

MODELING THE OPTIMAL IRON CONTENT IN Zr-1%Nb ALLOY BY SET-MEMBERSHIP IDENTIFICATION

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This paper addresses the problem of identifying the optimal iron content in Zr-1%Nb alloy that minimises the corrosion rate of WWER-1000 fuel rod cladding under primary-circuit conditions (350 °C, 16.5 MPa). Based on seven interval-valued corrosion-rate measurements of specimens with Fe=0.012...0.192 wt.%, we show that ordinary least-squares (OLS) regression is structurally inadequate: no polynomial of degree $m \leq 4$ is compatible with all measurement intervals, and OLS estimates of the optimal iron content (0.108...0.117 wt.%) carry a systematic bias of $\Delta\text{Fe}=0.006\ldots0.015$ wt.%. A set-membership (bounded-error) identification framework is applied instead. The feasible parameter set P^* – all 5th-degree polynomial coefficients simultaneously compatible with every measurement interval – is characterised via linear programming. The resulting LP envelope localises the corrosion-rate minimum at Fe $\in [0.101; 0.102]$ wt.% with $\bar{V} = 0.02975$ mg/(dm²·h), an order of magnitude more precisely than OLS. The identified systematic OLS error corresponds to a corrosion-rate increase of up to 22% above the achievable minimum – an unacceptable margin for cladding with a 60-year design service life.

INTRODUCTION

Zirconium alloys are among the most widely used high-purity structural metals for fuel rod cladding, guide tubes, and structural components in nuclear reactor cores. Their broad application rests on a characteristically low thermal-neutron absorption cross-section, adequate mechanical strength, and relatively high corrosion resistance in high-temperature aqueous environments [1, 2].

Corrosion and the associated hydrogen uptake are the critical degradation processes that limit the service life of zirconium-alloy cladding in both Western pressurised-water reactors (PWR) and Soviet-design WWER units, including the WWER-1000 reactors operating at all four Ukrainian nuclear power plants. Accordingly, considerable attention has been devoted to the effect of alloying elements on oxide-film growth kinetics, film stability, and hydrogen uptake [1, 3, 4].

Among the alloying elements – tin (Sn), niobium (Nb), chromium (Cr), and iron (Fe) – iron occupies a special position. Fe acts primarily through the formation of second-phase intermetallic particles (SPP): discrete microscopic inclusions in the zirconium matrix with a composition and crystal structure distinct from the solid solution. These particles arise from the limited solubility of iron in zirconium and play an important role in microstructure formation, influencing corrosion behaviour, stress distribution, and hydrogen uptake capacity. The oxidation behaviour of SPPs substantially affects both ZrO₂ film growth kinetics and the fraction of hydrogen absorbed by the metal [5, 6]. This feature is beneficial while SPPs remain stable and potentially detrimental after their dissolution under neutron irradiation, making iron the most ambiguous alloying element in zirconium metallurgy.

Noteworthy international results include STEM/EELS analysis of Zr(Fe,Cr)₂ particles in Zircaloy-4 [7], which revealed a fundamental difference between Fe and Cr behaviour: iron remains in the metallic state much longer than chromium and oxidises predominantly after the corrosion transition, when water penetrates

through nanopores and cracks. Reference [8] modelled oxide-growth kinetics in simulated WWER coolant (KOH+H₃BO₃, 300 °C) by in-situ EIS, demonstrating that compressive stresses in the oxide govern the ionic transport properties that determine the long-term oxidation rate. In BWR reactors using Zircaloy-2, the hydrogen pick-up fraction (HPU) correlates directly with Fe content: cladding with higher Fe shows up to 50 % thinner oxide and lower HPU at equivalent irradiation dose [9]. The physical link between Fe and HPU acts through the electronic conductivity of the oxide: in-situ EIS data reviewed in [10] demonstrate a linear relationship between oxide resistivity and HPU fraction.

A significant body of results bearing on the present study was produced at National Science Center “Kharkiv Institute of Physics and Technology” (NSC KIPT, Ukraine, Ukraine) through research on nuclear-grade alloys E110 (Zr-1%Nb) and E635 (Zr-1Nb-1.2Sn-0.35Fe) for WWER-type reactors [11]. In E110, the standard Fe content is very low (≤ 0.05 wt.%), so SPP formation is limited. NSC KIPT research showed that deliberate Fe micro-alloying to levels sufficient to produce Laves-phase Zr(Fe,Nb)₂ precipitates substantially improves corrosion resistance under WWER-1000 conditions [5, 12], opening a route for optimising E110-type alloys for long-term safe reactor operation.

