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Heat Transfer in Micro Direct Methanol Fuel Cell

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Iran

1. Introduction

1.1 The micro-fuel cell power supply

This invention is a simple high energy per unit mass fuel cell electrical power system for cellular phones, portable computers and portable electrical devices. We believe this is the best initial consumer niche market for fuel cell technology, rather than larger power systems. The micro-fuel cell utilizes vacuum thin film deposition techniques to coat pattern etched-nuclear-particle-track plastic membranes. The process forms catalytically active surface hydrogen/oxygen electrodes on either side of a single structured proton-exchange-membrane electrolyte. A series stack of cells is built onto a single structured membrane by geometrically engineering the cells on the membrane to allow through-membrane contacts, through-cell water control, thin film electrodes, and electrode breaks. These production techniques are well suited to roll-to-roll production processes and minimize the use of expensive catalysts. To improve reliability, an integrated system of fault correction is used to ensure the operation of the cell stack if there is cell damage. The fuel cells will be directly fueled with liquid hydrocarbon fuels such as methanol and ethanol, by incorporating new direct conversion catalysts. The Micro-Fuel Cell bridges the final gap in portable electronics with an energy source that is smaller, lighter, simpler, cleaner, and less expensive.

Comment on this chapter is that first a brief explanation about the methods of prediction methods for computing fluid dynamics analysis (CFD) is one of them is be provided.

Among the applications considered finite volume and finite element software for the calculation of the FLUENT CFD May be used with more ability and are more and more wide spread, so familiar with this part of the software are presented. Simulation for the micro fuel cell design to optimal dimensions for the design of channels was brought to get. Also, a heat transfer analysis was performed for the cell. At the end of the simulation the result can be validity.

2. Prediction methods

Predicting heat transfer and fluid flow processes into two main methods are performed:

1. Laboratory
2. Theoretical calculations

Accurate information about a physical process often determine by Experimental measurement. Laboratory researches on a system that exactly the same size as that real dimensions use to predict that how similar work version of the system under these same conditions, but in most cases do such experiments due to large size of the device being very

expensive and is often impossible, so tests on models with a smaller scale can be done, though here the issue of expansion of information obtained from ever smaller samples of all aspects of the device the original simulation does not often important aspects such as the combustion of model experiments to be excluded. These limits are further decreased useful results. Finally, should be remembering that in many cases, exist serious problems measurement and measurement instruments also not are out of error.

A theoretical prediction, use maximum application of mathematical model to comparison with the experimental results will be less used to. We are looking for physical processes; mathematical model essentially follows a series of differential equations. If the classical mathematical methods used in solving these equations, not exist predicting the possibility for many Utility phenomena. With little attention to a classic text on fluid mechanics or heat transfer can be determined that there are a few numbers of scientific problems that can count indefinite parameters with the equations needed to find. Moreover, these results often are include unlimited series, special functions, algebraic equations, specific values etc. So that may be, their numerical solution is not easy. Fortunately, numerical methods development and availability of large processors to ensure there has, for almost every issue of the practical implications of a mathematical model can be used.

3. Advantage of the theoretical calculation

3.1 Low cost

The most important point of a predictive computational cost is low. In most applications, the cost of applying a computer program costs far less than the same research laboratory, the physical status of the agent when the study is large and more complex, gaining more importance and that while the price of items currently being much more. The computational cost will be less likely in the future.

3.2 Speed

One study calculated that a can significantly speed is performed, the designer can concepts combining hundreds of different conditions in less than a day to study, to select the optimum design. On the other hand, simply can well imagine maturity or laboratory research will require much time.

3.3 Complete information

Computer Solution a problem give me the necessary information and complete details and will give value all the dependent variables (such as velocity, pressure, temperature, chemical concentration samples, turbulence intensity) across the field to your favorite loses. Unlike adverse conditions that are happen also during test, inaccessible places in a low computational job are decrease and don't exist flow turbulence due to measurement devices.

