Application of hydrogen as a reductant in metal production: Modelling and experimentation

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07/04/2025

About Mintek

- South African science council conducting research, development, and technology transfer for the minerals beneficiation industry
  - Established 1934
  - Annual budget ~ZAR 500M
  - Diversified commercial and public funding sources (~70/30)
  - Multiple technical and support divisions with domain-specific expertise



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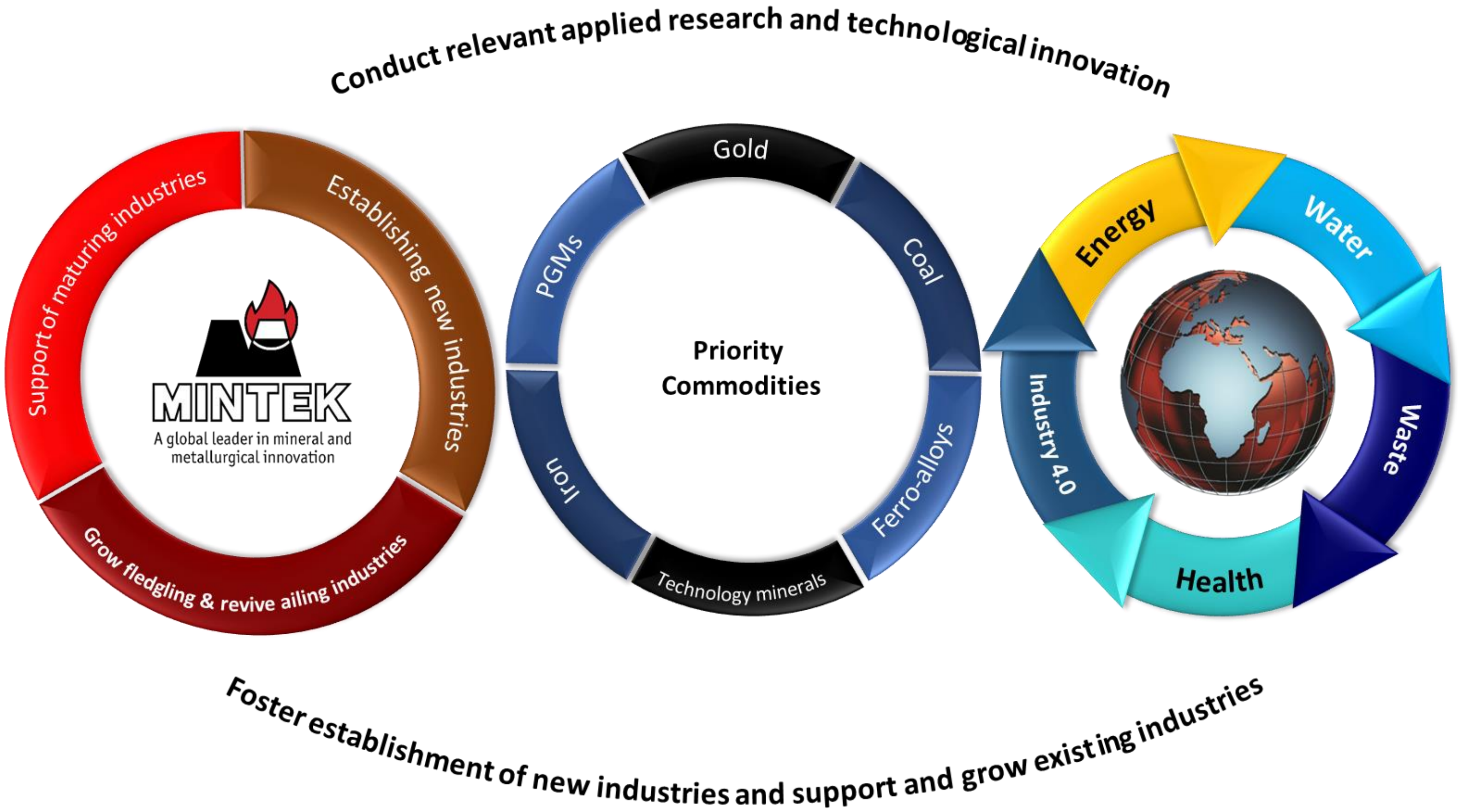
About Mintek



Introduction

- Metal production is generally carried out using carbon-based reductants in furnaces
- Conventional reductants constitute fossil carbon and this renders metal production carbon dioxide emissions intensive
- Reductants such as hydrogen, wherein water is the only by-product, have become attractive potential alternatives in metal production in addressing the high greenhouse gas emissions
- Unlike the carbon-based metal production processes, hydrogen-based metal production processes have not achieved widespread application in industry

Hydrogen as a reductant in metal production

- The use of hydrogen in metal production is based on pre-reduction, direct-reduction and plasma smelting with hydrogen
- As a first step towards designing hydrogen-based metal production processes, it is crucial to carry out comprehensive studies based on a combination of modelling and experimentation
- E.g., Before designing a pre-reduction reactor, it is crucial to investigate and understand the process kinetics and their influence on the overall pre-reduction reactor performance
- Computational fluid dynamics (CFD) reacting flow models are used to predict the influence of kinetics, geometry and flow field on the chemical reaction rates

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Hydrogen as a reductant for pre-reduction of chromite manganese ores

- Fe-oxide part of chromite is easily reducible with hydrogen, while the Cr-oxide component has a low degree of reduction
- Longer residence times are needed to achieve high metallization of Fe in the pre-reduction of chromite with hydrogen
- Hydrogen as a reductant for the carbonate containing manganese ores accelerates the decomposition of carbonates, reduces the iron oxide contained in the ore to metallic iron and reduces the higher manganese oxides to MnO
- Pre-reduction with hydrogen contributes to energy consumption reduction in the downstream smelting because it completes the endothermic carbonate decomposition