The role of iron in corrosion behaviour can be further appreciated by comparison with Western fuel cladding alloys. Zircaloy-4 (Zr-1.5Sn-0.2Fe-0.1Cr), the standard PWR cladding material, contains substantially more iron (0.18...0.24 wt.%) than standard E110, and its corrosion performance is governed primarily by the oxidation behaviour of Zr(Fe,Cr)₂ Laves-phase precipitates [1, 7]. Zircaloy-2 (Zr-1.5Sn-0.15Fe-0.1Cr-0.05Ni), used in BWR reactors, contains a similar Fe level and additionally benefits from nickel-containing SPPs that influence hydrogen pick-up [9]. The advanced alloy M5® (Zr-1%Nb, ≤ 0.015 wt.% Fe), developed for PWR service, deliberately minimises iron to suppress irradiation-induced SPP dissolution, achieving excellent

corrosion resistance through high Nb solid-solution content and a fine oxide microstructure. ZIRLO™ (Zr-1Nb-1Sn-0.1Fe) takes an intermediate approach, retaining a moderate Fe level to benefit from SPP strengthening while limiting irradiation-induced precipitate dissolution. These contrasting strategies highlight that there is no universal optimum iron content: it depends on the alloy system, reactor type, coolant chemistry, and irradiation conditions. For E110 operating in WWER-1000 primary coolant, the optimisation problem is non-trivial precisely because the beneficial Laves-phase precipitation occurs in a narrow Fe range, motivating the rigorous identification approach developed in this work.

1. PROBLEM STATEMENT AND EXPERIMENTAL DATA

We consider the problem of identifying the optimal iron content in the Zr-1%Nb alloy that minimises the

corrosion rate under primary-circuit operating conditions of a nuclear power plant (temperature 350 °C, pressure 16.5 MPa) [12].

The dataset consists of long-term corrosion tests of Zr-1%Nb specimens with Fe content from 0.012 to 0.192 wt.%, conducted at the NSC KIPT; a subset limited to the 1000-hour test is summarised in Table 1.

Corrosion rates are given as intervals $[V_i, \overline{V}_i]$ of hourly specimen mass-gain, not as point values. This is a fundamentally important feature of the dataset: the intervals are not a processing artefact but the primary form of the result. They reflect the true scatter among specimens with the same nominal Fe content, instrumental error and possible effects of test conditions. This feature distinguishes the present modelling task from a standard regression problem and calls into question the direct application of classical least squares [13].

Table 1

Corrosion tests results for Zr-1%Nb spicemens (1000 h)

Iron content Fe, wt.%	0.012	0.042	0.072	0.102	0.132	0.162	0.192
Weight gain, $\frac{mg}{dm^2}$, [min; max]	[35.3, 36.3]	[33.3, 36.6]	[31.8, 32.8]	[28.7, 29.9]	[31.3, 31.5]	[32.4, 33.3]	[32.54, 33.98]
Corrosion rate, $\frac{mg}{(dm^2 \cdot h)}$, [min; max]	[0.0353, 0.0363]	[0.0333, 0.0366]	[0.0318, 0.0328]	[0.0287, 0.0299]	[0.0313, 0.0315]	[0.0324, 0.0333]	[0.03254, 0.03398]

2. LIMITATIONS OF OLS FOR INTERVAL DATA

The OLS method constructs an approximating polynomial

$$f(x) = a_n x^n + \dots + a_1 x + a_0$$

by minimising the sum of squared deviations between model values and the midpoints of each interval pair $[V_i, \overline{V}_i]$, $\forall i = \overline{1, N}$.

2.1. OLS MODELS AND OPTIMUM-ESTIMATE BIAS

In our previous study [13], we constructed three polynomials of degrees $m = 2, 3, 4$ by OLS. The minima of the corresponding curves (Fig. 1) are located as follows: quadratic – $Fe \approx 0.117 \text{ wt.}\%$, $V_{\min} \approx 0.03096 \frac{mg}{dm^2 \cdot h}$; cubic – $Fe \approx 0.120 \text{ wt.}\%$, $V_{\min} \approx 0.03091 \frac{mg}{dm^2 \cdot h}$; 4th-degree – $Fe \approx 0.108 \text{ wt.}\%$, $V_{\min} \approx 0.02994 \frac{mg}{dm^2 \cdot h}$. The experimentally observed minimum $V = [0.0287, 0.0299] \frac{mg}{dm^2 \cdot h}$ corresponds to $Fe = 0.102 \text{ wt.}\%$. All three models overestimate the optimal iron content and underestimate the achievable corrosion minimum.

