Solutions

1. The sensible heat required to raise the temperature of a material is given by:

= sensible heat [J/s]
*m* = mass [kg]
*c*p = specific heat capacity [J/kg·K]
= change in temperature [K]

* We will assume that both processes start at room temperature, 25°C. We must look up the heat capacity of silica, which is 847 J/ kg·K at room temperature (NIST Chemistry WebBook, SRD 69).
* We will also assume that the heat capacity of silica is constant with temperature

In order to calculate the mass of silicon produced, we must know something about the efficiency of the chemical reactions and purifications. Max mentioned 80% reaction efficiency. He did not say whether it was mass or molar efficiency; but a reasonable guess is that he used mass efficiency because you can directly measure mass with a balance, whereas you cannot directly measure the number of moles.

* Assume 80% mass conversion

To obtain 1 kg of silicon via magnesiothermic reduction, we need 1 kg/0.8 = 1.25 kg of silica. *m* = 1.25 kg

We can now calculate the heat required to raise the temperature of silica to the magnesiothermic reduction temperature:

NB: DT°C = DTK because the factor of 273 cancels, this is ONLY true of differences in temperature.

Next we must find the cost of energy generation via coal-fired plants. This information is not readily available, so we will base our estimate on the cost of coal and its combustion efficiency.

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| --- | --- | --- |
| cost, *C*c | $29.72/t bituminous coal  | Reference: U.S. Energy Information Administration. “Coal explained: Coal Prices and Outlook,” 2019. Available at: <https://www.eia.gov/energyexplained/coal/prices-and-outlook.php> [Accessed 23 June 2020]. |
| heating value, *LHV* | 34,000 kJ/kg for bituminous | Reference: P. v. Zedtwitz and A. Steinfeld. Thermal gasification of coal — energy conversion efficiency and CO2 mitigation potential. *Energy*, (2003) **28**, pp. 441–456. |
| oxidation efficiency, *h*ox  | 0.98 | Reference: IPCC (2006) IPCC Guidelines for national greenhouse gas inventories. |
| furnace efficiency, *h*f | 80%-90% | Towler, G.P. [*Chemical Engineering Design: principles, practice and economics of plant process and design, 2nd ed*](https://find.shef.ac.uk/permalink/f/15enftp/44SFD_ALMA_DS51235977050001441). Oxford: Butterworth-Heineman **2013**, pp. 1183.  |

We know the energy required to produce one kilogram of Si using magnesiothermal reduction; we use this to calculate the mass of coal needed:

The cost of heating for one kilogram of silicon is:

This estimate is not very good because it neglects:

* The cost of heating Mg to 650°C
* Ancillary costs of running a coal furnace, like employee time, electricity for control and instrumentation, transport and storage of coal
* Heat losses from the reactor
* Enthalpy of magnesiothermal reduction
* Changes in heat capacity due to temperature

For our next iteration of these calculations, we might start by considering the last point, that heat capacity is not constant with temperature. It can be written empirically as:

The constants are found from the same NIST website, [a link is here](https://webbook.nist.gov/cgi/cbook.cgi?ID=C14808607&Type=JANAFS&Table=on).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| A | B | C | D | E |
| -6.076591 | 251.6755 | -324.7964 |

|  |  |
| --- | --- |
| 168.5604 |  |

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|  |  |
| --- | --- |
| 0.002548 |  |

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We will rewrite the equation above in a differential form so that we can apply this mathematical form of heat capacity:

We could begin by integrating this expression from 25°C to 650°C and seeing what the fraction effect is on our original estimate. We repeat this ‘correction’ process for each factor that we neglected, improving the accuracy of our estimate as we go.

Follow a similar methodology to calculate the cost of using convention manufacturing to produce silicon and the cost of using electrical energy instead of coal energy.

1. The heating stage (furnace), which is where the magnesiothermic reduction occurs, and the dissolution stage, where aqueous purification reactions solubilize the
2. Reactions:
	1. Reaction byproducts: MgO, Mg2Si
	2. Dissolution byproducts: MgCl, H2, H20, Mg2Cl2, SiH4, SiO2
	3. SiH4 is pyrophoric…it can autoignite in the air! We need to react away all of this gas to prevent a safety hazard.
3. A lab-scale furnace is stationary whilst an industrial furnace rotates to prevent the evolution of hotspots or a non-uniform temperature profile.
4. A low concentration of acid costs more to use because i) the lower concentration results in slower dissolution kinetics for the magnesium species (longer processing time) and ii) extra heating costs apply to remove the excess water. On balance, lower concentrations may significantly reduce the rate at which the reactor vessel corrodes, potentially saving significant capital costs. In addition, lower concentrations of acid could prevent serious injury if workers are accidentally exposed.
5. The higher the selectivity of silicon production, the higher the value of the final product and the greater the net profits because chemical value increases with purity.
6. Conduct an internet search for average operational hours in chemical plants. Many chemical plants are benchmarked against a standard of 8,000 hours/year.
7. Required purity of the final silicon product, reaction residence time/degree of conversion, temperature of reaction, etc.