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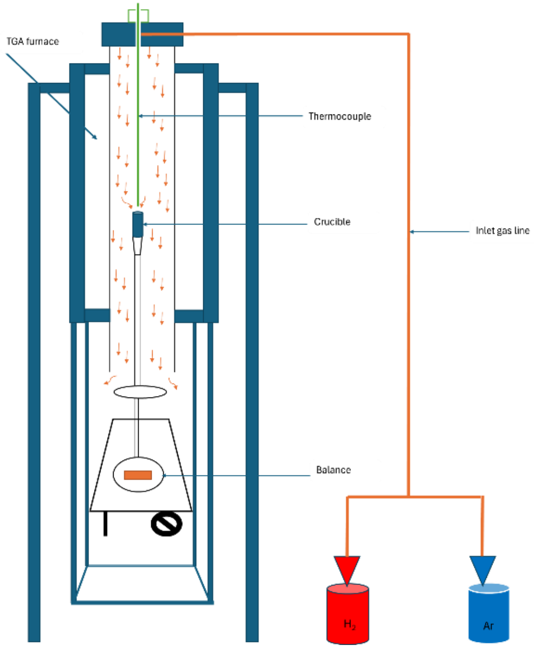
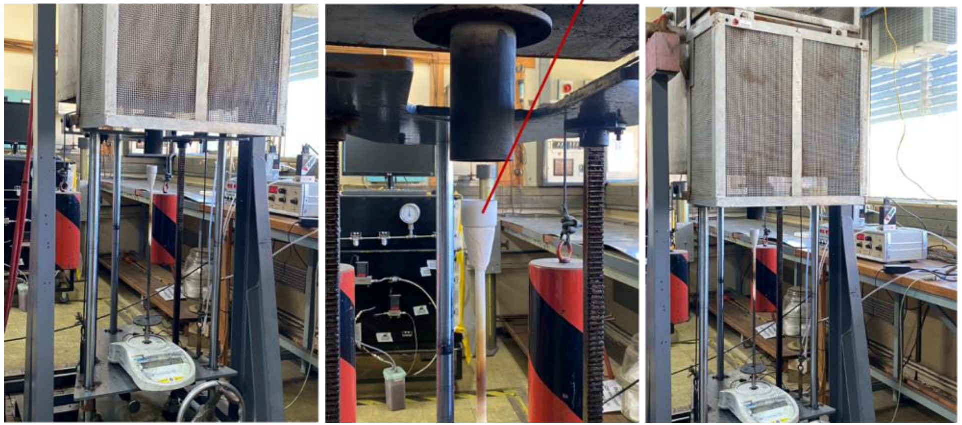
Pre-reduction of chromite pellets with hydrogen

- The isothermal and non-isothermal reduction experiments were conducted with hydrogen at 1200°C, 1350°C , 1400°C and 1500°C



A crucible cut to 2.5 cm height prior to tests



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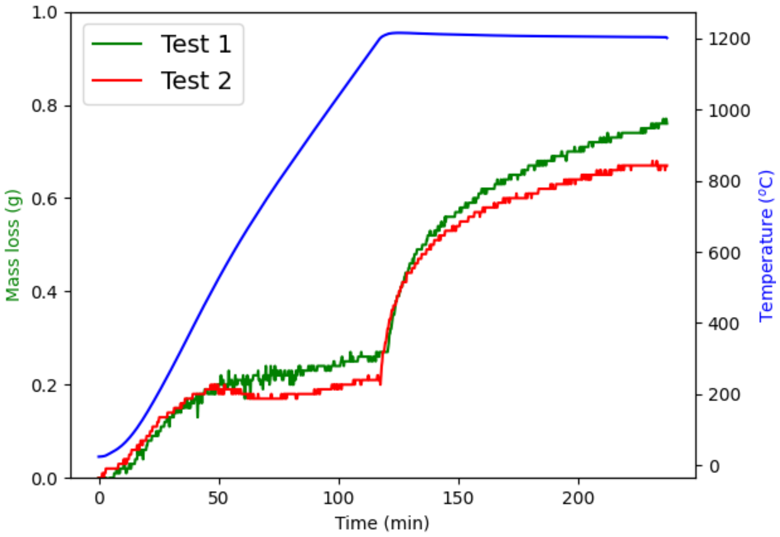
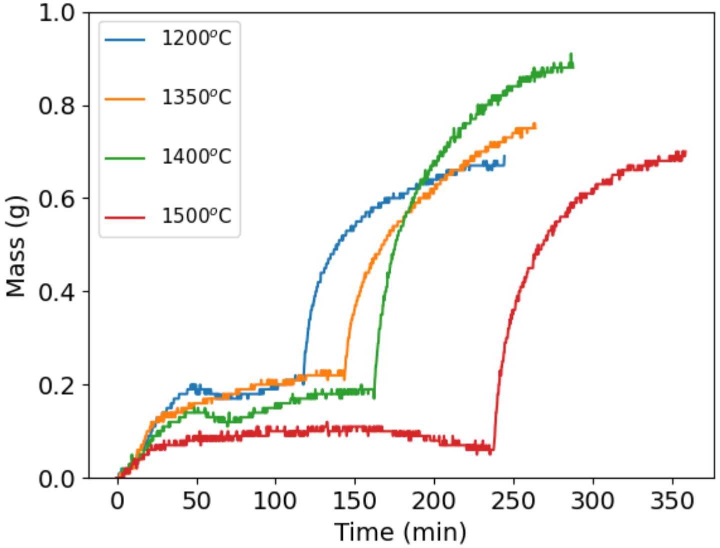
Results and discussions

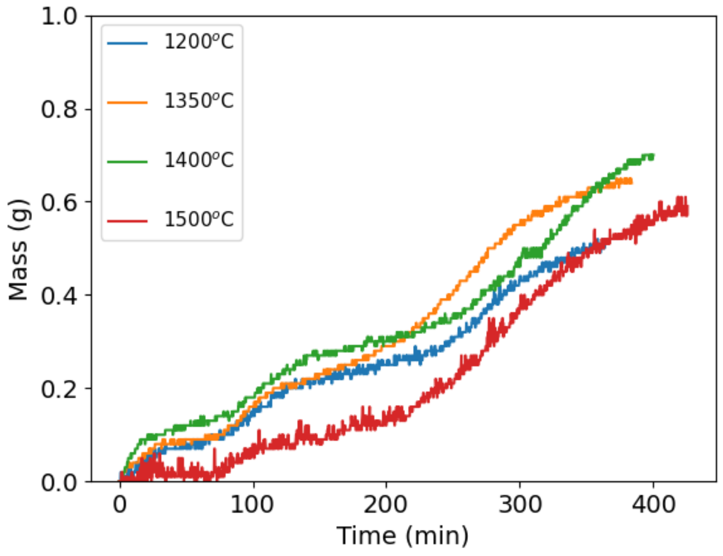
- Mass loss data from isothermal pre-reduction experiments