3.4 Ability to real simulate conditions

In a theoretical calculation, since the actual conditions can easily be simulated, there is no need to model the small scale and we resort to cold flow. For a computer program, having geometric dimensions too small or too big, apply very low or very high temperatures, to act with flammable or toxic materials, processes follow very fast or very slow to does not create a major problem.

3.5 Ability to simulate the ideal conditions

Sometimes a prediction method is used for studying the base phenomenon instead a complex engineering application. To study the phenomenon, the person concerned on a few main parameters focused and will be removed other aspect. Thus, under ideal conditions as much may be considered optimal conditions, for example, it can be two dimensional, constant densities, despite an adiabatic surface, or having an unlimited rate interplay named in a computational work, these conditions are easily and precisely can be established. Moreover, even in a practical test can be accurate to the near ideal conditions hardly.

4. Inadequacy of the theoretical calculation

According above, prominences are effective enough that the person encourage computer analysis. However, creation blind interest to any cause is not desirable. So that would be helpful to be aware of the obstacles and limitations. As previously mentioned, the computer analyzes used to concepts of a mathematical model. So a mathematical model importance, is limited the usefulness of the computational work. It should be noted, the final results of the person who used computer analysis, depend on the mathematical model and the numerical method. So that applying a mathematical model is inappropriate up can cause a numerical technique ideal to produce uncertainly results.

5. Choice prediction method

Discussion about relative suitability of the computer analysis and laboratory researches is not recommendations for laboratory work. Recognize the strong and weaknesses of these are essential to select the proper technique. Indubitable, test is the method of research about a new fundamental phenomenon. In this case, test leads and calculating will follow. In combination of some phenomenon known and effective to apply the calculation is useful. Even in these conditions also required to give validity to the results of calculations are compared with experimental calculations. On the other hand, to design a device through the experiment, the initial calculations were most helpful and if you practical research, is added the calculation, can often be decrease significant number of experiments. Therefore, the appropriate volume of activity should be combined a prediction to perform of rational calculations and test. Value of each of these compounds depends on the nature of problem and predictive purposes, economic issues and other specific conditions.

6. What is CFD?

In theory methods, in first, with the observation of physical phenomenon beginning the expression of the relevant differential equations and then extend to the algebraic equations governing the issue outlines. There is a problem that unlike phenomena which mathematical models suitable for them are offered (such as laminar flow), there are some phenomena mathematical model that still has not found suitable for them (such as two-phase flows). Hence use of the numerical methods as a third way to solve their problems. So on the other division into fluid dynamics can be divided into three parts:

- Experiment Fluid dynamics
- Theory Fluid dynamics

- Computational Fluid Dynamics

Computational fluid dynamics or CFD analysis of expression systems include fluid flow, heat transfer and associated phenomena such as chemical reactions, based on computer simulation that is CFD method can be very able, so that include a wide range of industrial applications in the industrial. Some examples include:

- Aircraft aerodynamic and vehicles
- Ship Hydrodynamic
- Power: combustion motor and gas turbines

And...

Therefore, a CFD has been as a major component in industrial production and design process increasingly. In addition, CFD fluid system designs of multi a unique advantage compared to the experimental methods have:

- Major reduction time and cost in new design
- Ability to study a system that tests on them are difficult or impossible (such as very large systems)
- Ability study systems under randomized more than usual about them
- Very high level of detail results.

6.1 CFD program

Structure of the CFD program is numerical method. There are general three methods for separate numerical methods that include:

1. Finite difference
2. Finite element
3. Spectral methods

6.2 Capability of program

FLUENT software can be able to simulation and modeling the following:

- Flow in complex geometry of two dimensional and three dimensional with the possible resolution of network optimization,
- Current density, compressibility and non-reversible,
- Persistent or transient analysis,
- Flows slimy, slow and turbulent,
- Newtonian and non-Newtonian fluids,
- Heat transfer, free convection or forced,
- Combined heat transfer / guidance,
- Radiation heat transfer,
- Rotating frames or static models,
- Slider and the network of networks by moving,
- Chemical reactions, including combustion and reaction models,
- Add optional volume terms of heat, mass, momentum, turbulence and chemical composition,
- Flow in porous media,
- Heat exchangers, blower, the radiators and their efficiency,
- Two-phase and multiphase flows
- Free surface flows with complex surface shapes.