The quadratic regression at $Fe = 0.102 \text{ wt.}\%$ predicts $\approx 0.0318 \frac{mg}{dm^2 \cdot h}$, overestimating the measurement by $\Delta \approx 0.0019 \frac{mg}{dm^2 \cdot h}$ – exceeding the interval width ($0.0012 \frac{mg}{dm^2 \cdot h}$) itself. No point on any OLS curve is compatible with the guaranteed measurement bounds at $Fe = 0.102 \text{ wt.}\%$.

The 4th-degree polynomial gives a better approximation at this point (predicts $\approx 0.0295 \frac{mg}{dm^2 \cdot h}$, which falls within $V = [0.0287, 0.0299] \frac{mg}{dm^2 \cdot h}$), but generates an unphysical additional minimum at low Fe and oscillates strongly between nodes. Ridge regularisation smooths the curve by reducing high-degree coefficients but substantially shifts the minimum towards larger Fe values, introducing a regularisation bias and causing the optimum to almost vanish. OLS thus provides no reliable identification of the optimal Fe content in either position or value of the corrosion minimum.

2.2. GAUSS-MARKOV HYPOTHESIS CHECKS FOR THE DATASET

Classical OLS theory rests on the Gauss-Markov assumptions, which are necessary conditions for unbiasedness, efficiency, and consistency of estimates. Based on the facts above, we show that none of these assumptions can be reliably verified for the Zr-1%Nb corrosion dataset.

Sample size. With $N=7$ and a 4th-degree polynomial (5 parameters), only 2 degrees of freedom remain – insufficient for a reliable estimate of residual variance and stable coefficient estimates (evidenced by unphysical curve oscillations between nodes).

Normality and independence of errors. The distribution within intervals $[V_i, \overline{V}_i]$, $i = \overline{1, N}$ is unknown and cannot be established from seven points, although each interval characterises real measurement scatter. Applying OLS to midpoints assumes a uniform distribution and independent errors, which is unverified.

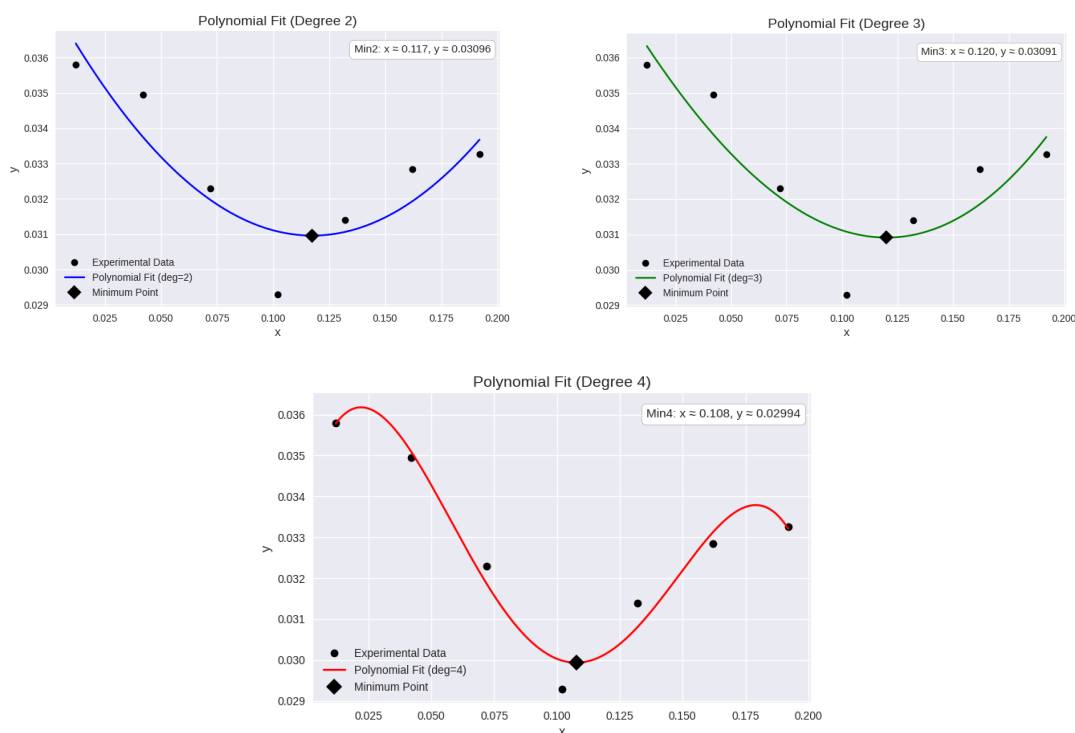


Fig. 1. Systematic bias of OLS polynomial models in locating the corrosion-rate minimum of Zr-1%Nb as a function of iron content

Small errors. At $Fe=0.042$ wt.% the relative interval width is $\approx 9.4\%$. At such magnitudes, linearised error-propagation theory produces significant systematic deviations, especially on the nonlinear portion of the corrosion-rate curve: underestimation in the central region and overestimation at the interval edges.

