. Higher temperatures during this period cause the modules to heat up, reducing efficiency. However, the figure also shows that efficiency is consistently higher when

wind effects are considered, confirming that wind helps cool the modules and minimize efficiency losses caused by high temperatures.

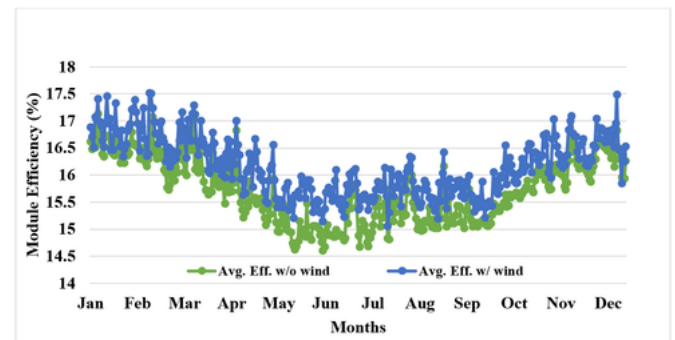


Figure 9. Module efficiency without (w/o) and with (w/) wind effect.

The energy generated by the solar cell was calculated using the given equations and analyzed with and without wind effects, as shown in Figure 10. The results clearly show that energy generation is higher when wind cooling is considered. Since PV module temperature directly affects efficiency, higher temperatures lead to reduced power output. The modeling results confirm that wind helps lower module temperatures, improving overall energy production. This effect is most noticeable during the hot summer months when high ambient temperatures would otherwise cause significant efficiency losses. By enhancing convective cooling, wind prevents excessive heating of the module, leading to greater energy generation compared to still-air conditions.

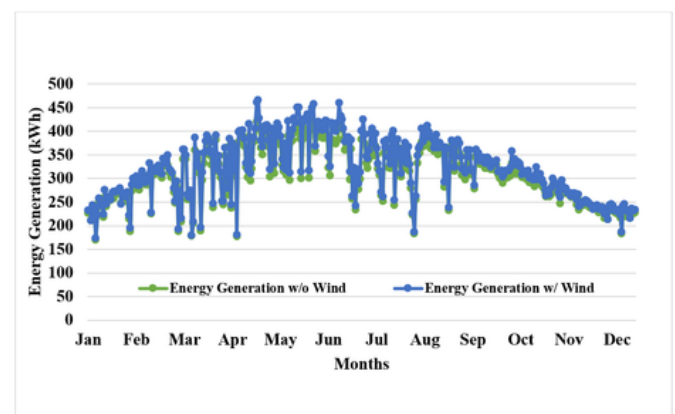


Figure 10. Energy generation without (w/o) and with (w/o) wind effect.

The performance ratio (PR) of the solar cell was calculated and analyzed with and without wind effects, as shown in Figure 11. The results show that PR is consistently higher when wind is considered, highlighting the role of convective cooling in improving PV performance. The performance ratio measures how efficiently a solar module converts available sunlight into usable energy, relative to its theoretical output under standard test conditions (STC). Since higher temperatures reduce energy generation, modules operating without wind experience greater efficiency losses. In this study, each 1°C rise in temperature led to a 0.45% decrease in energy output, which lowers the performance ratio in windless conditions. Wind helps offset these losses by keeping module temperatures lower, ultimately enhancing system efficiency and reliability.

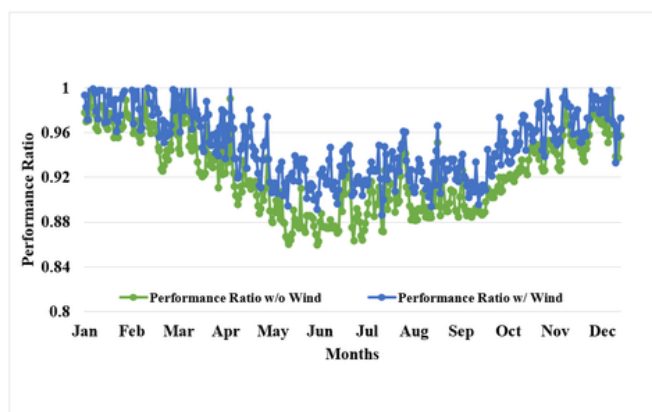


Figure 11. Performance Ratio without (w/o) and wind (w/) wind effect.

The impact of module temperature on the performance ratio (PR) of the PV cell was analyzed with and without wind effects over a year, as shown in Figure 12 and 13. The results clearly show that PR decreases as module temperature increases, which is expected since higher temperatures reduce solar cell efficiency. The performance ratio compares the actual energy generated to the theoretical energy output under STC, with STC values taken from the

manufacturers data sheet. Since energy generation is affected by both temperature and wind speed, modules operating without wind experience higher temperatures, leading to greater efficiency losses and a lower PR. These findings highlight the role of wind in cooling PV modules, helping to reduce thermal losses and improve overall performance.

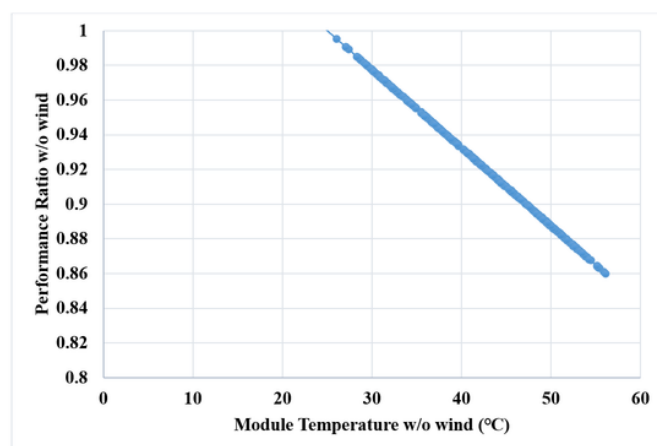


Figure 12. Effect of module temperature on performance ratio without (w/o) wind effect.

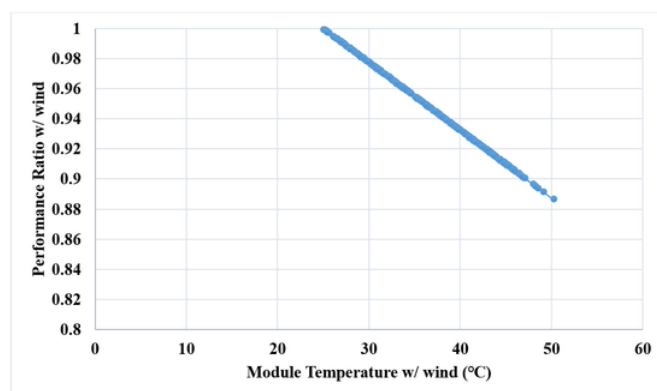


Figure 13. Effect of module temperature on performance ratio with (w/) wind effect.

Annual Energy Generation and capacity factor can be calculated from the above-mentioned relations.

Annual Energy Generation (AEG) without wind for daily basis calculation = 112.57MWh

Annual Energy Generation (AEG) with wind for daily basis calculation = 116.402MWh

Annual Increase in energy generation considering the wind effects = 3.832MWh

city Factor Without Wind
 $=112571460.7/(50000 \times 365 \times 24) = 25.70$
 CapacitFactorrr WithouWind
 $=116402616.1/(50000 \times 365 \times 24) = 26.58$
 Increase in capacity factor by considering
 the air = 0.88

3.3 Levelized Cost of Energy

The Levelized Cost of Energy (LCOE) represents the cost of electricity production over the operational lifetime of the energy system, typically corresponding to the plant's warranty period. In this study, LCOE is used to evaluate the cost of solar energy generation over 25 years. The calculation requires two main parameters: the total system cost, which includes both capital and operational expenses, and the total energy output over the plant's lifetime, considering efficiency losses and system degradation. The total system cost includes expenses related to solar panels, mounting structures, land acquisition, installation, and electrical infrastructure. In this case, the solar power plant is designed for a 50-kW capacity, using Copper Indium Gallium Selenide (CIGS) PV modules with a rated power of 305 W per panel, requiring 164 panels to meet the target capacity. The price of a 305 W CIGS solar panel in Pakistan is Rs. 20,000 per unit, resulting in a total module cost of Rs. 3,280,000. To support the panels, two stands per panel are required, with each stand costing Rs. 700, leading to a total expenditure of Rs. 229,600 for mounting structures.

