



NRC Publications Archive Archives des publications du CNRC

Use of computational fluid dynamics and virtual reality for design of fuel cell stacks

Beale, Steven; Jerome, Ronald; Ginolin, Anne; Perry, Martin; Ghosh, Dave

This publication could be one of several versions: author's original, accepted manuscript or the publisher's version. /
La version de cette publication peut être l'une des suivantes : la version prépublication de l'auteur, la version acceptée du manuscrit ou la version de l'éditeur.

Publisher's version / Version de l'éditeur:

Proceedings of the Eighth Conference of the CFD Society of Canada - CFD2K, 1, pp. 489-494, 2000

NRC Publications Record / Notice d'Archives des publications de CNRC:

<https://nrc-publications.canada.ca/eng/view/object/?id=5a36ee14-6f4e-4f43-bd91-3ceb2e96d727>
<https://publications-cnrc.canada.ca/fra/voir/objet/?id=5a36ee14-6f4e-4f43-bd91-3ceb2e96d727>

Access and use of this website and the material on it are subject to the Terms and Conditions set forth at

<https://nrc-publications.canada.ca/eng/copyright>

READ THESE TERMS AND CONDITIONS CAREFULLY BEFORE USING THIS WEBSITE.

L'accès à ce site Web et l'utilisation de son contenu sont assujettis aux conditions présentées dans le site

<https://publications-cnrc.canada.ca/fra/droits>

LISEZ CES CONDITIONS ATTENTIVEMENT AVANT D'UTILISER CE SITE WEB.

Questions? Contact the NRC Publications Archive team at

PublicationsArchive-ArchivesPublications@nrc-cnrc.gc.ca. If you wish to email the authors directly, please see the first page of the publication for their contact information.

Vous avez des questions? Nous pouvons vous aider. Pour communiquer directement avec un auteur, consultez la première page de la revue dans laquelle son article a été publié afin de trouver ses coordonnées. Si vous n'arrivez pas à les repérer, communiquez avec nous à PublicationsArchive-ArchivesPublications@nrc-cnrc.gc.ca.





National Research
Council Canada

Conseil national
de recherches Canada

Institute for Chemical Process
and Environmental Technology

Institut de technologie des procédés
chimiques et de l'environnement

NRC · CNRC



Use of Computational Fluid Dynamics and Virtual Reality for Design of Fuel Cell Stacks

Steven Beale, Ron Jerome,
National Research Council,
Ottawa, Ontario, Canada

Anne Ginolin
Institut Catholique d'Arts et Métiers,
Toulouse, France

Martin Perry, Dave Ghosh
Global Thermoelectric Inc.
Calgary, Alberta, Canada

Proceedings of the Eighth Conference of the CFD Society of Canada - CFD2K,
Montreal, 11–13 June 2000, Vol.1, pp. 489-494.

NRC. No. 42011

USE OF COMPUTATIONAL FLUID DYNAMICS AND VIRTUAL REALITY FOR DESIGN OF FUEL CELL STACKS

S. Beale, R. Jerome,
*National Research Council,
Ottawa, Ontario, Canada*

A. Ginolin,
*Institut Catholique d'Arts et Métiers
Toulouse, France*

M. Perry, D. Ghosh,
*Global Thermoelectric,
Calgary, Alberta, Canada*

Ce document présente les résultats d'un projet en cours portant sur le design et la modélisation des phénomènes de transport dans des empilements de piles à combustible. On considère le flux de fluide dans les passages d'empilements de piles combustibles contenant de 10 à 50 piles. Des calculs numériques détaillés ont été réalisés en utilisant une grille tridimensionnelle fine pour valider un modèle simplifié basé sur une résistance distribuée analogue. Bien que la géométrie soit plutôt simple, le champ de flux dans le conduit d'entrée est complexe, et l'utilisation d'une application de Réalité Virtuelle pour afficher les résultats se prouve bénéfique. Les résultats des calculs ont été utilisés pour modifier le design de l'équipement avec une amélioration d'uniformité de la pression et du flux.