Absence of outliers. The point $Fe=0.102$ wt.% is statistically incompatible with the quadratic, cubic, and 4th-degree OLS curves (see Fig. 1), i.e., it is structurally inconsistent with these models. Physically, however, it is the most important point in the dataset: it is where the experimental corrosion minimum is reached, associated with the formation of Laves-phase precipitates $Zr(Fe,Nb)_2$.

3. INTERVAL IDENTIFICATION: CONCEPT AND ADVANTAGES

Interval analysis, whose foundations were laid by R. Moore [14] and extended towards parameter identification by Jaulin and Walter [15], rests on a fundamentally different principle. Instead of minimising the sum of squared deviations from midpoints, a model must be compatible with the guaranteed bounds of every measurement. Compatibility is the key concept: model parameters are admissible if, for each argument value $x_i, i = \overline{1, N}$ (here, the Fe content), the model value $f(x_i)$ falls within the measurement interval $[V_i, \overline{V}_i], i = \overline{1, N}$. The set of all parameters compatible with the experimental interval data forms the feasible parameter set P , containing every possible model consistent with the measurements and error bounds [15, 16]. Unlike classical statistical approaches, this set is determined without any assumptions about the error distribution and is based solely on guaranteed uncertainty bounds [14] – it is a deterministic analogue of a confidence region.

We systematically state and justify the key advantages of the interval approach for processing experimental data given as uncertainty intervals, illustrated with the Zr-1%Nb corrosion test data.

1. *No assumptions about the error distribution.* OLS implicitly assumes Gaussian, independent errors – assumptions virtually impossible to verify for $N = 7$. The interval approach requires only knowledge of the error bounds, i.e., the intervals $[V_i, \overline{V}_i], i = \overline{1, N}$, which are directly provided by the measurements without additional hypotheses. Consequently, the guaranteed bounds of the interval model remain correct for any error distribution.

2. *Explicit representation of measurement uncertainty.* OLS collapses each interval $[V_i, \overline{V}_i], i = \overline{1, N}$ to a midpoint and loses scatter information. The interval width carries physical meaning: it reflects variability among specimens with the same nominal Fe content, which may be caused by microstructural inhomogeneity, different recrystallisation degree, or differences in micro-chemical composition at SPP level. The interval model preserves this information as the bandwidth between $\underline{V}$ and $\overline{V}$. In our data: at $Fe = 0.042\text{wt.}\%$, $\Delta V = 0.0366 - 0.0333 = 0.0033 \frac{\text{mg}}{\text{dm}^2 \cdot \text{h}}$ (largest in the dataset); at $Fe = 0.132\text{wt.}\%$ – $\Delta V = 0.0315 - 0.0313 = 0.0002 \frac{\text{mg}}{\text{dm}^2 \cdot \text{h}}$ (smallest). The OLS curve treats both points identically.

3. *Correct handling of small samples.* With $N=7$ and a 4th-degree polynomial ($p=4$), there are only $7 - 5 = 2$ degrees of freedom, insufficient for reliable statistical inference. Leave-one-out cross-validation ($k=7$) showed that the 3rd-degree polynomial has the largest prediction error, while the apparent superiority of the 4th-degree polynomial by R^2 is a small-sample artefact. The interval

approach requires no residual variance estimation and is valid even for $N=7$.

4. *Natural detection of anomalous observations.* In the interval approach, an observation is said to reveal structural inadequacy of the chosen parametric form if no curve of that family passes through the corresponding measurement interval simultaneously with all others – i.e., if including it renders P empty. Unlike a statistical outlier, which is a property of the point relative to the sample, this is a property of the point relative to a specific model: the same observation may be incompatible with a low-degree polynomial yet fully compatible with a higher-degree one. This is precisely what occurs at $Fe=0.102$ wt.%: no polynomial of degree $m \leq 4$ passes through all seven intervals, including $[0.0287, 0.0299]$. Rather than signalling a measurement error, this signals that the parametric form is inadequate – and prompts a physical explanation: the structural transition associated with $Zr(Fe,Nb)_2$ Laves-phase precipitation at $Fe=0.102$ wt.%. OLS, by contrast, absorbs this physically significant point into the least-squares fit, shifting all polynomial coefficients and biasing the estimated optimum.