Results and discussions

- Mass loss data from non-isothermal pre-reduction experiments



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Modelling pre-reduction of manganese ore by Hydrogen

- The lumpy manganese ore particles in a thermogravimetric furnace are modelled as a fixed bed of particles and the flow in and around the fixed bed is resolved
- The fixed bed is described as a collection of tensor and scalar properties
- When the reduction reactions take place, the transformation from one phase to the other results in density changes and this leads to changes in porosity
- $$\frac{d}{dt}\epsilon = -(1-\epsilon)\sum_{i=1}^{N}\frac{1}{\rho_i^s}R_i$$
- The structural changes in the intermediates oxides may result in porosity changes which will affect the transport of reducing gases into the reaction sites

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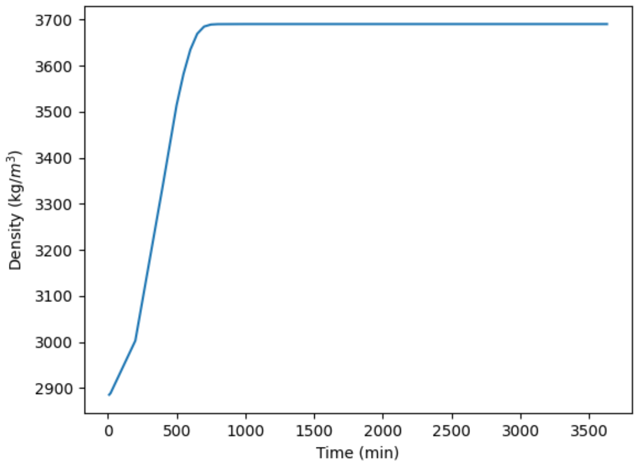
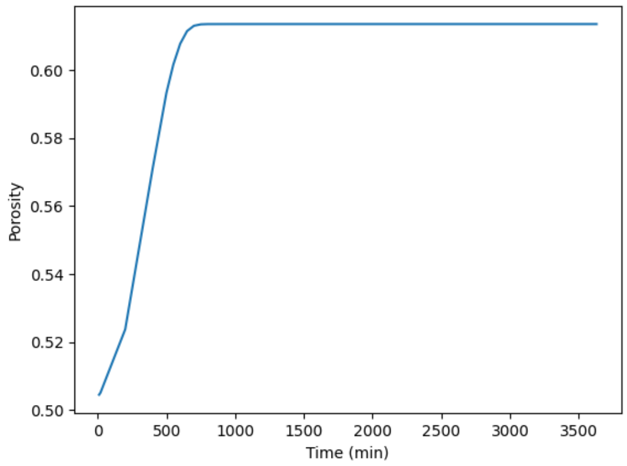
An example of density and porosity predicted by the model





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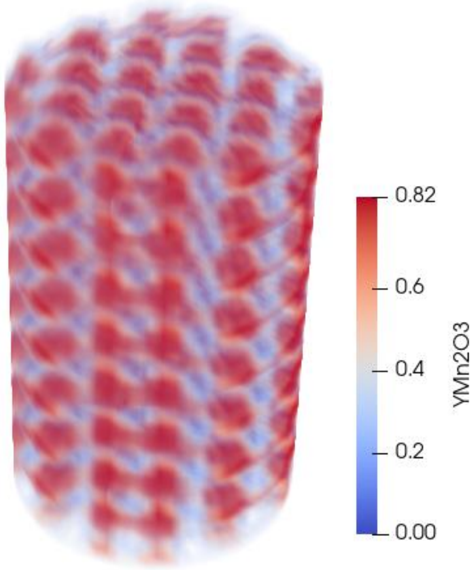
Results and Discussions

- Species mass fraction for a 0.3 m furnace with 0.175 m bed height



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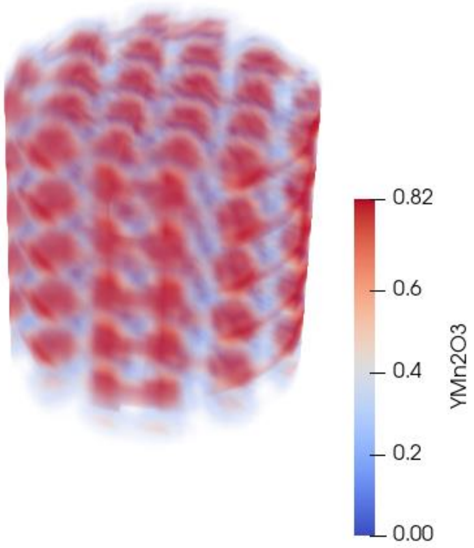

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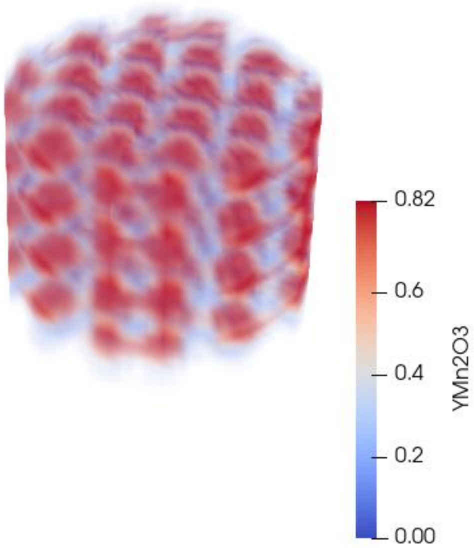

