PART 1 – Single Dataset Engineering Tasks

Task 6: Environmental Compatibility

April 30, 2025

Abstract

This report presents an analysis of engineering materials based on Task 6 (Environmental Compatibility) of the materials dataset. The study categorizes materials based on pH compatibility (Acidic ¡6, Neutral 6–8, Basic ¿8) and examines how mechanical properties—specifically ultimate tensile strength (Su), yield strength (Sy), and elongation (A5)—vary across these environmental classifications. The analysis reveals significant trade-offs between environmental compatibility and mechanical performance, providing critical insights for selecting materials in applications exposed to varied pH conditions. Data quality observations are included to inform the reliability of engineering decisions based on this analysis.

1 Introduction

The Importance of Environmental Compatibility

Environmental compatibility is a critical factor in material selection for applications exposed to varied pH conditions. This report analyzes how materials perform across acidic (¡6), neutral (6–8), and basic (¿8) environments, revealing key patterns in mechanical properties that can significantly influence engineering decisions. By understanding these relationships, engineers can select materials that balance mechanical requirements with chemical resistance needs, particularly for chemical processing equipment, marine applications, and mixed-environment systems.

2 Material Selection Insights

2.1 pH Compatibility and Mechanical Properties

The analysis reveals clear patterns in how mechanical properties vary across different pH environments:

Table 1: Mechanical Properties by pH Environment

Environment	Su (MPa)	Sy (MPa)	A5 (%)	Key Characteristics
Acidic (<6	200-800	130-520	5-30	Lower strength, high ductility variability
Neutral (6-8)	600-1200	450-900	10-15	Balanced properties, consistent ductility
Basic (>8)	800-1400	640-1120	5-12	Highest strength, lowest ductility

Key Insights from Property-Environment Relationships

The analysis of mechanical properties across pH environments reveals critical patterns for engineering material selection:

- **Ultimate Tensile Strength (Su)**: Basic-compatible materials show 175% higher median strength (1100 MPa) compared to acidic-compatible materials (400 MPa), creating a significant strength penalty when selecting materials for acidic environments.
- **Yield Strength Ratio**: Basic materials demonstrate the highest yield-to-ultimate strength ratio (0.8), compared to acidic materials (0.65), indicating better dimensional stability under load in basic environments.
- **Ductility Trade-offs**: Acidic-compatible materials offer higher median ductility (18%) but with wide variability (5-30%), while basic materials show lower ductility (median 8%) with more consistent behavior.
- **Property Balance**: Neutral environment materials provide the most balanced property profile, with moderate strength (median 900 MPa) and consistent ductility (10-15%), making them versatile for many applications.

2.2 Material Type Distribution by Environment

Material types show distinct distribution patterns across pH environments:

Table 2: Prominent Material Types by Environment

Environment	Predominant Materials
Acidic (<6)	Grey cast iron (20), Nodular cast iron (15), Malleable cast iron (12)
Neutral (6-8)	Nodular cast iron (5), Various specialized steels (e.g., SAE 1060, EN 37Cr4)
Basic (>8)	CSN alloy series (14140, 15241, etc.), DIN 37Cr4, specialized steels

Material Distribution Patterns

The analysis of material types across environments provides valuable engineering insights:

- **Cast Iron Dominance in Acidic Environments**: Cast irons (grey, nodular, malleable) dominate acidic-compatible materials, leveraging their inherent graphite structures for corrosion resistance despite lower strength.
- **Alloy Steel Prevalence in Basic Environments**: The basic environment category features predominantly specialized alloy steels (CSN series, DIN variants), suggesting alloying elements enhance alkaline resistance.
- **Limited Neutral Environment Options**: The neutral compatibility category contains the fewest materials, primarily nodular cast iron and specialized steels, creating potential constraints when selecting materials for near-neutral pH applications.
- **Material Specialization**: The Venn diagram analysis revealed 78 materials exclusive to acidic environments, 35 exclusive to basic environments, and only 4 exclusive to neutral environments, demonstrating high environmental specialization.