USE OF COMPUTATIONAL FLUID DYNAMICS AND VIRTUAL REALITY FOR DESIGN OF FUEL CELL STACKS

Steven Beale, Ron Jerome, *National Research Council, Ottawa, Ontario*
steven.beale@nrc.ca, ron.jerome@nrc.ca

Anne Ginolin, *Institut Catholique d'Arts et Métiers, Toulouse, France*

Martin Perry, Dave Ghosh, *Global Thermoelectric, Calgary, Alberta*
perrym@globalte.com, ghoshd@globalte.com

ABSTRACT

This paper presents the results of an ongoing project aimed at design and modelling of transport phenomena in stacks of solid-oxide fuel cells. Fluid flow in the passages of fuel cell stacks containing 10-50 cells is considered. Detailed numerical calculations were performed using fine three-dimensional meshes to validate a simplified model based upon a distributed resistance analogy. Although the geometry is quite simple, the flow field in the inlet manifold is complex, and the use of a Virtual Reality facility to display the results proved beneficial. The results of the calculations were used to re-design the equipment with improved uniformity of pressure and flow.

INTRODUCTION

Fuel cells are devices which convert chemical energy into electrical energy and heat (Appleby and Foulkes, 1989, Kordesh and Simader, 1996). There are three main parts to the fuel cell: Anode, cathode and electrolyte. The fuel, typically hydrogen or methane, is fed into the anode of the cell, while oxygen in the form of air, is supplied via the cathode. Oxygen ions are transported through the solid oxide electrolyte, reacting with H_2 at the anode to form water. Electrons flowing through an external circuit from anode to cathode provide a utilisable current. The reaction is exothermic, with the fuel cell operating at up to 1000°C. Solid Oxide Fuel Cells¹ (SOFC's) offer the potential advantage that methane or natural gas may be used in the place of hydrogen, as fuel. Under these circumstances internal reforming may occur, and endothermic reactions may also be present within the assembly.

Fuel cells are typically operated in stacks of cells. The configuration is similar to a single-pass cross-flow heat exchanger. Heat management is an

important concern: If the cell temperature is too low the chemical reaction will shutdown, while if it is too high mechanical failure of the system may occur; If just one cell in a stack fails, the entire stack is rendered useless. It is essential that the supply of air and fuel to each cell be uniform in order that the chemical reaction rate is the same at every cell in the stack, and thus the temperature distribution uniform.

Both air and fuel are being depleted within the passages of each cell assembly as a result of the chemical reaction, however it was ascertained that for a first analysis, the flow field would be analysed as a conservative field, in the absence of sinks due to chemistry, and with heat and mass transfer effects also neglected. The solution to this simpler design problem is prerequisite to progress when the latter effects are included, and provides a useful knowledge-base on which to develop more sophisticated tools in the future. A single-cell fuel cell model; into and out of a single multi-plate assembly, as well as a fuel cell stack model; within the inlet and exit headers (risers and downcomers) of the fuel cell array, of an entire stack assembly were therefore developed.

Mathematical Details

The problem to be solved is a steady three-dimensional (3-D) flow with air and/or methane as working fluids. These fluids are presumed to have constant properties. Two distinct approaches were considered.

(1) A direct numerical simulation (DNS) of the entire SOFC stack assembly, by means of the construction of a grid which is, not only large enough to cover the entire fuel-cell stack, but also fine enough to capture the detailed motion within the passages of each cell. While 10 years ago, a DNS approach would have been inconceivable, due to limitations of memory and speed, this is no longer the case. However such

simulations still require very large calculation times, and result in the creation of very large data sets.

