National Institute of Technology Karnataka, Surathkal

Production of Iron and Ferro Alloys, MT300

Report On

Reduction Kinetics Of Iron Oxide Pellets

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1 Theory

The general features of the kinetics and mechanism of iron oxide reduction by CO and H_2 are similar. Their difference is that reduction by H_2 is 5-10 times faster than that by CO. Lump ores, sinters, and pellets contain iron oxide primarily as Fe_2O_3, but in some ore bodies, the oxide is in the form of magnetite. The gangue minerals primarily contain SiO_2 and Al_2O_3, along with other minor compounds. In the stack region, CO and H_2 can reduce only the oxides of iron. The fundamental measure of the extent of reduction is the Degree of Reduction (F_0) defined as:

$$F_0 = \frac{\text{loss of mass of the ore due to removal of oxygen}}{\text{total mass of removable oxygen in ore}} \quad (1)$$

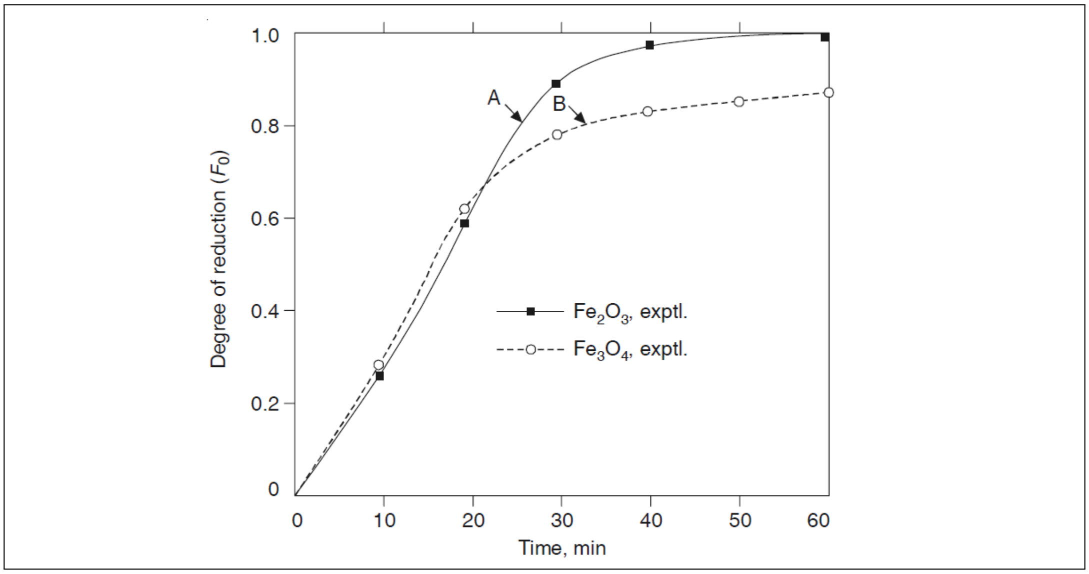


Figure 1: F_0 vs. time plots for reduction of Fe_2O_3 and Fe_3O_4 in H_2 at 900°C. [1]

Note:

- Lump ore, sinter and pellets are porous solids.
- Reduction is characterised by the formation of a porous product layer.
- Fe_2O_3 is reduced in stages, viz. $Fe_2O_3 \rightarrow Fe_3O_4 \rightarrow Fe_xO \rightarrow Fe$.
- Additional porosity develops during reduction owing to density differences of the products.
- The relative volumes per unit mass of Fe are:

$$\text{Fe} : \text{Fe}_x\text{O} : \text{Fe}_3\text{O}_4 : \text{Fe}_2\text{O}_3 = 1 : 1.79 : 2.08 : 2.14$$

