Transport Properties of an MnO/H_2 Based Thermal Plasma

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Abstract: Replacing carbon with hydrogen in the reduction of manganese ore to metallic manganese will require the development of novel plasma-based processes. Mathematical modelling of reactor operation will provide invaluable insight with respect to optimization and design choices. This paper reports from the computation of essential model input data, i.e. temperature-dependent transport properties for an MnO/H_2-based thermal plasma.

1. Introduction

At SINTEF (Trondheim, Norway), novel processes are developed for carbon-free reduction of metal ores [1]. Hydrogen (H_2) is a promising alternative to carbon (C), as its use as a reductant generates water vapor (H_2O) instead of carbon dioxide (CO_2). While some ores can be reduced by H_2, thermodynamic limitations prevent the reduction of others. This challenge can be overcome by leveraging more reactive hydrogen species, such as monoatomic (H) or ionized (H^+) hydrogen, found in hydrogen plasma. Aarnæs *et al.* [2] demonstrated that metallic manganese (Mn) can be produced from manganese oxide (MnO) using this approach.

Mathematical modelling, such as Computational Fluid Dynamics (CFD), plays an important role in the design and development of plasma reactors. However, key input for such models, e.g. plasma gas material properties, is often unavailable. To address this, we are developing frameworks to compute temperature-, pressure-, and composition-dependent material properties for arbitrary plasma gas mixtures, using established methodologies.

At ISPC25 in Kyoto [3], we presented computed temperature-dependent chemical equilibrium compositions for MnO/H_2 feeds and thermodynamic properties (specific heat capacity, adiabatic index, and speed of sound) at thermodynamic equilibrium. Here, we report transport coefficients (viscosity, thermal and electrical conductivities, and net emission coefficient) under the same equilibrium conditions.

2. Methods

The computation of equilibrium compositions and material properties assumes thermodynamic equilibrium, equipartition of energy, and ideal mixtures of thermally perfect gasses, employing standard methods from statistical physics [3]. The methods closely follow classical textbooks by e.g. Boulos *et al.* [4] and Anderson [5], as well as the computation framework by Reynolds *et al.* [6].

The equilibrium composition was computed for a mixture consisting of electrons and twenty-two tri-/di-/monoatomic and ionic species based on hydrogen, oxygen, and manganese nuclei. While rotational and vibrational excitations were restricted to ground states, electronic excitation data was utilized for all species. A detailed list of species, chemical reactions, and data sources is available in [3].

Viscosity and thermal and electrical conductivities were determined using gas kinetic theory, accounting for all possible species-species collisions.

The net emission coefficient was computed by integrating emission spectrum lines across all wavelengths for each species and summing the results

3. Results and Discussion

Using established methods from gas kinetic theory and statistical physics, temperature-, pressure-, and composition-dependent transport coefficients (viscosity, thermal and electrical conductivity, and net emission coefficient) were computed for MnO/H_2 based thermal plasma.

4. Conclusion

The developed computational framework can be used to provide essential input data for CFD simulations, enabling CFD-assisted design and development of novel plasma reactors for hydrogen based, carbon-free metal production.

Acknowledgement

This work was funded by SINTEF, Trondheim, Norway.

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