J. Min. Metall. Sect. B-Metall. 62 (1) (2026) 41 - 52

Journal of Mining and Metallurgy,
Section B: Metallurgy

Supplementary material

Supplementary material to
OPTIMIZATION OF SMELTING PROCESS OF MAGNESIUM BASED ON MACHINE LEARNING

Xin Li [a, **], Junhua Guo [b, *], Jianglei Fan [a], Yongbiao Wang [a], Yanyan Li [c], Xiaoguang Zhou [d], Shuxia Tian [a], Feng Mao [e], Kunlin Miao [f], Shizhong Wei [a, g]

[a] Zhengzhou University of Light Industry, College of Mechanical and Electrical Engineering, Zhengzhou, China
[b] China Academy of Machinery Zhengzhou Research Institute of Mechanical Engineering Co., Ltd., State Key Laboratory of High Performance & Advanced Welding Materials, Zhengzhou, China
[c] Zhengzhou University of Light Industry, School of Materials and Chemical Engineering, Zhengzhou, China
[d] Northeastern University, State Key Laboratory of Digital Steel, Shenyang, China
[e] Longmen Laboratory, Luoyang, China
[f] Zhengzhou University of Light Industry,School of Computer Science and Technology, Zhengzhou, China
[g] Henan University of Science and Technology,School of Materials Science and Engineering, Luoyang, China; Henan Engineering Technology Research Center for Wear Resistant Materials, Luoyang, China

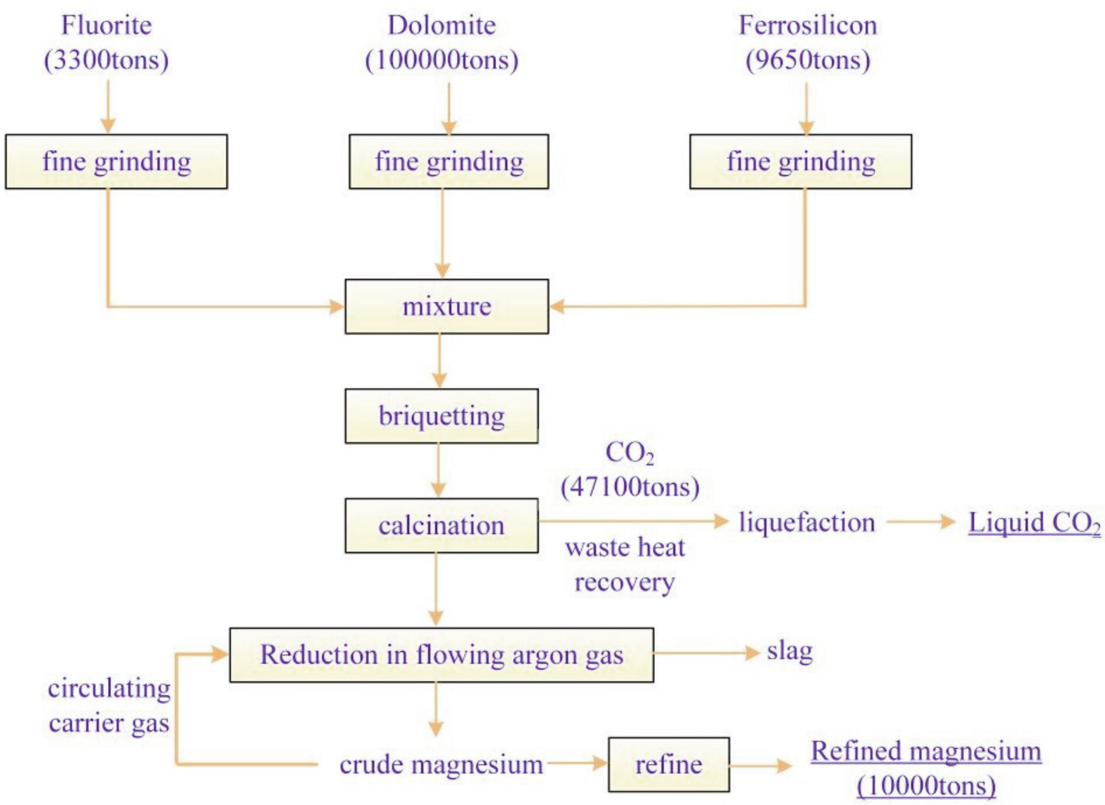

Figure S1. *Flow chart of continuous magnesium refining under flowing argon atmosphere*