5. *Guaranteed character of results.* Classical OLS regression yields a point estimate of the optimal Fe content with unknown posterior guarantee: 0.117 wt.% (quadratic) or 0.108 wt.% (4th-degree). These estimates differ substantially depending on the chosen polynomial degree – a subjective choice. The interval model yields guaranteed bounds: the optimal Fe content lies in the range x where the lower bounding curve $\underline{V}(x)$ reaches its minimum. Since $\underline{V}(x)$ is a lower bound for any realised value, its minimum is a guaranteed lower bound on the achievable corrosion rate – a property absent from OLS models.

4. SET-MEMBERSHIP IDENTIFICATION: LP-METHOD

Let a series of N measurements of a dependent variable y as a function of independent argument x be performed. Each measurement result y_i , due to instrument and experimental error, is not an exact value but belongs to a guaranteed interval:

$$y_i \in [\underline{y}_i, \overline{y}_i], i = \overline{1, N}.$$

No assumptions are made about the character of the error distribution within the interval. The identification problem is to find the set P of all parameter vectors $\overline{\theta} = (\theta_0, \theta_1, \dots, \theta_m)$ of the model $f(x; \overline{\theta})$ for which the model is compatible with all measurement intervals:

$$P = \{\overline{\theta} \in R^{m+1}: \underline{y}_i \leq f(x_i; \overline{\theta}) \leq \overline{y}_i, \forall i = \overline{1, N}\}.$$

P is the feasible set. Unlike the OLS point estimate, P is convex (when the model is linear in parameters) and provides a complete characterisation of identification uncertainty – the entire collection of parameters compatible with the experimental data without any assumptions about error distribution. The feasible set is formed by successive intersection of regions corresponding to individual interval measurements; each

additional constraint narrows the admissible parameter space.

For polynomial regression

$$f(x; \overline{\theta}) = \theta_0 + \theta_1 \cdot x + \dots + \theta_m \cdot x^m$$

the compatibility condition is linear in parameters:

$$\underline{y}_i \leq A^i \cdot \overline{\theta} \leq \overline{y}_i,$$

where $A^i = (1, x_i, x_i^2, \dots, x_i^m)$ is the Vandermonde row at x_i . The collection of N such conditions forms a system of $2N$ linear inequalities in $(m+1)$ unknowns – a linear programming (LP) problem.

The LP method in interval identification solves two sequential tasks: verifying the compatibility of the chosen parametric form with all measurement intervals, and constructing the envelope of admissible curves – the exact projection of P onto the function-value space.

Before building the envelope, one must confirm that P is non-empty – i.e., that at least one parameter vector θ makes the model simultaneously compatible with all N measurement intervals. This is checked via the Chebyshev-centre problem [17]:

find $\max_{\overline{\theta}, r}$ subject to

$$\begin{cases} \underline{y}_i \leq A^i \cdot \overline{\theta} - r \cdot \|A^i\|, \\ A^i \cdot \overline{\theta} + r \cdot \|A^i\| \leq \overline{y}_i, \\ \overline{\theta} \in R^{m+1}, \forall i = \overline{1, N}, \end{cases}$$

where $\|A^i\|$ – euclidean norm of a Vandermonde row.

If the optimal $r > 0$, then P is non-empty and the Chebyshev central curve $\overline{\theta}$ passes strictly inside all measurement intervals with guaranteed margin r . A negative r indicates structural inadequacy of the chosen parametric form – no curve of that degree is compatible with all intervals without widening them.

The envelope is the pair $\underline{f}(x)$ and $\overline{f}(x)$, defining for each argument x the smallest and largest value attainable by any curve in P :

$$\begin{aligned} \underline{f}(x) &= \min_{\overline{\theta} \in P} \{A(x) \cdot \overline{\theta} : \underline{y}_i \leq A^i \cdot \overline{\theta} \leq \overline{y}_i, \forall i = \overline{1, N}\}, \\ \overline{f}(x) &= \max_{\overline{\theta} \in P} \{A(x) \cdot \overline{\theta} : \underline{y}_i \leq A^i \cdot \overline{\theta} \leq \overline{y}_i, \forall i = \overline{1, N}\}, \end{aligned}$$

where $A(x) = (1, x, x^2, \dots, x^m)$ – is the Vandermonde row at x .

For each fixed x , two LP problems are solved – minimization and maximization of the linear function $A(x) \cdot \overline{\theta}$ subject to linear constraints.

