Optimizing Corrosion Resistance of Low-Alloy Steel for the Petrochemical Industry by Corrosion Big Data Methods

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中 石 化 安 全 工 程 研 究 院 有 限 公 司
SINOPEC Research Institute of Safety Engineering Co.，Ltd.

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1 Background

Brief Introduction

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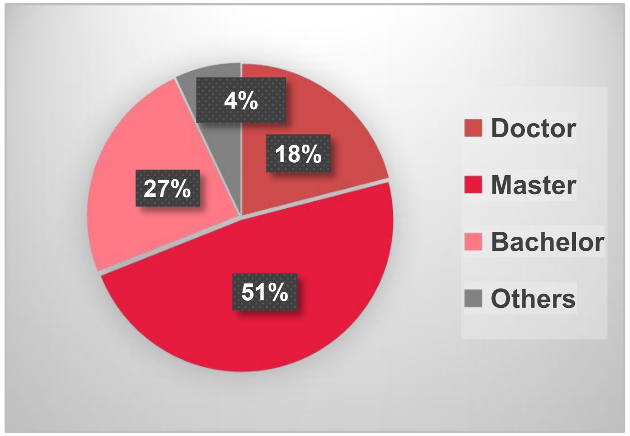
- Research Institute of Safety Engineering Co., LTD., SINOPEC Group
- National Key Laboratory of Chemical Safety——3 national key laboratories
- Chemical safety risk warning and intelligent management and control technology——8 provincial and ministerial key laboratories

SEARCH FORTUNE

RANK	NAME	REMOVE ✖ REVENUES ($M)	REMOVE ✖ REVENUE PERCENT CHANGE	REMOVE ✖ PROFITS ($M)	REMOVE ✖ PROFITS PERCENT CHANGE
1	Walmart	$648,125	6%	$15,511	32.8%
2	Amazon	$574,785	11.8%	$30,425	-
3	State Grid	$545,947.5	3%	$9,204.3	12.4%
4	Saudi Aramco	$494,890.1	-18%	$120,699.3	-24.1%
5	Sinopec Group	$429,699.7	-8.8%	$9,393.4	-2.7%
6	China National Petroleum	$421,713.6	-12.7%	$21,294.7	1%
7	Apple	$383,285	-2.8%	$96,995	-2.8%
8	UnitedHealth Group	$371,622	14.6%	$22,381	11.2%
9	Berkshire Hathaway	$364,482	20.7%	$96,223	-



Brief Introduction

- Dr. Mindong Chen

- Graduated from University of Science and Technology Beijing in 2018, advisor: Pro. Xiaogang Li
- （2018-present）SINOPEC Research Institute of Safety Engineering
- （2020-2021）Held a temporary position in a 18 million tons/year refining and chemical enterprises

- Responsible for research projects funded by：

National Natural Science Foundation of China

National key research and development plan

Science and Technology Department of Sinopec Group

Petrochemical Safety Administration of Sinopec Group

Brief Introduction

- Dr. Mindong Chen

Responsible for big data monitoring technology of chemical process corrosion, realized accurate perception of hidden process flow and equipment damage through multi-dimensional and multi-module data modeling and deep learning of equipment material and corrosion potential.

First prize of scientific and technological progress ——Chinese Society for Corrosion and Protection Society

Responsible for the dynamic monitoring and early warning model of major hazard safety production risk based on event tree, protective layer and Bayesian method, and applied to the national hazardous chemical safety risk monitoring and early warning system.

Second prize of management innovation ——Sinopec Group

Responsible for the research and development of equipment status intelligent monitoring and preventive maintenance technology, established the typical characteristics of dynamic and static equipment failures, and realized the online monitoring and early warning of typical equipment.

Third prize of Technical invention award ——Sinopec Group

Second prize in Management and Technology innovation——China Equipment Management Association

Background

- In China, refining industry mainly processes crude oil, which guarantees China's energy supply, but also brings severe corrosion problems to low-alloy steel.
- The refining industry demands materials with high corrosion resistance to withstand harsh conditions.

- Data Collection and Integration.
- Data Analysis and Modeling.
- Material Optimization.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REVIEW ARTICLE OPEN

Integrated computational materials engineering of corrosion resistant alloys

Christopher D. Taylor[1,2], Pin Lu[3], James Saal[3], G. S. Frankel[1] and J. R. Scully[4]

Structure, composition and surface properties dictate corrosion resistance in any given environment. The degrees of freedom in alloy design are too numerous in emerging materials such as high entropy alloys and bulk metallic glasses for the use of high-throughput methods or trial and error. We review three domains of knowledge that can be applied towards the goal of corrosion resistant alloy (CRA) design: (a) the aggregation of knowledge gained through experience in developing CRAs empirically, (b) data-driven approaches that use descriptive metrics for alloy composition optimization, and (c) first-principles models of elementary processes that regulate corrosion informed by theory and inspired by phenomenological models in the literature. A path forward for integrated computational materials engineering (ICME) of CRAs that unites these three knowledge domains is introduced.

npj Materials Degradation (2018)2:6 ; doi:10.1038/s41529-018-0027-4

Ref:

Xiaogang Li, Materials science: Share corrosion data, Nature, 2015, 527(7579): 441

Christopher D. Taylor, Integrated computational materials engineering of corrosion resistant alloys, npj Materials Degradation, 2018,2, (6)

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2 Case Study

Case 1 - offshore oil construction

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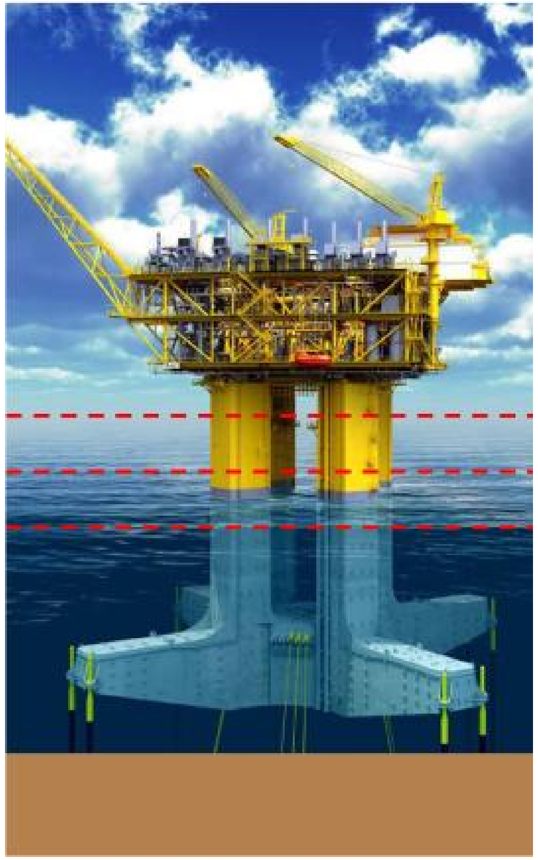
- **Corrosion problems in the application of low alloy steel in offshore petroleum engineering**
- **High chloride ion content and periodic changes in environmental factors**



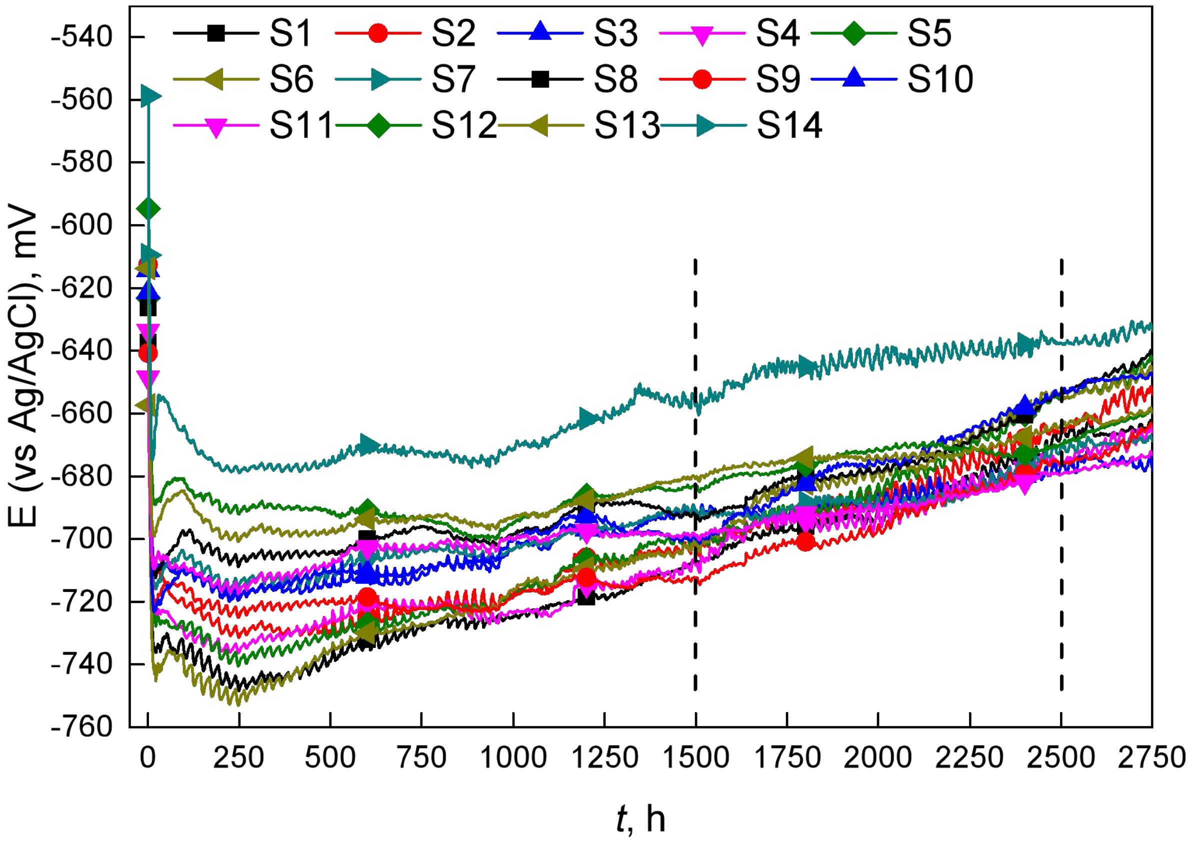
IoT devices used for big data monitoring