Land acquisition is a significant component of the cost. Each panel covers 1.65 m², but additional space is required for system components, bringing the total land area needed to 300 m². Given that land in Khuzdar costs Rs. 2,000,000 per m², the total land cost amounts to Rs. 600,000,000. Other infrastructure-related costs, including installation, labor, and electrical

connections, are estimated at Rs. 50,000,000. Additionally, inverters for the system are expected to cost Rs. 500,000. The tariff structure for the assigned power capacity of the plant is based on publicly available documents detailing tariff rates for existing solar plants in Pakistan, referenced in [28]. Since solar power plants have no fuel costs, ongoing operational expenses remain low, primarily consisting of maintenance and occasional component replacements. The detailed LCOE calculations are presented in Table 3, summarizing the overall cost structure and projected energy output over the plant's lifetime.

Table 3. Calculation of LCOE

Cost of Panels	Rs. 3,280,000/-
Cost of Land	Rs. 2,000,000/-
Cost of Inverters	Rs. 500,000/-
Cost of Stands	Rs. 229,600/-
Extras	Rs. 5,000,000/-
Total Capital Cost	Rs. 11,009,600/-
Average Discount rate	10%
Tariff rate	Rs. 8.6065/kWh
O & M Rate	Rs. 2.5797/kWh
Insurance	Rs. 1.0081/kWh
Levelized Cost of Energy	Rs. 9.16596/kWh

3.4 Social, Economic, and Environmental Benefits of Solar Energy

Solar energy is abundant and sustainable, making it a viable option for electricity generation in Pakistan. The assigned location receives substantial solar radiation, sufficient to support multiple solar power plants. One of the primary advantages of solar energy is its potential to reduce electricity costs, as solar-generated power is cheaper than conventional sources such as coal and hydroelectric power. With solar panel installations, households and industries can generate their own electricity, leading to lower utility bills and greater energy independence. Additionally, solar power plants have minimal operational costs after installation, primarily limited to staff salaries and scheduled maintenance. Selling surplus electricity to industries can

further improve financial returns, making solar energy a profitable long-term investment.

For a developing country like Pakistan, transitioning to solar energy is crucial for addressing energy crises and fostering economic growth. Solar energy projects create employment opportunities, with an estimated 200-300 jobs generated annually per installation. Furthermore, expanding solar power production contributes to GDP growth by reducing reliance on imported fossil fuels and stabilizing the electricity supply for industries and businesses. From an environmental perspective, solar energy significantly reduces greenhouse gas emissions. Unlike fossil fuels, solar power does not produce carbon dioxide (CO₂), nitrogen oxides (NO_x), or sulfur dioxide (SO₂), which contribute to global warming and air pollution. Studies indicate that solar power plants can prevent the emission of approximately 1.4 kg of CO₂ per kWh of electricity generated [29]. Additionally, integrating solar energy into the national grid can reduce the need for extensive transmission infrastructure and help preserve water resources, which are often depleted by conventional power plants.

Despite these benefits, solar power technology has some challenges. The manufacturing of photovoltaic (PV) cells involves toxic chemicals, and certain solar thermal power plants use hazardous heat-transfer fluids, which pose environmental risks if leaked. Proper disposal and recycling of solar panels at the end of their lifespan remain critical concerns. Beyond economic and environmental aspects, solar energy can improve the quality of life in regions like Khuzdar, Pakistan, where the Life Quality Index (LQI) and Human Development Index (HDI) are significantly low. The LQI of Khuzdar is 0.33, while its HDI is approximately 0.299, reflecting

limited access to essential services, low life expectancy, and poor economic conditions. Expanding solar energy in such regions can enhance air quality, provide reliable electricity, and support local industries, ultimately improving living standards. In summary, investing in solar energy in Pakistan offers multiple advantages, including lower electricity costs, reduced greenhouse gas emissions, job creation, and improved energy security. While some environmental challenges exist, they are manageable with proper regulations and disposal practices. Given its potential to support economic growth and environmental sustainability, solar energy should be a key focus for Pakistan's energy transition strategy.

4. Conclusion

This research presents a comprehensive investigation of the impacts of ambient temperature and wind speed on the performance of PV cells in Khuzdar, Baluchistan. The study showed the importance of wind speed in increasing PV performance via reduced losses caused by high module temperatures due to convective heat transfer. In particular, the efficiency of the PV module falls by 0.45% with the rise in temperature for each additional degree Celsius, which confirms the relevance of temperature regulation in reaching the maximum potential of PV systems. The comparison of the cases with and without considering the wind effect showed that wind increases the capacity factor from 25.70 to 26.58 and, thus, enhances the system's general performance. Besides the technical performance of the solar plant, this study also assesses the levelized cost of electricity and tariffs for solar power based on NEPRA numbers. Moreover, the assessment of social and environmental

impacts makes it evident that harnessing solar energy can help achieve the sustainable development goal of combating climate change by discontinuing greenhouse gas emissions while assisting customers to access affordable energy goods and services. In conclusion, with the results of studying the possibility of integrating wind into PV system design, the findings indicate that it is possible to enhance both the efficiency of solar panels and the economic profitability of their use in regions where wind conditions are like Khuzdar's.

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Imtiaz Ul Hasan received his M.Sc. degree in Chemical Engineering from KFUPM, Saudi Arabia. His research interests include heterogeneous catalysis, renewable energy, process simulation, carbon capture, and sustainable fuel production. He has authored and co-authored several peer-reviewed publications in catalysis, clean energy, and process engineering and has presented his research at international conferences.

Qamar Abbas received his M.Sc. degree in Mechanical Engineering from KFUPM, Saudi Arabia. His research interests include photovoltaic systems, renewable energy, thermal engineering, heat transfer, and energy system performance analysis. He has authored and co-authored several peer-reviewed publications in solar energy, thermal management, and photovoltaic technologies.

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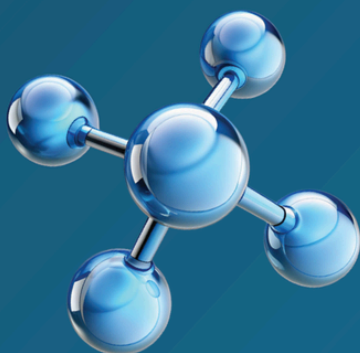


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Microbial and Mineral Fouling of Reverse Osmosis Membranes in Gas Plants: Insights from Rietveld XRD and MIC Diagnostics

Husam S. Khanfar*, Husin Sitepu, Ibrahim Al-Zahrani, Wala Algozeeb
Research and Analytical Services Department, Saudi Aramco, P.O. Box 62, Dhahran
31311, Kingdom of Saudi Arabia

*Corresponding authors: husam.khanfar@aramco.com

1. Abstract

Reverse osmosis (RO) membranes are prone to prematurely fouling in gas plant water utilities but the joint mechanisms of mineral scales and microbes are not yet well understood for this operation context. In this study, the mechanisms for physical, chemical and microbiological fouling of RO membranes from Saudi Aramco facilities were evaluated, to design efficient combined monitoring and control solutions. Fouled and virgin membranes were characterized using environmental scanning electron microscopy with energy-dispersive X-ray spectroscopy (ESEM-EDS), Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), Rietveld-based X-ray diffraction (XRD) and microbial culture and quantitative Polymerase chain reaction (qPCR).

Fouled membranes exhibited up to 130 wt% increase of weight, predominantly formed by calcium carbonate deposits of calcite phase on internal membrane surfaces.