The LP-box [16] – the minimal hyperrectangle containing P – is obtained by solving $2(m+1)$ LP problems, one per coefficient bound:

$$\theta_j = \min \{\theta_j : \underline{y}_i \leq A^i \cdot \overline{\theta} \leq \overline{y}_i, \forall i = \overline{1, N}\},$$

$$\bar{\theta}_j = \max \{ \theta_j : y_i \leq A^i \cdot \bar{\theta} \leq \bar{y}^i, \forall i = \overline{1, N} \}.$$

The LP-box

$$B_{\{LP\}} = [\underline{\theta}_0, \bar{\theta}_0] \times [\underline{\theta}_1, \bar{\theta}_1] \times \dots \times [\underline{\theta}_m, \bar{\theta}_m]$$

is an outer approximation of P in parameter space and may contain points not in P ; the envelope $[f(x), \bar{f}(x)]$ is the exact projection of P onto the function-value space and contains no superfluous curves. The least squares confidence interval is a probabilistic construct that relies on the assumption of Gaussian errors. The LP envelope provides a deterministic guarantee: any curve consistent with the measurement intervals lies inside the envelope, and any point of the envelope is attainable by some admissible curve.

Since $\underline{f}(x)$ is the lower envelope of all compatible curves, the point $x = \operatorname{argmin} \underline{f}(x)$ is a guaranteed lower bound on the optimal Fe content. Similarly, the minimum of $\bar{f}(x)$ gives the upper bound of the optimal range. Thus, the optimal Fe content is localized not by a single point, but by an interval

$$[\operatorname{argmin} \underline{f}(x), \operatorname{argmin} \bar{f}(x)],$$

which is fundamentally a more correct result for a problem with interval data.

5. RESULTS AND DISCUSSION

Let us present the results of applying interval methods to solve the problem of modeling the effect of the iron (Fe) content on the corrosion rate in the zirconium alloy Zr-1%Nb.

All computations were performed in Python 3 using NumPy and SciPy: LP problems (Chebyshev centre, LP-box, and envelope) were solved with `scipy.optimize.linprog` and the HiGHS solver.

5.1. PARAMETRIC FORM SELECTION

The key problem is to identify a model $V(x; \bar{\theta})$ that passes through all seven measurement intervals. The Chebyshev-centre compatibility check showed that for polynomial degrees $m = 2, 3, 4$ the optimal value r is negative (for the quadratic model $r \approx -0.0009 \frac{\text{mg}}{\text{dm}^2 \cdot \text{h}} < 0$), i.e., no low-degree curve passes through all seven measurement intervals without widening them. This is quantitative confirmation of the structural inadequacy of models with $m \leq 4$ – not a noise artefact, but a consequence of the real physical transition at $Fe = 0.102 \text{ wt.}\%$ associated with Zr(Fe,Nb)_2 Laves-phase precipitation.

The 5th-degree polynomial, as shown by the LP approach, is the first model compatible with all 7 measurement intervals without widening, with $r > 0$: $r = 0.000048 \text{ mg} / (\text{dm}^2 \cdot \text{h})$.

This confirms the structural adequacy of the chosen parametric form, guarantees the existence of a non-empty feasible set P , and is a necessary condition for correct construction of the envelope of admissible curves. The quantitative value of the guaranteed margin demonstrates extremely tight compatibility with the data.

5.2. LP ENVELOPE AND OPTIMAL Fe CONTENT

The envelope $[V(x), \bar{V}(x)]$ was constructed on a uniform grid of $K=500$ points on $[0.000, 0.205] \text{ wt.}\% \text{ Fe}$. Two LP minimisation and maximisation problems were solved at each grid point.

The Chebyshev central curve has parameters

$\bar{\theta} = (0.0291, 0.7382, -20.6925, 209.53, -893.12, 1361.40)$ and passes strictly inside all measurement intervals; it is the geometric centre of the envelope in the Chebyshev L_∞ norm.

The upper panel of Fig. 2 shows the LP envelope of admissible curves: the shaded region contains all 5th-degree polynomials compatible with the interval data; dashed and dotted curves are the lower $\underline{V}(x)$ and upper $\bar{V}(x)$ bounds of the envelope; the solid curve is the Chebyshev central solution.

The vertical orange marks the LP-optimal range $[0.101, 0.102] \text{ wt.}\%$, at which the lower-bound minimum $\underline{V} = 0.02975 \text{ mg}/(\text{dm}^2 \cdot \text{h})$ is attained.