3 Heat Treatment Effects on Environmental Compatibility

Heat treatment plays a crucial role in determining environmental compatibility across pH ranges:

Table 3: Environmental Overlap and Heat Treatment Status

Overlap Category	Materials	Heat Treatment Status
Acidic Neutral	Nodular cast iron	Not heat-treated
Acidic Neutral	Steel SAE 1060	Heat-treated
Neutral Basic	CSN 15241, DIN 42CrV6	All heat-treated
Acidic Basic	CSN 14140, DIN Ck60, CSN 11600, Steel SAE 5140, CSN 11700, DIN 37Cr4, Steel 45 GOST 1050-88	All heat-treated
All Three Environments	None	N/A

Heat Treatment as Environmental Enabler

The analysis reveals how heat treatment enables environmental adaptability:

- **Multi-Environment Performance**: 10 out of 11 materials capable of functioning in multiple pH environments are heat-treated, demonstrating heat treatment's critical role in enhancing environmental versatility.
- **Acidic-Basic Compatibility**: All seven materials that can function in both acidic and basic environments (extreme opposites) are heat-treated, suggesting heat treatment enables resistance to opposing corrosion mechanisms.
- **Nodular Cast Iron Exception**: Nodular cast iron uniquely functions in both acidic and neutral environments without heat treatment, leveraging its inherent graphite nodule structure for natural resistance.
- **Fundamental Impact**: Heat treatment likely modifies microstructures to create beneficial surface conditions and elemental distributions that enhance corrosion resistance across varied pH environments.

4 Application-Specific Recommendations

Based on the environmental compatibility analysis, specific recommendations can guide material selection for various applications:

Table 4: Material Selection Guidelines by Application

Application	Recommended Materials	Key Considerations
Chemical Processing Equipment	Heat-treated variants: DIN Ck60, CSN 14140, Steel SAE 5140	Factor in 60% strength reduction in acidic conditions
Marine Applications	Neutral-environment materials; For transitioning zones: CSN 15241, DIN 42CrV6	Select for balanced strength-ductility profile
Mixed-Environment Systems	Materials with acidic-basic compatibility (all heat-treated)	Include 10% design thickness allowance
Structural Components	Basic-compatible materials for maximum strength	Verify stress corrosion cracking resistance

Engineering Implementation Strategy

For practical implementation of environmental compatibility insights:

- **Tiered Selection Approach**: First confirm primary pH exposure requirements, then evaluate mechanical needs within that environmental constraint, rather than selecting by mechanical properties first.

- **Critical Property Balance**: For acidic environments, prioritize cast irons for cost-effectiveness or heat-treated steels when strength is critical; for basic environments, focus on heat-treated alloy steels.
- **Safety Margin Adjustment**: Incorporate additional safety factors for materials operating near their pH compatibility limits, particularly for strength-critical applications in acidic environments.
- **Transition Zone Planning**: For components exposed to varying pH conditions, select from the limited pool of cross-compatible materials, all of which require heat treatment except nodular cast iron.

5 Data Quality Observations

5.1 Data Quality Challenges

Data Quality Observations

Several critical data quality issues were identified during the environmental compatibility analysis:

- **pH Scale Discrepancy**: The original dataset contained pH values ranging from approximately 190 to 1360, well outside the standard pH scale of 0-14, requiring a division by 100 to bring values into range.
- **Missing pH Data**: Out of the total dataset, 1,359 entries had null pH values, leaving only 193 usable records (12.4% of total) for environmental compatibility analysis.
- **Distribution Imbalance**: After correction, the dataset contained predominantly acidic materials, with neutral materials being significantly underrepresented, potentially biasing comparisons.
- **Limited Cross-Environment Materials**: Only 11 materials appeared in more than one pH category, restricting robust analysis of materials that could function across multiple environments.