Calcium carbonate (Ca-C-O) as a typical dense scale was identified by ESEM-EDS. TGA analyses indicated significant amount of inorganic residues of the foulants. High Microbial cell densities, up to 10^5 cells/cm², composed of a variety of bacterial and archaeal species (including some

acid-producing and iron-oxidizing types) was observed. Significant correlation existed between microbial load and mineral scales accumulation.

Such correlation suggested a feed forward role of the microbial contamination by favoring an environment conducive for inorganic scaling, that leads to a synergistic fouling scenario.

Based on this multidisciplinary understanding, integrated Fouling Monitoring and Mitigation strategies should be developed in RO systems to enhance system reliability and reduce operational costs.

2. Introduction

The intersection of microbiologically influenced corrosion (MIC)^{1,2} and quantitative phase analysis of X-ray diffraction (XRD) data via the Rietveld method³⁻⁹ has emerged as a critical research area in industrial reliability, especially within the oil and gas sector. MIC poses increasing threats to equipment integrity, operational safety, and cost-efficiency. Identifying and characterizing microbial communities that induce corrosion is essential for developing effective mitigation strategies.

Previous investigations into deposits from crude coolers and reboilers at a Saudi

Aramco refinery revealed significant correlations between microbial activity and material degradation. Key microbial contributors included sulfate-reducing bacteria (SRB) and iron-oxidizing bacteria (IOB). Deposits contained microbial loads up to 10^3 cells/L in crude cooler samples and over 10^3 cells/g in reboiler samples. Complementary Rietveld analysis identified crystalline phases such as anhydrite, calcite, dolomite, and quartz, critical to understanding both chemical and microbial degradation pathways.

These findings have informed predictive maintenance strategies and enhanced asset reliability in refinery and gas plant operations¹⁰⁻¹³.

Reverse Osmosis (RO) and Biofouling in Harsh Environments

Similar to MIC challenges in refinery equipment, reverse osmosis (RO) membranes used in gas plants face persistent fouling issues. In water-scarce regions such as the Arabian Gulf, desalination by RO is vital for industrial and domestic water supply. The reliance on desalinated water for oilfield operations, including enhanced oil recovery, underscores the importance of maintaining RO membrane integrity.

Despite technological advances, RO membranes remain vulnerable to fouling—a multifactorial phenomenon involving physical, chemical, and biological factors. Biofouling accounts for over 45% of membrane fouling incidents^{14,15}, causing increased pressure drop, decreased permeate quality, and frequent maintenance, ultimately impacting process efficiency and costs.

Balancing microbial colonization with membrane performance requires detailed diagnostic approaches. Comprehensive

evaluation of fouled membranes enables identification of root failure causes, informing cleaning protocols, operational modifications, and replacement schedules¹⁶⁻¹⁸

Linking MIC and RO Fouling Mechanisms

Building on previous MIC studies, this research extends the analytical framework to investigate membrane fouling in gas plant RO systems. The integrated approach combining microbiological analysis and phase characterization offers a holistic understanding of failure mechanisms and supports development of tailored mitigation strategies.

3. Experimental Work

The below comprehensive experimental methods, which are described in turn, support the study's goals by delivering the findings obtained from the:

1. Quantifying microbial colonization and biofouling mechanisms
2. Identifying crystalline and elemental foulants affecting membrane performance
3. Assessing structural and chemical integrity of prematurely failed membranes
4. Linking feed water chemistry to fouling patterns
5. Developing a diagnostic framework to mitigate MIC and scaling

Subsequently, these data along with the reproducibility experimental results provide collectively a holistic understanding of RO membrane degradation under gas plant operational conditions.

3.1 Reverse Osmosis Membranes

Eight spiral-wound RO membrane elements were collected from four Saudi Aramco-operated water treatment plants. Membranes were selected due to premature failure, defined by an operational life of less than one year, accompanied by

increased differential pressure, reduced product flow, and elevated permeate conductivity.

Four virgin (unused) membrane elements and corresponding feed water samples from the same plants served as controls. All membranes were polyamide-based, operated under standardized conditions: 80% recovery and antiscalant dosing (3–5 ppm) per manufacturer guidelines.

Each fouled membrane underwent systematic external visual inspection, autopsy, internal structural evaluation, and integrity testing. Virgin membranes provided baseline references.

3.2 External Visual Inspection

A detailed visual inspection assessed physical features such as weight, dimensions, color, and surface texture, alongside external damage signs—cracking, discoloration, abrasion—on the fiberglass casing, O-rings, and ports. Observations were compared to virgin membranes.

3.3 Internal Inspection and Membrane Autopsy

Membrane autopsy involved removing anti-telescoping devices (ATDs), longitudinally cutting the fiberglass casing, and aseptically unrolling membrane sheets to minimize contamination.

Assessed parameters included:

- Number and arrangement of membrane sheets and spacers
- Sheet dimensions and glue-line integrity
- Texture, odor, and appearance
- Nature and distribution of surface deposits

3.4 Membrane Material Integrity Testing

Square samples (5 × 5 cm) from membrane sheets and spacers were excised aseptically for chemical and material characterization.

3.4.1 Fujiwara Test

Used to detect chemical damage, particularly from oxidizing agents like chlorine, performed on fouled, virgin, and sodium hypochlorite-treated membranes¹⁹.

3.5 Spectroscopic and Thermal Analyses

3.5.1 Environmental Scanning Electron Microscopy and Energy-Dispersive X-ray Spectroscopy (ESEM–EDS)

Surface morphology and elemental composition of membranes and deposits were examined via ESEM at 20 kV, 0.23 Torr (low vacuum). EDS mapping identified foulant composition.

3.5.2 Fourier Transform Infrared Spectroscopy (FTIR)

FTIR spectra were collected over 4000–700 cm^{−1} (128 scans, 4 cm^{−1} resolution) to detect functional group changes between fouled and virgin membranes.

3.5.3 Thermogravimetric Analysis (TGA)

TGA was performed from 25°C to 900°C at 20°C/min under ambient air to assess thermal stability and foulant composition.

3.6 Foulant Characterization

3.6.1 X-ray Powder Diffraction (XRD)

Crystalline phases were analyzed using a PANalytical X'Pert PRO diffractometer (CoK α radiation)^{2,19,12,20}. Patterns were interpreted with HighScore Plus and ICDD-PDF-4+ databases²¹ to identify mineral phases including polymorphs of calcium carbonate^{3–9}.

3.6.2 Microbiological Investigation (qPCR)

Quantitative PCR targeting 16S rRNA gene regions quantified microbial populations—total bacteria, archaea, acid-producing bacteria (APB), iron-oxidizing bacteria (IOB), sulfate-reducing bacteria (SRB)—on membranes and in feed water².

3.7 Feed Water Characterization

Feed water from each plant was analyzed for physicochemical parameters by ICP-OES and standard ASTM methods. Pretreatment processes (filtration, antiscalant dosing, disinfection) were noted. Water chemistry was correlated with fouling and scaling tendencies ²².

Collectively, these data provide a holistic understanding of RO membrane degradation under gas plant operational conditions.

4. Results

4.1 Physical Characteristics of Fouled RO Membranes

External Inspection and Weight Gain

Visual inspection of all membrane elements revealed no external damage—such as ruptures, discoloration, or cracks (Table 1). However, significant internal fouling was inferred from weight increases of up to 130% compared to virgin membranes, particularly in second-stage and tail-end modules.

Table 1.

External and internal physical characteristics of reverse osmosis (RO) membranes from different manufacturers used at water utility plants operated by Saudi Aramco.