The lower panel shows the envelope width across the full Fe range: in the optimum zone $0.156 \cdot 10^{-3} \text{ mg}/(\text{dm}^2 \cdot \text{h})$ – an order of magnitude smaller than at the range edges (up to $0.004376 \text{ mg}/(\text{dm}^2 \cdot \text{h})$). This narrowing is not a method artefact but reflects the real data structure: near the global minimum, all compatible curves converge into a narrow bundle, confirming the physical significance of this point and the reliability of the LP optimum estimate.

The LP envelope localises the optimal Fe content in $[0.101; 0.102] \text{ wt.}\%$ (see Fig. 2), consistent with the experimentally observed minimum at $Fe = 0.102 \text{ wt.}\%$. OLS estimates ($0.108 \text{ wt.}\%$ for the 4th-degree polynomial, $0.117 \text{ wt.}\%$ for the quadratic) exceed the upper bound of the LP range by $Fe = 0.006 \dots 0.015 \text{ wt.}\%$. This error corresponds to a corrosion-rate increase of up to 22% above the achievable minimum $\underline{V} = 0.02975 \text{ mg}/(\text{dm}^2 \cdot \text{h})$.

For WWER-1000 fuel rod cladding with a design service life of 60 years, such a deviation from the optimal alloy composition may lead to unacceptable consequences from the standpoint of effective and safe nuclear plant operation.

CONCLUSIONS

Based on the results obtained from constructing the LP envelope of admissible curves for modeling the dependence of the corrosion rate on the iron content in the Zr-1%Nb alloy, we have arrived at the following conclusions:

1. Low-degree polynomial models are structurally inadequate. No smooth curve of degree $m \leq 4$ passes through all seven observation intervals, including the critical point $Fe = 0.102 \text{ wt.}\%$, where the corrosion minimum associated with Zr(Fe,Nb)_2 Laves-phase precipitation is reached. This reflects a real structural transition, not measurement noise.

2. The 5th-degree polynomial is the first parametric form compatible with all data. The Chebyshev margin $r = 0.000048 \text{ mg}/(\text{dm}^2 \cdot \text{h}) > 0$ confirms structural adequacy

and is a necessary condition for correct envelope construction.

3. The LP envelope provides an exact deterministic characterisation of model uncertainty. Unlike the probabilistic OLS confidence interval, the envelope $[V(x), \bar{V}(x)]$ contains only curves compatible with the measurement intervals, without any error-distribution assumptions. The envelope width narrows from up to 0.004376 mg/(dm²·h) in at the range edges to 0.000156 mg/(dm²·h) in the optimum zone, reflecting the real convergence of admissible curves near the global minimum.

4. The LP envelope localises the optimal Fe content in [0,101; 0,102]wt.‰: the lower-bound minimum

$\underline{V}=0.02975$ mg/(dm²·h) is attained at $Fe=0.1011$ wt.‰ the upper-bound minimum 0.0299 mg/(dm²·h) at $Fe=0.1020$ wt.‰. The result is consistent with the experimental minimum and is an order of magnitude more precise than OLS estimates (0.108...0.117 wt.‰).

5. The OLS systematic bias $\Delta Fe = 0.006 \dots 0.015$ wt.‰ corresponds to a corrosion-rate increase of up to 22% above the achievable minimum. For WWER-1000 fuel rod cladding with a 60-year design service life such a deviation is unacceptable. The LP-envelope method provides a rigorous non-probabilistic basis for certified composition optimisation of Zr-1%Nb alloy.