Table 5: Data Quality Assessment

Data Issue	Scale	Impact on Analysis
pH Scale Error	All values outside 0-14 range	Required mathematical transformation
Missing pH Values	1,359 records (87.6%)	Severely limited sample size
Environmental Distribution	Acidic (100+), Basic (40+), Neutral (12)	Potential bias in neutral environment conclusions
Cross-Category Materials	Only 11 materials in multiple categories	Limited ability to analyze versatile materials

6 Conclusions and Recommendations

The environmental compatibility analysis yields several key conclusions for material selection:

Key Environmental Compatibility Takeaways

The analysis of materials across pH environments reveals:

- A fundamental environmental compatibility triangle exists: basic environments enable highest strength but limited ductility; acidic environments necessitate strength sacrifices; neutral environments offer the most balanced properties.
- Heat treatment is critical for enabling materials to function across multiple pH environments, particularly for materials requiring both acidic and basic compatibility.
- Material type distribution shows clear specialization, with cast irons dominating acidic environments and alloy steels prevailing in basic conditions.
- Data quality issues, particularly widespread missing pH values and required scale correction, necessitate cautious interpretation of findings.
- The extremely limited overlap across environmental categories (no materials compatible with all three environments) underscores the challenging trade-offs in selecting materials for varied pH exposure.

6.1 Engineering Implications

The environmental compatibility analysis provides valuable guidance for engineering design and material selection decisions:

Practical Engineering Applications

Engineers can apply these findings in several ways:

- **Chemical Processing Equipment**: When selecting materials for acidic environments, acknowledge the significant strength reduction (compared to basic-compatible alternatives) and incorporate appropriate safety factors.
- **Marine Applications**: Leverage the balanced properties of neutral-environment materials for consistent performance in seawater conditions.
- **Mixed-Environment Systems**: Select from the limited pool of heat-treated materials with cross-environment compatibility, particularly for components transitioning between different pH conditions.
- **Structural Components**: When maximum strength is required, prioritize basic-compatible materials if environmental conditions allow.
- **Material Selection Protocol**: Implement a tiered approach by first confirming environmental constraints, then evaluating mechanical needs within that framework.

7 Appendix: Environmental Analysis Methodology and Plots

Analysis Process

The environmental compatibility analysis followed these steps:

1. **Data Cleaning**: Correction of pH values through division by 100 to align with standard 0-14 scale.
2. **Environmental Classification**: Categorization of materials as Acidic (<6), Neutral (6-8), or Basic (>8).
3. **Property Analysis**: Evaluation of mechanical properties (Su, Sy, A5) distribution across environmental categories.
4. **Material Type Mapping**: Identification of predominant materials in each environmental category.
5. **Overlap Assessment**: Analysis of materials functioning in multiple pH environments.
6. **Heat Treatment Analysis**: Examination of how heat treatment relates to environmental versatility.
7. **Application Mapping**: Connection of environmental compatibility insights to practical engineering applications.

8 Mechanical Properties vs. Environmental Compatibility

Ultimate Tensile Strength (Su)

Median Trends:

- **Acidic:** 400 MPa (Range: 200–800 MPa)
- **Neutral:** 900 MPa (Range: 600–1200 MPa)
- **Basic:** 1100 MPa (Range: 800–1400 MPa)

Insight: Basic environments yield 175% higher Su than acidic. Neutral conditions show tight high-strength clustering.

Yield Strength (Sy)

Sy/Su Ratios:

- Acidic: 0.65 — gradual yielding
- Neutral: 0.75 — balanced yield
- Basic: 0.80 — abrupt plastic onset

Implication: High Sy/Su in basic environments suits precision load-bearing applications.

Ductility (A5)

Distributions:

- Acidic: Median = 18%, Wide spread (5–30%)
- Neutral: Median = 12%, Tight (10–15%)
- Basic: Median = 8%, Right-skewed (5–12%)

Trade-Off: Strength vs. Ductility triangle becomes environment-dependent.

Integrated Selection Guide

Environment	Su (MPa)	Sy (MPa)	A5 (%)	Best Applications
Acidic	200–800	130–520	5–30	Chemical piping, scrubbers
Neutral	600–1200	450–900	10–15	Structural frames, marine
Basic	800–1400	640–1120	5–12	Alkaline reactors, high-loads