2 Mechanism of reduction

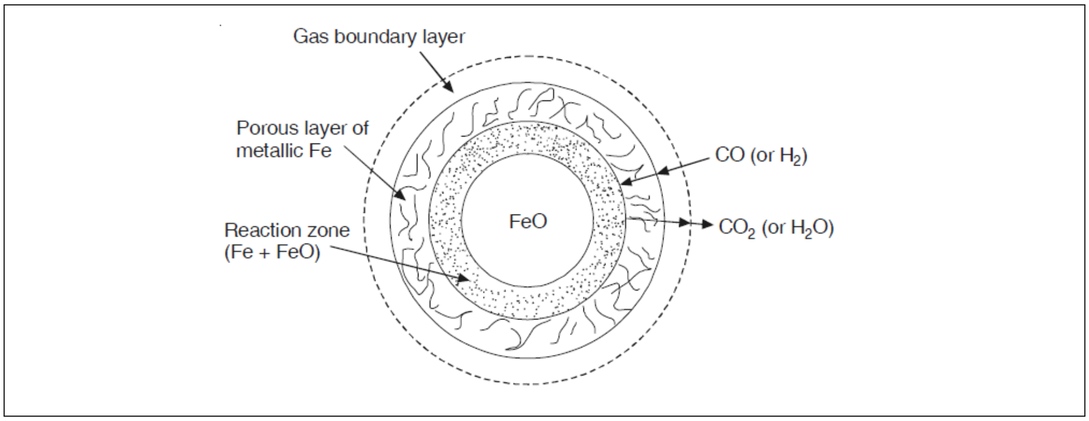


Figure 2: Sketch of a partially reduced FeO sphere showing layers and kinetic steps. [1]

Steps involved in reduction of a pellet are:

- Transfer of reactant gas to the solid surface (CO or H2) across the gas boundary layer around the piece of solid.
- Inward diffusion of reactant gas through the pores of the solid.
- Chemical reaction at the interface.
- Outward diffusion of the product gas (CO2 or H2O) through the pores
- Transfer of the product gas from the solid surface into the bulk gas across the boundary layer.

Chemical Reaction Control: The chemical reaction at the oxide-metal interface is the slowest step and controls the overall reduction rate. The rate per unit area of remaining oxide is constant with time. This mechanism dominates when gas diffusion through the product layer is fast, typically at the start of reduction or for small porous particles.

Diffusion Control: The diffusion of reducing gas inward and product gas outward through the porous metallic iron layer controls the overall reduction rate. Gas concentration decreases at the reaction interface as diffusion becomes slower than the chemical reaction. This mechanism dominates at high temperatures for large particles, particularly when the iron layer is significantly thick.

3 Mathematical Equations

Chemical Control:

$$F = 1 - (1 - t/\tau)^3$$

and:

$$\tau = \frac{\rho_0 R_0}{b k_s C_g}$$

Diffusion Control:

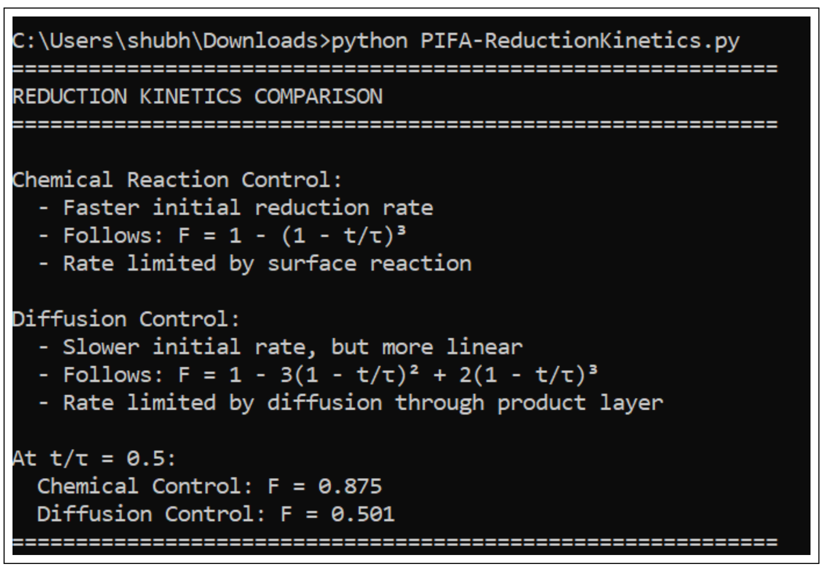
$$F = 1 - 3(1 - t/\tau)^2 + 2(1 - t/\tau)^3$$

and:

$$\tau = \frac{\rho_0 R_0^2}{6bD_eC_g}$$

Where, for a spherical pellet:

- F = degree of reduction;
- t = actual time;
- τ = total time for complete reduction;
- t/τ = normalized time.
- R_0 = initial pellet radius (m)
- ρ_0 = molar density of oxygen in the oxide (mol/m^3)
- k_s = surface reaction rate constant (m/s)
- D_e = effective diffusivity of gas through product layer (m^2/s)
- C_g = gas concentration (mol/m^3)
- b = stoichiometric coefficient



```
C:\Users\shubh\Downloads>python PIFA-ReductionKinetics.py
============================================================
REDUCTION KINETICS COMPARISON
============================================================

Chemical Reaction Control:
  - Faster initial reduction rate
  - Follows: F = 1 - (1 - t/τ)³
  - Rate limited by surface reaction

Diffusion Control:
  - Slower initial rate, but more linear
  - Follows: F = 1 - 3(1 - t/τ)² + 2(1 - t/τ)³
  - Rate limited by diffusion through product layer

At t/τ = 0.5:
  Chemical Control: F = 0.875
  Diffusion Control: F = 0.501
============================================================
```

Figure 3: Snapshot of successful program execution. Code Listing 1

4 Code

Listing 1: Python code used for plotting degree of reduction of a spherical pellet.

```
'''
MT300: PIFA
Reduction Kinetics
Python Programming Group Project

Team Members:
1. Anindith B. L. - 231MT008
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2. Shubhang S. Galagali - 231MT049
3. Suhas Gowda M. - 231MT053
'''

import numpy as np
import matplotlib.pyplot as plt

# Normalized dimensionless time array initialized:
time = np.linspace(0, 1, 1000)

# Degree of reduction (F) as a function of time

# For spherical pellets:

# 1. Chemical Reaction Control (Shrinking Core Model)
# F = 1 - (1 - t)^3

F_chemical = 1 - (1 - time)**3

# 2. Diffusion Control through Product Layer (Shrinking Core Model)
# F = 1 - 3(1-t)^2 + 2(1-t)^3
F_diffusion = 1 - 3*(1 - time)**2 + 2*(1 - time)**3

# Create the plot
plt.figure(figsize=(10, 6))
plt.plot(time, F_chemical, 'green', linewidth=2.5, label='Chemical Reaction
    Control')
plt.plot(time, F_diffusion, 'purple', linewidth=2.5, label='Diffusion Control')

# Formatting
plt.xlabel('Normalized Time (t/  )', fontsize=12, fontweight='bold')
plt.ylabel('Degree of Reduction (F)', fontsize=12, fontweight='bold')
plt.title('Reduction Kinetics of Spherical Pellet:\nChemical vs Diffusion
    Control',
          fontsize=14, fontweight='bold')
plt.legend(fontsize=11, loc='lower right')
plt.grid(True, alpha=0.3, linestyle='--')
plt.xlim(0, 1)
plt.ylim(0, 1)

# Add annotations to highlight differences
plt.annotate('Faster initial rate', xy=(0.3, 0.7), xytext=(0.15, 0.85),
            arrowprops=dict(arrowstyle='->', color='green', lw=1.5),
            fontsize=10, color='green')
plt.annotate('Slower initial rate,\nlinear region', xy=(0.5, 0.5), xytext
    =(0.65, 0.3),
            arrowprops=dict(arrowstyle='->', color='purple', lw=1.5),
            fontsize=10, color='purple')

plt.tight_layout()
plt.show()

# Print key characteristics
print("=" * 60)
print("REDUCTION KINETICS COMPARISON")
print("=" * 60)
```

```
print("\nChemical Reaction Control:")
print("  - Faster initial reduction rate")
print("  - Follows: F = 1 - (1 - t/  )  ")
print("  - Rate limited by surface reaction")
print("\nDiffusion Control:")
print("  - Slower initial rate, but more linear")
print("  - Follows: F = 1 - 3(1 - t/  )   + 2(1 - t/  )  ")
print("  - Rate limited by diffusion through product layer")
print("\nAt t/   = 0.5:")
print(f"  Chemical Control: F = {F_chemical[500]:.3f}")
print(f"  Diffusion Control: F = {F_diffusion[500]:.3f}")
print("=" * 60)
```