RO element characteristics	Water utility plant											
	A				B			C		D		
Membrane number	1	2	3	4	5	6	7	8	9	10	11	12
RO Stage	1 st	2 nd	2 nd	-	1 st	1 st	-	2 nd	-	1 st	1 st	-
Location	Tail	Front	Tail	New	Front	Tail	New	Tail	New	Front	Tail	New
Weight (Kg)	22.9	32.4	33.3	13.9	19.2	24.7	14.4	21.8	14.5	15.3	19.4	13.2
External Abnormality	No	No	No	No	No	No	No	No	No	No	No	No
Number of membrane sheets	20	20	20	20	20	20	20	26	26	25	25	25
Sheet size (cm)	103 x 95	103 x 95	103 x 95	103 x 95	103 x 95	103 x 95	103 x 95	97 x 80	97 x 80	97 x 85	97 x 85	97 x 85
Internal feature	Thick layer of white rough scales				Layer of white rough scales			Layer of white rough scales		Layer of white rough scales		

Key site-specific weight increases:

- Plant A: Second-stage membranes up to 130% heavier.
- Plant B: Tail-end membrane 72% heavier than virgin equivalent.
- Plant C: Second-stage tail membrane 50% heavier.
- Plant D: Tail element 47% heavier than its front counterpart.

These trends are consistent with flow dynamics and concentration polarization, where later-stage membranes face higher fouling risks.

Internal Observations

Internal autopsies revealed:

- Thick, white, rough deposits on membrane surfaces and feed spacers in all fouled elements.
- Variations in sheet count and sheet dimensions by manufacturer.
- No signs of biofilm slime or odor.
- Irregular glue application (2–6 cm) across some units, suggesting variable manufacturing quality.

These findings indicate inorganic fouling as the dominant mechanism, with possible compounding effects from manufacturing inconsistencies.

4.2 Chemical Stability of Membranes: Fujiwara Integrity Test

The Fujiwara test was performed to detect oxidative degradation of the polyamide membrane layer. No red coloration (indicative of N-chlorinated polymers) was observed in any fouled samples, in contrast to positive controls treated with sodium hypochlorite.

This confirms:

- 1.No chemical damage from oxidizing agents.
- 2.Membrane degradation is not due to chlorination, but due to external fouling layers.

4.3 Microstructural and Elemental Analysis (ESEM-EDS)

Surface Morphology

Environmental SEM images revealed rosette-shaped crystalline deposits across all fouled membranes, regardless of plant origin, suggesting a uniform mineral scaling mechanism (Fig. 1).

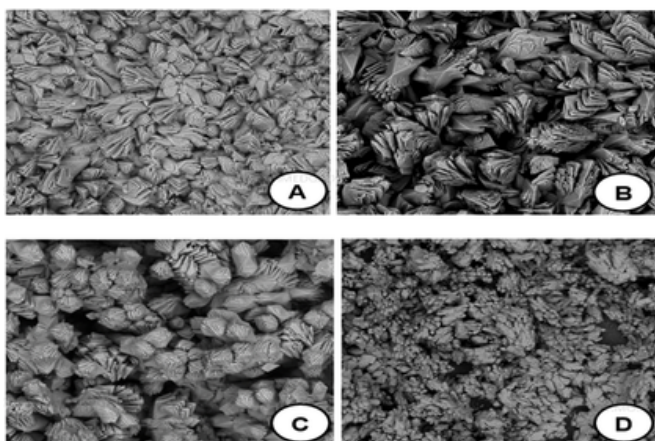


Figure 1. ESEM micrographs showing rosette-shaped crystalline deposits on fouled reverse osmosis membranes from utility Plant A (A), Plant B (B), Plant C (C), and Plant D (D).

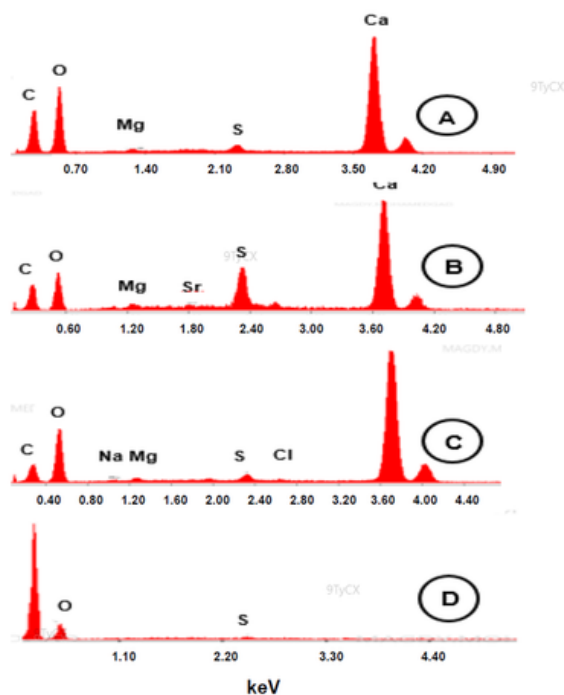


Figure 2. EDS spectra showing elemental composition of fouling materials on reverse osmosis membranes from Plant A (A), Plant B (B), Plant C (C), and comparison with a virgin (reference) membrane (D).

Elemental Composition

EDS spectra showed deposits composed primarily of **calcium (Ca)**, **carbon (C)**, and **oxygen (O)**—consistent with **calcium carbonate**. Trace amounts of magnesium (Mg), sodium (Na), sulfur (S), and strontium (Sr) were also present, suggesting **co-precipitation** of minor elements (see Figure 2). Cross-sectional ESEM-EDS confirmed:

- No delamination or thinning of membrane structure.
- Uniform deposition patterns, except for localized sulfur enrichment in one membrane (Sample 3).

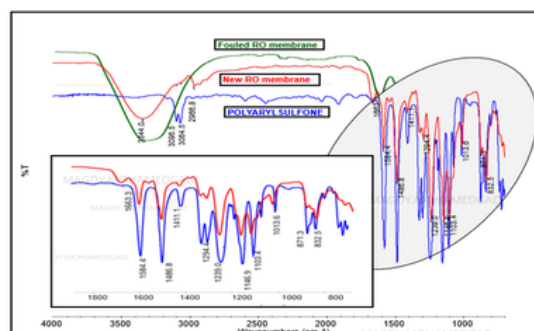


Figure 3. FTIR spectra of the upper and lower layers of a new RO membrane showing sulfonated polysulfone structure.

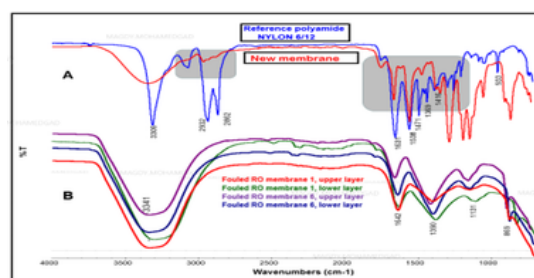


Figure 4. Comparison of FTIR spectra between new and fouled membrane layers highlighting polyamide-associated peaks and chemical modifications.

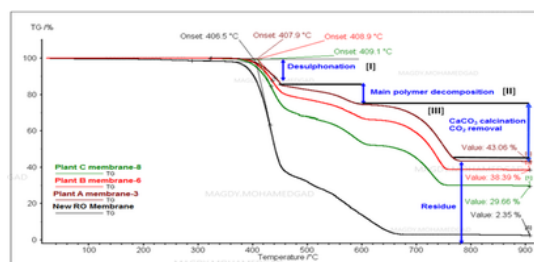


Figure 5. TGA curves of virgin and fouled RO membrane samples showing multi-stage decomposition patterns.

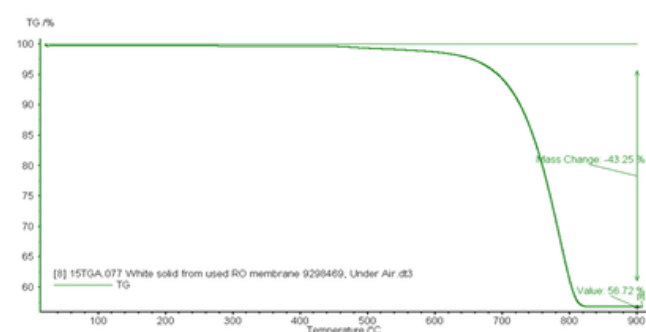


Figure 6. TGA curve of inorganic scale recovered from fouled membranes indicating high thermal residue.

Table 2. Summary of TGA decomposition stages and residual mass for virgin and fouled RO membranes.