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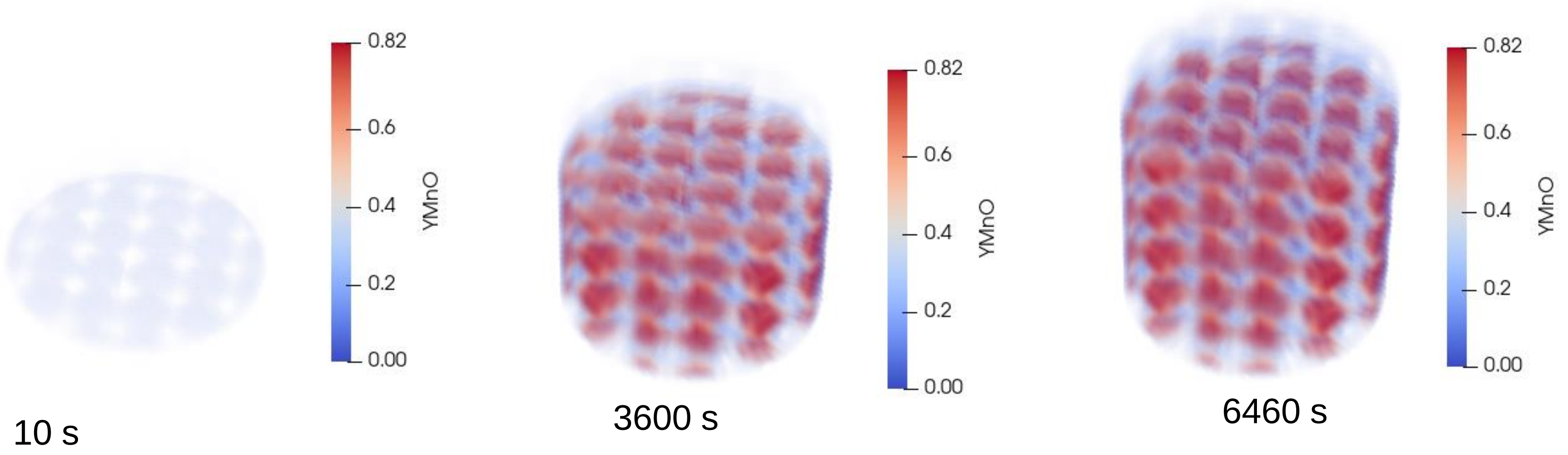
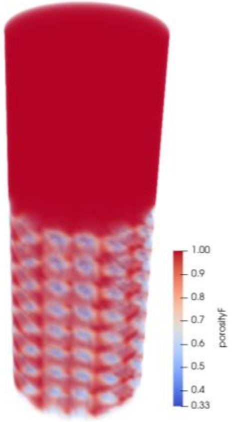
Results and Discussions

- Species mass fraction profiles



Results and Discussions

- Porosity and density fields



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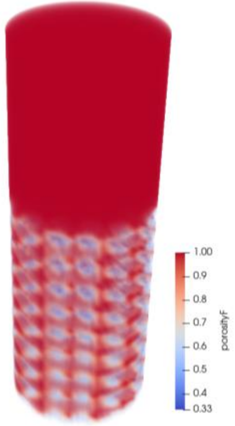

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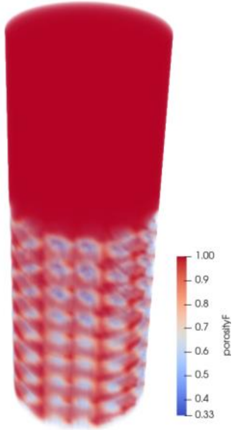

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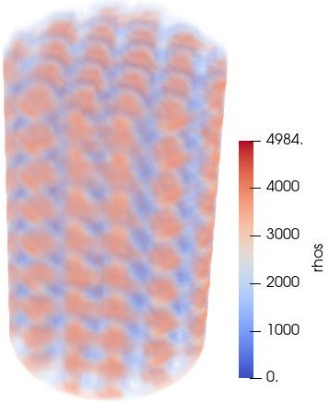

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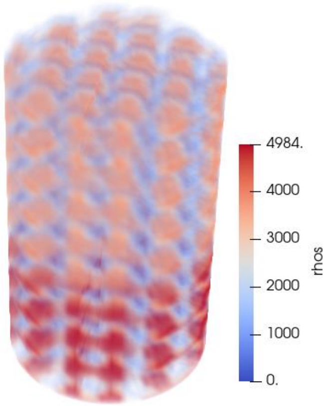

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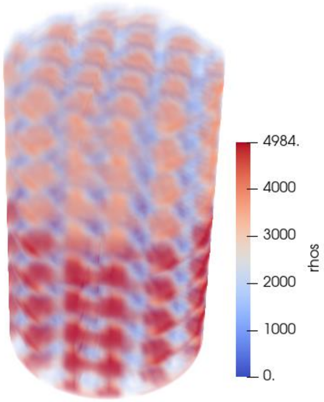