This capabilities allows that the FLUENT to be used in the wide range in many industries

- Application Process Equipment in chemistry, energy (power), oil, gas,
- Applications of environmental (change climate conditions), air space,
- Turbo machine, car,
- Heat exchangers, electronics (semiconductors and electronic components cooling)
- Air conditioning and refrigeration, process materials and fire investigation and design architects.

In other words, FLUENT a suitable choice for modeling compressibility and non compressibility fluid flow can be complex.

7. Numerical analysis of a micro direct methanol fuel cell

7.1 Assumptions for flow and pressure distribution analysis

As was expressed in the anode, reaction begins when produce the CO_2 bubbles, so our actual flow will be two-phase. According to the process for production parts the surface quality of spark is not perfectly polished level. The pump flow is completely uniform because not using a pressure circuit breakers, was not to provide the desired flow.

But in this analysis were the following assumptions:

1. Fluid phase is Single and the gas in the fluid was regardless.
2. Fluid resistance with surface channels was regardless.
3. Inlet flow rate was considered uniform completely.

Full analysis was performed as symmetrical. Therefore, analysis was performed on half the model. The line of symmetry is aligned with 135 degrees angle line. For network selected triangular elements and are used 378,640 elements totally in the model. Mesh models is given in figure (1).

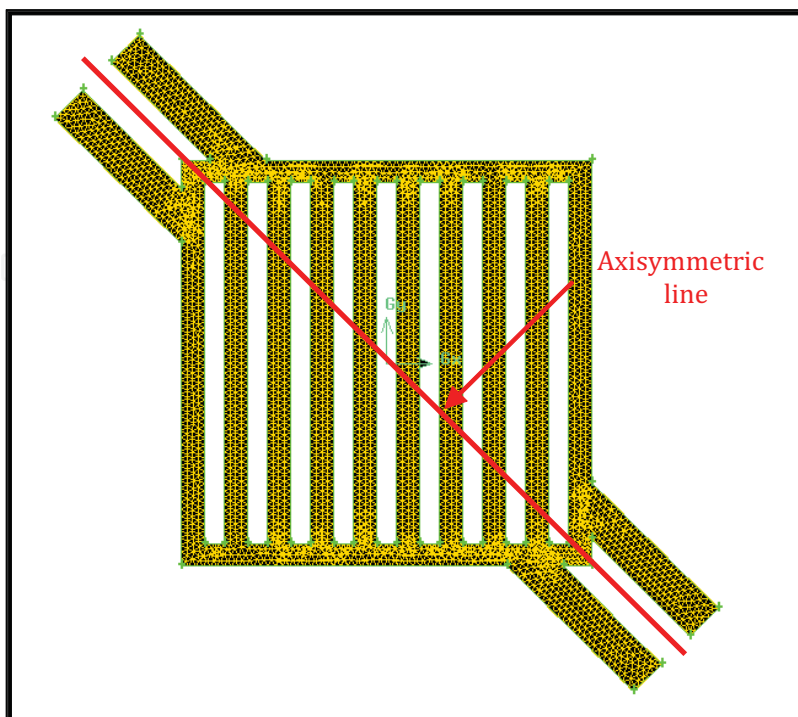


Fig. 1. Meshing model and axisymmetric line

For this simulation model is used the second order momentum equation that is given in formula (4-1) and the momentum coefficient have been used 0.7.