Samples ID	TGA Results					
	t (°C)	Total weight loss @ 900°C (wt%)	Residue @ 900°C (wt%)	wt% loss due to desulfonation (380°C-460°C)	wt% loss due to CO ₂ release (600°C - 800°C)	Calculated CaCO ₃ (wt%)
New RO membrane	404.1	98	2	NA	NA	NA
Plant A membrane-3	413.9	57	43	11	30	68
Plant B membrane-6	405.5	62	38	14	31	70
Plant C membrane-8	406.5	70	30	22	26	59

4.4 FTIR Spectroscopy: Polymer Composition and Surface Changes

FTIR analysis confirmed the intact chemical structure of virgin membranes, with characteristic peaks for sulfonated polysulfone and trace polyamide coatings (Figs. 3–4). In fouled membranes, additional peaks and band broadening were observed, indicating:

- Presence of adsorbed organics and/or carbonate scale.
- No evidence of core polymer degradation.

4.5 Thermogravimetric Analysis (TGA)

TGA provided thermal decomposition profiles of both virgin and fouled membranes (Fig. 5, Table 2):

All four membranes exhibit excellent initial stability up to around 400°C, with minimal

weight loss. Virgin membranes showed 98% mass loss, with minimal residue. It also exhibits the highest thermal stability, with a higher onset temperature for desulphonation and main polymer decomposition. Fouled membranes retained up to 43% residue, confirming significant inorganic scale content. The distinct decomposition stages matched carbonate decomposition temperatures ($\geq 600^\circ\text{C}$), supporting CaCO_3 identification. Moreover, isolated scale samples exhibited similar thermal behavior, further validating the presence of carbonate-based fouling (Fig. 6).

The TGA results suggest that the New RO Membrane exhibits the highest thermal stability, followed by Plant C membrane-8 and Plant B membrane-6, and then Plant A membrane-3. These findings can inform the selection and application of these membranes in various industrial processes.

4.6 Microbial Profiling by qPCR

Quantitative PCR revealed:

- Feed water had bacterial counts of 10^3 – 10^4 cells/mL; archaea were 10^1 – 10^2 cells/mL.
- Fouled membranes had 10–100x higher microbial loads, with 10^4 – 10^5 bacteria/cm² and up to 10^3 archaea/cm².
- Virgin membranes showed minimal contamination.

Functionally relevant microbial groups included:

- Acid-producing bacteria (APB)
- Iron-oxidizing bacteria (IOB)
- Sulfate-reducing bacteria (SRB) and archaea (SRA)

These microbes likely contributed to biofilm initiation and mineral deposition, even in the absence of visible biofilms (Fig. 7).

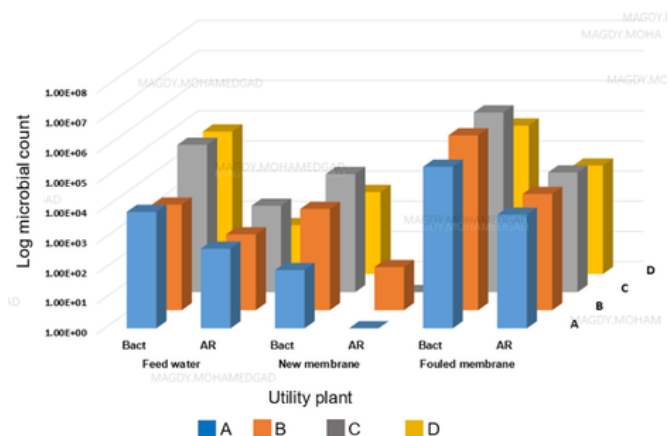


Figure 7. Microbial load (cells/mL or cells/cm²) in feed water, fouled, and virgin RO membranes across all utility plants, as determined by qPCR.

4.7 Feed Water Chemistry

All feed waters were classified as brackish, with TDS ranging from ~950 to 1700 mg/L (Table 3). Common features across plants:

- Alkaline pH (7.7–8.2)
- Elevated calcium (106–199 mg/L) and bicarbonate (204–520 mg/L) — conducive to calcite scaling
- High sulfate in Plant D (720 mg/L) — potential support for SRB activity

Despite low salinity, these ionic profiles support a geochemical environment favorable to CaCO₃ precipitation and microbial colonization.

Table 3. Physicochemical composition of pretreated feed water from different utility plants.

Parameter	Unit	Plant A	Plant B	Plant C	Plant D
Bicarbonate	mg/L	204	246	520	282
Carbonate	mg/L	0	0	0	0
Hydroxide	mg/L	0	0	0	0
Barium	mg/L	<1	<1	<1	<1
Calcium	mg/L	111	122	106	199
Chloride	mg/L	314	328	318	282
Potassium (# excluded from TDS)	mg/L	12	15	10	17
Magnesium	mg/L	42	48	56	53
Sodium	mg/L	158	179	151	135
Silicon	mg/L	9	9	7	8
Sulfate	mg/L	240	250	318	720
Strontium	mg/L	2	2	2	2
Total Phosphorus	mg/L	<1	<1	<1	<1
pH	—	7.8	8.0	8.2	7.7
Total Dissolved Solids (TDS)*	mg/L	1,069	948	1,459	1,671
Conductivity	µS/cm	1,763	1,464	1,653	3,112
Specific Gravity	g/cm ³	1.0001	1.0007	1.0002	1.0005

*Note: Potassium not included in TDS.

4.8 X-ray Diffraction (XRD) Analysis

XRD identified **calcite (CaCO₃)** as the **sole crystalline** phase in fouling deposits across all membranes (Fig. 8). No gypsum or silica was detected.

Refined crystal parameters:

·a = b = 4.988 Å; c = 17.068 Å

·Space group: R-3c

These results confirm **feed water-derived scaling**, aligned with ESEM-EDS and TGA data, and support a **universal fouling mechanism** across plant sites.

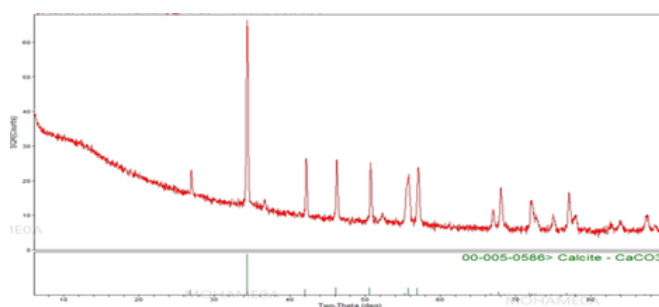


Figure 8. X-ray diffraction pattern of the crystalline scale recovered from fouled RO membranes. The sharp peaks correspond to calcium carbonate in the form calcite (CaCO₃), confirming its presence as the dominant mineral phase. Calcite was identified by its characteristic hexagonal crystal structure, classified within the space group R-3c (No. 167). The refined lattice parameters were: a = b = 4.988 Å, c = 17.068 Å, α = β = 90°, γ = 120°. These values are consistent with standard crystallographic references.^{7,8,23,25} The source of calcium (Ca) in the scale formation was attributed to the feed water.

5. Discussion

The findings from this study provide a comprehensive understanding of membrane fouling mechanisms, emphasizing the predominance of calcium carbonate scaling as the primary factor leading to membrane failure. Notably, the membrane materials themselves remained chemically and structurally unaltered throughout the process, indicating that fouling was

predominantly external. An integrated diagnostic approach—comprising autopsies, chemical assays, and microbiological analyses—facilitated a multi-dimensional assessment of fouling progression, revealing the complex interplay between inorganic deposits and microbial activity.

The characterization techniques, including X-ray diffraction (XRD), environmental scanning electron microscopy with energy dispersive spectroscopy (ESEM-EDS), and thermogravimetric analysis (TGA), consistently identified calcite as the principal foulant. The water chemistry profile—particularly alkaline pH, elevated calcium (Ca^{2+}), and bicarbonate (HCO_3^-) concentrations—created favorable conditions for calcium carbonate nucleation and crystal growth. This phenomenon was most pronounced in the tail-end and second-stage membranes, consistent with the effects of concentration polarization that amplify mineral precipitation at these locations.