The composition of 14 types of low-alloy steels

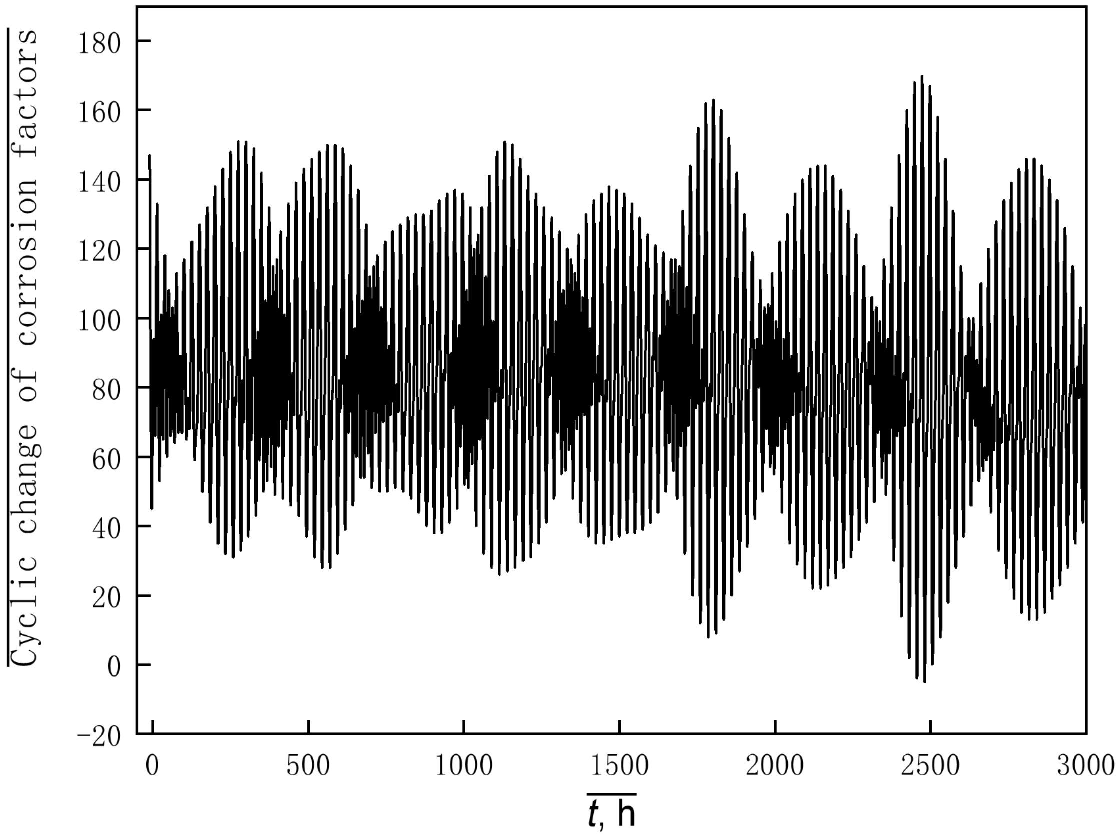
Alloy steels	Compositions/wt%												
	Fe	C	Si	Mn	P	S	Ni	Cr	Cu	Al	Ti	Nb	Others
S1	99.38	0.042	0.18	0.35	0.008	0.003	0	0	0	0.029	0	0	
S2	99.27	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0.0496	0.0205	0	0	
S3	99.20	0.091	0.21	0.4	0.013	0.016	0	0	0.04	0	0	0	N:0.028
S4	98.68	0.17	0.22	0.88	0.018	0.005	0	0	0	0.023	0	0	
S5	98.48	0.072	0.1388	1.2186	0.0124	0.0034	0	0	0	0.0394	0.0178	0.015	
S6	98.18	0.1	0.28	1.42	0.01	0.002	0	0	0	0	0	0	
S7	98.07	0.064	0.22	1.18	0.008	0.005	0	0	0.32	0	0.014	0.035	V:0.049,N:0.033
S8	97.83	0.04	0.3	1.79	0.013	0.001	0	0.025	0	0	0	0	
S9	97.81	0.0672	0.181	1.5407	0.0131	0.0027	0	0.2075	0	0.0382	0.0176	0.063	Mo:0.0575
S10	97.65	0.097	0.26	1.64	0.01	0.006	0	0	0.2	0	0.017	0.048	V:0.067,N:0.004
S11	97.44	0.0697	0.3257	1.0426	0.0167	0.0079	0.1299	0.6239	0.2636	0.0288	0.017	0.0264	
S12	97.08	0.06	0.17	1.5	0.014	0.002	0.4	0.25	0.26	0.026	0.012	0.02	Mo:0.2
S13	96.81	0.11	0.29	1.12	0.013	0.003	0.41	0.46	0.27	0.036	0.019	0	N:0.41, V:0.03, B:0.015
S14	94.97	0.12	0.33	0.37	0.08	0.04	2.72	1.05	0	0	0	0	Mo:0.24,V:0.08

Case 1 - offshore oil construction

- **High-frequency, long-term, multi-channel corrosion potential data obtained using IoT monitoring devices.**

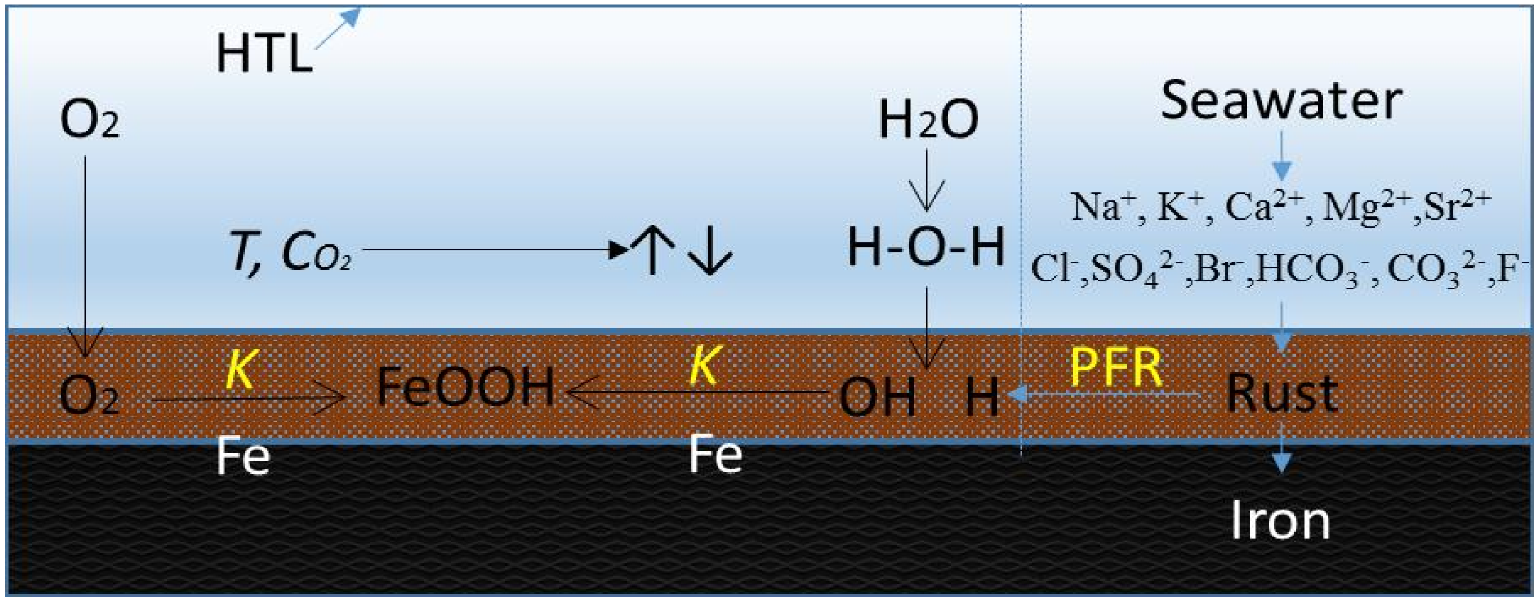


Hourly measured corrosion potential data.



Changes in a specific environmental factor.

- **Principles for establishing corrosion resistance indicators**



$$E = \frac{RT}{zF} \ln K^{\ominus} - \frac{RT}{zF} \ln K$$

PFR: The inverse of the standard deviation of the open-circuit potential fluctuation resulting from environmental changes

Ref:

IVERSON W P. Transient voltage changes produced in corroding metals and alloys [J]. Journal of The Electrochemical Society, 1968, 115(6).

MELCHERS R E. Effect of small compositional changes on marine immersion corrosion of low alloy steels [J]. Corrosion Science, 2004, 46(7): 1669-91.

MELCHERS R. Modeling of marine immersion corrosion for mild and low-alloy steels—Part 1: Phenomenological model [J]. Corrosion, 2003, 59(4): 319-34.

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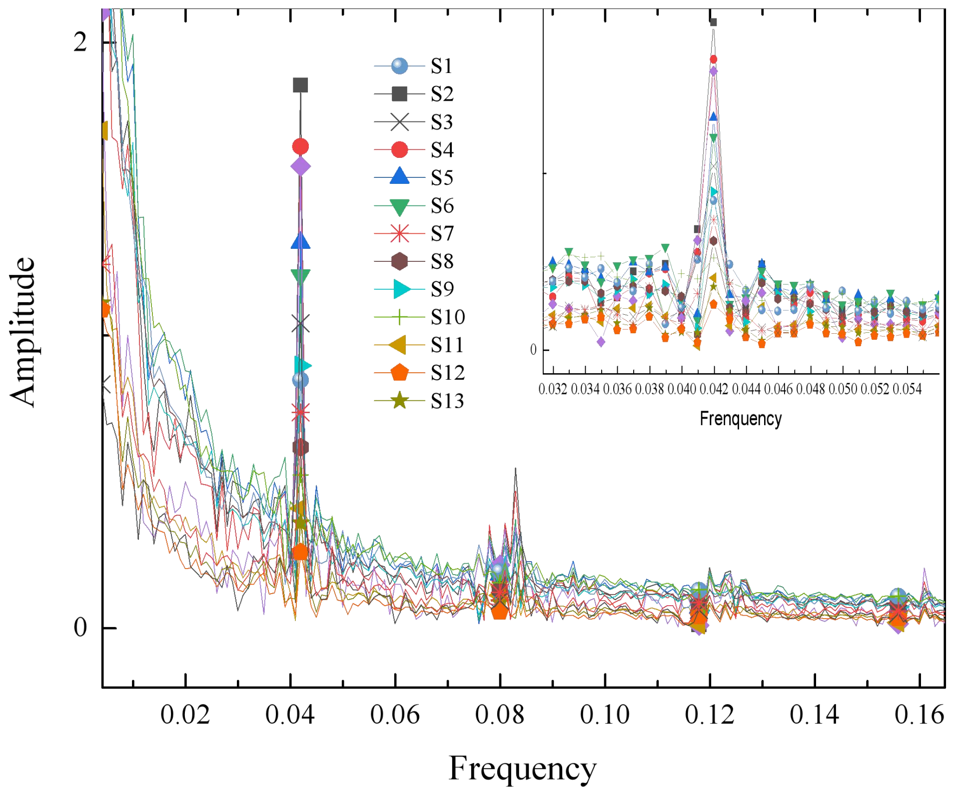
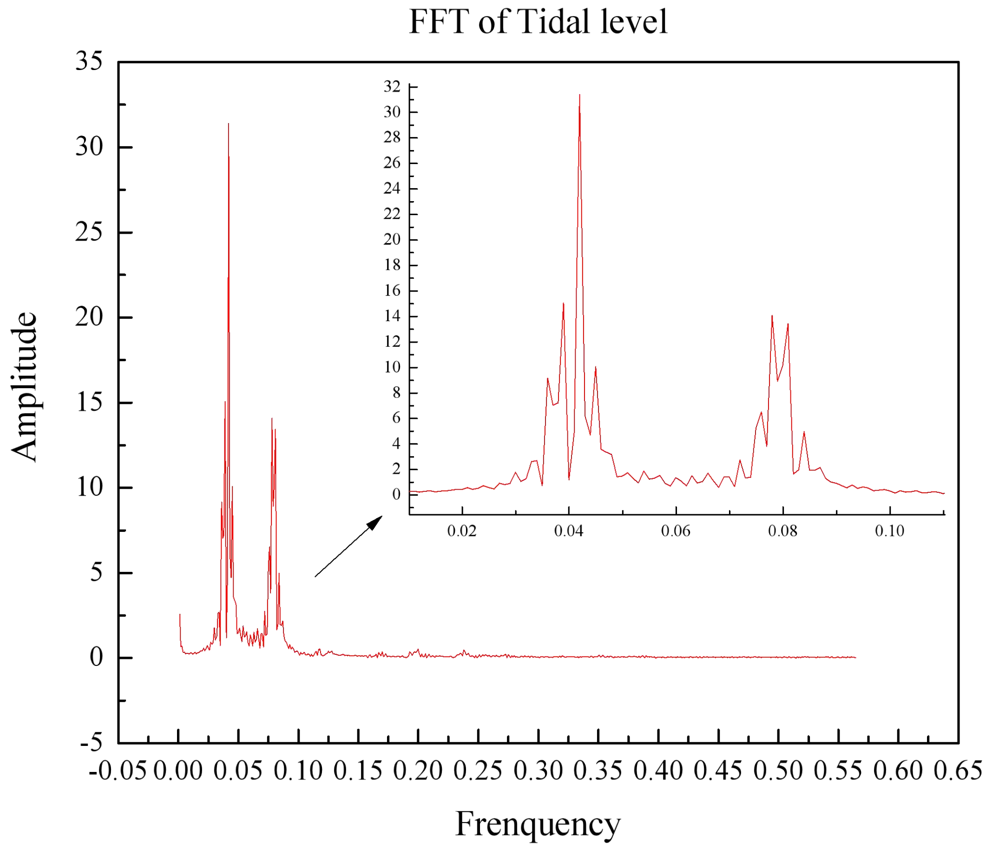
- **Verify that the corrosion potential fluctuations are caused by variations in the specific environmental factor.**
- **The skewed part of the graph on the left is the result of long-period trends.**