The full Python script is available online at this GitHub repository.

5 Output

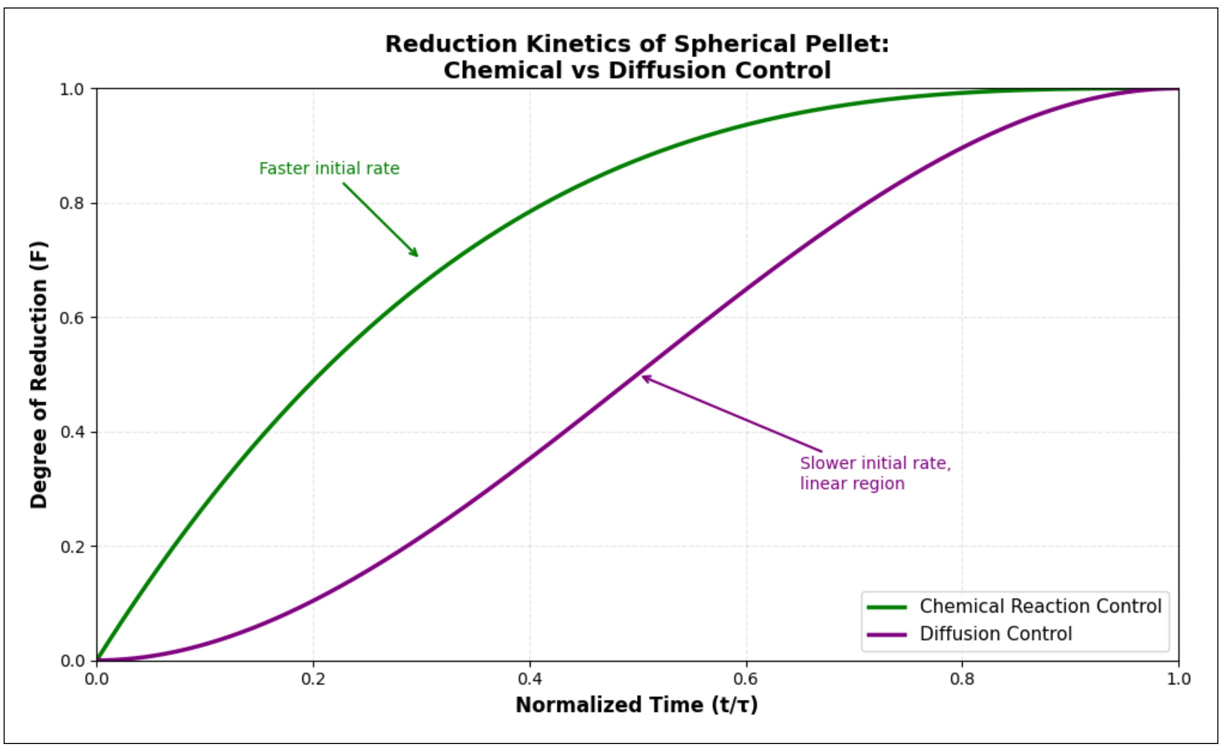

Figure 4: Degree of reduction as a function of time for a spherical pellet considering chemical control and diffusion control. [Code Listing 1]

References

[1] A. GHOSH and A. CHATTERJEE, *IRON MAKING AND STEELMAKING: THEORY AND PRACTICE*. Eastern economy edition, PHI Learning, 2008.