*Corresponding author: guojunhua92@163.com *; XinLi1384051@163.com**;*

1. Material balance calculation

Composition of dolomite: MgO 20.60%, CaO 31.05%, Al_2O_3 0.16%, SiO_2 0.44%, Na 0.02%, K 0.005%

The raw material used in the experiment is dolomite, and the ingredients are prepared according to chemical equation (1).

$$2\left(CaO\cdot MgO_{(s)}\right)+Si\left(Fe\right)_{(s)}= \\ 2Mg_{(g)}+2CaO\cdot SiO_{2(s)}+Fe\left(Si\right)_{(s)} \quad (1)$$

It is calculated based on 1mol MgO, and MgO/CaO=1, Si/2MgO=M. The fluorite powder added is 3% of the mass of the raw materials used.

Ferrosilicon is added in excess of 15% according to the theoretical value of reaction with MgO

Fluorite powder dosage 3%

The actual yield of magnesium is: 85% (Pure magnesium content/agglomerate magnesium content in crystalline magnesium);

Refined magnesium yield 95%

According to the annual production of 10000 tons of magnesium, the material balance sheet is shown in Table S1.

The main technical and economic indicators are shown in Table S2.

2. Comprehensive energy consumption analysis:

2.1. Calculation of main production equipment selection:

(1) Mixing mill

The ground ferrosilicon powder, fluorite powder, and calcined white are added to the mixing mill according to the proportion of ingredients. The total amount of mixed material is 113000 ton (calculated based on an annual output of 10kt magnesium). Running in 3 shifts per day, with an actual running time of 8 hours per shift, the utilization rate of the grinding machine is 70%.

Hourly grinding amount: $\frac{113000}{3\cdot 8\cdot 330\cdot 0.7}=20.38\ (t/h)$

Select 2 sets of Φ 1830×6400 ball mills with a production capacity of 12t/h.

Ball mill motor power is 17.5kwh/t.

(2) Rolling machine

Produce 113000 tons of pellets annually, with a required equipment capacity of:

$$\frac{113000}{3\cdot 8\cdot 330\cdot 0.7}=20.38\ (t/h)$$

Therefore, 6 compaction machines with a production capacity of 5t/h were arranged, with 5 in operation and 1 standby.

Using a Φ 430×250 ball press, the power consumption of the ball press motor is 3.7 kwh/t.

3. Thermal equilibrium calculation

3.1. Gas composition:

Using water gas as the heating fuel, its chemical composition (%) is: CO_2 10.5, CO 30.5, H_2 52.5, CH_4 1.0, N_2 5.5.

3.2. Composition of pellet material:

According to the actual production situation,

Table S2. *Main raw material consumption and annual demand for magnesium production*

No.	Project Name	Unit	Unit consumption per ton of magnesium	Annual demand of 10kt
1	dolomite	t	10	100
2	ferrosilicon	t	0.965	9.65
3	fluorspar	t	0.33	3.3
4	Restoration tank	t	0.063	630

Table S1. *Annual input output quantity of materials required for main production processes*

process	Input			Output		
	Project Name	Unit	Number	Project Name	Unit	Number
Prepared raw material	dolomite	kt/a	100	pellet	kt/a	113
	ferrosilicon	kt/a	9.65			
	fluorite	kt/a	3.3			
Reduction	pellet	kt/a	113	Liquid CO_2	kt/a	47.1
				Crystalline magnesium	kt/a	10.53
				Reduction slag	kt/a	55.37

walnut shaped pellets are selected, with a composition (%) of: $MgCO_3$ 38.28, $CaCO_3$ 49.07, ferrosilicon 8.54%, CaF_2 2.9%.

