Appendix 1: Solution Conditions

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Appendix 2: Data
Each “Point” refers to the similarly numbered experimental condition as shown in Table 2.2.1. Each graph depicts all replicates for each sampled point. The data for concentration v. time of Fe(II) and HS⁻ are shown.
Point 6 [S\(^2\)-]

Point 7 [Fe(II)]
Point 9 [$S^{2-}$]

Point 10 [Fe(II)]
Point 11 \([S^2^-]\)

Point 12 \([\text{Fe(II)}]\)
Point 12 [S²⁻]

![Graph of S²⁻ concentration over time]

Midpoint [Fe(II)]

![Graph of Fe(II) concentration over time]
Point 13 $[S^{2-}]$

Point 14 $[\text{Fe(II)}]$
Point 17 \([S^2^-]\)

Point 18 \([\text{Fe(II)}]\)
Appendix 3: Plots of $\ln(A/A_0)$

Each “Point” refers to the similarly numbered experimental condition as shown in Table 2.2.1. Each graph depicts all replicates for each sampled point. The data for $\ln(A/A_0)$ vs time for both Fe(II) and HS$^-$ are shown.

![Point 1 $\ln(\text{Fe}(\text{II})/\text{Fe}(\text{II})_0)$](image)

![Point 1 $\ln(S/S_0)$](image)
Point 2 $\ln(\text{Fe(II)}/\text{Fe(II)}_0)$

- $y = -9.9774 \times 10^{-4}x - 3.5611 \times 10^{-1}$
  - $R^2 = 9.2119 \times 10^{-1}$
- $y = -1.4750 \times 10^{-3}x - 7.8759 \times 10^{-1}$
  - $R^2 = 7.4810 \times 10^{-1}$
- $y = -1.0095 \times 10^{-3}x - 7.0133 \times 10^{-1}$
  - $R^2 = 8.9976 \times 10^{-1}$

Point 2 $\ln(S/S_0)$

- $y = -9.9774 \times 10^{-4}x - 3.5611 \times 10^{-1}$
  - $R^2 = 9.2119 \times 10^{-1}$
- $y = -1.4750 \times 10^{-3}x - 7.8759 \times 10^{-1}$
  - $R^2 = 7.4810 \times 10^{-1}$
- $y = -1.0095 \times 10^{-3}x - 7.0133 \times 10^{-1}$
  - $R^2 = 8.9976 \times 10^{-1}$
Point 3 $\ln(\text{Fe(II)/Fe(II)}_0)$

\begin{align*}
\ln(\text{Fe(II)/Fe(II)}_0) &= -1.1772 \times 10^{-3}x - 9.5374 \times 10^{-1} \\
R^2 &= 9.1929 \times 10^{-1}
\end{align*}

\begin{align*}
\ln(\text{Fe(II)/Fe(II)}_0) &= -2.6065 \times 10^{-3}x - 1.8657 \times 10^{-1} \\
R^2 &= 9.6992 \times 10^{-1}
\end{align*}

Point 3 $\ln(S/S_0)$

\begin{align*}
\ln(S/S_0) &= -2.0916 \times 10^{-3}x - 3.3858 \times 10^{-1} \\
R^2 &= 8.6517 \times 10^{-1}
\end{align*}

\begin{align*}
\ln(S/S_0) &= -2.0916 \times 10^{-3}x - 3.3858 \times 10^{-1} \\
R^2 &= 9.6992 \times 10^{-1}
\end{align*}
Point 4 $\ln(\text{Fe}(\text{II})/\text{Fe}(\text{II})_0)$

- $y = -1.2265E-03x - 8.9590E-01$
  - $R^2 = 9.6995E-01$

Point 4 $\ln(S/S_0)$

- $y = -1.6131E-03x - 7.7715E-01$
  - $R^2 = 6.0531E-01$
- $y = -1.2265E-03x - 8.9590E-01$
  - $R^2 = 9.6995E-01$
Point 5 \( \ln(\text{Fe(II)}/\text{Fe(II)}_0) \)

\[ y = -1.2254 \times 10^{-03}x - 6.0139 \times 10^{-01} \]
\[ R^2 = 8.9116 \times 10^{-01} \]

Point 5 \( \ln(S/S_0) \)

\[ y = -2.0461 \times 10^{-03}x - 4.1479 \times 10^{-01} \]
\[ R^2 = 8.2355 \times 10^{-01} \]

\[ y = -1.1961 \times 10^{-03}x - 7.2885 \times 10^{-01} \]
\[ R^2 = 9.4317 \times 10^{-01} \]
Point 8 $\ln(\text{Fe(II)}/\text{Fe(II)}_0)$