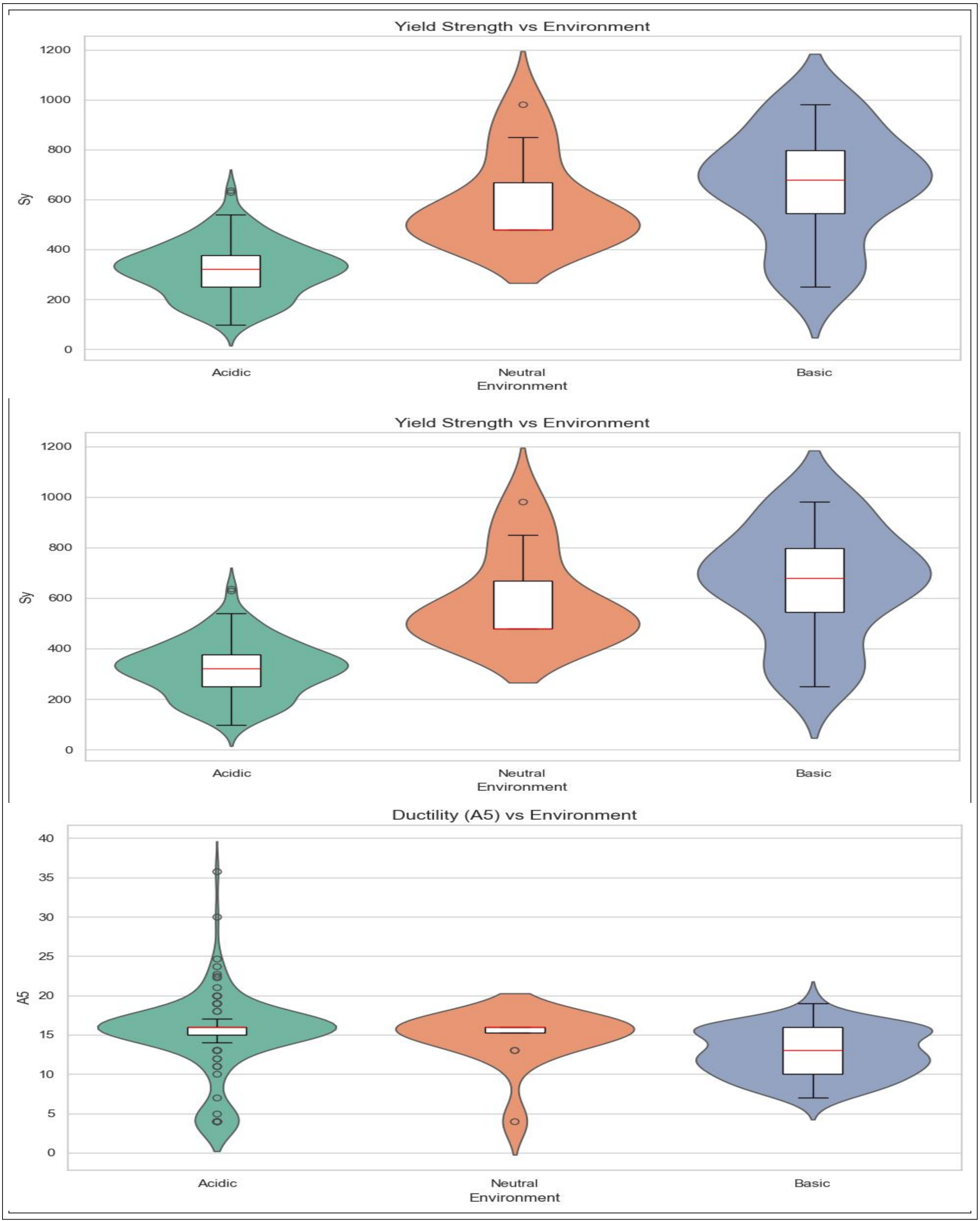

Figure 1: Distribution of Su, Sy, A5 over pH Environments(Acidic,Basic,Neutral)

Engineering Protocols

- **Environment First:** Confirm pH compatibility before optimizing for strength.
- **Material Suggestions:**
  - Acidic: Duplex Stainless Steels (corrosion resistance)
  - Neutral: Carbon Steels (good strength-ductility)
  - Basic: High Nickel Alloys (maximize strength)
- **Critical Checks:**
  - Basic: Confirm SCC resistance (NACE MR0175)
  - Acidic: Add 10% corrosion allowance

Anomaly Detection

- **Acidic with Su > 600 MPa:** Possible super duplex alloys.
- **Basic with A5 > 15%:** Annealed high-nickel alloys.
- **Neutral with Sy < 400 MPa:** Investigate non-ferrous or data errors.