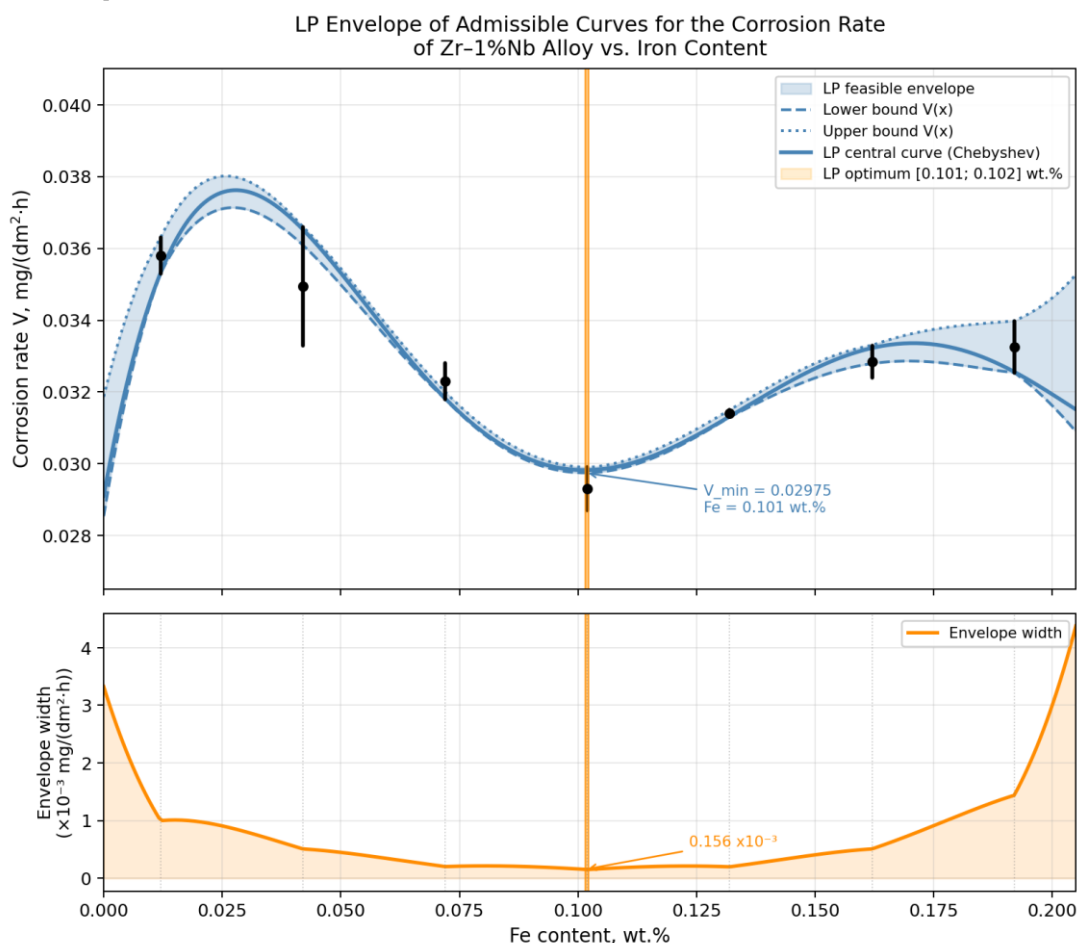


Fig. 2. LP envelope of admissible curves for the corrosion-rate of Zr-1%Nb Alloy as a function of iron content (upper panel) and envelope width (lower panel)

Envelope characteristics are summarised in Table 2.

Table 2

Characteristics of the exact LP envelope

Characteristic	Value
Minimum of lower bound $\underline{V}(x; \bar{\theta})$	$Fe=0.1020$ wt.‰ at $Fe=0.1011$ wt.‰
Minimum of upper bound $\bar{V}(x; \bar{\theta})$	0.029900 mg/(dm ² ·h) at $Fe=0.1020$ wt.‰
Envelope width (minimum, optimum zone)	0.000156 mg/(dm ² ·h)
Envelope width (maximum, range edges)	0.004376 mg/(dm ² ·h)
LP-optimal Fe range	[0.101, 0.102] wt.‰

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МОДЕЛЮВАННЯ ОПТИМАЛЬНОГО ВМІСТУ ЗАЛІЗА В ЦИРКОНІЄВОМУ СПЛАВІ Zr-1%Nb МЕТОДАМИ ІНТЕРВАЛЬНОЇ ІДЕНТИФІКАЦІЇ

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Розглядається задача визначення оптимального вмісту заліза у сплаві Zr-1%Nb, що мінімізує швидкість корозії оболонок паливних стрижнів реакторів ВВЕР-1000 за умов першого контуру (350 °C, 16,5 МПа). На основі семи інтервальних вимірювань швидкості корозії зразків із вмістом Fe = 0,12...0,192 мас.% показано, що класичний метод найменших квадратів (МНК) є структурно неадекватним: жоден поліном ступеня $m \leq 4$ не сумісний з усіма інтервалами вимірювань, а оцінки МНК оптимального вмісту заліза (0,108...0,117 мас.%) містять систематичну похибку $\Delta Fe = 0,006...0,015$. Застосовано підхід інтервальної (set-membership) ідентифікації. Множина допустимих параметрів P^* – усі коефіцієнти полінома 5-го ступеня одночасно сумісні з кожним інтервалом вимірювань – охарактеризована методами лінійного програмування. LP-конверт локалізує мінімум швидкості корозії при $Fe \in [0,101; 0,102]$ мас.% із $\underline{v} = 0,02975$ мг/(дм² · год) на порядок точніше за оцінки МНК. Виявлена систематична похибка МНК відповідає збільшенню швидкості корозії до 22% відносно досяжного мінімуму – неприйнятна величина для оболонок із розрахунковим терміном служби 60 років.