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Toward computational models of metallurgical converting processes

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Abstract

In many flowsheets used for high-temperature metallurgical processing, alloy converting is required as a secondary treatment stage in order to refine products from primary smelting furnaces to acceptable quality. This process entails contacting molten metal alloy with oxygen in a converter unit. Oxygen reacts chemically with undesirable and less noble components of the alloy to produce metal oxides, forming a separate slag phase which is generally discarded from the converter as a waste product. Alloy converting is applied extensively in the production of intermediate products such as low carbon ferromanganese and ferrochromium, as well as in treatment of the complex alloys arising from pyrometallurgical processing of e-wastes and related processes.

In the present paper an initial computational modelling study of a particular converter unit design, the Top Blown Rotary Converter (TBRC), is presented. The TBRC consists of a cylindrical vessel which is lined with insulating refractory materials, inclined at an angle, and rotated about its axis. Material to be converted is batch-fed to the unit, and a combustion lance fed with propane and oxygen is inserted into the mouth of the vessel. The lance flame is generally controlled to produce an excess of oxygen, thereby providing both thermal energy and available oxygen for the alloy converting process.

To advance the state of the art and improve design and operability of TBRC units, the capabilities of computational models of the fluid flow, heat transfer, and chemical reactions occurring in the lance flame of the converter were explored. Models were implemented and executed using transient combustion flow solvers available in the OpenFOAM® open-source computational mechanics platform, and the impact of chemical reaction mechanism complexity on solver performance and accuracy was assessed. The distributions of energy and reaction products through the interior of the TBRC were examined as a function of the flowrates of oxygen and propane to the lance at different stoichiometric ratios, and converting rates for the various conditions were estimated from the flux of oxygen to the boundaries representing the molten alloy.

Computational fluid dynamics; combustion; chemical reaction; metallurgy; converting
1. Introduction

Converting processes make up a substantial portion of secondary pyrometallurgical unit operations and are used extensively for intermediate chemical treatment and product refinement in industries ranging from platinum-group metals to ferroalloys [1, 2].

A number of different converter designs may be used depending on the primary commodity being treated. They share the common traits that they are refractory-lined containment vessels holding molten metal alloy, into which oxygen (either pure, as air, or mixed with other gases) is blown. Certain components of the alloy react preferentially with the oxygen to produce metal oxides forming a separate liquid phase (slag), which may then be easily separated from the refined alloy. By necessity converters operate at temperatures above the melting point of the alloys being treated, usually between 1200 and 1700°C. In recent years the demand for small-scale, flexible, easily-operated converter units capable of handling the metallurgically complex and variable streams encountered in processes such as cathode-ray tube and electronic waste recycling has been growing rapidly. The Top-Blown Rotary Converter (TBRC) design addresses many of these needs [2].

A typical TBRC unit is shown in Figure 1, and consists of a cylindrical, inclined vessel containing a batch of alloy to be refined. The vessel is rotated about its axis and is heated using a removable gas combustion lance. The lance is fed with oxygen and a hydrocarbon fuel, typically methane or propane, and produces a subsonic combustion flame. This flame enters the converter vessel and provides both thermal energy as well as the ideal furnace atmosphere conditions for the particular refining process being performed. Specifically, the ratio of oxygen to fuel may be adjusted to produce a reducing (excess fuel) or oxidising (excess oxygen) environment as needed.

Fig. 1. (l) TBRC pilot plant in operation, (r) high-speed camera image of TBRC lance flame in air

TBRC operations are generally controlled using simplified calculations of both the combustion efficiency in the lance as well as the energy input and losses. In order to improve the design, operation and efficiency of such units, a computational modelling study was deemed to be of some value in developing a better fundamental understanding of their behaviour. Computational methods have been applied extensively in the study of other designs such as Ausmelt® [3] and Peirce-Smith [4] converters, but the focus has generally been on multiphase fluid flow effects and gas-liquid stirring in the molten bath rather than combustion chemistry in the gas phase which is peculiar to the TBRC operation. With this in mind the present paper focuses on the development of methods for modelling of the coupled fluid flow, heat transfer, and chemical combustion phenomena in the TBRC lance flame, and presents some preliminary analysis of how these phenomena affect the transfer of oxygen from the gas phase to the molten process material inside the TBRC vessel. More detailed experimental validation of the results will follow in future work.