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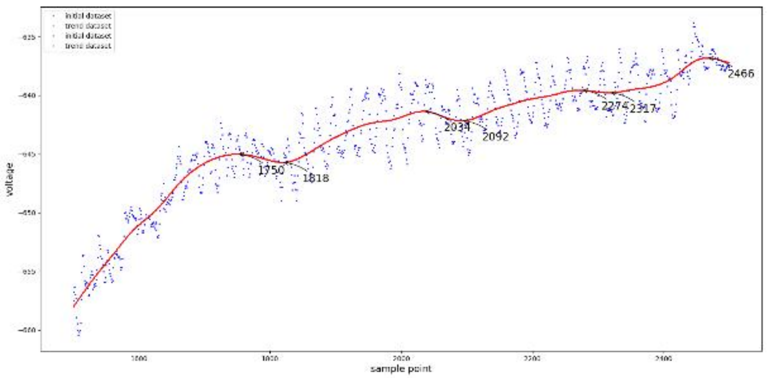
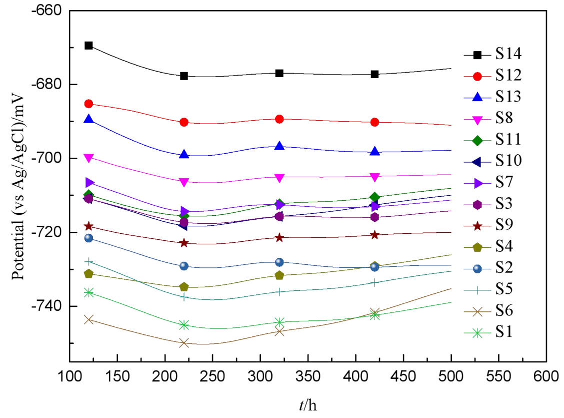
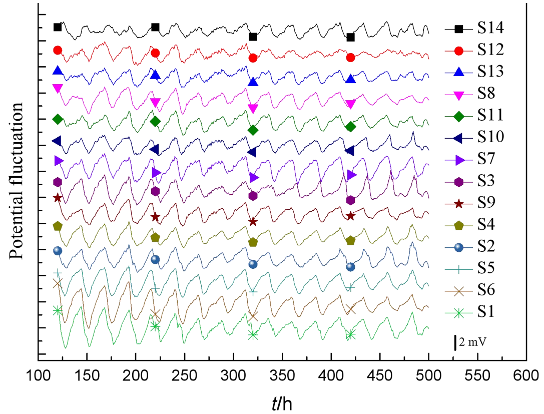
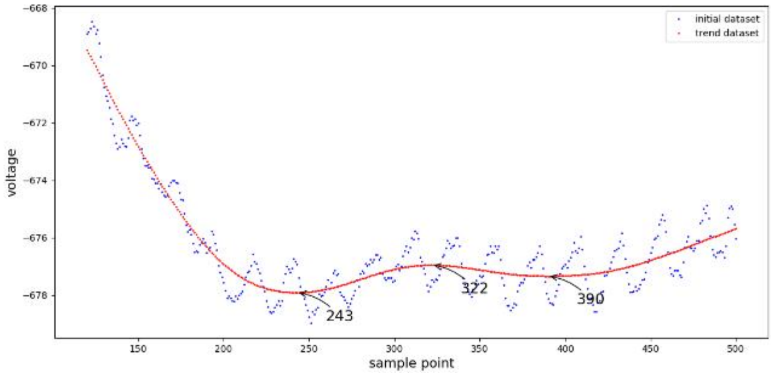
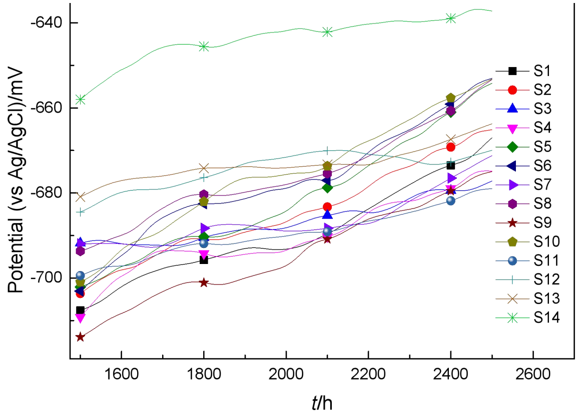
- **Decomposition of Fluctuation and Trend Components**
- **After testing various methods, the Hodrick-Prescott Filter was selected for decomposing the fluctuation and trend components.**

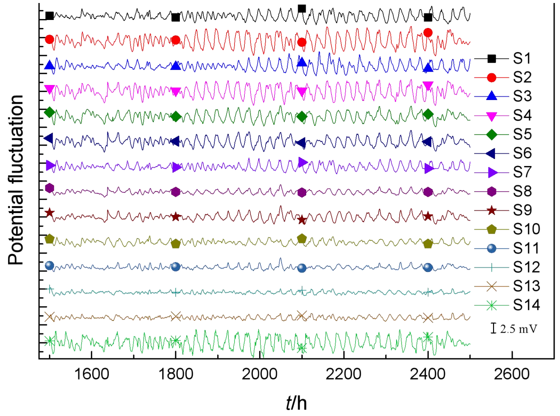












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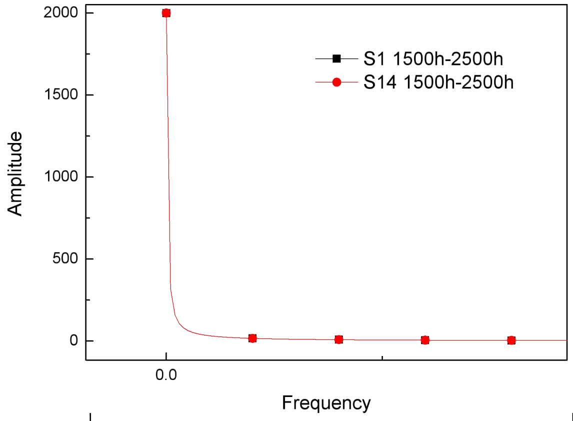
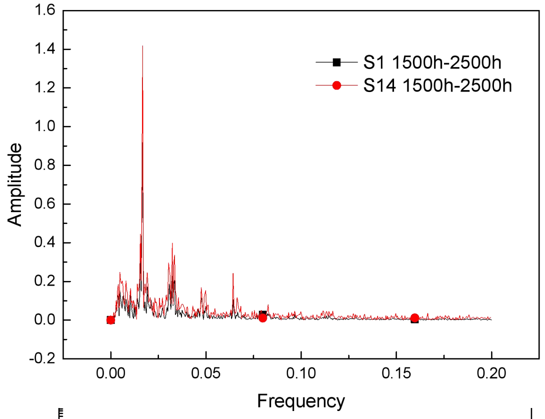
- **The decomposed data was subjected to Fourier Transform, confirming that the Hodrick-Prescott Filter can effectively extract potential fluctuation data caused by environmental variations.**

Trend

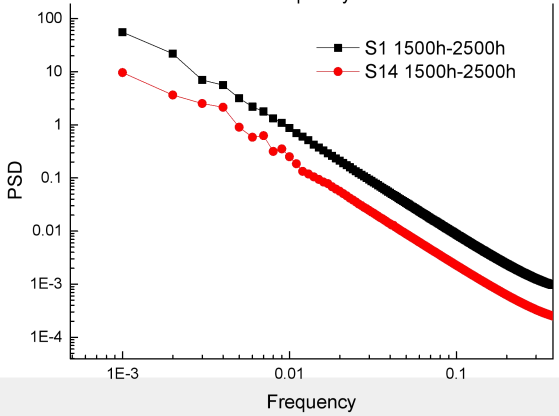


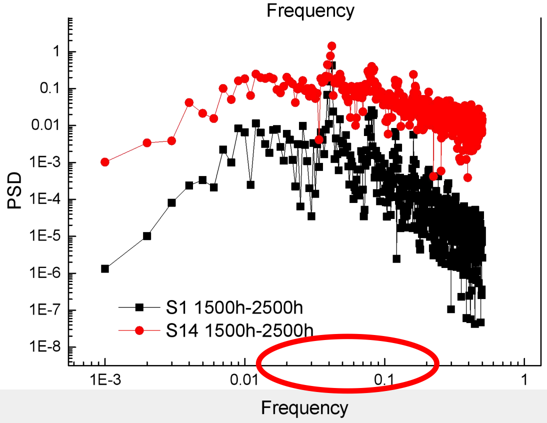
Fluctuation



HP filter→Potential Fluctuation

Amplitude Density





Power Spectral Density (PSD)

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- **Results of the correlation analysis between PFR and alloy element composition**
- **highly correlated results，conclusions consistent with empirical knowledge**
- **leading to new insights**

PFR of different carbon steels in the 120h-500h interval.

Series	PFR	Series	PFR
S6	0.738	S8	1.201
S1	0.797	S4	1.207
S5	0.894	S11	1.3
S7	0.925	S10	1.362
S3	0.991	S13	1.504
S2	1.082	S14	1.525
S9	1.18	S12	1.574

PFR of different carbon steels in the 1500h-2500h interval.

Series	PFR	Series	PFR
S2	0.587	S9	1.17
S14	0.632	S7	1.189
S4	0.635	S10	1.617
S5	0.857	S8	1.868
S4	0.88	S11	1.979
S3	0.894	S13	2.194
S1	0.985	S12	2.687

The correlation between alloy composition and PFR in the 120h-500h interval.

Compositions	ρ	MIC
Fe	**-0.7890**	0.6894
C	0.1736	0.0754
Si	0.3784	0.3705
Mn	0.1429	0.1601
P	**0.5952**	0.3949
S	0.1477	0.2570
Ni	**0.7095**	0.4028
Cr	**0.7064**	0.5087
Cu	0.3497	0.2570
Al	-0.0069	0.1601
Ti	0.2256	0.1601
Nb	0.1485	0.1281
Mo	**0.6552**	0.5178
V	0.4129	0.2963
N	-0.1499	0.1601
B	0.3096	0.1745

The correlation between alloy composition and PFR in the 1500h-2500h interval.

Compositions	ρ	MIC
Fe	**-0.5341**	0.6894
C	**-0.5912**	0.2578
Si	0.2486	0.1613
Mn	**0.5604**	0.5087
P	-0.2655	0.321
S	**-0.4719**	0.257
Ni	0.1767	0.4028
Cr	0.2793	0.3705
Cu	**0.575**	0.5087
Al	0.151	0.257
Ti	**0.5005**	0.4083
Nb	0.4211	0.5087
Mo	0.2781	0.306
V	0.0661	0.1239
N	0.1009	0.1593
B	0.3784	0.2284

Here are the algorithms used in the previous procedures

Fourier Transform $$F(\omega)=\mathcal{F}[f(t)]=\int_{-\infty}^{\infty} f(t)e^{-iwt}dt$$

Hodrick-Prescott Filter $$\min_{\tau_t} \sum_{t=1}^{T}((y_t-\tau_t)^2+\lambda((\tau_{t+1}-\tau_t)-(\tau_t-\tau_{t-1}))^2)$$

The Hodrick-Prescott Filter (HP Filter) is a method used for analyzing time series data. It minimizes the variance of fluct uations in a time-varying sequence over time.

