COMPUTER MODELLING OF A NOVEL TUBULAR SOFC CONCEPT

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ABSTRACT

Computer modelling is currently being used to assist in the development of a small diameter tubular solid oxide fuel cell (SOFC) technology. Finite element modelling is being undertaken with the ANSYS analysis package. Initial work is directed at validating the accuracy of ANSYS with regard to the proposed design. To this end, a verification model has been designed, to allow a comparison between physical and computational data. Modelling has yielded credible thermal and mass flow distributions, however, physical results are currently unavailable for comparison.

INTRODUCTION

Computer modelling is an invaluable tool in technological research, providing indications of the feasibility and change in performance of design and operation modifications. This, in turn, assists the development and optimisation of new technologies. Over recent years, there has been a significant growth in the use of computer modelling, corresponding to an increase in computing power to the extent that much modelling can be undertaken on an average home computer. This growth can also be attributed, in part, to the increased acceptance of the validity of computer simulations.

Solid oxide fuel cells (SOFCs) are perceived as a promising development for the efficient use of fossil fuels. Earlier designs of fuel cells are gradually being integrated into commercial applications and SOFCs are expected to follow. Current SOFCs use an oxygen ion conducting electrolyte and come in a range of geometries. Development has focused on the tubular design of Siemens Westinghouse and various planar configurations, in particular, the cross-flow arrangement. Recently, a new design was proposed, based around small diameter tubes, with fuel flowing inside the tubes (1). Benefits of this design include improved mechanical properties (2), rapid thermal cycling, and ease of fabrication (3). Computer modelling is required to assist in the determination of many operating parameters.

ANSYS, a generic computer modelling (finite element) analysis package, is being used for current modelling activities. As it is a generic modelling environment, it is desirable to validate the results ANSYS produces or, at least, quantify the errors. To this end, a physical “verification cell” is under construction, as shown in Figure 1. The verification cell will be constructed from 1.65 mm gauge stainless steel, and will approximate the mass and thermal flow fields from a proposed stack configuration. Initial modelling is aimed at simulating this system, with fuel and air being burnt in the
vessel, while the temperature distribution is examined through the use of thermocouples. Comparison will then be made between measured temperatures, and simulated values. The simulation has underlying mathematics, which are solved transparently by ANSYS.

**METHODOLOGY**

Computer modelling has been undertaken using the ANSYS Finite Element modelling package. A number of upgrades have been made to the programme, and this work has been undertaken, previously on version 5.2 and, currently on version 5.4. Computer platforms have also changed, present work using the Microsoft Windows operating systems (95, 98, and NT 4), on a range of Intel processors. The most computationally intensive tasks have been performed on a Pentium II-400 with 256 MB of RAM and 20 GB total disk storage. However, the greatest memory overhead has been approximately 140 MB, and the largest output files, from a single run, totalled 1.4 GB.

**Figure 1.** Schematic and section views of the verification cell.
Theory

The primary equations used by ANSYS are detailed below. The first equation in fluid dynamics is the equation of continuity [1], which describes conservation of mass.

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
\]

\[\left(\nabla \cdot \rho \mathbf{u} = \frac{\partial \rho \mathbf{u}_x}{\partial x} + \frac{\partial \rho \mathbf{u}_y}{\partial y} + \frac{\partial \rho \mathbf{u}_z}{\partial z}\right)\]  

[1]

It is useful, from a finite element modelling perspective, to substitute the rate of change of density, in equation 1 and elsewhere, with a rate of change of pressure expression [2]. ANSYS allows the derivation of \( \frac{\partial \theta}{\partial t} \) from either, the ideal gas law (for a compressible gas) or, a constant (for the incompressible solver).

\[
\frac{\partial p}{\partial t} = \frac{\partial \rho}{\partial p} \frac{\partial p}{\partial t}
\]

\[
\rho = \frac{p}{RT} \Rightarrow \frac{\partial \rho}{\partial p} = \frac{1}{RT} \quad \text{or} \quad \frac{\partial \rho}{\partial p} = \frac{1}{\beta}
\]

[2]

Conservation of momentum, in turn, leads to the three momentum (or motion) equations [3], in which 'i' represents one of the three orthogonal directions in the coordinate system (ie. x, y, and z).

\[
\frac{\partial \rho \mathbf{u}_i}{\partial t} + \nabla \cdot (\rho \mathbf{u}_i \mathbf{u}) = \rho g_i - \frac{\partial \rho}{\partial i} + \nabla \cdot (\mu \nabla \mathbf{u}_i) + R_i + \tau_i
\]

[3]

\( \tau_i \), in this equation, is a term accounting for viscous losses, which has further differential equations, omitted here due to the limited contribution of viscous losses in this system. A user defined source term can be entered, as \( R_i \), and this may later allow us to simulate the “flow” through the electrolyte.