2. Model Development

A numerical model of the lance flame and vessel interior gas space of a propane-fired pilot-scale TBRC unit at Mintek was constructed using the OpenFOAM® open source computational mechanics framework [5]. The standard rhoReactingBuoyantFoam finite-volume method solver was used (with minor modifications to permit accurate...
calculation of chemical species fluxes at boundary surfaces and extend the capabilities of the radiation model), and implements the following features:

- Compressible fluid flow and pressure calculations on unstructured meshes using a combined PISO-SIMPLE algorithm suitable for highly transient flow under laminar or turbulent conditions
- Coupled heat transfer including buoyancy effects and thermal radiation
- Coupled chemical species transport and reaction kinetics

The geometry of the problem is presented in Figure 2. The region modelled consists of the lance tip, including an inlet boundary for a pre-mixed combination of propane fuel and oxygen, and solid surfaces representing the water-cooled jacket of the lance. It should be noted that the use of a pre-mixed inlet is an approximation in this case, as actual TBRC lances typically inject fuel and oxygen separately through concentric annular nozzles. The gas space is initially filled with a stoichiometric mixture of combustion products CO₂ and H₂O, and the outlet of the vessel is assumed to be open to an atmosphere of the same composition. The vessel walls and alloy pool are treated as solid surfaces due to the short time periods modelled (< 200 ms) and are held at a fixed temperature representative of typical TBRC process conditions. All vessel boundaries are treated as zero-gradient boundaries for the chemical species concentration fields, with the exception of oxygen atoms and molecules for which the alloy pool is set to a concentration of zero (representing a rapid metal oxidation reaction occurring at the surface). In this study models were limited to 2D planar slices to retain manageable run times, however, the implementation extends naturally to 3D with little or no modification.

Model results were post-processed to obtain the average mass flux of oxygen at both the vessel outlet \( q_{\text{outlet}} \) and the alloy pool \( q_{\text{pool}} \) at each time step, per relationships shown in equation (1).

\[
q_{\text{pool}} = \frac{1}{A_{\text{pool}}} \sum_{i=1}^{n} \left( D_0 \nabla x_O + D_{O_2} \nabla x_{O_2} \right)_i \cdot \mathbf{n}_i \delta A_i \quad q_{\text{outlet}} = \frac{1}{A_{\text{outlet}}} \sum_{i=\text{outlet}} \left( x_O + x_{O_2} \right) \rho_i \mathbf{u}_i \cdot \mathbf{n}_i \delta A_i
\]  

Here, \( D_0 \) and \( D_{O_2} \) are the diffusion coefficients of oxygen atoms and molecules in the gas mixture, \( x_O \) and \( x_{O_2} \) are the mass fraction fields of oxygen atoms and molecules, \( \mathbf{n}_i \) is the normal of the \( i \)th surface element in the boundary being considered, \( \delta A_i \) is its area, \( \rho_i \) is the density of the gas mixture, and \( \mathbf{u}_i \) is the velocity field at the surface element.