Spearman Correlation Coefficient Analysis：Linear Correlation

$$\rho=\frac{\sum_i (x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\sum_i (x_i-\bar{x})^2 \sum_i (y_i-\bar{y})^2}}$$

Maximal Information Coefficient (MIC) Analysis: Nonlinear Correlation

$$\mathrm{MIC}[x,y]=\max \frac{I(x,y)}{\log_2(\min(n_x,n_y))}$$

Ref:

COGLEY T, NASON J M. Effects of the Hodrick-Prescott filter on trend and difference stationary time series Implications for business cycle research [J]. Journal of Economic Dynamics and Control, 1995, 19(1): 253-78.

RAVN M O, UHLIG H. On adjusting the Hodrick-Prescott filter for the frequency of observations [J]. Review of economics and statistics, 2002, 84(2): 371-6.

D.N. Reshef, Y.A. Reshef, H.K. Finucane, S.R. Grossman, G. McVean, P.J. Turnbaugh, E.S. Lander, M. Mitzenmacher, P.C. Sabeti, Detecting novel associations in large data sets, Science, 334 (2011) 1518-1524.

J.B. Kinney, G.S. Atwal, Equitability, mutual information, and the maximal information coefficient, Proceedings of the National Academy of Sciences, 111 (2014) 3354-3359.

Case 1 - offshore oil construction

- Some elements exhibit a strong linear correlation with PFR. Aside from linear relationships, no significant nonlinear correlations are observed based on MIC.

- In the 120h-500h interval:
- Fe content shows a negative correlation with PFR.
- Ni, Cr, Mo, and P show positive correlations with PFR.

- In the 1500h-2500h interval:
- Fe, C, and S are negatively correlated with PFR.
- Mn, Cu, and Ti are positively correlated with PFR.

Case 1 - offshore oil construction

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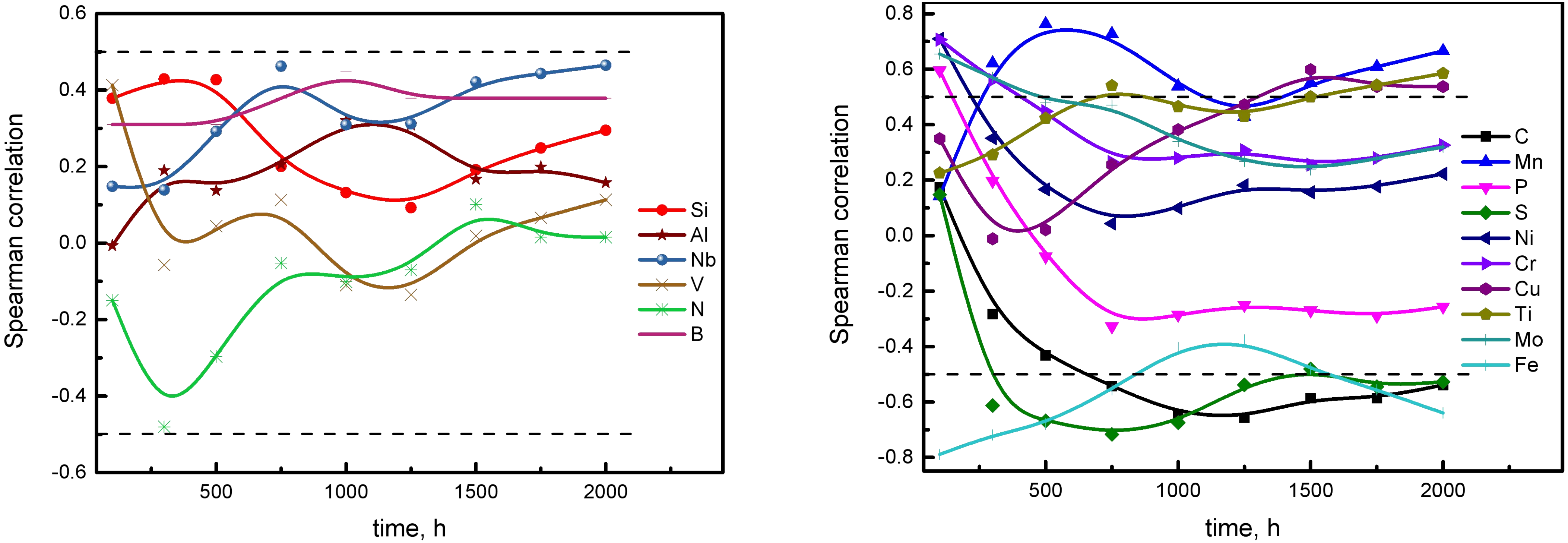
● Analysis and Obtained Resuls

The evolution of the correlation between the corrosion resistance indicator PFR and alloy elements over time.



The conclusions have been used to guide the development of metal materials for offshore oil construction.

More information:

Mindong Chen, etc., An electrochemical method based on OCP fluctuations for anti-corrosion alloy composition optimization, Anti-Corrosion Methods and Materials, 65/3 (2018) 325–330

Mindong Chen, Corrosion behaviors and evolution of marine engineering E690 steel in marine splash zones (doctoral thesis) ,University of Science and Technology Beijing, 2018

Case 1 - offshore oil construction

- **AI for Science**

Investigate how the correlation between PFR and alloy elements evolves over time to understand long-term material performance.

- **Conclusion Validation:**

Compare analytical results with empirical knowledge to confirm the validity of findings.

Use independent experimental data to cross-check the conclusions.

- **Material Development Guidance:**

Translate findings into actionable insights for optimizing alloy compositions for offshore oil construction.

Focus on improving corrosion resistance under specific marine environmental conditions.

- **Optimization and Prediction:**

Develop predictive models to forecast PFR based on alloy composition and environmental factors.

Use these models to design new metal materials with enhanced corrosion resistance for offshore applications.

Case 1 - offshore oil construction

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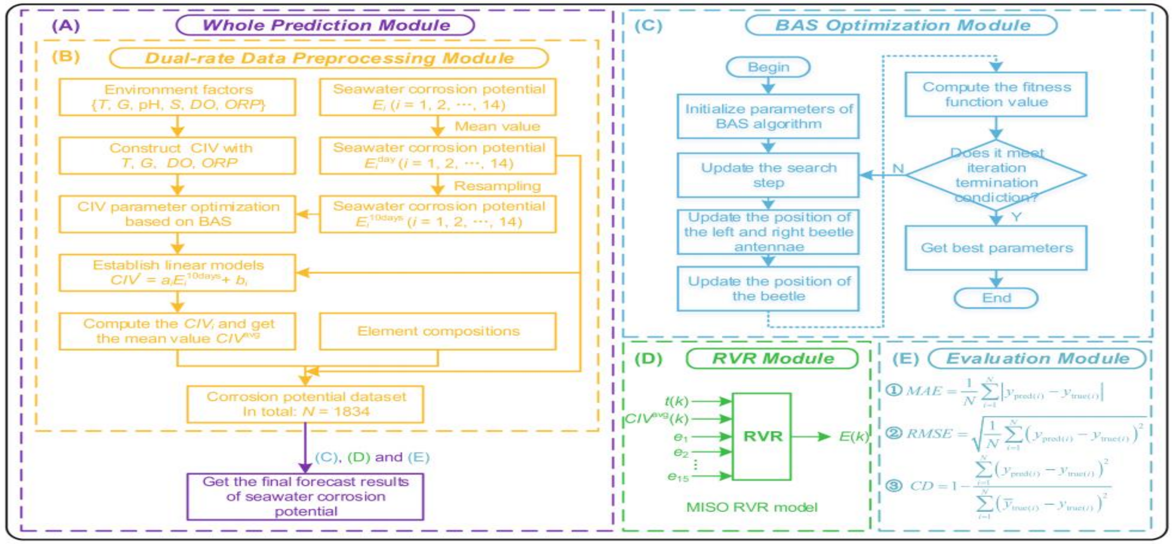
- **AI for Science**
- **Construct the CIV-RVR model**

$$E(k) = f(t(k), \mathrm{CIV}^{\mathrm{avg}}(k), e_1, e_2, \cdots e_{15}), \quad k = 1, 2, \ldots, N$$

$$K = m \exp\left(-\frac{\left\|x_i - y_j'\right\|^2}{\sigma_1^2}\right) + n(x_i y_j' + \sigma_2^2)^2$$

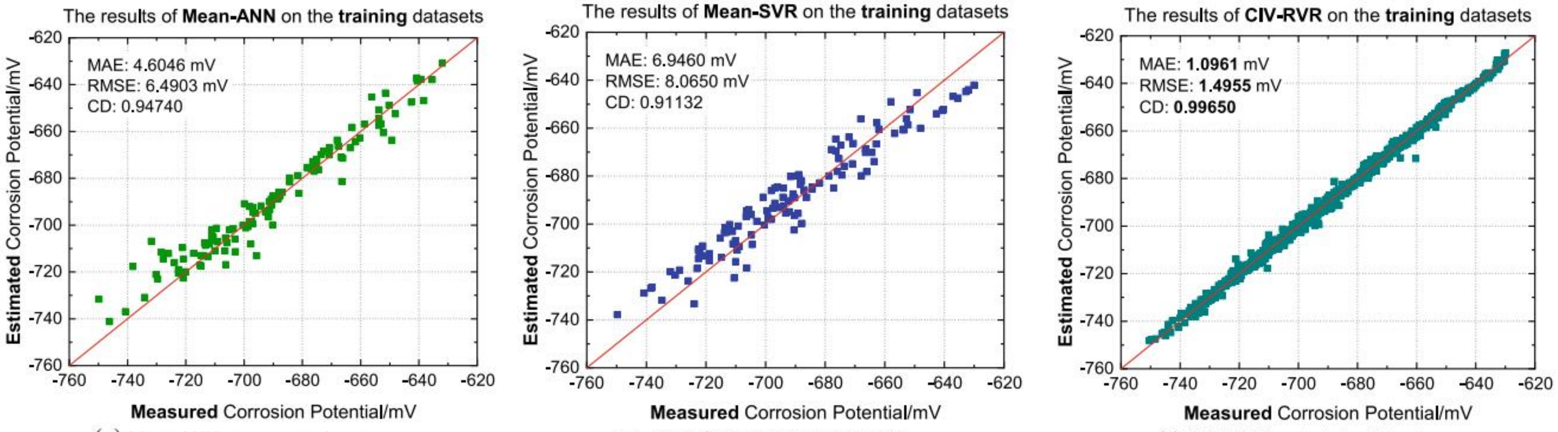


- **Evaluation Criteria**

$$\mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}\left|y_{\mathrm{pred}(i)} - y_{\mathrm{true}(i)}\right|$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(y_{\mathrm{pred}(i)} - y_{\mathrm{true}(i)}\right)^2}$$

$$\mathrm{CD} = 1 - \frac{\sum_{i=1}^{N}\left(y_{\mathrm{pred}(i)} - y_{\mathrm{true}(i)}\right)^2}{\sum_{i=1}^{N}\left(\bar{y}_{\mathrm{true}(i)} - y_{\mathrm{true}(i)}\right)^2}$$



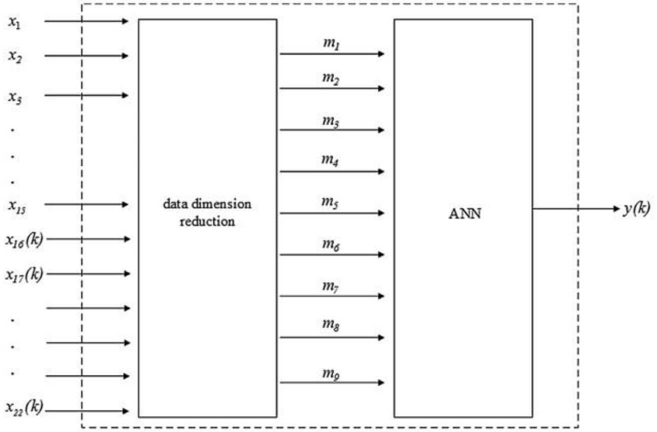
(a) Mean-ANN on training datasets. (c) Mean-SVR on training datasets. (e) CIV-RVR on training datasets.

