Experimental and Numerical Studies on a One-step Method for the Production of Mg in the Silicothermic Reduction Process

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This file contains:

Table S1 Chemical analysis of qualified dolomite (wt %)

MgO	CaO	SiO_2	Fe_2O_3	Al_2O_3	Ignition
21.07	32.44	0.58	0.09	0.06	45.76

Table S2 Chemical analysis of 75% ferrosilicon alloy (wt %)

Si	Fe	Al	Ca	Mn	Cr	C
76.08	21.75	0.88	0.72	0.33	0.14	0.10

Table S3 Solid-Solid chemical kinetics models and corresponding equations

Model	Mechanism	Equation
F1	One dimensional nuclei growth (n=1)	$-\ln(1-\alpha)=k_{F1}\tau$
F2	Two dimensional nuclei growth (n=2)	$[-\ln(1-\alpha)]^{1/2}=k_{F2}\tau$
F3	Three dimensional nuclei growth (n=3)	$[-\ln(1-\alpha)]^{1/3}=k_{F3}\tau$
D1	One dimensional diffusion	$\alpha^2/2=k_{D1}\tau$
D2	Two dimensional diffusion	$\alpha+(1-\alpha)\ln(1-\alpha)=k_{D2}\tau$
D3	Three dimensional diffusion	$1-2/3\alpha-(1-\alpha)^{2/3}=k_{D3}\tau$
R1	Chemical reaction Zero order equation (n=0)	$\alpha=k_{R1}\tau$
R2	Chemical reaction (cylindrical geometry)	$1-(1-\alpha)^{1/2}=k_{R2}\tau$
R3	Chemical reaction (spherical geometry)	$1-(1-\alpha)^{2/3}=k_{R3}\tau$

In the one-step technology, the mixture containing qualified dolomite, 75% ferrosilicon alloy and calcium fluoride powder was pulverized to 200 mesh in a ball mill and briquetted in a plunger press at 150 MPa. The density of the briquettes was measured to 2800 kg/m^3. In the briquettes, there are about 1185 kg carbon dioxide and 323 kg magnesium per cubic meter. Then in the dolomite decomposition stage, the density of the briquettes can be expressed as follows:

$$\rho_{bd}=2800-1185\alpha \tag{S1}$$

In the magnesium reduction stage, the density of the briquettes can be expressed as follows:

$$\rho_{br}=1615-323\beta \tag{S2}$$

The thermal conductivity of the briquettes was measured to 0.9 W/(m·K). When the dolomite decomposition process was completed, the thermal conductivity of the briquettes was measured to 0.7 W/(m·K); When the magnesium reduction process was completed, the thermal conductivity of the briquettes was measured to 0.55 W/(m·K). For convenience of calculations, the extent-dependence thermal conductivity was simplified as a linear relationship in the two processes. Then in the dolomite decomposition stage, the thermal conductivity of the briquettes can be expressed as follows:

$$\lambda_{bd} = 0.9 - 0.2\alpha \tag{S3}$$

In the magnesium reduction stage, the thermal conductivity of the briquettes can be expressed as follows:

$$\lambda_{br} = 0.7 - 0.15\beta \tag{S4}$$

Table S4 showed specific heat of the reactants and products and we could find that the specific heat changed with temperature. For convenience of calculations, we assumed a linear relationship between the specific heat and temperature. Then the expression of the specific heat of $CaCO_3 \cdot MgCO_3$ is:

$$C_{b-CaCO_3 \cdot MgCO_3} = 0.0944T + 138.24 \tag{S5}$$

The expression of the specific heat of CaO·MgO is:

$$C_{b-CaO \cdot MgO} = 0.0194T + 82.657 \tag{S6}$$

The expression of the specific heat of $2CaO \cdot SiO_2$ is:

$$C_{b-2CaO\cdot SiO_2} = 0.055T + 125.62 \quad \text{(S7)}$$

Then in the dolomite decomposition stage, the specific heat of the briquettes can be expressed as follows:

$$\begin{aligned} C_{bd} &= (0.0944T + 138.24)(1-\alpha) + (0.0194T + 82.66)\alpha \\ &= 0.0944T + 138.24 - (0.075T + 55.58)\alpha \end{aligned} \quad \text{(S8)}$$

In the magnesium reduction stage, the specific heat of the briquettes can be expressed as follows:

$$\begin{aligned} C_{br} &= (0.0194T + 82.66)(1-\beta) + (0.055T + 125.62)\beta \\ &= 0.0194T + 82.66 + (0.0081T - 19.85)\beta \end{aligned} \quad \text{(S9)}$$

Table S4 Specific heat of the reactants and products[1]

Temperature, K	Specific heat C_b, J/(mol·K)		
	$CaCO_3\cdot MgCO_3$	$CaO\cdot MgO$	$2CaO\cdot SiO_2$
300	156.351	79.85	129.02
400	174.895	89.483	145.827
500	187.803	94.353	155.795
600	198.492	97.349	163.072
700	208.133	99.459	169.077
800	217.216	101.097	174.405
900	225.974	102.461	179.339
1000	234.53	103.654	184.029
1100	242.955	104.737	188.559
1200	251.29	105.743	189.887
1300	259.561	106.696	194.497
1400	267.787	107.611	199.108
1473	273.77	108.26	202.474

References

(1) Kubaschewski, O.; Catterall, J. A., *Thermochemical data of alloys*. Pergamon Press: London, 1956.