Microbial contributions, although not visually evident through biofilm formation, were significant. Quantitative assessments indicated higher microbial populations on fouled membranes, including aerobic and anaerobic bacteria such as aerobic plate bacteria (APB), iron-oxidizing bacteria (IOB), sulfate-reducing bacteria (SRB), and sulfate-reducing archaea (SRA). These microorganisms are known to influence local pH fluctuations, ion exchange processes, and nucleation sites, thereby facilitating calcite deposition. It is plausible that a bio-mineral feedback loop exists wherein microbial activity promotes mineral scaling, which subsequently enhances microbial retention and proliferation.

Importantly, membrane integrity assessments—via Fujiwara tests, Fourier-transform infrared spectroscopy (FTIR), and TGA—confirmed the absence of oxidative degradation or polymer breakdown. The fouling mass was external and did not compromise the membrane's polymer layers, indicating that the primary issue resides in external fouling management rather than intrinsic membrane material deterioration.

The root cause analysis points to feed water chemistry as a critical factor. Despite relatively low total dissolved solids (TDS), specific water profiles—characterized by high bicarbonate and calcium levels in certain plants—created supersaturation conditions conducive to mineral precipitation. The presence of sulfate further supported microbial activity, particularly sulfate-reducing microbes, which contribute to corrosive and fouling processes. These chemical and biological factors collectively fostered mineral deposition and microbial colonization on membrane surfaces.

In terms of operational implications, these insights necessitate a multidisciplinary approach to fouling mitigation. Strategies should include real-time monitoring of feed water chemistry and microbial indicators, optimized antiscalant dosing calibrated to feed variability, and the application of validated biocides to control microbial activity. Routine membrane autopsies and advanced diagnostics are also essential to detect early signs of fouling, enabling proactive intervention.

6. Conclusion

In conclusion, this study underscores the complex synergism between inorganic

scaling and microbial activity in RO membrane fouling. An integrated diagnostic framework—combining physical inspection, chemical analysis, and microbiological profiling—is vital for sustainable membrane operation. The findings highlight that calcite scaling is the dominant fouling mechanism, subtly amplified by microbial processes, with membrane materials remaining unaffected. Ultimately, feed water composition is central to fouling risk, and implementing systematic, interdisciplinary monitoring is crucial for preserving long-term membrane performance in industrial applications.”

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Authors

Dr. Husam S. Khanfar is a Senior Research Scientist at Saudi Aramco's Research and Analytical Services Department. He holds a Ph.D. and M.S. from the Arab University of Bahrain, where his research focused on microbiology-induced corrosion, and a B.Sc. from the University of Jordan. Dr. Khanfar specializes in materials characterization to support failure analysis investigations and catalyst development. He has authored and co-authored over 20 journal articles.

Dr. Husin Sitepu, recently retired from Saudi Aramco, is an expert in applied crystallography and diffraction science. His research focused on advanced materials characterization using XRF, XRD, and the Rietveld method, supporting catalyst development, QA/QC, and failure analysis. With 70+ publications, he holds a Ph.D. in Physics and is active in the International Center for Diffraction Data, International Union of Crystallography, and Neutron Scattering Society of America.

Ibrahim M. Al-Zahrani is a Senior Research Consultant at Saudi Aramco's RASD. He earned his Ph.D. and M.Sc. from KFUPM and a B.Sc. from King Saud University, specializing in catalyst synthesis and characterization using TGA, FTIR, and Raman spectroscopy. With expertise in materials characterization, he has published 20+ papers and holds over 10+ U.S. patents.

Dr. Walaa Algozee is a Lead Scientist at the Saudi Aramco Research & Development Center (R&DC). She earned her Ph.D. from Rice University, an M.Sc. from the University of Manchester, and a B.Sc. from the University of Colorado. Her research focuses on plastic waste conversion, hydrocarbon characterization, and hydrogen production. She has authored over 30 publications and holds more than 20 U.S. patents.

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Intrinsically Conducting Polymers (ICPs) in Energy Technology: Fundamentals, Applications, and Experimental Progress

Maha Hamed Alenazi, Abdul-Rahman Al-Betar*

Chemistry Department, King Fahd University of Petroleum & Minerals

*Corresponding authors: abetar@kfupm.edu.sa

1. Introduction

The ongoing global energy transition has intensified the demand for advanced materials capable of enabling efficient, sustainable, and economically viable energy technologies. Despite significant progress in renewable energy deployment, fossil fuels still account for nearly 80% of the global primary energy supply, while worldwide energy demand is projected to increase by approximately 14% by 2040.[1] This growing disparity between rising energy demand and the urgent need to reduce greenhouse gas emissions has heightened concerns over long-term energy security, climate change, and resource sustainability, thereby accelerating the search for clean and reliable energy solutions.[2] Although substantial advances have been achieved in energy technologies, no single energy source can independently satisfy the diverse requirements of modern energy systems in terms of reliability, scalability, energy density, and infrastructure compatibility.[3-5] Instead, future energy systems are expected to rely on an integrated energy portfolio that combines renewable electricity, hydrogen technologies, and advanced energy storage systems. Within this framework, the development of high-performance functional materials has become a fundamental research priority, as breakthroughs in materials design directly

determine the efficiency, durability, stability, and commercial viability of next-generation energy conversion and storage technologies.[6] Among the emerging classes of functional materials, the discovery of electrically conducting polymers fundamentally transformed the perception of organic polymers from electrically insulating materials into a versatile class of electroactive materials with broad technological potential. Over the past four decades, continuous advances in polymer chemistry, molecular engineering, and nanostructure fabrication have significantly expanded the functionality of intrinsically conducting polymers (ICPs). The modern history of ICPs was truly sparked by Shirakawa and co-workers, who demonstrated a dramatic increase in electrical conductivity upon oxidizing polyacetylene with iodine.[7] This discovery transformed organic polymer research and established the modern foundation for conducting polymer science. The outstanding performance of intrinsically ICPs is attributed to their unique π -conjugated molecular architecture, in which alternating single and double bonds create delocalized electronic states along the polymer backbone. This conjugated framework enables electrical conductivity that can be precisely tuned through reversible oxidation or reduction (doping),

allowing ICPs to bridge the gap between conventional insulating polymers and inorganic electronic materials. The most widely used ICPs in energy systems include polyaniline (PANI),[8] polypyrrole (PPy),[9] polythiophene (PT),[10] and poly(3,4-ethylenedioxythiophene) (PEDOT).[7] ICPs can be synthesized through a variety of approaches, including chemical oxidative polymerization, electrochemical polymerization, vapor-phase polymerization, interfacial polymerization, and template-assisted methods.[11] Their characteristics include lightweight nature, mechanical flexibility, chemical versatility, and scalable processing, with the ability to conduct electrical charges, enabling substantial improvements in their electrical conductivity, electrochemical activity, environmental stability, and mechanical properties. ICPs have been extensively explored in numerous energy-related applications, including electrochemical supercapacitors,[12] rechargeable batteries,[13] fuel cells,[14] and solar cells.[15] Additionally, depending on the device architecture, they may function as electroactive electrode materials, conductive matrices, interfacial layers, catalyst supports, or protective coatings.[6] Regardless of these significant advances, the practical implementation of ICP-based energy Technologies continues to face several challenges.[16] Long-term electrochemical stability, structural degradation during repeated redox cycling, limited conductivity retention under operating conditions, and scalable manufacturing remain important barriers to widespread commercialization.[17] Addressing these limitations requires a deeper understanding of the fundamental structure–property relationships governing ICP behavior, together with continued

advances in molecular design, nanostructure engineering, and composite fabrication. This article provides a comprehensive review of the fundamentals, applications, and recent experimental progress of intrinsically conducting polymers; it also presents experimental insights to bridge the gap between current literature and practical implementation in energy technologies. By integrating critical literature analysis with representative experimental observations, this review provides a more comprehensive perspective on the structure–property–performance relationships governing ICP-based energy devices.