(2) For this reason a second approach based on a distributed resistance analogy (DRA) was developed. Fine-scale simulations are conducted within the inlet and exit manifolds, however the SOFC core is treated as if it were a porous media using local volume averaging with a distributed resistance, F , defined (Patankar and Spalding, 1972) as,

$$\bar{\nabla} p = F \bar{U} \quad (1)$$

where the 'filter' or 'superficial' velocity, $\bar{U} = r \bar{u}$, \bar{u} is a 'pore' or 'interstitial' velocity, and r the volume fraction of the working fluid. Inertial effects may be introduced, for example, as,

$$\frac{\partial(r_i \rho_i)}{\partial t} + \bar{\nabla} \cdot (r_i \rho_i \bar{u}_i) = 0 \quad (2)$$

$$\frac{\partial(\rho_i r_i \bar{u}_i)}{\partial t} + \bar{\nabla} \cdot (\rho_i r_i \bar{u}_i; \bar{u}_i) = -r_i \bar{\nabla} p_i - F r_i^2 \bar{u}_i \quad (3)$$

Various other forms are also possible. The resistance term, F , may be evaluated; (i) using an analytical solution, (ii) experimentally from data of friction coefficient, f , vs. Reynolds' number, or (iii) from the results of detailed fine-scale numerical calculations for flow in 'typical' passages. The former (i) was employed here. For many fully-developed laminar duct flows, $f = a/\text{Re}$ with Re based on a hydraulic diameter*, D_h , $\text{Re} = D_h \rho u / \mu$. Under these circumstances,

$$F = \frac{2a}{r} \frac{\mu}{D_h^2} \quad (4)$$

The Appendix contains an analysis appropriate for plane ducts, see Kays and Crawford, 1966, for other geometries. The code PHOENICS² was used to perform all flow-field calculations. The geometry and boundary conditions were constructed with an OpenGLTM based virtual-reality (VR) editor. For the DRA, the viscous-diffusion terms were turned off and the distributed resistance introduced as a momentum

sink (i.e. as a source-term). The results were then displayed, as described further below.

RESULTS

The NASA Flow Analysis Software Toolkit³ (FAST), Walatka et al., 1992, and the Visual Toolkit⁴ (VTK), Schroeder et al., 1997, were used for visualisation and animation. Immersion techniques were employed to render the results, in stereo, on a virtual reality (VR) wall. This environment consisted of a 10' by 8' screen, rear projection system, two-processor Silicon Graphics Onyx2 machine with a graphic pipe; and stereo glasses. In addition display of 3-D plots of vector and scalar fields in Virtual Reality Markup Language (VRML) allowed for the simultaneous viewing of results in Ottawa and Calgary via a secure web site. MPEG files of the animated sequences, observed on the VR wall were also constructed for display on personal computers. Figure 1 is an image of one such sequence, while Fig. 2 shows scientists observing the results of the work in the immersive environment.

Calculations were performed for single cells, 10-cell and 50-cell stacks. For the latter, the inlet is located in the side of the inlet manifold, whereas the outlet is located in the bottom of the exit manifold. Figures 3 and 4 show velocity and pressure distributions, obtained using a DRA, on a vertical plane-of-symmetry: It can be seen that the pressure distribution and hence the flow is quite uniform across the central core of the stack, in spite of the complex nature of the flow within the inlet manifold. A step is situated at the bottom of the stack core, as a design requirement. Parametric studies were conducted to ascertain the influence of various geometric parameters; channel height, H , pitch, P , width, b (see Appendix, for details).

Figures 5(a) and 5(b) show pressure distributions obtained using DNS and DRA methods in the stack core for a second SOFC design. It can be seen that agreement between the two methods is good. Inspection of the pressure contours and velocity vectors, Fig. 5(c), reveal that for this design, flow uniformity is far from satisfactory in comparison to the results of Figs. 3 and 4.

Calculations performed to assess the measure of grid independence achieved for the results of this study, are illustrated below in Fig. 6. It can be seen that a reasonable independence of the pressure distribution from the grid size has been achieved.

* Some authors introduce a hydraulic 'radius', $r_h = D_h/4$. This is not logical, however, since for a circular pipe the radius is $D_h/2$. According to Kays, 1996, usage appears to have propagated from the early text by McAdams, 1942.