More information:
Chen L, Fu D, Chen M. Modeling and mining dual-rate sampled data in corrosion potential online detection of low alloy steels in marine environment[J]. Journal of Materials Science, 2020, 55(27): 13398-13413.

Case 1 - offshore oil construction

- **AI for Science**
- **Mining of corrosion resistance model of key alloying elements**

Id	t (day)	T (°C)	σ (S/cm)	PH	S (%)	DO (mg/L)	v (m/s)	C (%)	Mn (%)	S (%)	P (%)	Si (%)	Ni (%)	Cr (%)	Mo (%)	V (%)	Cu (%)	Nb (%)	Ti (%)	Al (%)	B (%)	N (%)	E (%)
1	1	23.26	52168	8.14	34.37	7.03	0.95	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
2	10	23.69	51536	8.11	33.89	5.3	1.11	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
3	20	24.79	51816	8.08	34.08	6.59	1.32	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
4	30	25.75	51811	8.12	33.9	4.08	1.53	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
5	40	26.37	52413	8.16	34.05	4.15	1.36	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
6	50	27.2	52721	8.09	33.91	4.91	1.49	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
7	60	27.57	52700	8.18	33.97	4.89	1.23	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
8	70	28.72	53574	8.18	34.03	5.38	1.01	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
9	80	28.55	53265	8.23	33.81	6.36	1.28	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
10	90	29.41	52995	8.24	33.63	4.41	1.08	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
11	100	30.1	53357	8.3	33.64	4.72	1.02	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
12	110	30.3	51110	8.05	33.83	5.47	0.98	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
13	120	28.5	51510	8.12	34.03	6.58	0.75	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
14	130	29.33	51110	8.22	33.78	6.46	1.32	0.1554	0.0959	0.3193	0.0241	0.0086	0.0145	0.0415	0	0.0496	0	0	0	0.0205	0	0	-
15	1	23.26	52168	8.14	34.37	7.03	0.95	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
16	10	23.69	51536	8.11	33.89	5.3	1.11	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
17	20	24.79	51816	8.08	34.08	6.59	1.32	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
18	30	25.75	51811	8.12	33.9	4.08	1.53	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
19	40	26.37	52413	8.16	34.05	4.15	1.36	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
20	50	27.2	52721	8.09	33.91	4.91	1.49	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
21	60	27.57	52700	8.18	33.97	4.89	1.23	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
22	70	28.72	53574	8.18	34.03	5.38	1.01	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
23	80	28.55	53265	8.23	33.81	6.36	1.28	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
24	90	29.41	52995	8.24	33.63	4.41	1.08	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
25	100	30.1	53357	8.3	33.64	4.72	1.02	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
26	110	30.3	51110	8.05	33.83	5.47	0.98	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
27	120	28.5	51510	8.12	34.03	6.58	0.75	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
28	130	29.33	51110	8.22	33.78	6.46	1.32	0.042	0.18	0.35	0.008	0.003	0	0	0	0	0	0	0	0.029	0	0	-
29	1	23.26	52168	8.14	34.37	7.03	0.95	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
30	10	23.69	51536	8.11	33.89	5.3	1.11	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
31	20	24.79	51816	8.08	34.08	6.59	1.32	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
32	30	25.75	51811	8.12	33.9	4.08	1.53	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
33	40	26.37	52413	8.16	34.05	4.15	1.36	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
34	50	27.2	52721	8.09	33.91	4.91	1.49	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
35	60	27.57	52700	8.18	33.97	4.89	1.23	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
36	70	28.72	53574	8.18	34.03	5.38	1.01	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
37	80	28.55	53265	8.23	33.81	6.36	1.28	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
38	90	29.41	52995	8.24	33.63	4.41	1.08	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
39	100	30.1	53357	8.3	33.64	4.72	1.02	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
40	110	30.3	51110	8.05	33.83	5.47	0.98	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
41	120	28.5	51510	8.12	34.03	6.58	0.75	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
42	130	29.33	51110	8.22	33.78	6.46	1.32	0.17	0.22	0.88	0.018	0.005	0	0	0	0	0	0	0	0.023	0	0	-
43	1	23.26	52168	8.14	34.37	7.03	0.95	0.1	0.28	1.42	0.01	0.002	0	0	0	0	0	0	0	0	0	0	-
44	10	23.69	51536	8.11	33.89	5.3	1.11	0.1	0.28	1.42	0.01	0.002	0	0	0	0	0	0	0	0	0	0	-
45	20	24.79	51816	8.08	34.08	6.59	1.32	0.1	0.28	1.42	0.01	0.002	0	0	0	0	0	0	0	0	0	0	-
46	30	25.75	51811	8.12	33.9	4.08	1.53	0.1	0.28	1.42	0.01	0.002	0	0	0	0	0	0	0	0	0	0	-
47	40	26.37	52413	8.16	34.05	4.15	1.36	0.1	0.28	1.42	0.01	0.002	0	0	0	0	0	0	0	0	0	0	-



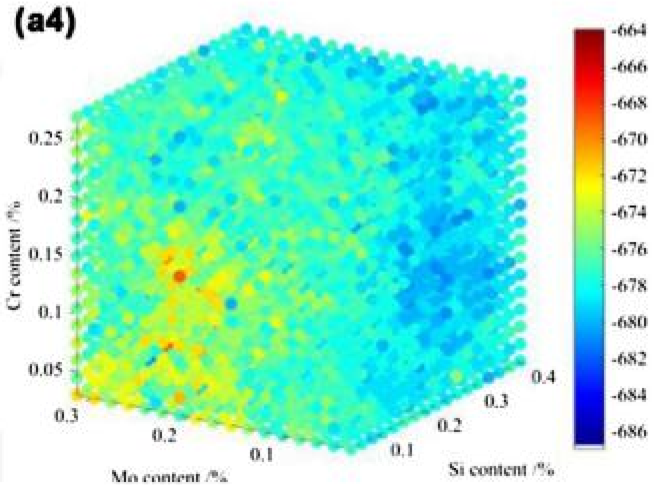
Step1: Building y（k）=f（x1k，x2k，。。。，x22k）

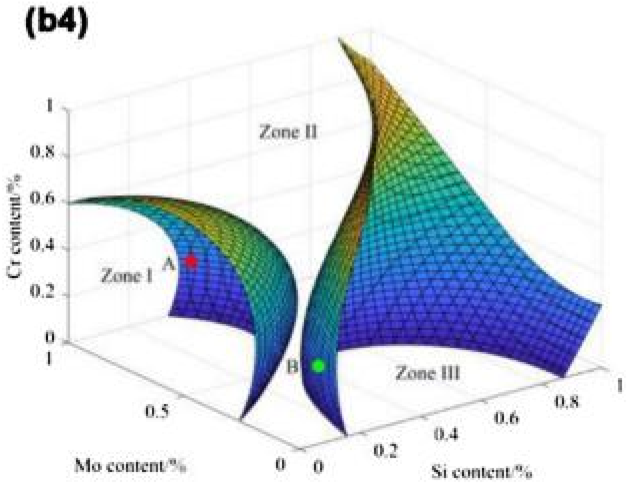
Step2: Calculate the average y (k) from the initial stage to the stable stage

Step3: Visualize the relationship between y(k) and any 3 xnk

Step4: Three grades are obtained using K-means

Step5: The alloy element composition interval is used to judge the corrosion resistance





More information:

Wei X, Fu D, Chen M, et al. Data mining to effect of key alloying elements on corrosion resistance of low alloy steels in Sanya seawater environmentAlloying Elements[J]. Journal of Materials Science & Technology, 2021, 64: 222-232.

Case 2 - petrochemical plant

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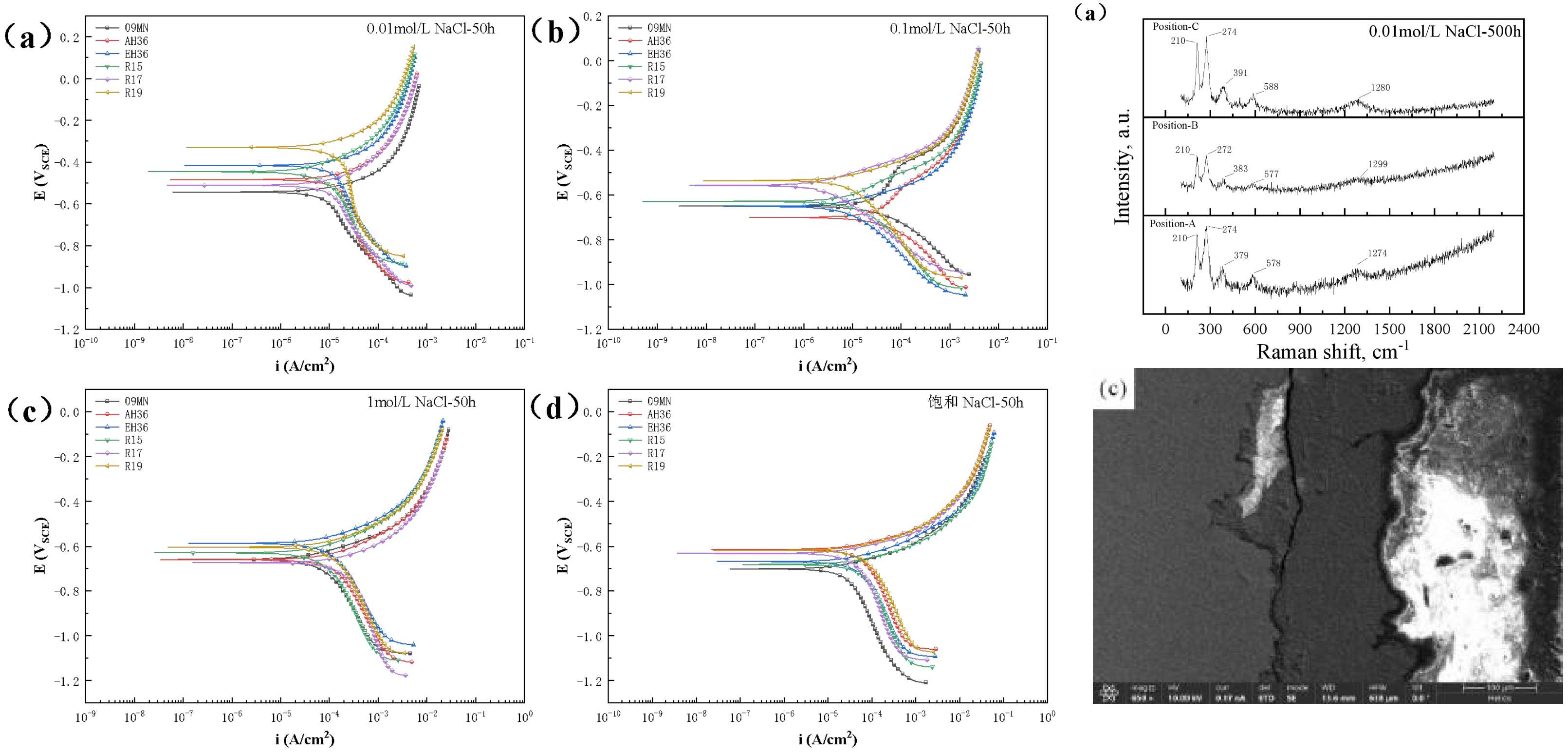
- **Low alloy steel materials used extensively in refining and chemical plants**
- **Different source of imported crude oil，equipment material seriously corrodes**