$y = -1.5484E-03x - 7.6315E-01$

$R^2 = 5.8582E-01$

Point 8 $\ln(S/S_0)$

$y = -1.9263E-03x - 4.5732E-01$

$R^2 = 9.4380E-01$
Point 9 \( \ln(\text{Fe(II)}/\text{Fe(II)}_0) \)

- \[ y = -7.3887 \times 10^{-4}x - 1.0667 \times 10^0 \]
  \( R^2 = 5.4572 \times 10^{-1} \)

Point 9 \( \ln(S/S_0) \)

- \[ y = -7.3887 \times 10^{-4}x - 1.0667 \times 10^0 \]
  \( R^2 = 5.4572 \times 10^{-1} \)

- \[ y = -1.3071 \times 10^{-3}x - 3.8470 \times 10^{-1} \]
  \( R^2 = 8.8381 \times 10^{-1} \)

- \[ y = -1.1264 \times 10^{-3}x - 4.9905 \times 10^{-1} \]
  \( R^2 = 6.7216 \times 10^{-1} \)
Point 10 $\ln(\text{Fe(II)}/\text{Fe(II)}_0)$

![Graph of $\ln(\text{Fe(II)}/\text{Fe(II)}_0)$ vs. Time(s)](image)

Point 10 $\ln(\text{S}/\text{S}_0)$

![Graph of $\ln(\text{S}/\text{S}_0)$ vs. Time(s)](image)

- $y = -8.0674 \times 10^{-4}x - 5.4871 \times 10^{-1}$
  $R^2 = 9.8074 \times 10^{-1}$

- $y = -5.2947 \times 10^{-4}x - 6.2368 \times 10^{-1}$
  $R^2 = 9.6099 \times 10^{-1}$

- $y = -1.3887 \times 10^{-3}x - 3.0462 \times 10^{-1}$
  $R^2 = 9.7638 \times 10^{-1}$
Point 11 $\ln(\text{Fe(II)}/\text{Fe(II)}_0)$

$y = -1.1656E-03x - 9.5954E-01$

$R^2 = 9.5748E-01$

Point 11 $\ln(S/S_0)$

$y = -6.7797E-04x - 8.0152E-01$

$R^2 = 5.4948E-01$

$y = -6.7518E-04x - 7.9088E-01$

$R^2 = 2.9043E-01$
Point 12 $\ln(\text{Fe(II)} / \text{Fe(II)}_0)$

Point 12 $\ln(S / S_0)$

Equations:

- $y = -9.8604E-04x - 5.7228E-01$
  $R^2 = 9.0109E-01$

- $y = -6.1142E-04x - 1.2791E+00$
  $R^2 = 4.5771E-01$

- $y = -8.5558E-04x - 3.6157E-01$
  $R^2 = 6.3341E-01$
Point 13 \( \ln(\frac{\text{Fe(II)}}{\text{Fe(II)}_0}) \)

\[ y = -8.3190 \times 10^{-04}x - 5.2842 \times 10^{-01} \]
\[ R^2 = 8.5913 \times 10^{-01} \]

Point 13 \( \ln(\frac{S}{S_0}) \)

\[ y = -1.1028 \times 10^{-03}x - 6.6489 \times 10^{-01} \]
\[ R^2 = 7.8456 \times 10^{-01} \]
Point 14 \( \ln(\text{Fe(II)}/\text{Fe(II)}_0) \)

\[ y = -5.6256 \times 10^{-4} x - 3.9099 \times 10^{-1} \]
\[ R^2 = 9.1566 \times 10^{-1} \]

Point 14 \( \ln(\text{S}/\text{S}_0) \)

\[ y = -9.2535 \times 10^{-4} x - 7.8236 \times 10^{-1} \]
\[ R^2 = 6.3940 \times 10^{-1} \]

\[ y = -1.7748 \times 10^{-3} x - 4.9733 \times 10^{-1} \]
\[ R^2 = 9.0786 \times 10^{-1} \]
Point 16 $\ln(\text{Fe(II)}/\text{Fe(II)}_0)$

![Graph of $\ln(\text{Fe(II)}/\text{Fe(II)}_0)$ vs. Time(s)](image)

Equations:
- $y = -1.3448E-03x - 8.0590E-01$ (R² = 7.5341E-01)
- $y = -2.4856E-03x - 8.6181E-01$ (R² = 8.4883E-01)

Point 16 $\ln(S/S_0)$

![Graph of $\ln(S/S_0)$ vs. Time(s)](image)