It is important to note that the inclusion of chemical kinetic mechanisms in fluid dynamics solvers requires the solution of a set of ordinary differential equations for each cell in the numerical mesh at each time step, as well as solution of a separate transport equation for the spatial and temporal distribution of each species present. This represents substantial computational overhead; the net result is that chemistry calculations dominate the time to solution in OpenFOAM® and comparable solvers, and must be handled carefully to avoid significant performance penalties. Simplified chemistry models using empirical single-step or double-step mechanisms [6], infinitely fast reaction rates (local thermodynamic equilibrium) and similar can afford considerable improvements in solver performance, but should always be cross-checked against simulation results using full mechanisms and kinetics. The present study therefore focuses only on methods dealing with full mechanism models – the exploration of simplified chemistry models for the TBRC case is left to future work.
2.1. Reduced-order combustion mechanisms

In most modern combustion chemistry mechanisms [6, 7, 8, 9], reaction of propane with oxygen proceeds initially via thermal decomposition, oxidation, or dehydration reactions to produce shorter-chain molecules of which C2H4, C2H2, and CH4 are the most abundant, followed by C2H6 and short-chain aldehydes. These act as secondary fuels, combusting via their own mechanisms into methane and other single-carbon radicals before being fully oxidised to CO and H2O. A sub-mechanism describing reactions between O2, CO, CO2, H2, and H2O plus the radicals O, H, and OH then acts to govern the relative concentrations of the final combustion products.

The GRI-MECH 3.0 mechanism [7] was selected as the basis for this study. This mechanism is optimised primarily for methane combustion but does contain species up to and including propane and its radicals. Although it is recommended by the authors of the mechanism that it not be used for simulations of propane combustion where a high degree of quantitative accuracy is required, it is nonetheless a useful test case as the reaction pathways included are representative of more detailed and complex mechanisms. It is also anticipated that the majority of TBRC units – including the Mintek pilot plant under consideration in the present work – will be converted to operate with natural gas in the future, and experience with this mechanism will be of some value.

The full GRI-MECH 3.0 mechanism comprises 53 species and 325 reactions. As the combustion chemistry under consideration in the present work is focused primarily on propane and oxygen, a methodology to generate static reduced-order mechanisms (ROMs) for specific cases given a more complex and general base mechanism was developed. In this method, the chemFoam solver included in OpenFOAM® was used to simulate the concentration of various species over time in a fully-mixed reactor at fixed pressure, for a variety of initial C3H8/O2 mixtures and temperatures, using the full mechanism. The composition and temperature of the mixture at each time step in the chemFoam simulation was used to calculate the reaction rates of each reaction in the full mechanism. All reactions above a certain rate relative to the fastest reaction were flagged and combined across all simulations into a subset of the full mechanism. The subset of reactions was then used to identify a corresponding subset of participating species, forming the ROM. By varying the relative rate limit, smaller or larger ROMs may be generated. In order to choose an appropriate reduced model for the current case, chemFoam simulations were performed using both the ROM under consideration and the full mechanism. Selected results are shown for two different rate limits, 2% and 1%, in Figures 3 and 4 respectively.

Reducing the relative rate limit down to 1% results in a markedly better fit to the original mechanism. In this ROM the behaviour of propane reacting with oxygen is captured sufficiently accurately across all major species and an appropriate range of initial compositions and temperatures to act as a surrogate for the full mechanism while including only 31 species and 66 reactions. As will be seen later this has an appreciable impact on the performance of OpenFOAM® models for the TBRC case.

Fig. 3. Temperature and combustion products as functions of time for reaction of a 65% O2/35% C3H8 mixture by volume at 1273 K (solid lines show GRI-MECH 3.0 results, dashed lines ROM at 2% relative rate limit)
2.2. Thermal radiation considerations

In combustion chemistry models the distribution of temperature and various species through the flame volume is often highly complex and non-isotropic. As fuel-oxygen flames can operate at very high temperatures (over 3000 K), thermal radiation is a dominant energy transfer mode in some parts of the geometry and must be taken into account using an appropriate model. Numerical solution of the full radiation problem requires discretisation in both wavelength of light emitted and absorbed by the species present, and in the direction in which any given beam points. Although the spectra of many combustion species are quite complex grey gas approximations [10], which integrate out the wavelength dependence of the absorption spectrum to obtain a wavelength-independent absorption coefficient, retain good accuracy in many cases and significantly reduce the complexity of the radiation calculations. To treat the directional discretisation, the discrete ordinate method [11] was applied using 32 rays in the x-y plane of the 2D models.