The modelling of thermal phenomena is central to the analysis of SOFCs, thus an energy balance is required. To this end, the principle of conservation of energy leads to the energy equation [4].

\[
\frac{\partial}{\partial t} \left( \rho c_p T_0 \right) + \nabla \cdot (\rho c_p T_0 \mathbf{u}) = \nabla \cdot (K \nabla T_0) + \dot{q} + \frac{\partial}{\partial t} P + \Phi + W^r + E^k
\]

[4]
Where \( T_0 \) (the total or stagnation temperature) is the temperature of the fluid after it has been brought isentropically to a zero velocity (4). This is calculated at the inlet, from known temperature and velocity via the relation in equation [5]. Due to the low inlet velocity in this problem (0.02 m.s\(^{-1}\)) we have specified the stagnation temperature to be equal to the reference temperature (293 K).

\[
T_0 = T_{\text{static}} + \frac{|v|^2}{2c_p} \tag{5}
\]

The full energy equation is solved for a compressible fluid, while an incompressible fluid eliminates the terms for viscous work (\( W^v \)), viscous heat generation (\( \Phi \)), kinetic energy (\( E_k \)), and pressure work (\( \oint P \)). Neglecting turbulence, the final equation is the pressure equation [6], which ANSYS renders in the shown form for reasons of numerical accuracy.

\[
\rho \frac{Dv}{dt} = (\rho - \rho_0) \bar{g} - \nabla P_{\text{rel}} + \mu \nabla^2 v
\]

\[\bar{P}_{\text{abs}} = P_{\text{ref}} + P_{\text{rel}} - \rho_0 \bar{g} \cdot \mathbf{r}\]  

The solution process, in a finite element method, then involves solving each degree of freedom, at each node, in an iterative process. Each analysis tool implements this differently, with a number of different solution algorithms being available, each suited to a particular set of problems. ANSYS takes advantage of a number of different solution schemes, which can be selected by the operator, but its iterative process (Table 1) is always the same.

| Table I. ANSYS Iteration Structure (4) |
|--------------------------------------|
| Formulate - Solve VX equation approximately – Calculate \( \dot{V}_x \) |
| Formulate - Solve VY equation approximately – Calculate \( \dot{V}_y \) |
| Formulate - Solve VZ equation approximately – Calculate \( \dot{V}_z \) |
| Formulate pressure equation using \( \dot{V}_x, \dot{V}_y, \) and \( \dot{V}_z \) |
| Solve pressure equation for relative pressure |
| Update velocities based on \( \dot{V}_x, \dot{V}_y, \dot{V}_z \) and relative pressure |
| Formulate - Solve energy equation for temperature |
| Solve species transport equations |
| Update temperature dependent properties |
| Solve turbulence equations for ENKE and ENDS |
| Update Effective Properties based on Turbulence Solution |
| Check Rate of Change of the Solution (Convergence Monitors) |
| End of Global Iteration |

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Modelling and Meshing

A number of different finite element meshes have been tried, although the ANSYS meshing routine has proven difficult to manipulate. The model (Figure 2) takes advantage of the evident rotational symmetry about the central axis. Two significant problems with meshing of the model domain have included: too few elements in some of the thinner sections of the model, and total number of elements becoming too great for efficient solution times, especially in transient (time-dependant) analyses. Additional work is being undertaken on refining the mesh to improve solution times and, it is expected, accuracy of results.

Figure 2. Finite Element Meshes produced by ANSYS (refined mesh on right).