Equations:
- $y = -1.4622E-03x - 5.9671E-01$ (R² = 6.9885E-01)
- $y = -1.3448E-03x - 8.0590E-01$ (R² = 7.5341E-01)
- $y = -2.4856E-03x - 8.6181E-01$ (R² = 8.4883E-01)
Point 17 $\ln(\text{Fe(II)}/\text{Fe(II)}_0)$

![Graph showing $\ln(\text{Fe(II)}/\text{Fe(II)}_0)$ vs. Time(s)]

Point 17 $\ln(S/S_0)$

![Graph showing $\ln(S/S_0)$ vs. Time(s)]

- $y = -1.5477E-03x - 9.3204E-01$
  - $R^2 = 8.2690E-01$
- $y = -1.9446E-03x - 2.5435E-01$
  - $R^2 = 9.7186E-01$
- $y = -1.5310E-03x - 4.9880E-01$
  - $R^2 = 8.4013E-01$
Point 18 $\ln(\text{Fe(II)/Fe(II)}_0)$

$y = -5.0443E-03x - 1.2778E+00$
$R^2 = 9.9039E-01$

Point 18 $\ln(S/S_0)$

$y = -1.1835E-03x - 1.0920E+00$
$R^2 = 7.6689E-01$

$y = -1.3437E-03x - 7.5186E-01$
$R^2 = 8.6494E-01$
Point 20 $\ln(\text{Fe(II)/Fe(II)}_0)$

![Graph of $\ln(\text{Fe(II)/Fe(II)}_0)$ vs. Time(s)]

Point 20 $\ln(S/S_0)$

![Graph of $\ln(S/S_0)$ vs. Time(s)]

Equations:

- $y = -7.6946E-04x - 8.0104E-01$
  $R^2 = 6.5812E-01$

- $y = -6.0192E-04x - 7.9777E-01$
  $R^2 = 4.3921E-01$

- $y = -8.1473E-04x - 7.8398E-01$
  $R^2 = 6.5180E-01$
Point 23 \(\ln(\text{Fe(II)/Fe(II)}_0)\)

\[
y = -2.8442E-04x - 1.1190E+00
R^2 = 5.6848E-02
\]

\[
y = -1.5948E-03x - 3.4953E-01
R^2 = 9.5240E-01
\]

\[
y = -1.0440E-03x - 8.1591E-01
R^2 = 8.0971E-01
\]

Point 23 \(\ln(S/S_0)\)

\[
y = -2.8442E-04x - 1.1190E+00
R^2 = 5.6848E-02
\]

\[
y = -1.5948E-03x - 3.4953E-01
R^2 = 9.5240E-01
\]

\[
y = -1.0440E-03x - 8.1591E-01
R^2 = 8.0971E-01
\]
Point 24 $\ln(\text{Fe(II)}/\text{Fe(II)}_0)$

$$y = -1.0936 \times 10^{-3} x - 1.2070 \times 10^0$$
$$R^2 = 6.1904 \times 10^{-1}$$

Point 24 $\ln(\text{S}/\text{S}_0)$

$$y = -1.5241 \times 10^{-3} x - 1.7956 \times 10^{-1}$$
$$R^2 = 9.0695 \times 10^{-1}$$

$$y = -2.2827 \times 10^{-3} x - 4.2503 \times 10^{-1}$$
$$R^2 = 7.3781 \times 10^{-1}$$
Appendix 4: Design Expert© Input

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<th>Run</th>
<th>ln(Fe(II)/Fe(II)_0) = -1</th>
<th>ln(Fe(II)/Fe(II)_0) = -0.5</th>
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*Where cells are highlighted, an average of two of the replicates replaced the third due to the third being an outlier. The averaged data has only one cell in the row highlighted, whereas the replaced data has the entire row highlighted.*
Appendix 5: Box-Cox Plots, Response Surfaces, and Model Coefficients

Square root(mole S oxidized at the time when \( \ln(\text{Fe(II)}/\text{Fe(II)}_0) = -0.5 \))

Design-Expert® Software
Sqrt(R1)

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<tr>
<th>Factor</th>
<th>Beta</th>
<th>F-Value</th>
<th>p-Value</th>
<th>% Contribution</th>
<th>Significant?</th>
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</thead>
<tbody>
<tr>
<td>Intercept</td>
<td>7.87E-03</td>
<td>1.410E+02</td>
<td>&lt; 0.0001</td>
<td>50.64%</td>
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<td>A-Iron</td>
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<td>B-Sulfide</td>
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</table>
Square root(Time when ln(Fe(II)/Fe(II)₀) = -0.5)

Design-Expert® Software
Sqrt(R1)