3.3. Material flow rate

According to the actual production situation, the material flow rate is: 120kg of pellets per can, 18720kg of pellets per furnace per day (52 cans per furnace), 780kg of pellets per furnace hour, 3120kg of calcination per furnace per hour, and a smelting cycle of 3 cycles per day, including 2 hours of calcination and 6 hours of reduction per cycle. The daily production of magnesium is 32 tons, and the daily magnesium production of each furnace is 1684kg. The material magnesium ratio is 10.76, requiring 19 furnaces.

3.4. Calcination reduction temperature

The calcination temperature is 1000 °C, and the reduction reaction temperature is 1200 °C.

3.5. Fuel combustion calculation

Pre made pellet calcination and temperature rise:

Calcination per hour: $MgCO_3$:1194.44Kg/h, $CaCO_3$:1530.91, Si:199.83, Fe:66.61, CaF_2 91.12

$$Q_{\substack{\text{Heating of}\\ \text{furnace materials}}} = \begin{pmatrix} 1194.44 \cdot 1.27 + 1530.91 \cdot 0.84 + \\ 199.83 \cdot 0.98 + 66.61 \cdot 0.82 + 91.12 \cdot 1.34 \end{pmatrix} \cdot 1000$$

$$Q_{\text{Furnace materials}} = 317.5457 \cdot 10^4 \text{kJ / h}$$

$$V_{\text{Heating}} = \frac{\overset{\text{Magnesium consumption per ton}}{(\text{mass of dolomite}) \cdot Q_{divide}}}{Q_{\text{gas}}} =$$

$$\frac{11300 \cdot 317.5457 \cdot 10^4}{3120 \cdot 9455.84} = 1216.27 \text{ m}^3$$

Q_{gas}=9455.84kJ/m^3 (it is calculated based on water gas composition)

3.6. Thermal equilibrium calculation during calcination process:

The amount of CO_2 generated during the pellet calcination process is:

Table S3. Thermodynamic data of each substance

substance name	-ΔH$_{298}$/(kJ/mol)	specific heat/(kJ/kg·°C)
$MgCO_3$		1.27
$CaCO_3$		0.84
Si	0	0.98
Fe	0	0.82
CaF_2	0	1.34

$$V_{CO_2} = \frac{3120 \cdot 41.64\%}{44} \cdot 22.4 = 661.39 \text{ m}^3 \text{ / h}$$

41.64% is the theoretical calcination rate, and 3120kg/h is the theoretical calcination mass per furnace per hour.

(1) Hot income portion:

Q_{gas}=9455.84kJ/m^3 (it is calculated based on water gas composition)

(2) Heat expenditure portion:

Carbonate decomposition in pellets, theoretical calculation based on pellet composition

$MgCO_3$=MgO+CO_2 (calcination) ΔH=20.801kJ/mol(1000°C)

$CaCO_3$=CaO+CO_2 (calcination) ΔH=163.207kJ/mol(1000°C)

A 1kg pellet contains 383g of magnesium carbonate and 491g of calcium carbonate. It decomposes and absorbs heat at 1000 °C is:

$$Q_{\text{divide}} = \frac{383}{84} \cdot 20.801 + \frac{491}{100} \cdot 163.207 \text{ kJ / kg}$$

Therefore: Q_{divide} is 896.189kJ/kg. If calculated based on the production of tons of magnesium, the consumption of water and gas during calcination is:

$$V_{\text{Calcination}} = \frac{\overset{\text{Magnesium consumption per ton}}{(\text{mass of dolomite}) \cdot Q_{divide}}}{Q_{\text{gas}}} =$$

$$\frac{10000 \cdot 896.189}{9455.84} = 947.76 \text{ m}^3$$

V_{total}=1216.27+947.76=2164.03m^3

(3) waste heat recovery

Waste heat generated from tons of magnesium producing CO_2 Q_{CO2}

$$Q_{\text{CO2}} = C \cdot m \cdot \Delta t = 1.003 \cdot 4.71 \cdot 1000 \cdot (200 - 50) =$$
$$7.086 \cdot 10^5 \ KJ = 74.93 \ m^3 gas$$