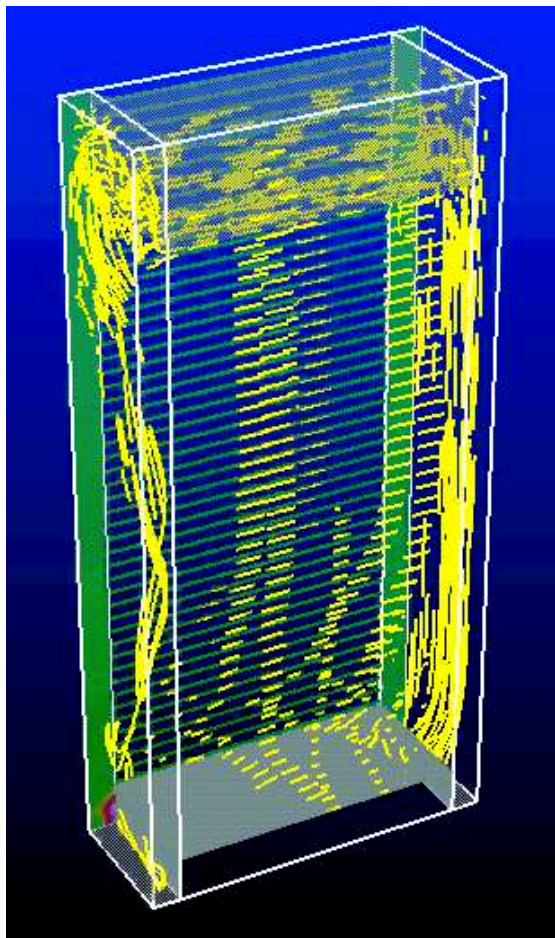


Figure 1. Particle traces constructed using visualisation software.



Figure 2. Observing the results in the VR facility.

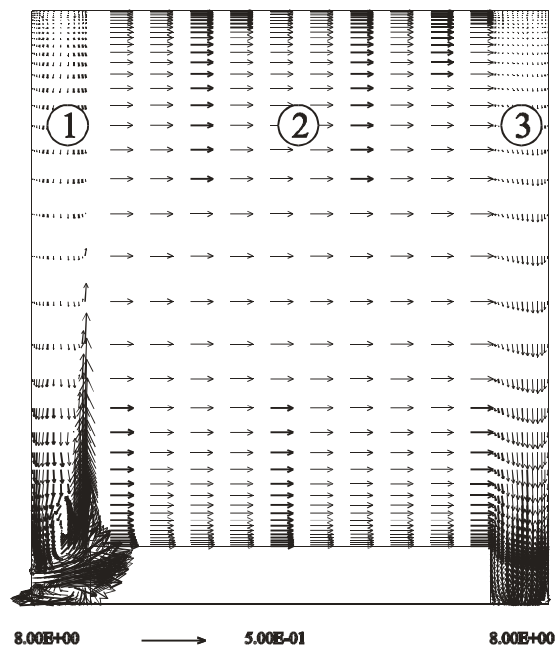


Figure 3. Velocity (m/s) in a 50-cell stack assembly: (1) Inlet manifold, (2) SOFC stack (3) outlet manifold. NB: Vector scales in SOFC stack and manifolds are different.

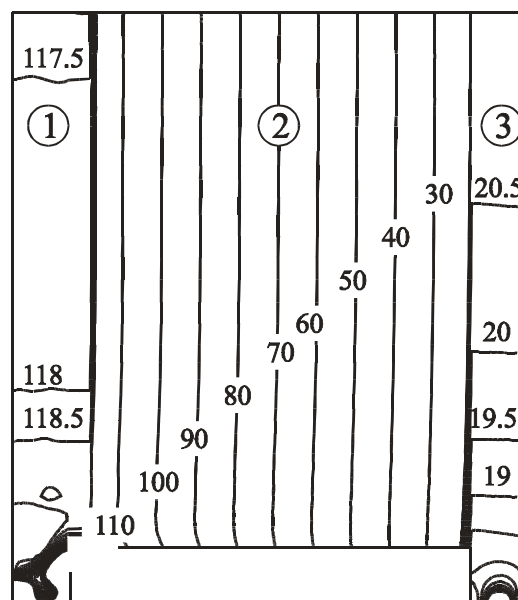


Figure 4. Pressure (Pa) in a 50-cell stack assembly.