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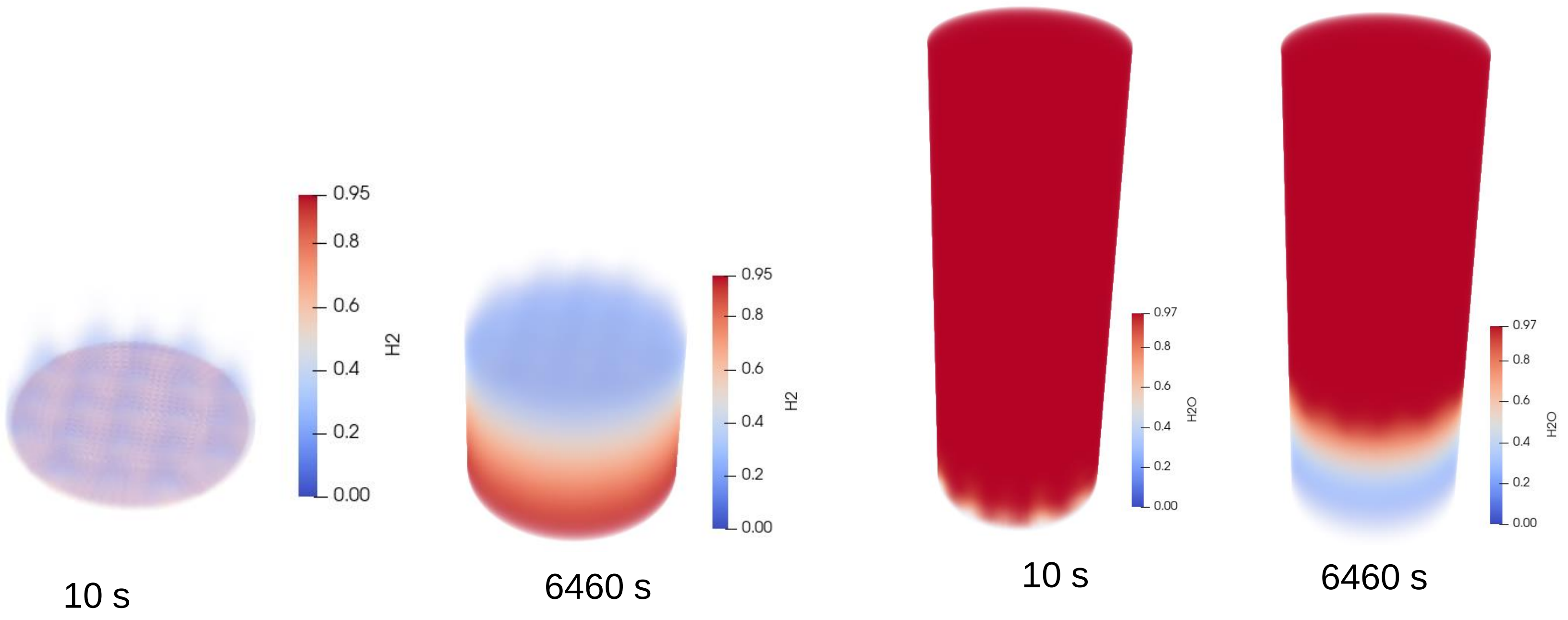
Results and Discussions

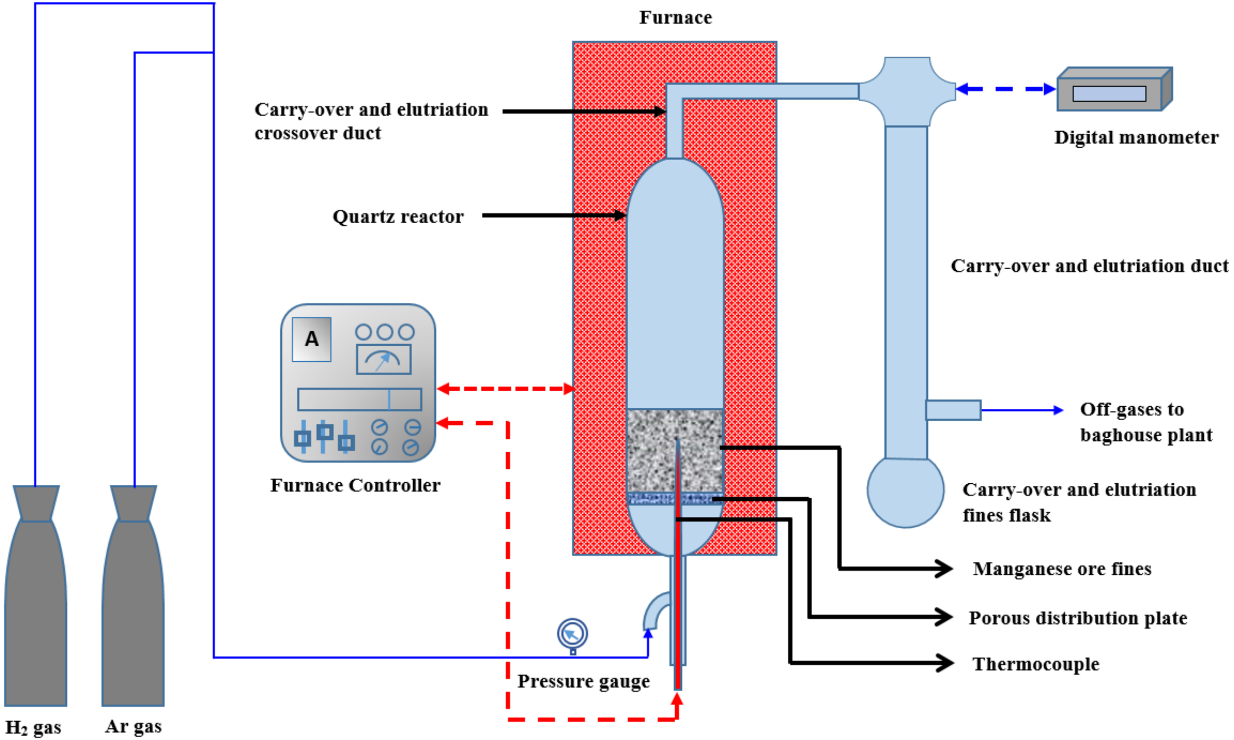
- Species mass fraction for a 0.3 m furnace with 0.175 m bed



Research on hydrogen by colleagues at Mintek

- This section presents the work done by other researchers at Mintek on the application of hydrogen as a reductant in metal production

Pre-reduction of manganese ore fines with hydrogen in a fluidised bed



Mchabe, D.; Tsebe, S.;Matinde, E. Evaluation of the Effects of Fluidization Conditions on Hydrogen Reduction in Manganese Ore Fines. Minerals 2025, 15, 368. https://doi.org/10.3390/min15040368

Results and discussions: Effect of temperature[1]

Respective mineral proportions in as-received Nchwaneng and Zambian manganese ores