3.7. Thermal equilibrium calculation during the reduction process:

(1) Hot income portion:

Q_{gas}=9455.84kJ/m^3 (Calculated based on gas composition)

(2) Heat expenditure portion:

Heat absorption of furnace materials:

$$Q_{\text{Furnace materials}} = \sum \left(C_i^{1200\,^\circ C} \cdot t_2 - C_i^{1000\,^\circ C} \cdot t_1 \right) G_i \ kJ / h$$

t_1 is the temperature at which the pellet calcination ends and the reduction begins: 1000°C;

t_2 is the reduction reaction temperature: 1200°C:

G_i is unit time flow rate of each substance in the pellet, kg/h.

It is calculated based on the original formula data:

MgO=568.78kg/h, CaO=857.31kg/h, Si:199.83 Fe:66.61 CaF_2 91.12.

C_i is the specific heat of each substance, the thermodynamic data of each substance are shown in the following Table S4:

Table S4. *Thermodynamic data of various substances*

substance name	$-\Delta H_{298}$/ (kJ/mol)	specific heat/ (kJ/kg·°C)
MgO	182.84	1.32
CaO	634.29	1
Si	0	0.98
Fe	0	0.82
CaF_2	0	1.34

Based on the above data, calculate the heat absorption of each substance, and the total heat absorption of the furnace charge is:

$$Q_{\text{Charge}} = \begin{pmatrix} 568.78 \cdot 1.32 + 857.31 \cdot 1 + 199.83 \cdot 0.98 \\ +66.61 \cdot 0.82 + 91.12 \cdot 1.34 \end{pmatrix} \cdot 200$$

$$Q_{\text{Charge}} = 39.61 \cdot 10^4 \ kJ / h$$

Heat absorbed by reaction:

According to the reaction equation:

$$2(MgO \cdot CaO) + Si = 2Mg + 2CaO \cdot SiO_2$$

$$\Delta H^{\theta}_{298} = 2626.7 \ kJ / mol$$

According to the magnesium production rate of 93kg per hour in the reduction furnace, the total reaction heat is:

$$Q_{\text{reaction}} = \frac{2626.7 \cdot 93 \cdot 10^3}{2 \cdot 24.305} = 502.588 \cdot 10^4 \ kJ / h$$

where, 24.305 is the molar mass of magnesium.

Therefore $Q_{Total\ \ expenditure} = Q_{charge} + Q_{reaction}$, assuming the hourly gas consumption is x, that is

$9455.84 \cdot x = 39.61 \cdot 10^4 + 502.588 \cdot 10^4$

$x = 573.40$

If the gas consumption during reduction is calculated based on the production of tons of magnesium, then it is:

$$\frac{544.75 \cdot 1000}{93} = 6165.59 \ m^3 / t$$

The various energy consumption in the production process of magnesium metal is converted to standard coal using the standard coal coefficient. As shown in Table S5.

4. The LCA calculation process of this manuscript

4.1. Basic parameters and data sources

Heating value of water gas: 9455.84 kJ/m³

Heating value of standard coal: 29307.6 kJ/kg (National standard, 7000 kcal/kg)

Conversion of electricity consumption to standard coal: 0.1229 kgce/kWh (GB/T 2589)

Ton magnesium calcined consume water gas: 2164.03 m³/t-Mg

Ton magnesium reduction consume water gas (1200 ℃ benchmark): 6165.59 m³/t-Mg

Total electricity consumption: 1042 kWh/t-Mg (Table S5, abrasive 200+pelletizing 42+others 800)

CO_2 from carbonate: 4.71 t/t-Mg (Table S1, 47.1kt÷10kt)

Temperature correction: Base 1200°C; Table 3 in manuscript: initial process 1400°C/optimized process 1398°C