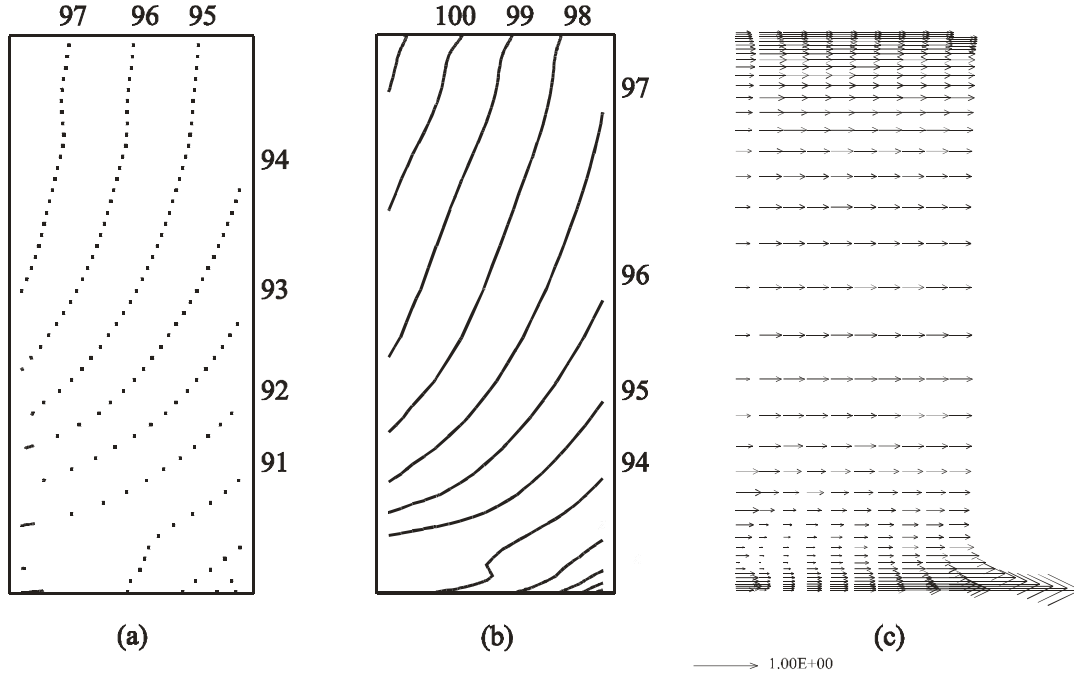


Figure 5. Pressure (Pa) contours in stack (a) DNS (b) DRA method; (c) Velocity (m/s) vectors DRA method.

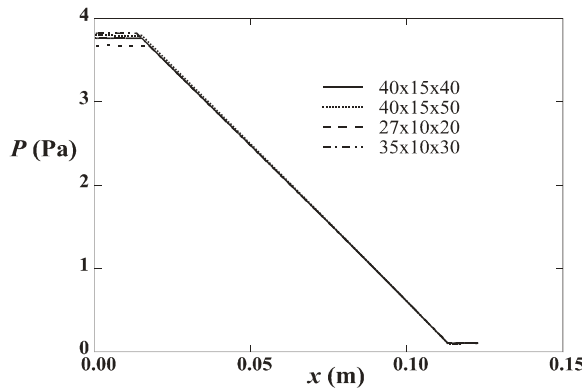


Figure 6: Grid dependence studies

DISCUSSION

Figure 3 shows vectors in (1) the inlet manifold, (2) the stack-core and (3) the outlet manifold. Although the geometry is quite simple, the flow regime within the inlet manifold is complex; the initially horizontal influent impinges on the step at the base of the assembly and then diverges in various directions in 3-D. Flow on the core-side of the inlet manifold is channel-like with downflow occurring in the upper regions. In spite of this, flow within the passages of the SOFC stack is quite uniform, suggesting the

design to be a good one. Note there is little variation in the vectors across the core, in spite of the complex re-circulating 3-D flow in the manifold: Because the core-flow is a low Reynolds number or creeping flow, it is the pressure gradient which drives the flow; inertial or convective influences are subordinate. Flow in the outlet manifold is less complex than that in the inlet; due to the upwind nature of convection; and the size and form of the fluid outlet is less critical than is the case for the inlet.