材料	Mn	P	Ni	Cr	Cu	Ti	Mo	Fe	C	S
Q345-R15	1.51	0.008	0.01	0.18	0.01	0.013	0.01	Bal	0.05	0.001
Q345-R17	1.55	0.008	0.01	0.19	0.01	0.012	0.01	Bal	0.05	0.001
Q345-R19	1.52	0.009	0.01	0.19	0.01	0.012	0.01	Bal	0.06	0.001
Q345-EH36	1.51	0.009	0.12	0.17	0.02	0.015	0.001	Bal	0.05	0.002
Q345-AH36	1.21	0.019	0.01	0.028	0.01	0.011	0.002	Bal	0.181	0.004
Q345-09Mn NiDR	1.36	0.013	0.36	0.06	0.05	0.001	0.026	Bal	0.09	0.0042
Q345-0	1.70	0.030	0.012	0.30	0	0.20	0.10	Bal	0.18	0.02

Chemical composition of low alloy steel materials wt. %



Potentiodynamic polarization, Raman and rust cross section test results

Case 2 - petrochemical plant

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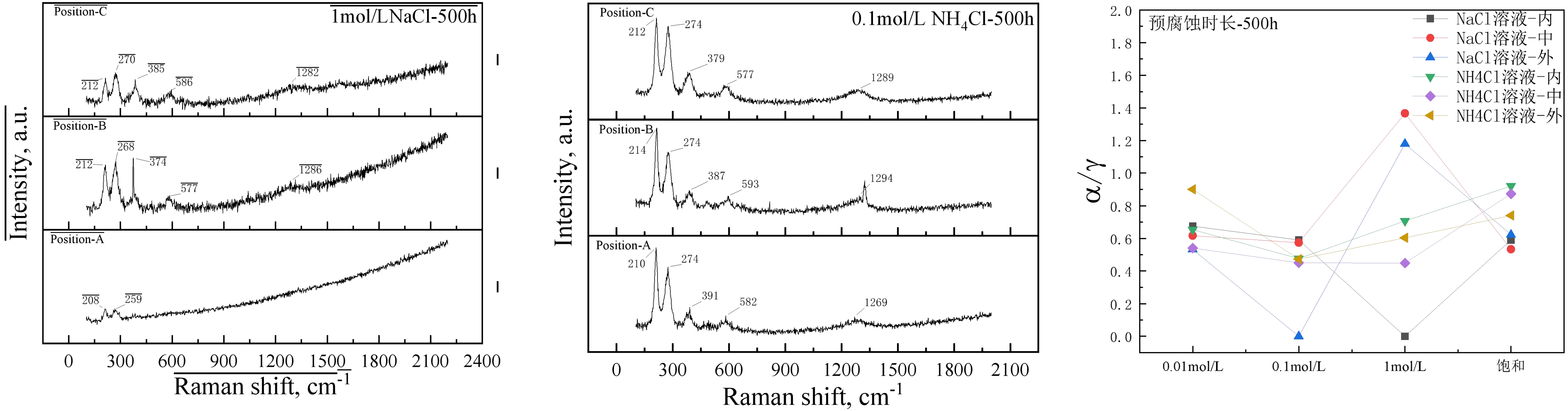
- **Raman spectrum**



Raman spectra and α/γ values of corrosion products of rust layer of Q345 steel in simulated refining corrosive solution environment

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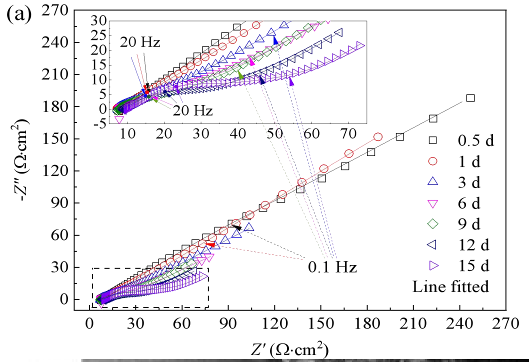
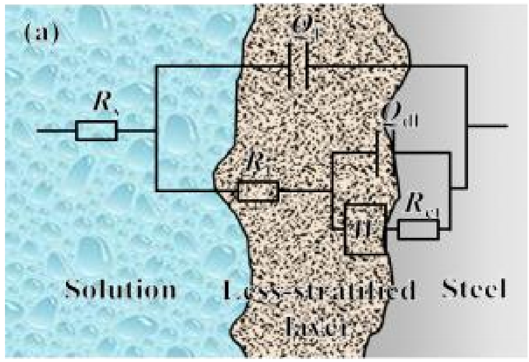
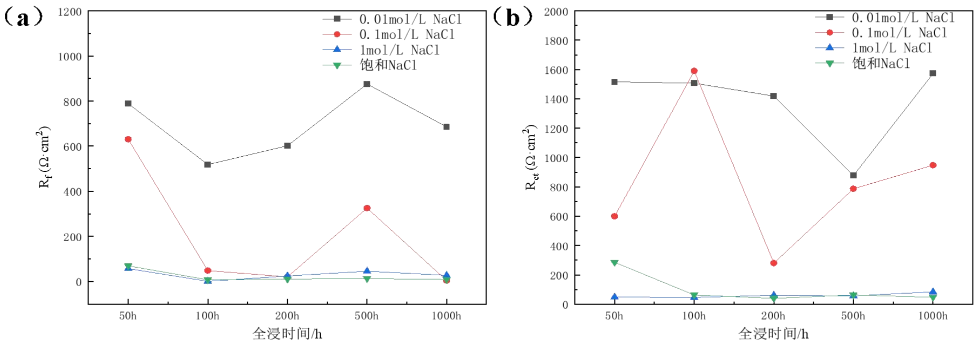
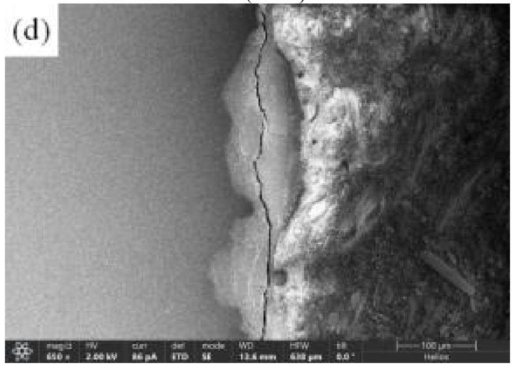
Electrochemical impedance and fitting

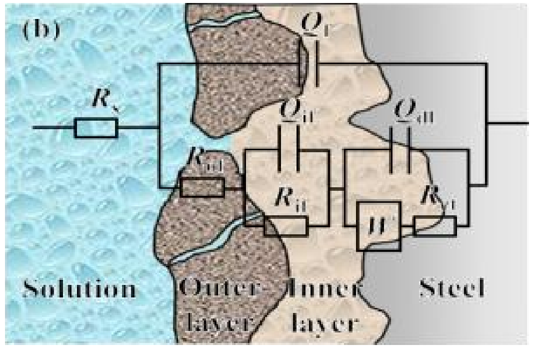


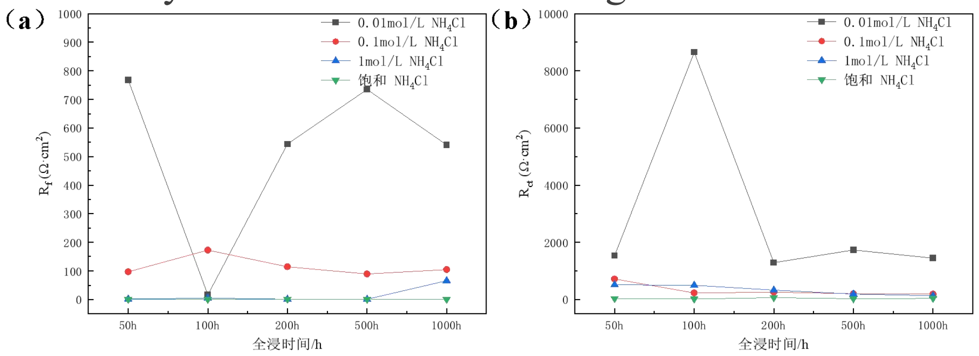




Rust layer resistance Rf and charge transfer resistance Rct





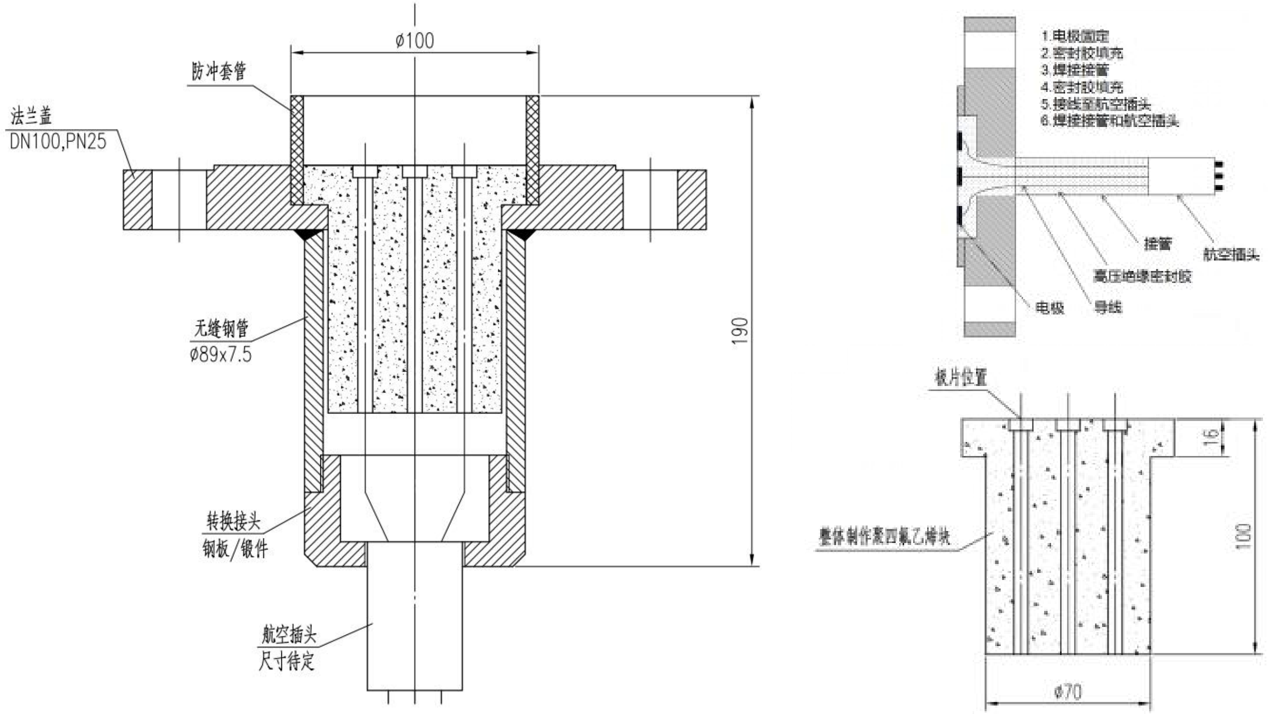


Electrochemical resistance and rust layer cross section morphology

Equivalent circuit diagram

Rust layer resistance Rf and charge transfer resistance Rct

- **Developed 8-channel array electrode probe**
- **Passed pressure and safety tests**