Mineral	Ideal Chemical Composition	Nchwaneng ore	Zambia ore
		%	%
Braunite	$Mn^{2+}Mn^{3+}{}_6SiO_{12}$	41.36	ND
Hausmannite	$Mn^{2+}Mn^{3+}{}_2O_4$	3.62	ND
Kutnohorite	$Al_2Mg_5(Si_3O_{10})\ (OH)_8$	3.49	ND
Bementite	$Mn_8Si_6O_{15}(OH)_{10}$	ND	ND
Jacobsite	$Mn^{2+}Mn^{3+}{}_2O_4$	ND	ND
Manganosite	MnO	ND	ND
Buixbyite	$Mn^{3+}{}_{1.5}Fe^{3+}{}_{0.5}O_3$	14.16	ND
Manganite	MnO	6.96	ND
Marokite	$CaMn^{3+}{}_2O_4$	2.7	ND
Rhodochrosite	$Mn^{2+}(CO_3)$	<1	ND
Romanechite	$(Ba,H_2O)_2(Mn^{4+},Mn^{3+})_5O_{10}$	ND	56.1
Pyrolusite	MnO_2	ND	21.44
Cryptomelane	$K(Mn^{4+},Mn^{2+})_8O_{16}$	ND	5.91
Hollandite	$Ba(Mn^{4+},Mn^{2+})_8O_{16}$	ND	2.19
Jacobsite	$Mn^{2+}Mn^{3+}{}_2O_4$	ND	2.04
Coronadite	$Pb(Mn^{4+},Mn^{2+})_8O_{16}$	ND	1.26
Galaxite	$(Mn,Mg)(Al,Fe^{3+})_2O_4$	ND	<1
Ankerite	$Ca(Fe^{2+},Mg)(CO_3)_2$	ND	1.26
Lizardite	$Mg_3(Si_2O_5)(OH)_4$	ND	<1
Hematite	Fe_2O_3	13.68	<1
Dolomite	$CaMg(CO_3)_2$	7.87	ND
Calcite	$CaCO_3$	5.61	ND
Quartz	SiO_2	ND	8.27

ND = not detected

Mineral phases of the products of Nchwaneng manganese ore that was reduced by hydrogen gas at 500 ◦C and 700 ◦C, respectively

Compound Name	Formula	Relative Abundance	
		500 °C	700 °C
Iron Manganese Oxide	$(FeO)_{0.198}(MnO)_{0.802}$	Major	Major
Calcium Manganese Oxide	$(MnO)_{0.877}(CaO)_{0.123}$	Minor	Minor
Manganosite	MnO	Intermediate	Intermediate
Iron Manganese	$Fe_{0.95}Mn_{0.05}$	Minor	Intermediate
Quartz	SiO_2	Minor	ND

Predominant (>50 mass %), major (30-50 %), intermediate (15-30 %), minor (5-15 %) and trace (<5 %)

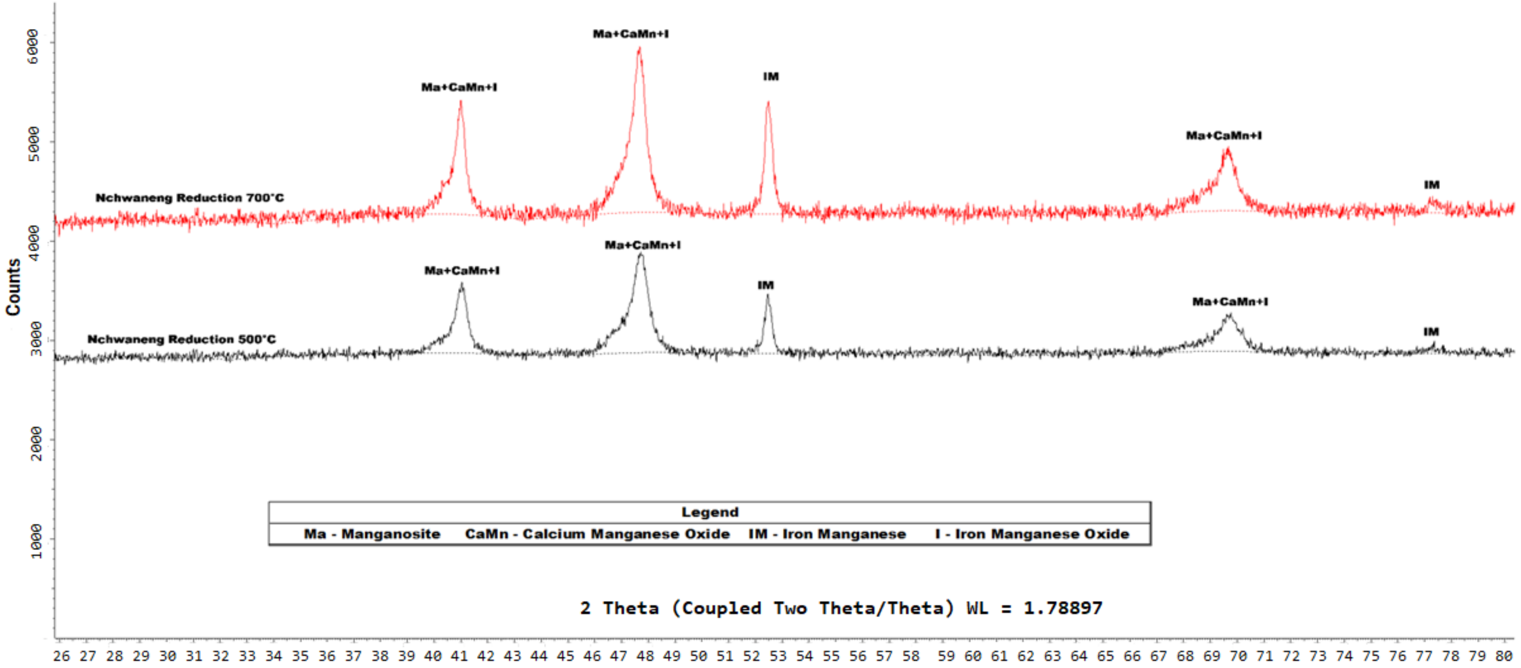
Mineral phases of the products of Zambian manganese ore that was reduced by hydrogen gas at 550 ◦C, 600 ◦C, 700 ◦C and 800 ◦C, respectively