7.2 Momentum equation

The equation is shown in equation (1):

$$\frac{\partial}{\partial t}(\rho_m v_m) + \nabla \cdot (\rho_m v_m v_m) = -\nabla p + \nabla \cdot [\mu_m (\nabla v_m + \nabla v_m^T)] + \rho_m g + F + \nabla \cdot \left(\sum_{k=1}^n \alpha_k \rho_k v_{dr,k} v_{dr,k} \right) \quad (1)$$

To evaluate the distribution flow in flow field, parallel and cross strip field of this analysis is given. Figure (2) contour flow distribution in parallel flow channel depth of $Z=0.3$ and flow rate $\dot{m} = 0.3 \text{ cc/min}$ is shown. Figure (3) contour of the current distribution in the cross strip flow field is shown. The figure denote uniformity and dispersal distribution cross strip flow field in comparison with the parallel flow field is much higher and this may seem at first glance appears one of the important factors in the high efficiency cell that is reactive. If the path of liquid methanol in the parallel flow field is traced, we observe that the area around the flow field path and center of flow field have a little velocity. However, if parallel compared to cross strip flow field, which is observed uniformity in all area of flow field except in the corner and it shows that in terms of flow field analysis. It can give higher efficiency compared with parallel the flow field. After simulation, cross strip flow field is superior to parallel. Figure (4) show flow vector in inlet and Figure (5) show flow vector in outlet channels cross strip flow field.