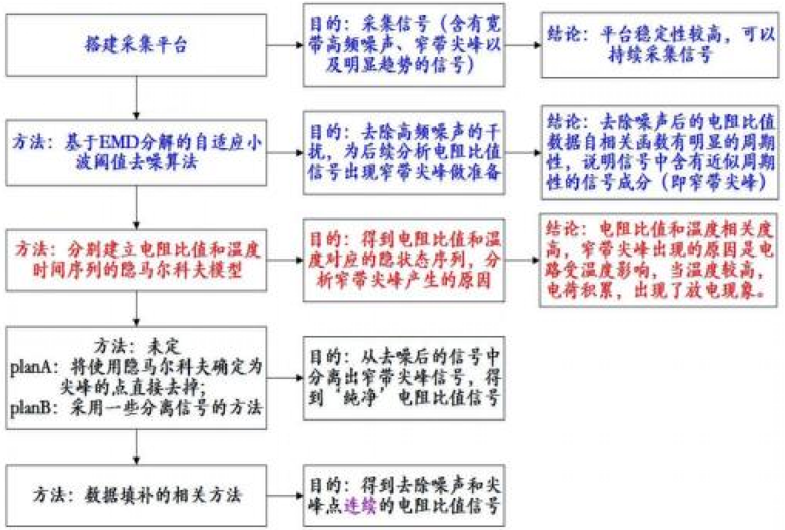
A high-flux multi-channel corrosion probe was established for refining and chemical environment

Pressure tolerance and safety testing

Case 2 - petrochemical plant

- **Probes for field applications, multi-channel and single-channel**
- **Field data acquisition method**

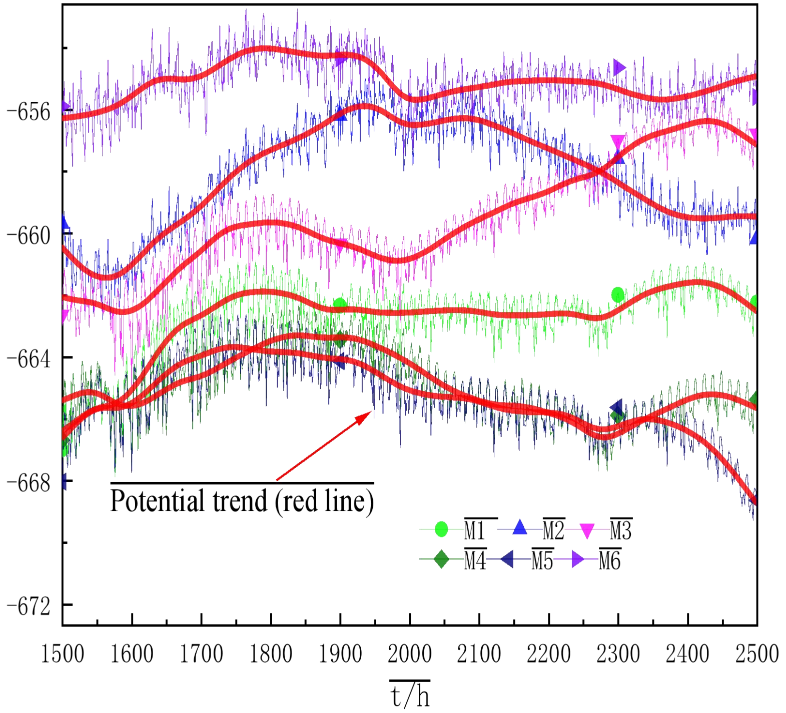
Flange probe



$$\min_{\tau_t} \sum_{t=1}^{T}\left((y_t-\tau_t)^2+\lambda\left((\tau_{t+1}-\tau_t)-(\tau_t-\tau_{t-1})\right)^2\right)$$

Preferred filtering method

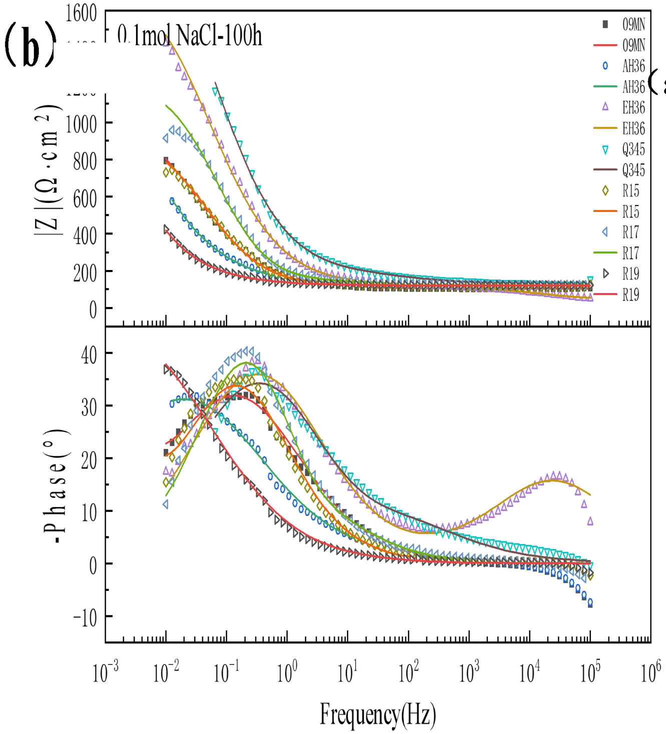
Field operation matters

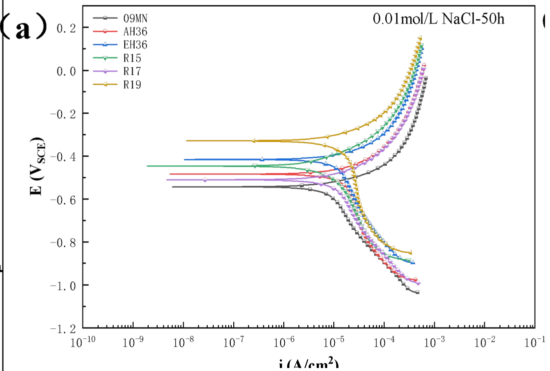


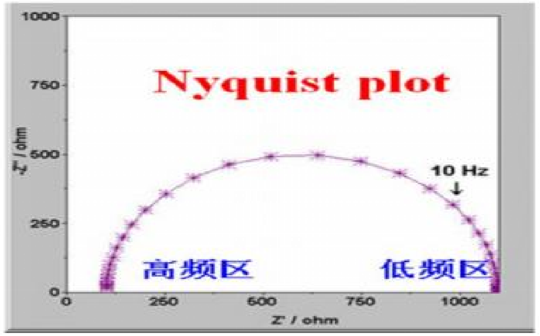
Measurement data

Case 2 - petrochemical plant

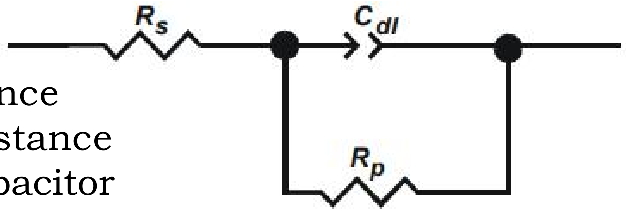
- **According to the characteristics of materials and environment, established the method of obtaining I_{corr}**
- **Principles for establishing corrosion resistance indicators——PFR & I_{corr}**







Rs: dielectric resistance
Rp: polarization resistance
Cdl: double layer capacitor



High frequency impedance: measured dielectric resistance Rs

Low frequency impedance: Measuring Rs+Rp

Polarization resistance Rp=(Rs+Rp)-Rs

According to Stern's equation: icorr=B/Rp

Case 2 - petrochemical plant

- **Quantitative data**
- **Database and digital twin space**

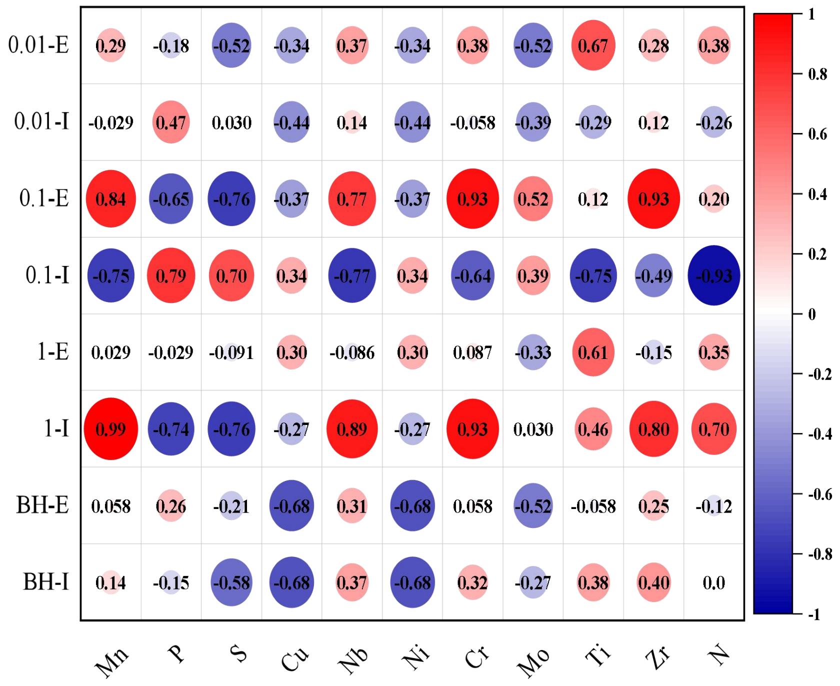
Quantitative indicators

- Traditional electrochemical characteristic quantity
- Two-dimensional corrosion morphology
- High throughput monitoring data
- test inside the device
- Alloying element composition