Compound Name	Formula	Relative Abundance			
		550 °C	600 °C	700 °C	800 °C
Iron Manganese Oxide	$(FeO)_{0.198}\ (MnO)_{0.802}$	Major	Predominant	Predominant	Predominant
Calcium Manganese Oxide	$(MnO)_{0.877}\ (CaO)_{0.123}$	ND	ND	Minor	ND
Lorenzenite	$Na_2(Ti_2Si_2O_9)$	ND	Minor	ND	ND
Sodium Manganese Iron Carbide Nitride	$Na_{1.8}FeMnC_6N_6$	Minor	ND	ND	ND
Srebrodolskite	$Ca_2Fe_2O_5$	Minor	ND	ND	ND
Andradite	$Ca_3Fe_2(Si_{1.58}Ti_{1.42}O_{12})$	Minor	ND	ND	ND
Forsterite	Mg_2SiO_4	Intermdiate	Minor	ND	ND
Akageneite	$Fe^{3+}O(OH)$	ND	Minor	Minor	ND
Ramsdellite	MnO_2	ND	ND	ND	Minor
Kurchatovite	$K_3(HAl_2Si_4O_{13})$	ND	ND	ND	Minor
Barium Oxide Peroxide	$Ba\ (O2)_{0.972}\ (O)_{0.027}$	ND	ND	ND	Trace
Quartz	SiO_2	Minor	Trace	Trace	Minor

Predominant (>50 mass %), major (30-50 %), intermediate (15-30 %), minor (5-15 %) and trace (<5 %)

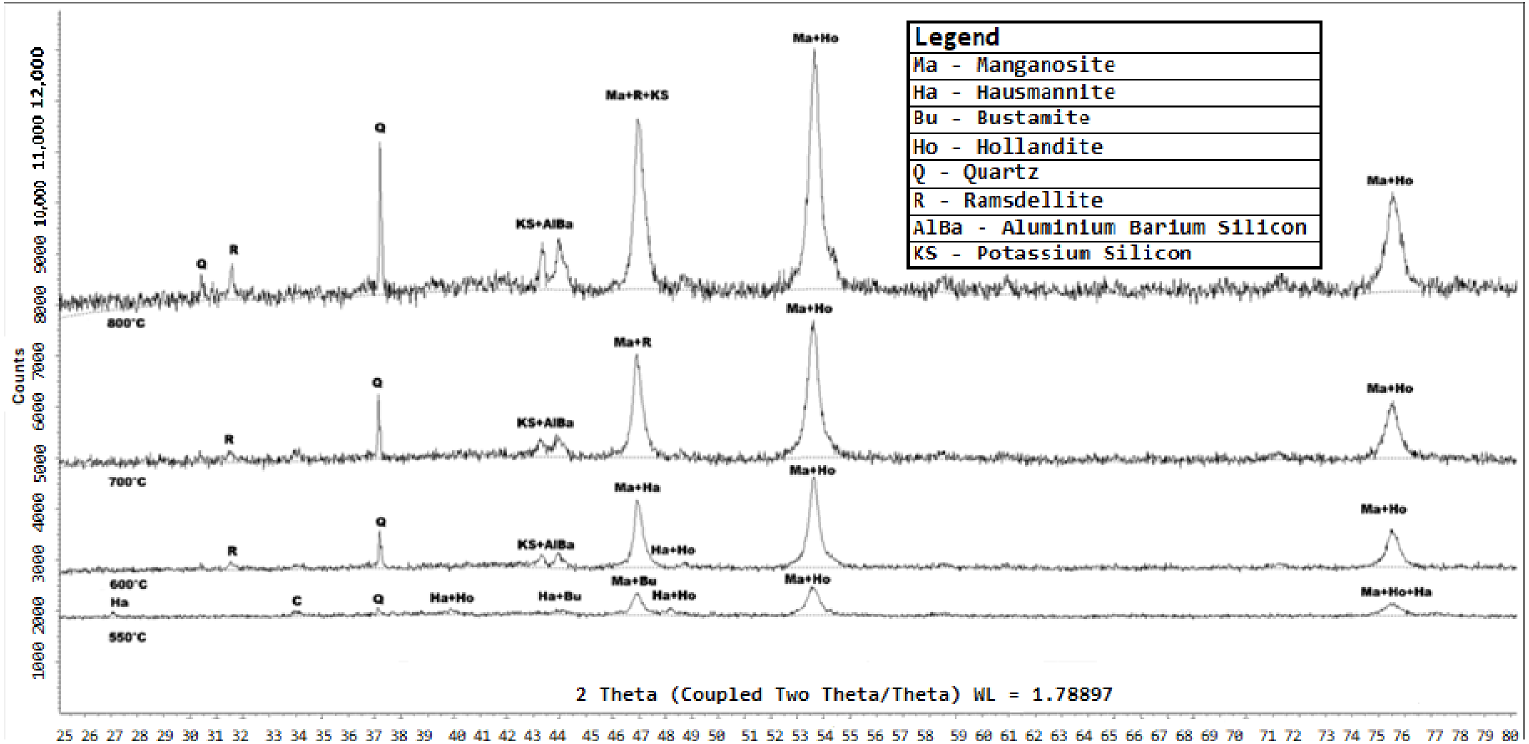
Mchabe, D.; Tsebe, S.;Matinde, E. Evaluation of the Effects of Fluidization Conditions on Hydrogen Reduction in Manganese Ore Fines. Minerals 2025, 15, 368. https://doi.org/10.3390/min15040368

Results and discussions: Effect of temperature



XRD diffractograms of the products of Nchwaneng manganese ore that was reduced by hydrogen gas at 500 ◦C and 700 ◦C, respectively. The analysis was conducted using a Bruker D8 diffractometer equipped with Fe-filtered Co Kα radiation. Data were collected over a 2θ range of 5–80° with a step size of 0.02° 2θ. Phase identification was performed using Bruker EVAR software, while quantitative phase analysis was conducted using TOPASR software.