4.2. Temperature correction coefficient

Base temperature: 1200°C

Initial process: 1400°C → ΔT +200°C

Table S5. *Process cost of prefabricated pellets*

No.	Project	Unit	Unit price (yuan)	Unit consumption
1	raw materials			
1.1	Dolomite	t	50	10
1.2	Ferrosilicon	t	5600	0.965
1.3	Fluorspar	t	2700	0.33
2	Fuel and power			
2.1	Abrasive power consumption	kWh	0.6	200
2.2	Pressure ball power consumption	kWh	0.6	42
2.3	Calcined water gas	m^3	0.5	2164.03
2.4	Reduced water gas	m^3	0.5	6165.59
2.5	Other electricity consumption	kWh	0.6	800
3	CO_2	t	600	-4.71
4	CO_2 waste heat recovery	m^3	0.5	-74.94

Optimized process: 1398℃ → ΔT +198℃

The restoration energy consumption is approximately linear with temperature, and the correction coefficient is proportional to the temperature difference:

Initial process coefficient: 1400/1200 = 1.1667

Optimized process coefficient: 1398/1200 = 1.165

4.3. Initial Process (Table 3: 1400℃/4h)

Energy consumption

Electricity consumption standard coal E_{elec} = 1042 · 0.1229 = 128.06 kgce/t-Mg

Standard coal quantity for calcining coal gas E_{calc} = 2164.03·9455.84÷29307.6 = 693.20 kgce/t-Mg

Gas used in the reduction process (temperature correction) V_{red} = 6165.59·1.1667 = 7193.39 m³/t-Mg

E_{red} = 7193.39·9455.84÷29307.6 = 2317.37 kgce/t-Mg

Total energy consumption E_{total} = 128.06+693.20+2317.37 = 3138.63 kgce/t-Mg

CO_2 Emission

Electric emissions CO_{2elec}: 1042·0.785÷1000 = 0.818 t/t-Mg

Calcination of coal gas combustion CO_{2calc_gas}: 2164.03·0.00112 = 2.424 t/t-Mg

Reduce gas combustion CO_{2red_gas}: 7193.39·0.00112 = 8.057 t/t-Mg

Carbonate decomposition $CO_{2carbonate}$: 4.71 t/t-Mg

Total consumption: 0.818+2.424+8.057+4.71 = 16.009 t/t-Mg

4.4. Optimized Process (Table 3: 1398℃/3.72h)

Time correction: 3.72/4 = 0.93

Energy consumption

Electricity consumption standard coal E_{elec}: 128.06 kgce/t-Mg

Calcined coal gas need standard coal E_{calc}: 693.20 kgce/t-Mg

Reduction gas need standard coal (temperature+time correction) V_{red} = 6165.59·1.165·0.93 = 6674.68 m³/t-Mg

E_{red} = 6674.68·9455.84÷29307.6 = 2150.22 kgce/t-Mg

Total energy consumption E_{opt} = 128.06+693.20+2150.22 = 2971.48 kgce/t-Mg

CO_2 Emission

Electric emissions CO_{2elec}: 0.818 t/t-Mg

Calcination of coal gas combustion CO_{2calc_gas}: 2.424 t/t-Mg

Reduce gas combustion CO_{2red_gas}: 6674.68×0.00112 = 7.476 t/t-Mg

Carbonate decomposition $CO_{2carbonate}$: 4.71 t/t-Mg

Total consumption: 0.818+2.424+7.476+4.71 = 15.428 t/t-Mg

4.5. Energy saving and carbon reduction range (entire process)

Energy reduction: (3138.63−2971.48)/3138.63·100% = 5.33%

CO_2 reduction: (16.009−15.428)/16.009·100% = 3.63%

4.6. LCA Results

Table S6 shows the total energy consumption and CO_2 emission results at initial process and optimized process.

Table S6. *Total energy consumption and CO_2 Emission results*

Item	Initial process	Optimized process	Reduction
Total energy consumption /kgce t^{-1} Mg	3138.63	2971.48	5.33%
CO_2 emission /t t^{-1} Mg	16.009	15.428	3.63%