Lambda
Current = 0.5
Best = 0.6
Low C.I. = 0.42
High C.I. = 0.78

Recommend transform:
Square root
(Lambda = 0.5)

Box-Cox Plot for Power Transforms

Square root(Time when ln(Fe(II)/Fe(II)₀) = -0.5)

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<th>Beta</th>
<th>F-Value</th>
<th>p-Value</th>
<th>% Contribution</th>
<th>Significant?</th>
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Power ($\lambda=0.88$) transform of moles of sulfide oxidized at time when

$$\ln(\text{Fe(II)}/\text{Fe(II)}_0) = -1$$

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<td>1.100E+00</td>
<td>0.2982</td>
<td>0.00%</td>
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<tr>
<td>AD</td>
<td>-2.87E-08</td>
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<td>BD</td>
<td>1.93E-09</td>
<td>3.122E+00</td>
<td>0.0821</td>
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<tr>
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<td>1.217E+00</td>
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<tr>
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<td>2.50E-09</td>
<td>2.176E-02</td>
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<tr>
<td>B$^2$</td>
<td>-4.17E-10</td>
<td>6.113E+01</td>
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<tr>
<td>C$^2$</td>
<td>4.42E-08</td>
<td>1.189E-01</td>
<td>0.7314</td>
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<td>no</td>
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<tr>
<td>D$^2$</td>
<td>8.36E-09</td>
<td>1.661E-01</td>
<td>0.6850</td>
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### Square root (time when ln(Fe(II)/Fe(II)_0) = -1)

<table>
<thead>
<tr>
<th>Factor</th>
<th>Beta</th>
<th>F-Value</th>
<th>p-Value</th>
<th>% Contribution</th>
<th>Significant?</th>
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<tbody>
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<td>Intercept</td>
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<td>1.969E+01</td>
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<td>3.569E-01</td>
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<td>no</td>
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<tr>
<td>B-Sulfide</td>
<td>4.64E-02</td>
<td>1.828E+02</td>
<td>&lt; 0.0001</td>
<td>34.09%</td>
<td>yes</td>
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<tr>
<td>C-Phosphate</td>
<td>-3.15E+00</td>
<td>1.685E+01</td>
<td>0.0001</td>
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<tr>
<td>D-Carbonate</td>
<td>-1.25E+00</td>
<td>9.800E+00</td>
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<tr>
<td>AB</td>
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<td>2.545E+01</td>
<td>&lt; 0.0001</td>
<td>4.75%</td>
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<tr>
<td>AC</td>
<td>9.01E-03</td>
<td>2.202E-01</td>
<td>0.6405</td>
<td>0.04%</td>
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</tr>
<tr>
<td>AD</td>
<td>5.72E-03</td>
<td>5.543E-01</td>
<td>0.4593</td>
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<tr>
<td>BC</td>
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<td>1.905E+00</td>
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<tr>
<td>BD</td>
<td>4.69E-04</td>
<td>1.183E+00</td>
<td>0.2810</td>
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<td>no</td>
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<tr>
<td>CD</td>
<td>2.15E-02</td>
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<tr>
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<td>4.334E+00</td>
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<tr>
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<td>4.190E+00</td>
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<td>0.78%</td>
<td>yes</td>
</tr>
</tbody>
</table>

### R²

| R²        | 0.9985 | Adjusted R² | 0.9981 |

**Design-Expert® Software**

- **Sqrt(R1)**
- **Lambda**
  - Current = 0.5
  - Best = 0.47
  - Low C.I. = 0.33
  - High C.I. = 0.61
- **Recommend transform:**
  - Square root
  - (Lambda = 0.5)

**Box-Cox Plot for Power Transforms**

- Lambda vs. Ln(ResidualSS)
- Values: 17.90, 22.59, 27.28, 31.97, 36.66
- Lambda range: -3 to 3

