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Exploring new ways to decarbonize metal production with multiphysics modelling and high-performance computing

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Direct-current (DC) electric arc furnaces are used extensively in the recycling of steel as well as primary production of many industrial commodities such as ferrochromium, titanium dioxide, cobalt, and platinum group metals. This typically involves a process called carbothermic smelting, in which raw materials are reacted with a carbon-based reductant such as metallurgical coke to make the desired product. Although it is one of humanity's oldest and most established technologies, carbothermic metal production is becoming increasingly unattractive due to its significant scope-1 emissions of carbon dioxide and other environmental pollutants. Because of this many alternatives to fossil carbon reductants are currently being researched, and in the context of broad initiatives to establish a sustainable hydrogen economy both in South Africa and internationally, the possibility of directly replacing coke with hydrogen as a metallurgical reductant is of particular interest. A DC arc furnace fed with hydrogen has the potential to reduce or eliminate carbon emissions provided renewable resources are used for both electrical power and hydrogen production.

Key to the operation of DC arc furnace is the electric arc itself – a high-velocity, high-temperature jet of gas which has been heated until it splits into a mixture of ions and electrons (a plasma) and becomes electrically conductive. The plasma arc acts as the principal heating and stirring element inside the furnace, and understanding its behaviour is an important part of operating an arc furnace efficiently and productively. However, due to the extreme conditions under which arcs operate, studying them experimentally can be difficult, expensive, and hazardous. Coupled multiphysics models which simulate arcs from first principles of fluid flow, heat transfer and electromagnetics are therefore of great value in conducting *in silico* numerical experiments and building an understanding of how they behave under different process conditions. This presentation will discuss the development of an arc modelling workflow incorporating aspects of process thermochemistry, plasma property calculation from fundamental physics, and computational mechanics models of the arc itself. This workflow is then used to explore the impact of introducing hydrogen gas as an alternative reductant in metallurgical alloy smelting processes.

In keeping with the theme of this year's CHPC National Conference, the critical role of HPC in plasma arc modelling will be discussed in terms of the data life cycle in plasma arc modelling – from input parameters through to raw simulation data, and finally to key insights which will help guide the next generation of clean metal production technologies.

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No. Not a student nor Postdoc.

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Yes

CHPC User

Yes

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