2. Applications in Energy Systems

The versatility of intrinsically conducting polymers has enabled their incorporation into a broad spectrum of energy technologies (Figure 1), where they perform distinct functions depending on the device architecture and operating mechanism. By acting as electroactive materials, conductive networks, charge-transport layers, or multifunctional composites, ICPs contribute to improved electrochemical performance and device efficiency. The following sections discuss their applications in supercapacitors, rechargeable batteries, fuel cells, and solar cells, highlighting their functional roles, recent experimental advances, and the key factors governing their performance.

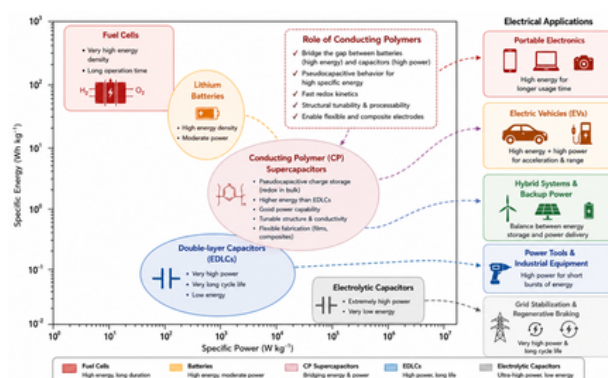


Figure 1. Ragone plot comparing the energy–power characteristics of major electrical energy-storage technologies, highlighting the intermediate performance of conducting polymer (CP)-based supercapacitors and their representative electrical applications.[18]

2.1 Supercapacitors

Supercapacitors are electrochemical energy storage devices that bridge the gap between conventional capacitors and rechargeable batteries by combining high power density, rapid charge–discharge capability, and long operational lifetime.[19] Based on their charge-storage mechanism, supercapacitors are classified into (1) Electrochemical double-layer capacitors (EDLCs) and (2) pseudo capacitors. EDLCs store energy through electrostatic ion adsorption at the electrode/electrolyte interface, whereas pseudo capacitors store charge through fast and reversible Faradaic redox reactions within electroactive materials, resulting in significantly higher capacitance and energy density. Among pseudocapacitive materials, **ICPs** have attracted considerable attention because of their high electrical conductivity, reversible redox activity, low cost, and facile synthesis. Unlike EDLCs, ICPs store charge throughout the bulk of the polymer via reversible doping/de-doping processes, thereby providing higher specific capacitance while maintaining rapid charge-transfer kinetics. Consequently, ICP-based supercapacitors are considered promising candidates for bridging the performance gap between high-energy batteries and high-power EDLCs. **Figure 2a** shows that reversible p-type and n-type doping processes govern the electrochemical behavior of ICPs.[20] During discharge, these reactions proceed in the reverse direction, enabling reversible energy storage. Depending on the electrode

configuration, conducting polymer supercapacitors are generally categorized into symmetric (Type I), asymmetric (Type II), dual-doped (Type III), and hybrid devices, as shown in **Figure 2b**. Indicating that increasing the operating voltage and capacitance directly enhances the energy density. Even their excellent pseudocapacitive performance, ICPs still suffer from structural degradation caused by repeated volume expansion and contraction during doping/de-doping cycles. Therefore, recent research has focused on nanostructured and composite electrodes incorporating carbon materials,[21] metal oxides,[22] MXenes,[23] and metal–organic frameworks (MOFs),[24] to improve conductivity, mechanical stability, and long-term cycling performance.

2.2 Batteries

Rechargeable batteries dominate electrochemical energy storage but face limitations such as sluggish kinetics, interface instability, and mechanical degradation during cycling.[25, 26] Unlike their role in supercapacitors, ICPs in batteries serve primarily as multifunctional engineering materials.[27] ICPs can enhance electron/ion transport and electrode kinetics by their mixed ionic–electronic transport. In addition, they are widely applied as conductive coatings, conductive binders, artificial interfacial layers, 3D conductive frameworks, and hybrid electrode hosts to improve connectivity, buffer volume expansion, and stabilize electrode architectures (Figure 3). [28–34] Recent battery designs increasingly exploit ICP-based hybrid architectures in which the conducting polymer serves as a multifunctional conductive matrix while secondary components provide complementary electrochemical functions.

Furthermore, nanostructured ICPs (1D, 2D, and 3D) provide high surface areas and shortened diffusion pathways, significantly boosting rate capability and cycling durability.[15, 35, 36] Regardless of these advantages, improving intrinsic electrochemical stability and large-scale processability remains essential for practical commercialization.

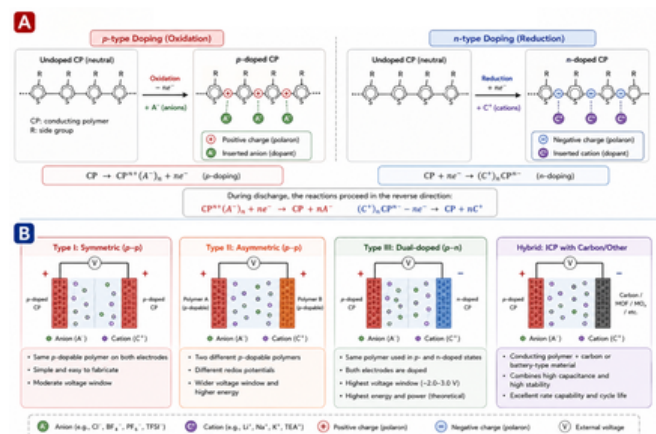


Figure 2. (a) Schematic illustration of p-type (oxidation) and n-type (reduction) doping processes in conducting polymers, showing the formation of positive and negative polarons accompanied by the insertion of anions and cations, respectively. (b) Typical configurations of conducting polymer supercapacitors: symmetric (Type I), asymmetric (Type II), dual-doped (Type III), and hybrid devices.

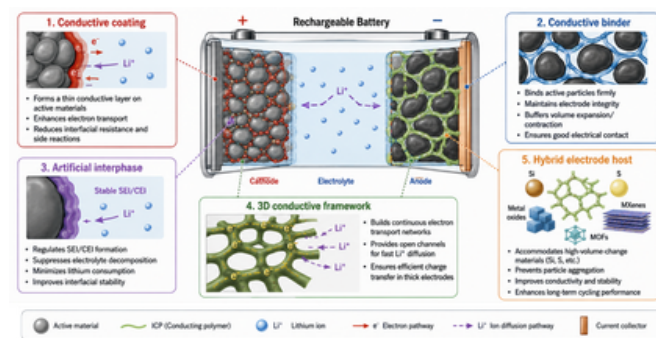


Figure 3. Schematic illustration of the primary application strategies and functional roles of intrinsically conducting polymers (ICPs) in rechargeable battery electrodes.

2.3 Fuel Cells & photovoltaic devices

Fuel cells and photovoltaic (PV) devices are among the most advanced electrochemical energy-conversion technologies, directly

converting chemical or solar energy into electricity with high efficiency and minimal environmental impact.[37, 38] Although fuel cells operate through electrocatalytic oxidation–reduction reactions and photovoltaic devices through photoinduced charge generation, both technologies rely on efficient charge transport across complex interfaces. Hence, their performance depends not only on the intrinsic activity of catalytic or photoactive materials but also on effective interfacial engineering that enables rapid charge transfer, proton transport, appropriate energy-level alignment, and long-term structural stability.[6, 39, 40] ICPs, particularly PANI, PPy, and poly(3,4-ethylenedioxythiophene) (PEDOT), have emerged as multifunctional materials owing to their π -conjugated backbones, tunable electrical conductivity, and versatile interfacial chemistry.[41, 42] Through molecular design, chemical doping, and hybridization, ICPs simultaneously improve electrical conductivity, ion transport, catalyst utilization, and interface stability, making them indispensable components in modern electrochemical energy-conversion devices.