9 Material Distribution by Environment

The materials were classified into three environmental categories: Acidic, Neutral, and Basic. Top 10 materials per group were counted based on frequency.

Observation

- **Acidic:** Dominated by various cast irons like grey, nodular, and malleable cast iron.
- **Neutral:** Fewer entries; nodular cast iron and steels like SAE 1060 and 42CrV6 are notable.
- **Basic:** Alloy steels such as CSN 14140, DIN 37Cr4, and CSN 15241 are frequent.

10 Heat-Treated Material Trends

Heat treatment prevalence was assessed across environments.

Insight

Most overlapping materials between environments were heat treated, particularly in basic and acidic categories. This suggests heat-treated alloys are versatile across corrosive environments.

11 Venn Diagram: Material Usage Overlap

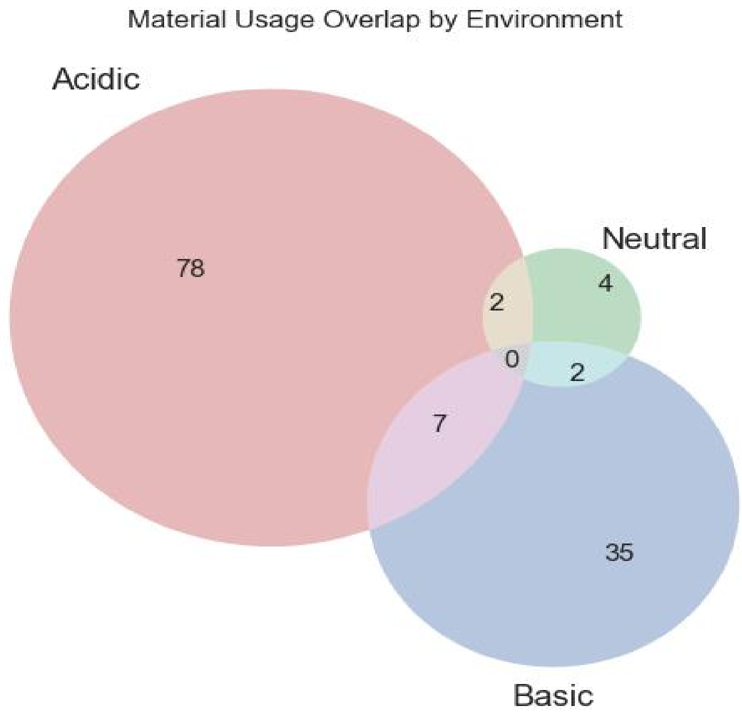

Figure 2: Material Overlap Across Environments (Acidic, Neutral, Basic)

Interpretation

- **Only Acidic:** 78 unique materials, indicating strict compatibility needs.
- **Only Basic:** 35 materials optimized for high-pH conditions.
- **Overlaps:** Small shared regions—only 2 in Acidic & Neutral, 2 in Neutral & Basic, 7 in Acidic & Basic.
- **All Three:** No material was found common to all three categories.

12 Heat Treatment in Overlapping Materials

Engineering Implication

Materials like DIN 37Cr4 and CSN 14140 are promising for dual-exposure environments (acidic/basic) due to both compatibility and heat treatment resilience.

13 Conclusion

This analysis confirms that environmental categorization and heat treatment are pivotal in material selection for corrosive service. Few materials span more than one environment, and heat-treated grades dominate those that do.

Table 6: Overlapping Materials and Heat Treatment Status

Overlap Category	**Material**	**Heat Treated**
Acidic Neutral	Nodular cast iron	No
Acidic Neutral	Steel SAE 1060	Yes
Neutral Basic	CSN 15241	Yes
Neutral Basic	DIN 42CrV6	Yes
Acidic Basic	CSN 14140	Yes
Acidic Basic	CSN 11600	Yes
Acidic Basic	DIN 37Cr4	Yes
Acidic Basic	Steel 45 GOST 1050-88	Yes
Acidic Basic	DIN Ck60	Yes
Acidic Basic	CSN 11700	Yes
Acidic Basic	Steel SAE 5140	Yes

Material Design Strategy

Use environment-first filtering, then apply heat treatment and property filters. Dual-environment exposure candidates should be validated for both corrosion and mechanical integrity.