In order to close the radiation calculations, expressions describing the absorption coefficient as a function of temperature for each species present must be supplied. The absorption spectra for major species C2H6, C2H4, C2H2, CH4, CO, CO2, H2O and OH were obtained from the HITRAN spectroscopic database via the HAPI interface [12], and integrated to find the Planck mean absorption coefficient at a range of temperatures between 300 and 3000 K. Polynomial functions in inverse temperature suitable for use in OpenFOAM® were then fitted to the results, and are shown in Table 1 ($R^2$ is the statistical coefficient of determination for the fit). Spectroscopic data for C3H8 is not available from HITRAN, but polynomial coefficients are published elsewhere [10].

Table 1. Polynomial fits for Planck mean absorption coefficient, $\alpha_P = a_0 + \frac{a_1}{T} + \frac{a_2}{T^2} + \frac{a_3}{T^3} + \frac{a_4}{T^4} + \frac{a_5}{T^5}$

<table>
<thead>
<tr>
<th>Species</th>
<th>$a_0$</th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$a_3$</th>
<th>$a_4$</th>
<th>$a_5$</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2H6</td>
<td>2.94 x 10^-4</td>
<td>4.32 x 10^-2</td>
<td>-1.46 x 10^-6</td>
<td>1.48 x 10^-9</td>
<td>-4.27 x 10^{-11}</td>
<td>3.77 x 10^{-13}</td>
<td>0.9981</td>
</tr>
<tr>
<td>C2H4</td>
<td>-1.04</td>
<td>7.11 x 10^{-1}</td>
<td>-1.55 x 10^{-7}</td>
<td>1.30 x 10^{-10}</td>
<td>-3.45 x 10^{-12}</td>
<td>2.88 x 10^{-14}</td>
<td>0.9997</td>
</tr>
<tr>
<td>C2H2</td>
<td>-1.75</td>
<td>1.13 x 10^{-4}</td>
<td>-2.36 x 10^{-7}</td>
<td>2.06 x 10^{-10}</td>
<td>-5.07 x 10^{-12}</td>
<td>3.90 x 10^{-14}</td>
<td>0.9999</td>
</tr>
<tr>
<td>CH4</td>
<td>1.54</td>
<td>-8.99 x 10^{-4}</td>
<td>1.58 x 10^{-7}</td>
<td>-7.98 x 10^{-9}</td>
<td>1.63 x 10^{-12}</td>
<td>-1.19 x 10^{-14}</td>
<td>0.9957</td>
</tr>
<tr>
<td>CO</td>
<td>0.475</td>
<td>-4.64 x 10^{-3}</td>
<td>1.25 x 10^{-7}</td>
<td>-7.76 x 10^{-9}</td>
<td>1.81 x 10^{-12}</td>
<td>-1.43 x 10^{-14}</td>
<td>0.9945</td>
</tr>
<tr>
<td>CO2</td>
<td>-0.421</td>
<td>-1.78 x 10^{-4}</td>
<td>8.23 x 10^{-7}</td>
<td>-5.53 x 10^{-10}</td>
<td>1.36 x 10^{-13}</td>
<td>-1.13 x 10^{-15}</td>
<td>0.9789</td>
</tr>
<tr>
<td>H2O</td>
<td>0.515</td>
<td>-5.65 x 10^{-3}</td>
<td>1.51 x 10^{-7}</td>
<td>-6.30 x 10^{-9}</td>
<td>1.44 x 10^{-12}</td>
<td>-1.03 x 10^{-14}</td>
<td>0.9999</td>
</tr>
<tr>
<td>OH</td>
<td>-0.344</td>
<td>1.42 x 10^{-3}</td>
<td>-1.20 x 10^{-6}</td>
<td>1.53 x 10^{-9}</td>
<td>-1.41 x 10^{-11}</td>
<td>7.79 x 10^{-12}</td>
<td>0.9999</td>
</tr>
</tbody>
</table>

All species not listed here were treated as optically transparent. As they are generally present in very small quantities, this assumption is not expected to significantly affect the heat transfer calculations in the model.