Digital twin data

- Volatility/trend data
- Relational data
- Evaluation index
- Trend data

Industrial application



Relation of alloying elements to electrochemical characteristic quantities

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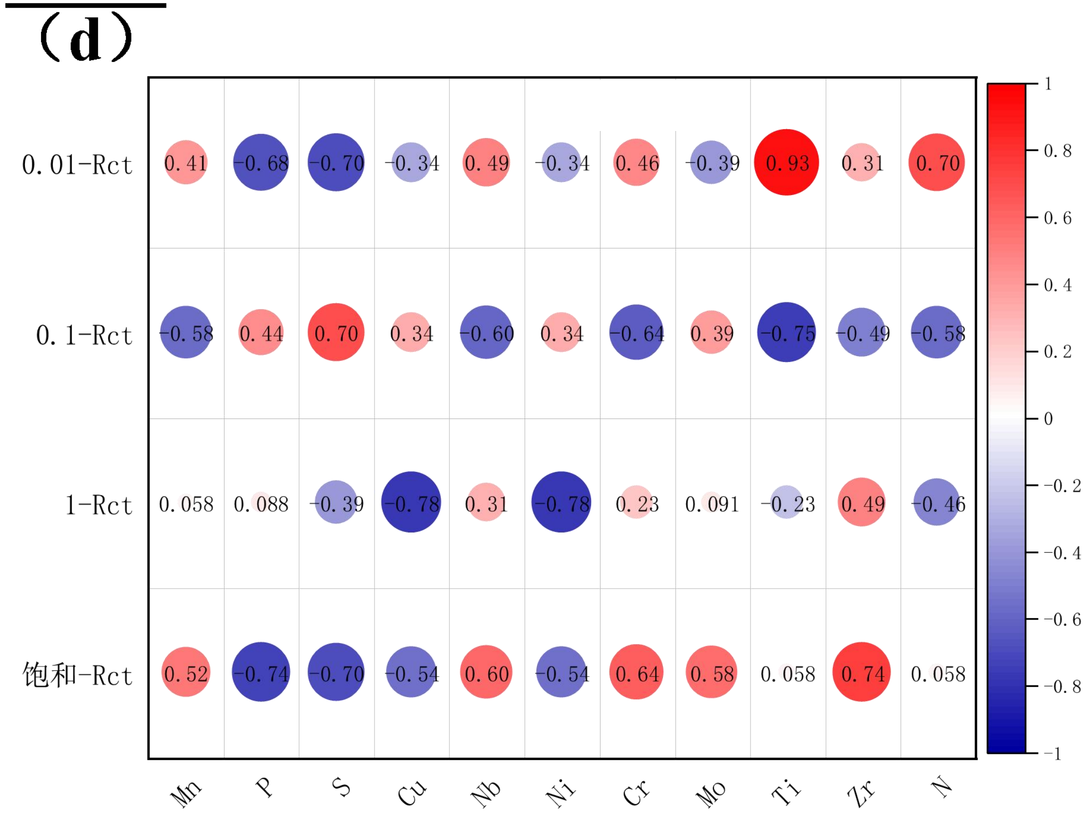
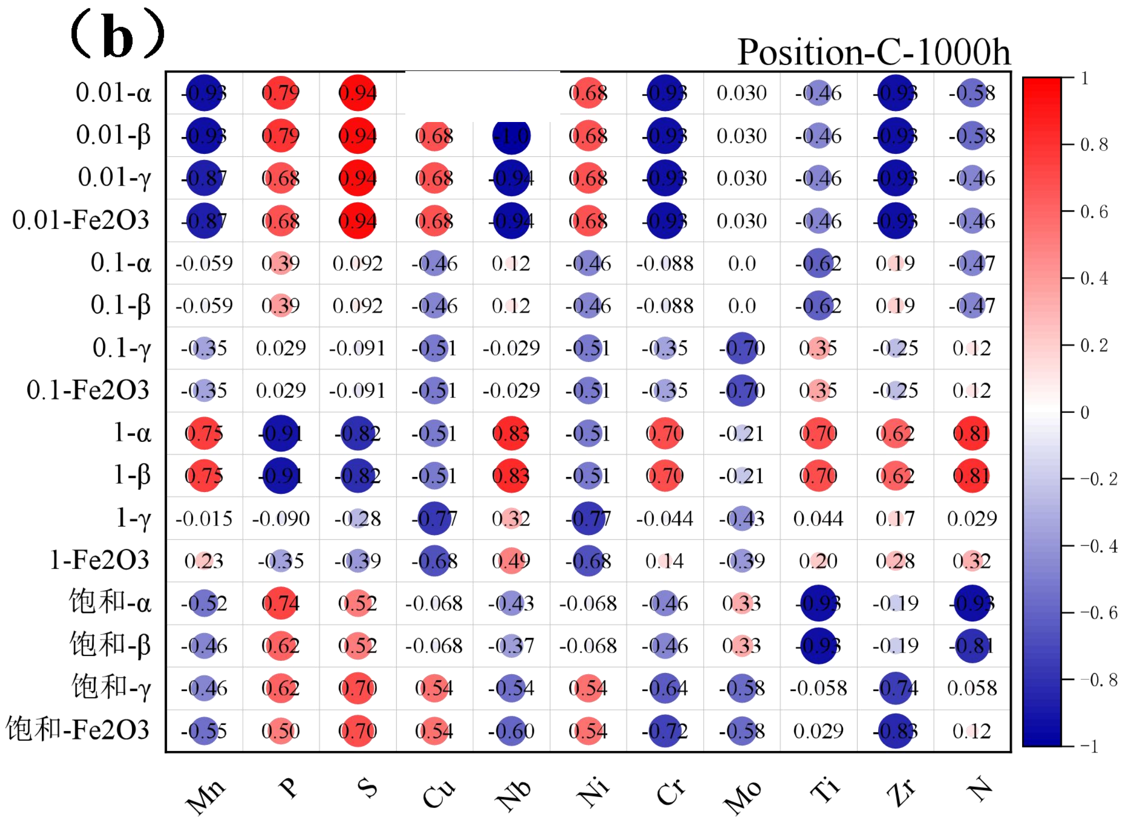
- **Spearman correlation between quantitative results and alloying element composition**



Spearman linear correlation between alloy elements and charge transfer resistance (Rct)



Spearman linear correlation between alloying elements and phase content of outer film

Case 2 - petrochemical plant

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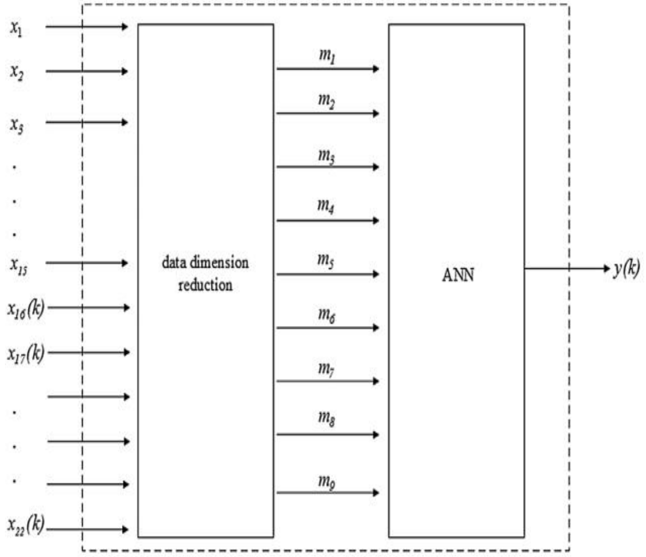
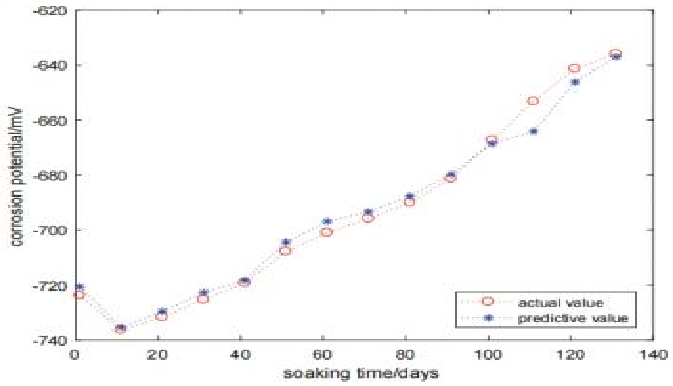
- Pressure data of the last point is taken and updated in real time.
- Lims data is aligned using Local Preserved Projection.
- The pitting data is collected intermittently and only maps other data at this time point.
- Alloying element data is fixed in the time series;
- The measured potential and high and low frequency impedance are updated in real time.



Time series	x1	x2-x3	x4-x6	x7-x9	x10-x12	x13-x22	y1	y2
kn	D103 (MPA)	t、humid、v	Cl、S、H_2O	x0、f（x0）、f'（x0）	Rust composition (or Rct、Rf)	Alloying element	Corrosion potential	Corrosion rate
k1:2021/06/01 00:00:00	1.40376051	a1	b1	–	–	e1	f1	g1
k2:2021/06/01 01:00:00	1.81615004	a2	b1	–	–	e1	f2	g2
k3:2021/06/01 02:00:00	1.93862413	a3	b1	–	–	e1	f3	g3
…	…	…	…	…	…	…	…	…
k2160: 2021/08/29 00:00:00	1.89268661	a2160	b90	c1	d1	e1	f2160	g2160



The predicted curve is compared with the actual curve

Evaluation index	MAE	RMSE	MAPE
Result	3.00	3.92	0.45%

Evaluation index result

Case 2 - petrochemical plant

- Microalloying composition design and two heat treatment processes
- complete the pipeline manufacturing, and carried out industrial tests in May 2023
- fixed point thickness measurement and pulse eddy current scan once a month

Case 2 - petrochemical plant

- the sulfur protection value of the atmospheric and vacuum equipment was effectively increased by 0.5%
- the average thinning rate of the pipe section in May 2023 after one year of use was 4%
- the test pipe section was 1.5%, reduced by about 60%

	Inspection location number	装置	检测设备/管线	Maximum measured value（mm）	Minimum measured value（mm）	备注/上次检测最小值（mm）	规格型号		Corrosion thinning percentage	Commissioning time
							管径	壁厚		
1	3	III焦化	顶循线 P3104A/B出入口管线	13.16	9.89	9.91	DN300	10.31	4.56%	2023.5
2	9	III焦化	顶循线 P3104A/B出入口管线	11.25	8.99	9.00	DN250	9.27	3.13%	2023.5
3	10	III焦化	顶循线 P3104A/B出入口管线	11.81	9.06	9.07	DN250	9.27	2.59%	2023.5
4	15	III焦化	顶循线 P3104A/B出入口管线	14.87	9.25	9.27	DN300	10.31	10.28%	2023.5
5	21	III焦化	顶循线 P3104A/B出入口管线	11.55	8.91	8.93	DN250	9.27	3.99%	2023.5
6	22	III焦化	顶循线 P3104A/B出入口管线	11.68	8.90	8.91	DN250	9.27	4.31%	2023.5
7	项目管段	III焦化	顶循线 P3104A/B出入口管线	13.10	12.57	12.59	DN400	12.7	1.50%	2023.5

Case 2 - petrochemical plant

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- **Other conclusions are used for material selection and material design of the equipment to enhance the operating life of the equipment**

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3 Vision

Application effect

- Material corrosion big data monitoring and early warning combined with real-time process status of the plant.
- Optimization and development of corrosion resistant equipment materials for refining and chemical process environment based on corrosion big data to improve process margin.
- Can be widely used in highly corrosive hazardous chemical storage tanks, pipelines, and high-chlorine coastal steel structure facilities.

Vision for future

- **AI for Science ——Principles for establishing corrosion resistance indicators**

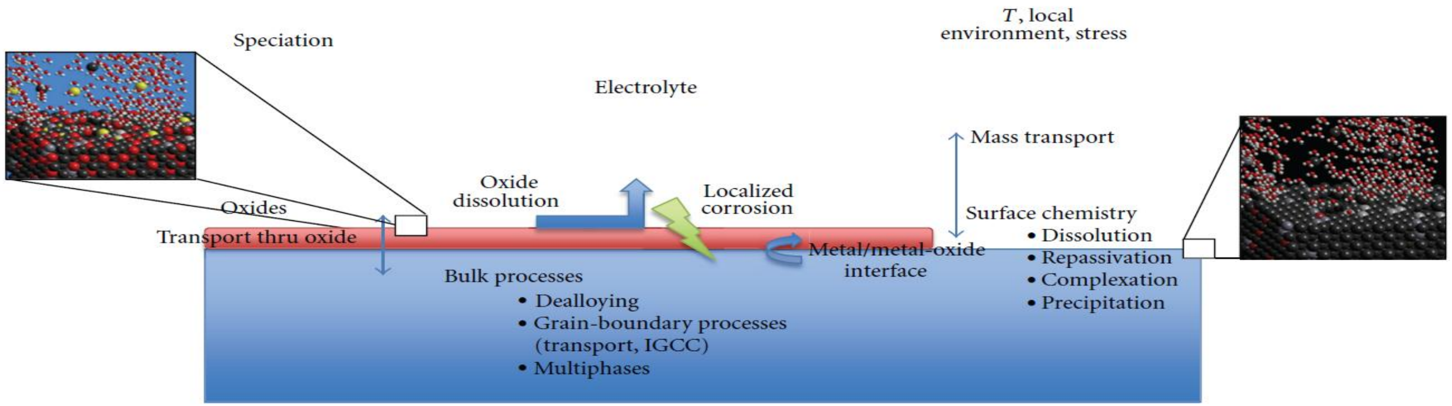
Use AI to discover empirically correlated data on corrosion resistance evaluation indicators

PFR、Icorr

- **AI for Science ——AI selects neural network models, predictive, deep correlation, and quantitative relationship methods**

Quantitative relationships, models,CIV-RVR model、α/γ、R_{ct}、etc.

- **AI makes decisions and managerial recommendations**



Vision for future

- CSCP and ICORR，Leading advances in the natural sciences and engineering
- We are glad to conduct academic exchanges and contacts with colleagues from ICORR and CSCP

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Thanks