---

87
Square root([time to phase change] + 30)

<table>
<thead>
<tr>
<th>Factor</th>
<th>Beta</th>
<th>F-Value</th>
<th>p-Value</th>
<th>% Contribution</th>
<th>Significant?</th>
</tr>
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<tbody>
<tr>
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<td>3.78E+01</td>
<td>1.888E+01</td>
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<td>51.43%</td>
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<tr>
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<td>-5.12E-01</td>
<td>1.194E-01</td>
<td>0.7309</td>
<td>0.02%</td>
<td>no</td>
</tr>
<tr>
<td>B-Sulfide</td>
<td>6.30E-02</td>
<td>1.718E+02</td>
<td>&lt; 0.0001</td>
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<tr>
<td>C-Phosphate</td>
<td>-1.30E+00</td>
<td>5.923E+00</td>
<td>0.0178</td>
<td>1.15%</td>
<td>no</td>
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<tr>
<td>D-Carbonate</td>
<td>-3.68E-01</td>
<td>1.252E+01</td>
<td>0.0008</td>
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<tr>
<td>AB</td>
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<td>7.464E+00</td>
<td>0.0082</td>
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<td>1.600E-01</td>
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<td>0.03%</td>
<td>no</td>
</tr>
<tr>
<td>BD</td>
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<td>4.308E-02</td>
<td>0.8363</td>
<td>0.01%</td>
<td>no</td>
</tr>
<tr>
<td>CD</td>
<td>-1.65E-02</td>
<td>1.977E+00</td>
<td>0.1646</td>
<td>0.38%</td>
<td>no</td>
</tr>
<tr>
<td>A^2</td>
<td>-4.49E-03</td>
<td>1.459E+00</td>
<td>0.2316</td>
<td>0.28%</td>
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</tr>
<tr>
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<td>2.516E+01</td>
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<td>R^2</td>
<td>0.8075</td>
<td>Adjusted R^2</td>
<td>0.7648</td>
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</table>
**k<sub>obs</sub> HS<sup>−</sup> oxidized**

<table>
<thead>
<tr>
<th>Factor</th>
<th>Beta</th>
<th>F-Value</th>
<th>p-Value</th>
<th>% Contribution</th>
<th>Significant?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intercept</td>
<td>3.30E-04</td>
<td>6.799E-01</td>
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<td>51.03%</td>
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<tr>
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<td>7.587E-02</td>
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<tr>
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<td>3.51E-07</td>
<td>3.747E-01</td>
<td>0.5427</td>
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<td>no</td>
</tr>
<tr>
<td>C-Phosphate</td>
<td>-3.52E-06</td>
<td>1.354E+00</td>
<td>0.2489</td>
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<td>no</td>
</tr>
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<td>1.409E+00</td>
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<tr>
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<td>1.131E+00</td>
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</tr>
<tr>
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<td>4.304E-05</td>
<td>0.9948</td>
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<tr>
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<td>3.891E-01</td>
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</tr>
<tr>
<td>A&lt;sup&gt;2&lt;/sup&gt;</td>
<td>-6.80E-08</td>
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<td>1.13%</td>
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<tr>
<td>B&lt;sup&gt;2&lt;/sup&gt;</td>
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<td>3.775E-02</td>
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<tr>
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<td>5.233E-03</td>
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<tr>
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<td>9.169E-01</td>
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<td>4.92%</td>
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</tr>
</tbody>
</table>

**R<sup>2</sup>** | 0.1313 | Adjusted R<sup>2</sup> | -0.0618 |
%HS oxidized at time when ln(Fe(II)/Fe(II)_0) = -0.5

%HS oxidized at time when ln(Fe(II)/Fe(II)_0) = -0.5

<table>
<thead>
<tr>
<th>Factor</th>
<th>Beta</th>
<th>F-Value</th>
<th>p-Value</th>
<th>% Contribution</th>
<th>Significant?</th>
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</thead>
<tbody>
<tr>
<td>Intercept</td>
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<td>9.467E+00</td>
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</tr>
<tr>
<td>B-Sulfide</td>
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<td>4.026E+01</td>
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<tr>
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<td>5.192E+00</td>
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<tr>
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<td>1.61E-01</td>
<td>4.635E-01</td>
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<tr>
<td>AB</td>
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<td>9.719E+00</td>
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<tr>
<td>AC</td>
<td>4.36E-03</td>
<td>6.123E-02</td>
<td>0.8054</td>
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<tr>
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</tbody>
</table>

Design-Expert® Software
R1
Lambda
Current = 1
Best = 3
Low C.I. = 
High C.I. =
Recommend transform:
None
(Lambda = 1)
%HS<sup>-</sup> oxidized at time when $\ln(\text{Fe(II)/Fe(II)}_0) = -1$

<table>
<thead>
<tr>
<th>Factor</th>
<th>Beta</th>
<th>F-Value</th>
<th>p-Value</th>
<th>% Contribution</th>
<th>Significant?</th>
</tr>
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<tbody>
<tr>
<td>Intercept</td>
<td>8.06E+01</td>
<td>1.324E+01</td>
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<td>55.96%</td>
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<tr>
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<td>0.2153</td>
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<td>D-Carbonate</td>
<td>-1.95E-01</td>
<td>1.270E+00</td>
<td>0.2641</td>
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<tr>
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<td>1.052E+00</td>
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<tr>
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