3. Results and Discussion

In order to assess the performance of the model and its sensitivity to selected TBRC operating parameters, a base case set of parameters was identified to represent a typical operating state of the Mintek unit (see Table 2). In all cases, models were initialised with the vessel interior at stagnant conditions and at a fixed temperature of 1573 K. Treating interior surfaces as having the same constant temperature is a simplifying approximation used in these initial tests – in
general, the interior surface temperatures will be controlled by the balance in heat transfer between interior and exterior of the TBRC vessel. Simulations were run for 200 ms of model time unless otherwise indicated.

Table 2. Base case parameters used for TBRC lance combustion model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vessel length</td>
<td>0.435 m</td>
<td>Pool temperature</td>
<td>1573 K</td>
</tr>
<tr>
<td>Vessel diameter</td>
<td>0.324 m</td>
<td>Inlet temperature</td>
<td>1573 K</td>
</tr>
<tr>
<td>Vessel outlet diameter</td>
<td>0.280 m</td>
<td>Vessel wall temperature</td>
<td>1573 K</td>
</tr>
<tr>
<td>Lance diameter</td>
<td>0.0483 m</td>
<td>Lance wall temperature</td>
<td>300 K</td>
</tr>
<tr>
<td>Oxygen/fuel inlet diameter</td>
<td>0.0158 m</td>
<td>Oxygen flowrate</td>
<td>6 Nm$^3$/h*</td>
</tr>
<tr>
<td>Vessel inclination angle</td>
<td>30°</td>
<td>Propane flowrate</td>
<td>1.2 Nm$^3$/h*</td>
</tr>
</tbody>
</table>

* Normal cubic meters per hour defined at 1 atm pressure and 20°C temperature

3.1. Model performance

In order to identify suitable numerical conditions for the TBRC model, a number of performance tests were conducted using the base case parameter set.

The first series of tests examined the parallel scaling of the model using a numerical mesh of quadrilateral elements with a maximum size of 2.5 mm, for a total mesh element count of 68,967. The model was run using between 1 and 48 processor cores at the CHPC Lengau high performance computing facility [13]. Performance relative to the single processor case was calculated and expressed as a speed-up factor. The results are shown in Figure 5.

Effective linear scaling was observed up to 24 processor cores, representing less than 3000 elements per core. Beyond this value parallel efficiency begins to fall off due to communication overheads, but it is expected that larger 3D models would scale effectively to hundreds of processors.

The second set of tests examined the impact of the chemical mechanism on the execution speed of the model. Two cases were run – one using the full GRI-MECH 3.0 mechanism, and one using the 31-species ROM generated earlier. In the GRI-MECH 3.0 case, automatic order reduction based on the dynamic adaptive chemistry method was activated in OpenFOAM® using a relative limit of 1% in order to enable fair comparison between the two mechanisms. Performance of the full mechanism case averaged 1046 s per millisecond of model time while performance of the ROM case averaged 267 s per millisecond, representing a factor of approximately four performance improvement in favour of the ROM case.

The third set of tests examined the effect of mesh resolution on the results of the model. Cases with maximum mesh element sizes from 2 to 5 mm were run for 50 ms of model time from initial conditions. The flux of oxygen to the alloy pool and vessel outlet boundaries were calculated and reported as functions of time for the duration of each simulation. The results are given in Figure 6.
It can be seen that although there is substantial local variation due to the nonlinear nature of the governing equations, the magnitude of the predicted oxygen flux as well as the gross model behaviour are largely independent of resolution in this range. High-frequency transient behaviour is however captured somewhat better at higher resolutions, as evidenced by the smoother curves with fewer rapid oscillations in the case of the 5 mm mesh. From these observations, a mesh resolution of 2.5 mm was selected for the remainder of the modelling cases in the study.