In fuel cells (**Figure 4a**), ICPs are incorporated as electrically conductive catalyst supports, protective coatings, hybrid composite matrices, and proton-exchange membrane components.[43, 44] These multifunctional roles improve catalyst dispersion, suppress catalyst agglomeration and poisoning, facilitate charge transfer, and enhance both the mechanical and electrochemical stability of the electrodes.[45] Hybrid systems

combining ICPs with carbon nanomaterials, transition-metal compounds, noble-metal nanoparticles, and polyoxometalates (POMs) further enhance fuel-cell performance through synergistic interactions.[46] The conducting polymer provides continuous electronic pathways, whereas the inorganic components contribute catalytic active sites and reversible redox centers, leading to faster oxygen reduction (ORR) and hydrogen evolution (HER) kinetics, lower charge-transfer resistance, and improved long-term durability.[47] In addition, ICP/POM-based proton-exchange membranes exhibit enhanced proton conductivity, improved thermal stability, and better water management, making them promising materials for next-generation PEM fuel cells.[48, 49]

In photovoltaic devices (**Figure 4b**), ICPs primarily function as charge-selective interfacial layers that promote efficient carrier extraction while suppressing charge recombination.[50, 51] Among them, PEDOT:PSS is the most widely employed hole-transport material because of its high electrical conductivity, optical transparency, favorable energy-level alignment, and excellent solution processability, resulting in improved power-conversion efficiency and operational stability.[52] The integration of ICPs with redox-active polyoxometalates (POMs) and semiconductor nanomaterials further enhances photovoltaic performance by creating highly efficient charge-transfer interfaces.[53] In these hybrid systems, POMs act as electron acceptors and reversible redox mediators that facilitate electron extraction, improve energy-level matching, and stabilize charge-separated states, thereby increasing photocurrent density, open-circuit voltage, conversion

efficiency, and long-term device stability.

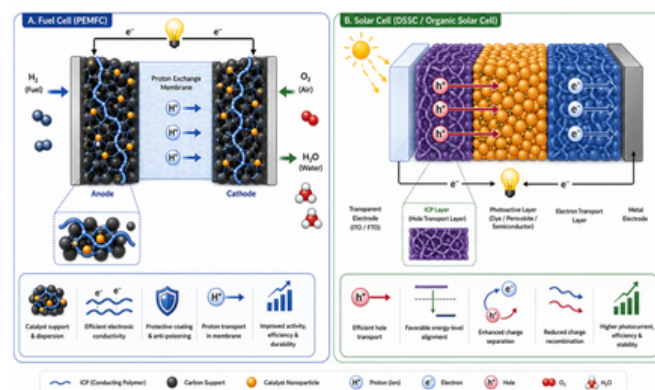


Figure 4. Schematic illustration of the multifunctional roles of intrinsically conducting polymers (ICPs) in (a) fuel cells and (b) photovoltaic devices.

3. Experimental

Polyaniline can be formed by electrochemical cycling of aniline (0.1 M) in H_2SO_4 solution between -0.2 V and 1.0 V. Figure 5 shows electrochemical polymerization of aniline in H_2SO_4 . The increase of current with cycling is an indication of polymer growth. The first cycle shows a nucleation loop as well as an overpotential current.

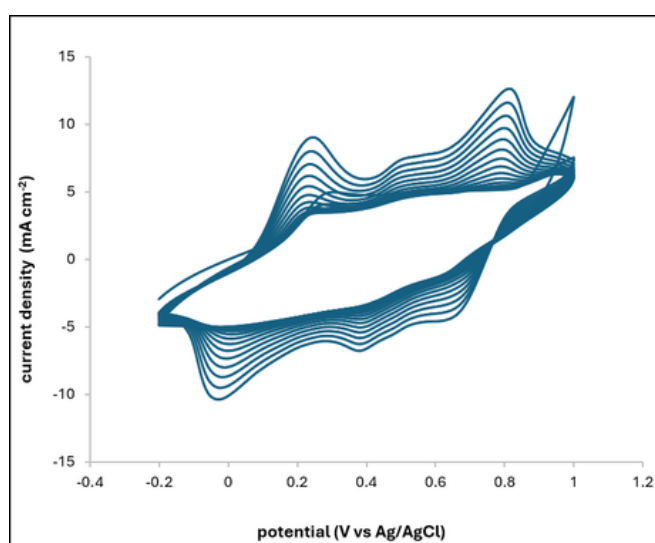


Figure 5. Electrochemical polymerization of aniline in 0.1 M H_2SO_4 at 0.1 V s^{-1} by cyclin between -0.2 V and 1.0 V on GCE.

4. Conclusion

Intrinsically conducting polymers (ICPs) combine organic mechanical flexibility with high electrical conductivity via conjugated π -bond backbones.

Reversible redox doping enables high-capacity bulk pseudocapacitance, making ICPs effective active materials in supercapacitor electrodes.

In rechargeable batteries, ICPs serve as multifunctional conductive matrices, artificial interphases, and strain-buffering binders during cycling.

For fuel cells and photovoltaics, ICPs accelerate charge extraction, improve catalytic support durability, and facilitate efficient proton transport.

Electrochemical polymerization offers a precise, controllable method for synthesizing uniform, electroactive polymer films directly onto electrodes.

To combat degradation from redox cycling, hybridizing ICPs with carbon nanomaterials, MXenes, MOFs, or polyoxometalates is crucial for scalability.

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Dr. Abdul-Rahman Al-Betar is an Associate Professor in the Department of Chemistry at King Fahd University of Petroleum and Minerals (KFUPM), Dhahran, Saudi Arabia. He earned his B.S. and M.S. degrees in Kinetics Chemistry from KFUPM and his Ph.D. in Electrochemistry of Conducting Polymers from Memorial University, Canada, in 2012. His research focuses on energy storage and supercapacitors. He is also actively involved in innovative science education for youth and instructor training, and has led KFUPM's gifted-students program during summer sessions.

Maha Hamed Alenazi is a Ph.D. student in Chemistry at King Fahd University of Petroleum and Minerals (KFUPM), Saudi Arabia. Her research focuses on advanced functional materials for hydrogen production, carbon capture, and clean energy applications. She holds an M.Sc. in Chemistry from King Khalid University and a B.Sc. from Imam Abdulrahman Bin Faisal University, with interests in catalysis and sustainable energy technologies.

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Dr. Shakeel Ahmed is a Research Scientist at the IRC for Refining & Advanced Chemicals at King Fahd University of Petroleum & Minerals. His primary areas of expertise include industrial catalysis, inorganic synthesis, and instrumental analysis. With over 200 publications and 77 co-invented patents to his name, Dr. Shakeel has made significant contributions to his field. He has been honored with numerous national and international awards and is recognized among the top 2% of scientists worldwide.

Dr. SK Safdar Hossain

Dr. SK Safdar Hossain is a Professor of Chemical Engineering at King Faisal University. He earned his Ph.D. in Catalysis from King Fahd University of Petroleum & Minerals (KFUPM). His research focuses on reaction engineering, energy storage devices, and chemical process control. He has published over seventy-five peer-reviewed articles and is a co-inventor on fifteen United States patents. Dr. Hossain is a Senior Member of the American Institute of Chemical Engineers (AIChE) and a Life Member of the Indian Institute of Chemical Engineers (IICChE).



Dr. Mansour Saleh Alturki

Dr. Mansour Saleh Alturki, Associate Professor of Medicinal Chemistry at Imam Abdulrahman Bin Faisal University, specializes in synthetic chemistry and drug discovery targeting metabolic disorders, infectious diseases, and cancer. With 23+ years of experience, his expertise includes computational drug design, ADMET profiling, molecular dynamics, and AI-driven research in human health innovations.

Ms. Hissah Alqahtani

Ms. Hissah Alqahtani is a Lecturer in Physical Chemistry at Al Yamamah University, specializing in electrochemistry and advanced materials for energy and environmental applications. With expertise in corrosion, supercapacitors, solar cells, and water treatment, she has published extensively and holds three patents in these fields. Ms. Alqahtani is also a reviewer for international scientific journals, including the Molecular Structure Journal and Springer Nature.

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