The use of boundary conditions is central to computer modelling, and significant time has been spent selecting and configuring appropriate boundary conditions for this simulation. The most obvious boundary condition is the rotational symmetry about the Y-axis, which is implemented by constraining the x-component of the velocity (V_x) to zero, at the Y-axis. Fluid dynamics also makes use of the “zero slip condition”, which simply states, that all velocity components are zero at any solid boundary. This is, of
course, expanded to all interior nodes of the solid areas. Fuel velocity is set at the fuel inlet, with the current simulation using 0.02 m.s$^{-1}$ (2 cm.s$^{-1}$). Pressure is set at the outlet to the reference pressure ($P_{ref}$) of 101325 Pa (~1 atm). Temperature is initially 293 K (20°C) with external, non-flow boundaries being adiabatic. Heat generation, of 10 MW.m$^{-3}$, is applied to a set of nodes above the fuel tube, simulating a flame, to approximate combustion. A later model will better account for heat generation, and is expected to incorporate a multiple gas species concentration solution.

RESULTS & DISCUSSION

Figure 3. Steady-state Temperature Profiles
Transient analysis has, so far, yielded minimal beneficial results, with several hours of computation yielding only fractions of a second of analysis. Steady state has, however, proven more productive, after extensive experimentation. Two plots of the temperature profile are shown in Figure 4. The entire system reaches at least 462 K (~190°C), but the flame temperature reaches a maximum of only 1096 K (~720°C). With the addition of more accurate heat generation, and a refined finite element mesh, it is expected that the temperatures will be significantly higher, with preliminary exploration supporting this.

Figure 4. Steady-state Velocity: Vectors (left) and Contours (right)
Due to the heat generated in the combustion region, air is drawn in, at velocities of up to 1.6 m.s$^{-1}$. The fuel inlet velocity of 0.02 m.s$^{-1}$ is insignificant compared to anywhere else in the stack. Buoyancy driven flow is enhanced by the conduction of heat through the top of the exhaust manifold and, given the velocities generated, free convection should provide ample oxygen to the system. Further analysis, and physical measurements, will provide perspective to these results.

**SUMMARY**

Significant effort has been expended to configure a generic finite element modelling programme to simulate the complex behaviour in a solid oxide fuel cell environment. Initial modelling has provided credible results, supporting the desirable feature of buoyancy driven air flow (free-convection). Further analysis will help to develop a configuration, which will deliver optimum thermal flow fields for cell operation and efficient running. It is anticipated that results obtained from the experimental work, and modelling simulations will help achieve these goals. However, until physical results are available, it is impossible to verify the validity of the computer model.

**SYMBOLS**

| Symbol | Description | Units |
|--------|-------------|-------|
| $\rho$ | density | kg.m$^{-3}$ |
| $v$ | velocity vector | m.s$^{-1}$ |
| $v_i$ | i-direction component of velocity | m.s$^{-1}$ |
| $P$ | pressure | Pa (= kg.m$^{-1}$.s$^{-2}$) |
| $P_{abs}$ | absolute pressure | Pa |
| $P_{rel}$ | relative pressure | Pa |
| $P_{ref}$ | reference pressure | Pa |
| $R$ | universal gas constant | kJ.kmol$^{-1}$.K$^{-1}$ |
| $T$ | temperature | K |
| $T_0$ | total (stagnation) temperature | K |
| $\mu$ | dynamic (bulk) viscosity | kg.m$^{-1}$.s$^{-1}$ |
| $\mu_e$ | effective viscosity | kg.m$^{-1}$.s$^{-1}$ |
| $K$ | thermal conductivity | W.m$^{-1}$.K$^{-1}$ |
| $c_p$ | specific heat | J.kg$^{-1}$.K$^{-1}$ |
| $g$ | acceleration due to gravity | m.s$^{-2}$ |
| $r$ | position vector | m |
| $q$ | volumetric heat source | W.m$^{-3}$ |

**ANSYS Specific Symbols**

- $\dot{V}_i$: approximate velocity (i-component) for subsequent calculations
- $\text{TKE}$: Turbulent kinetic energy
- $\text{ENDS}$: kinetic energy dissipation rate
- $\tau_i$: viscous loss term in momentum equation
- $R_i$: user source term (for distributed resistance)
- $\beta$: constant for rate of change of density with respect to pressure

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(for an incompressible fluid)

\[ \Phi \] \hspace{1em} \text{viscous heat generation term}

\[ E^k \] \hspace{1em} \text{turbulent kinetic energy}

\[ W^v \] \hspace{1em} \text{viscous work}

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