3.2. Base case results

Oxygen fluxes from the TBRC model at base case conditions are shown in Figure 7.

As the premixed flow from the lance tip ignites and the flow patterns in the flame establish themselves through the TBRC vessel, there are both rapid oscillations in the oxygen fluxes at periods of a few ms or less, as well as large-scale changes between high and low flux conditions at longer intervals of 50 to 100 ms. The latter are related to the jet dynamics of the flow out of the lance tip which cause it to move back and forth in a sinusoidal (helical in 3D) pattern, alternately playing across the surface of the alloy pool or bypassing to the vessel outlet. The faster oscillations are likely to be associated with short-lived vortices and other fluid dynamic structures in the flame plume.

Visualisations of the temperature field together with selected species concentration fields during a period of high flux to the alloy and low flux to the vessel outlet are shown in Figure 8. It can be seen that at this point the flame plume is strongly directed toward the pool boundary, pushing the excess oxygen remaining after combustion downward toward the surface where it can react with the molten alloy. At the same time flow at the outlet is mostly inward, drawing oxygen-poor combustion products back into the vessel.

Visualisations of the fields during a period of high flux to the vessel outlet and low flux to the alloy pool are shown in Figure 9. Comparing with Figure 8, at this point in the simulation the flame plume is directed away from the pool and flow from the vessel outlet is predominantly outward, carrying any excess oxygen out of the TBRC before it is able to contact and react with the molten alloy.
Fig. 8. Field visualisations for base case model at time 93 ms

Fig. 9. Field visualisations for base case model at time 180 ms
3.3. Sensitivity to inlet gas flowrate and composition

Adjustment of the flowrates of oxygen and propane to the lance are primary control actions on TBRC plants. It is therefore of some operational interest to examine the effect on the model’s behaviour of changing the total flowrate as well as the proportion of gases fed to the lance.

In order to study the effect of the total flow, the flowrates of oxygen and propane given in Table 2 were adjusted by factors from 30% lower to 30% higher. Both flowrates were adjusted by the same amount in order to maintain a constant composition in the inlet gas equivalent to that of the base case. The time-dependent oxygen fluxes from the lowest and highest flowrate models are compared to the base case in Figure 10.

![Fig. 10. Effect of changing total lance inlet flowrate on oxygen deportment – time-dependent behaviour](image1)

The observed dynamics are reasonably similar in all cases, with the overall levels of oxygen flux varying between high and low operating periods while exhibiting significant high-frequency oscillations. The peak oxygen fluxes are generally slightly higher at higher flowrates and occur sooner after model initialisation, in accordance with the higher mass flowrates (and therefore higher flowrates of combustion products including excess oxygen) through the vessel volume.

Time-averaged fluxes over the full 200 ms simulation period were calculated for all successful model runs and are reported in Figure 11.

![Fig. 11. Effect of total lance inlet flowrate on oxygen deportment to boundaries – time-averaged behaviour](image2)

Increasing the total flowrate of the fuel-oxygen mix from the lance results in increased oxygen fluxes to both the alloy pool and the vessel outlet. Multiplying the average fluxes by the surface areas of the boundaries they are associated with in the model permits the calculation of an “oxygen efficiency”, which expresses the fraction of excess oxygen available after combustion which reports to the alloy pool for converting reactions. This efficiency drops gradually with increasing flowrate, indicating increasing bypass of oxygen to the vessel outlet as the flowrates increase.

To study the effect of changing the composition of the fuel-oxygen mixture, the flowrate of oxygen from Table 2 was adjusted by factors from 30% lower or 30% higher while keeping all other parameters, including the propane flowrate, constant. Time-dependent oxygen fluxes from selected cases are shown in Figure 12.