Figure 4 shows isobars on the vertical symmetry plane. A pressure maximum occurs at the point-of-impingement at the step. The pressure gradient across the stack (2) is quite uniform in the horizontal direction. In the manifolds (1),(3) the gradient is relatively small and decreases with height, due to injection/suction of matter into and out of the SOFC stack.

The mean pressure difference across the stack-core was computed both from the data and from Eq. (7) assuming fully-developed uniform flow. In most cases, the mean pressure drop across the stack approaches theoretical values, i.e., local variations in velocity and pressure average out. The pressure difference between the inlet and outlet, $\Delta P_{\text{overall}} = \Delta P_{\text{stack}} + \Delta P_{\text{manifolds}}$, was also computed as a

measure of the required pumping power. Manifold losses are in many cases quite significant, with substantial variations being observed, depending on the particular configuration under consideration. For uniform flow the ratio of $\Delta P_{\text{stack}}/\Delta P_{\text{manifolds}}$ should be large. The results of the parametric studies, revealed which of the geometric parameters were important and allowed for the stack design to be optimised.

Comparison of DNS and DRA methods

Figure 5 is a comparison of a DNS approach with a DRA approach based on Eqs. (2)-(3). The dashed lines in Fig. 5(a) are due to the pressure not being defined in solid regions. It can be seen that the DRA and DNS results are similar with small systematic differences in the absolute values being observed: From Eq. (7), the slope of the pressure gradient, dP/dx is proportional to $1/H^3$, for constant \bar{U} , so the deviations are rather minor. The details of the velocity profile in the DNS model are, of course, lost with the DRA.

For the results of Fig. 5, the core resistance is small, and inertial effects cannot be excluded: The pressure and velocity distributions are less uniform than for the previous case. Figure 5(c) also shows velocity vectors across the SOFC core for this case. The flow fields tend to be fairly uniform over the central region of the core, with increased magnitude towards the bottom of the stack, and decreased values towards the top. For a large stack it is necessary to maintain sufficiently high viscous losses, and associated pressure gradient within the core, so that the inertial effect associated with suction and injection of the working fluid out of and into the two manifolds, does not lead to fuel starvation at the top of the core.

In Eq. (3), the 'convecting' term is the superficial velocity, $\bar{U} = r\bar{u}$, but the 'convected' term (dependent variables) are components of the interstitial velocity. DRA approaches, based on the original study of Patankar and Spalding, 1972, and also where solid regions were blocked and \bar{u} alone is present were also considered. Minor differences between various approaches may occur when inertia is significant; due treatment of the convection terms. Equations (2)-(3) are recommended, however the reader should be aware that a closure assumption, albeit a reasonable one, has been invoked. The main advantage of Eqs. (2)-(3) is that a coarse grid whose elements need not necessarily coincide with the interfaces between the fuel-cell interconnect devices

and the passages within which the working fluid flows may readily be employed.

The DRA approach is a reasonable facsimile for DNS, and may be considered as providing a balance between simple lumped-capacity hydrodynamic models, which are over-simplistic, and DNS calculations which are overly time-consuming, at present.

CONCLUSIONS

A DRA model may be used as an engineering tool to design SOFC's with a measure of confidence: Certain details of the flow field, such as the periodic viscous effects of the cells on the flow in the manifolds are suppressed with the DRA. However, as a basic tool, the DRA combines computational speed with a measure of accuracy, and is an acceptable method for modelling SOFC's for engineering purposes because of the associated economies of computer run-time and memory.

Numerical calculations of fluid flow within single fuel cells, 10-cell, and 50-cell stacks of the design prototypes suggested that certain models were superior. Salient features of the flow field were identified, and design improvements effected. For flow in large SOFC stacks, the back pressure across the stack assembly should be significantly larger than the hydraulic resistance in the inlet manifold in order to maintain uniformity of pressure and velocity across the core. The geometric features, by which this may be achieved were identified using parametric studies, and the SOFC design re-configured for uniformity, as a result of this CFD study.