Results and discussions: Effect of temperature



XRD diffractograms of the products of Zambian manganese ore that was reduced by hydrogen gas at 550 ◦C, 600 ◦C, 700 ◦C and 800 ◦C, respectively. The analysis was conducted using a Bruker D8 diffractometer equipped with Fe-filtered Co Kα radiation. Data were collected over a 2θ range of 5–80° with a step size of 0.02° 2θ. Phase identification was performed using Bruker EVAR software, while quantitative phase analysis was conducted using TOPASR software

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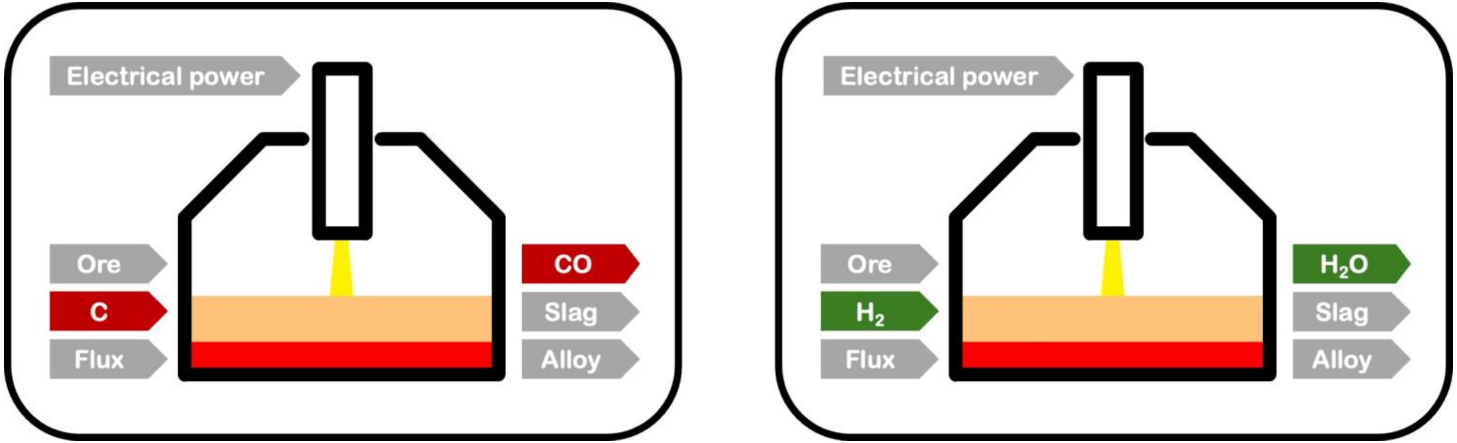
Modelling of Electric Arc Behaviour in Direct-Current Smelting Furnaces

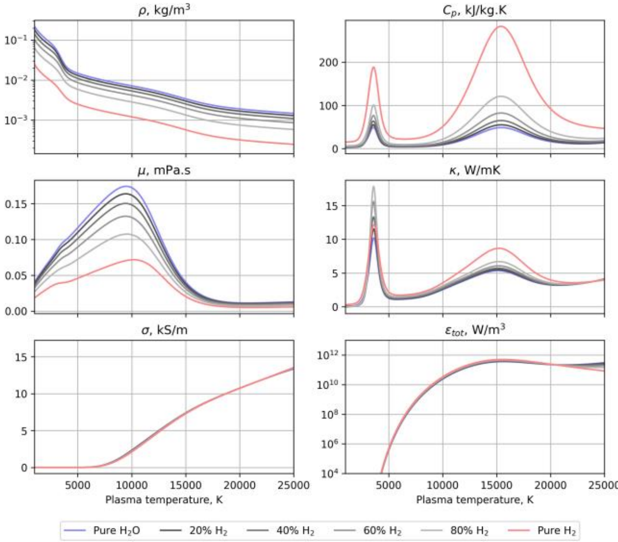
- Possibilities for carbon replacement with hydrogen

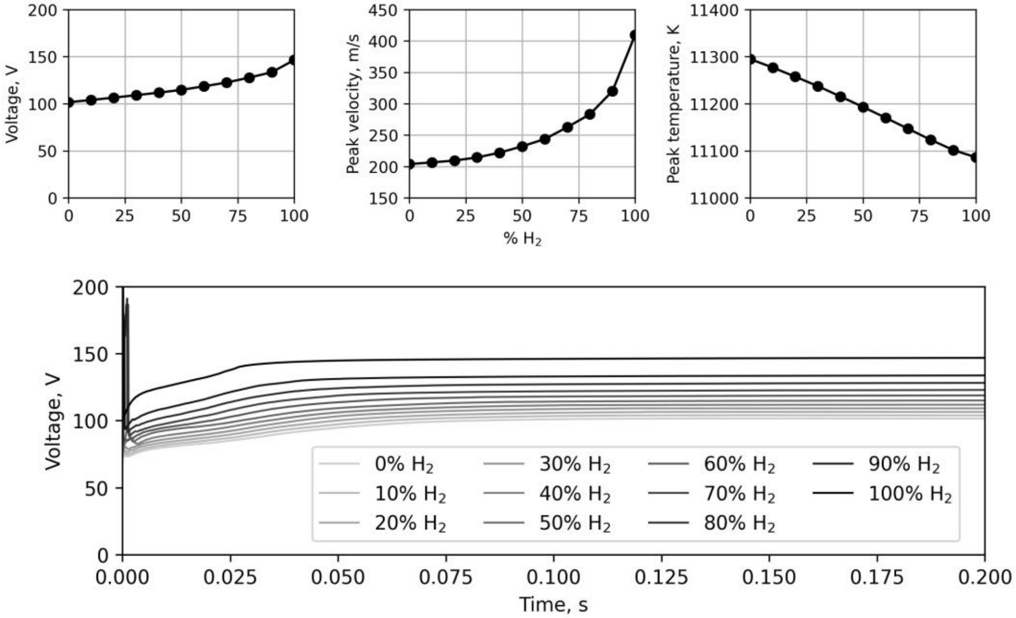


Reynolds, Q. G., Erwee, M. W., Geldenhuys, I. J., Haraldsson, H. V, Johnsen, S. G., Jones, R. T., Tesfahunegn, Y., & Xakalashe, B. S. (2024). Computational Modelling of Electric Arc Behaviour in Direct-Current Smelting Furnaces Using Hydrogen as a Reductant. 1–13.

Results and discussions

- LTE plasma properties for different H_2-H_2O gas compositions at 1 atm pressure





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Concluding remarks

- The isothermal and non-isothermal pre-reduction experiments showed that longer reduction times are required to achieve higher degrees of reduction
- CFD models for pre-reduction in a TGA revealed that the lower section of the bed gets pre-reduced before the top section and that the reaction front propagates from the particle surface inwards
- CFD modelling succeeded in highlighting some phenomena of interest in hydrogen smelting using DC arc furnaces, however, much work remains to be done and that includes experimental data from laboratory and pilot plant testing for direct validation of the model results
- Hydrogen is an attractive potential reductant in metal production

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Acknowledgements

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