![Available oxygen efficiency](image3)
Fig. 12. Effect of changing oxygen inlet flowrate on oxygen deportment – time-dependent behaviour

Altering the fuel-oxygen composition in the lance inlet gas has a significant impact on the oxygen fluxes to the boundaries in the model, with elevated oxygen compositions resulting in higher fluxes. This is largely to be expected, as models with greater oxygen content in the feed gas leave more excess oxygen available after completion of the propane combustion reaction for transport to the various boundaries of the TBRC vessel.

Time-averaged fluxes over the simulation period were calculated for all successful model runs and are shown in Figure 13.

Fig. 13. Effect of oxygen inlet flowrate on oxygen deportment to boundaries – time-averaged behaviour

Increasing the proportion of oxygen in the lance feed gas alters the oxygen fluxes in the model in a non-linear manner. At low oxygen concentrations, most or all of the oxygen supplied is consumed in the combustion reaction with propane and very little is left to circulate through the vessel and come into contact with the alloy pool – this reflects operation under reducing conditions. As the oxygen flowrate is increased beyond the stoichiometric limit required by propane combustion the fluxes rise rapidly, reflecting operation under oxidising conditions. It is interesting to observe that naïve calculation of the stoichiometric limit in accordance with equation 2 yields a critical oxygen flowrate of 6 Nm$^3$/h in this case. However, since the reactions are occurring at high temperatures it is more likely that CO rather than CO$_2$ is the primary combustion product as shown in equation 3 – this would give a critical oxygen flowrate of 4.2 Nm$^3$/h.

\[
\begin{align*}
\text{C}_4\text{H}_8 + 5\text{O}_2 & \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O} \\
\text{C}_3\text{H}_8 + \frac{7}{2}\text{O}_2 & \rightarrow 3\text{CO} + 4\text{H}_2\text{O}
\end{align*}
\]

(2)  
(3)

Per Figure 13, free oxygen is available in small quantities at flowrates below 6 Nm$^3$/h O$_2$. This confirms that the combustion of propane in the TBRC lance flame proceeds at least partially to CO rather than CO$_2$, and is supported to some degree by the reaction product species observed in Figures 8 and 9. It should be noted that this is a somewhat oversimplified analysis, and in reality a balance between various combustion reactions including (2), (3), and combustion to solid C would be expected to occur at different fuel:oxygen ratios.

4. Conclusions

Development of a preliminary computational model for the lance combustion component of TBRC pyrometallurgical converting operations was successful. Reduced-order mechanisms based on the GRI-MECH 3.0 mechanism for natural gas combustion were developed for propane combustion, and demonstrated substantial performance improvements.
over the full mechanism in coupled computational mechanics applications. Simple test cases run using two-dimensional approximations of the geometry of a TBRC pilot plant demonstrated the capabilities of the model in predicting oxygen deportment to the interior boundaries of the converter vessel, an important variable for design and operation of the unit. First-order sensitivity of the model to the flowrates of feed gases from the lance was also examined, with the chemistry of the vessel interior shown to be predominantly dependent on the relative concentrations of oxygen and propane in the lance feed gas.

This study is intended to be an initial exploration of the problem, and as such a great deal of work remains to be done. Validation against experimental results in terms of flame behaviour and converting efficiency is critical if such models are to be trusted in an industrial setting. Inclusion of converting kinetics at the alloy pool surface [14] would be of value in completing the chemical description of the coupled combustion-converting process. Comparison of full-mechanism solvers with one- or two-stage combustion models would also be of value to determine whether such simplified (but faster to simulate) models are appropriate for use in modelling the combustion stage of TBRC units. Finally, a more extensive exploration of turbulent combustion modelling including large eddy simulation and eddy dissipation concept approaches [15] is recommended in order to extend the capabilities of the present model to larger, more industrially-relevant scales.

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