FUTURE WORK

Research is now being conducted into SOFC's with planar and more complex passages. The flow of both working fluids, combined with inter-fluid heat transfer and Ohmic heating is being considered.

Concurrent (interactive) display and manipulation of graphics data, locally on VR walls, and across the country via the high-speed internet CA*net 3 is also the subject for research.

Experimental facilities are being built to gather empirical data and conduct flow visualisation studies for model validation purposes.

ACKNOWLEDGEMENTS

Financial support for this project was provided by Global Thermoelectric Inc., the Institute for Chemical Process and Environmental Technology, and the Environmental Management Office of the National Research Council. The authors wish to thank Dr. Pierre Boulanger of NRC's Institute for Information Technology for providing access to the VR facility, and to Dr. John Ludwig of CHAM for technical support.

APPENDIX: PLANE DUCT GEOMETRY

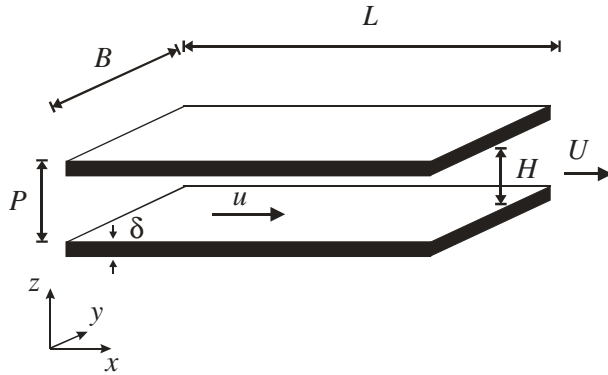


Figure 7. Schematic of a plane duct.

For fully-developed flow between parallel plates, Langlois, 1964, with $r = H/P$, it can readily be shown that the friction coefficient is given by,

$$f = \frac{\tau_w}{\frac{1}{2}\rho u^2} = \frac{12\mu}{\rho H u} \quad (5)$$

and the distributed resistance is obtained as,

$$F = \frac{12P\mu}{H^3} \quad (6)$$

In the z direction the velocity is presumed zero, $w = 0$. The pressure drop across the stack is just,

$$\Delta \bar{p} = \frac{12L\mu u}{H^2} = \frac{12L\mu \dot{Q}}{nBH^3} \quad (7)$$

where n is the number of cells in the stack, B is the width of the duct in the y -direction and $\dot{Q} = nBH u$ is the prescribed volumetric discharge, assuming uniform flow conditions.

REFERENCES

- Appleby, A.J., and Foulkes, F.R. *Fuel Cell Handbook*, Van Nostrand Reinhold, New York, 1989.
- Kays, W.M. Personal Communication, 1996.
- Kays, W.M. and Crawford, M.E. *Convective Heat and Mass Transfer*, 2nd ed., McGraw-Hill, New York, 1966.
- Kordesh, K., and Simader, G. *Fuel Cells and their Applications*, John Wiley, New York, 1996.
- Langlois, W.E. *Slow Viscous Flow*, MacMillan, London, 1964.
- McAdams, W.H. *Heat transmission*, 2nd ed. McGraw-Hill, New York, 1942.
- Patankar, S.V., *Numerical heat transfer and fluid flow*, Hemisphere, Washington, 1980.
- Patankar, S.V., and Spalding, D.B. A Calculation Procedure for the Transient and Steady-state Behaviour of Shell-and-tube Heat Exchangers, TR EF/TN/A/48, Imperial College of Science and Technology, London, 1972.
- Schroeder, W., Martin, K., and Lorensen, W. *The Visualisation Toolkit*, 2nd ed. Prentice Hall, Upper Saddle River, 1997.
- Walatka, P.P., Clucas, J., McCabe, R.K. and Plessel, T. *FAST User Guide*. RND-92-013. NASA. 1992.

USEFUL WEB SITES

- ¹ Global Thermoelectric web site : <http://www.globalte.com>
- ² CHAM web site : <http://www.cham.co.uk>
- ³ NASA FAST web site: <http://science.nas.nasa.gov/Software/FAST/>
- ⁴ The Visualization Toolkit web site: <http://www.kitware.com/vtk.html>