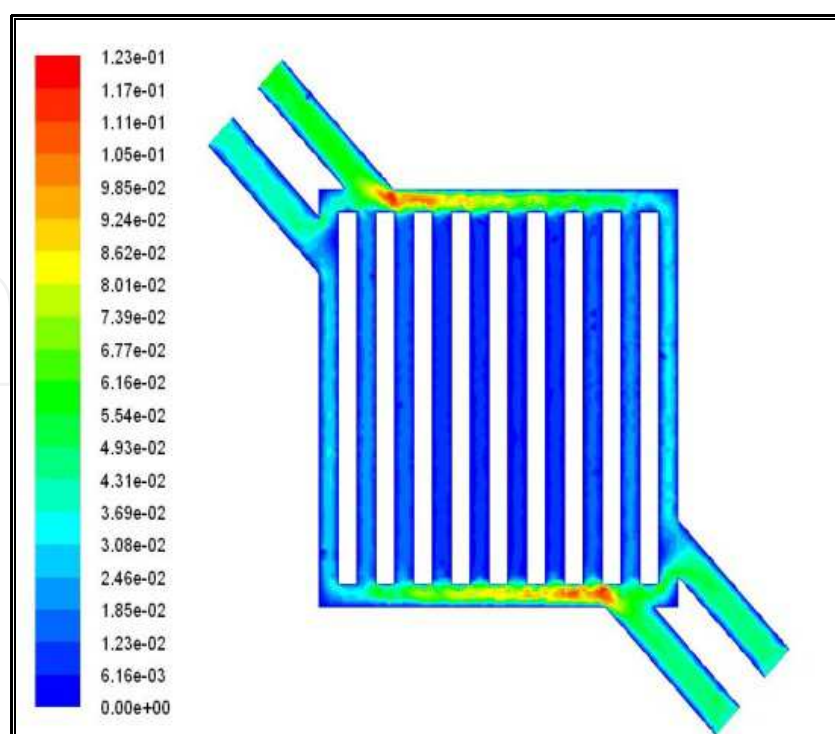


Fig. 2. Flow contour in parallel

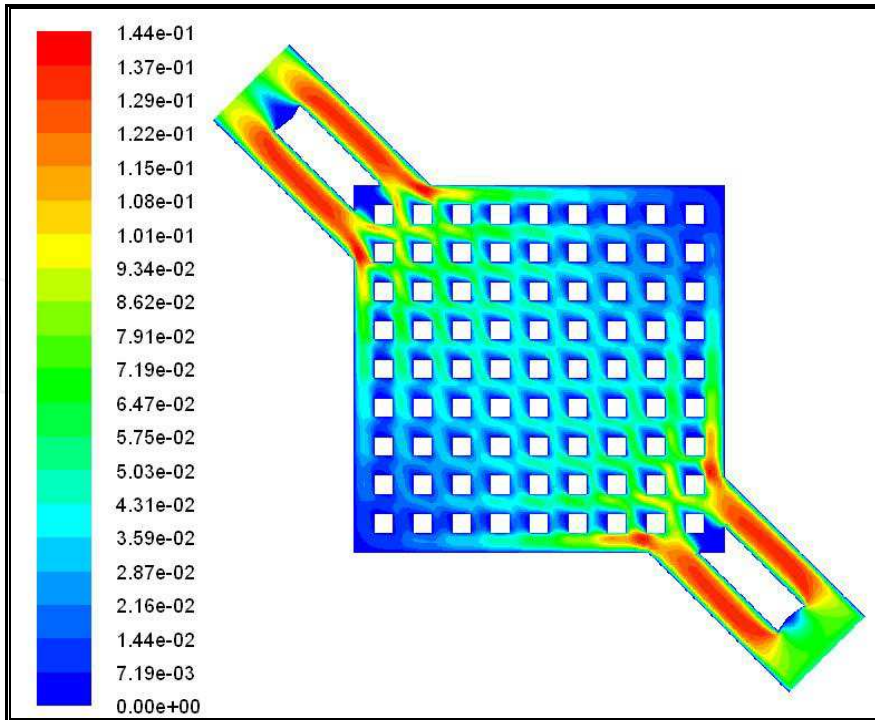


Fig. 3. Flow contour in cross strip

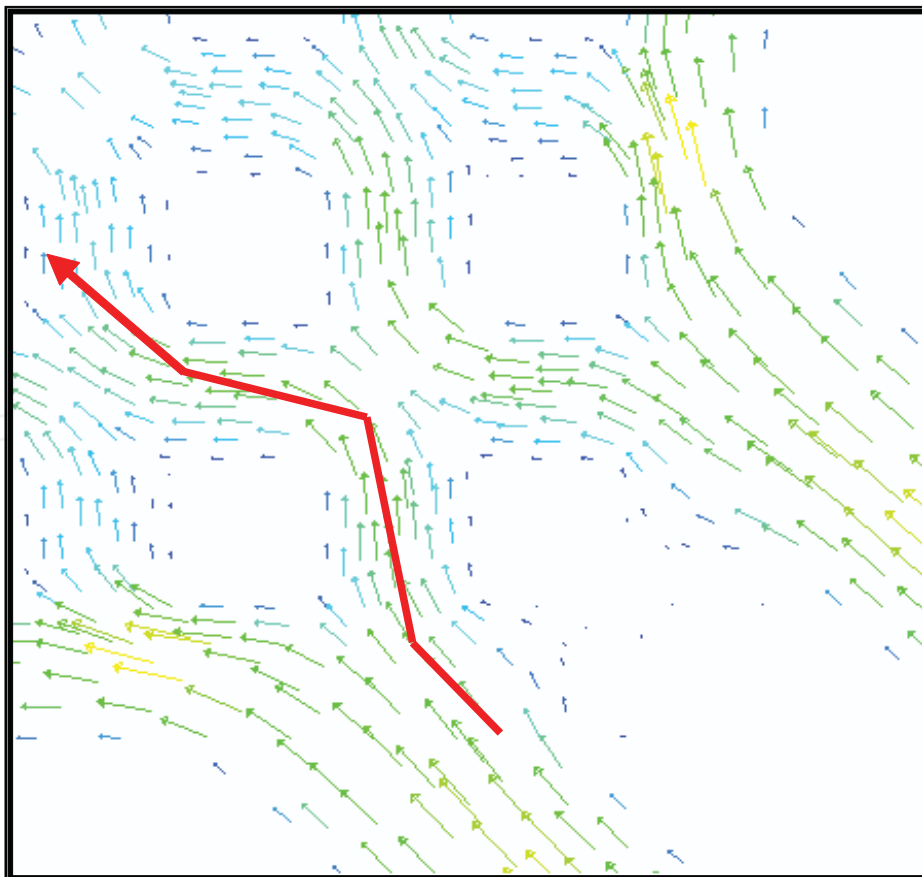


Fig. 4. Flow of parallel in inlet

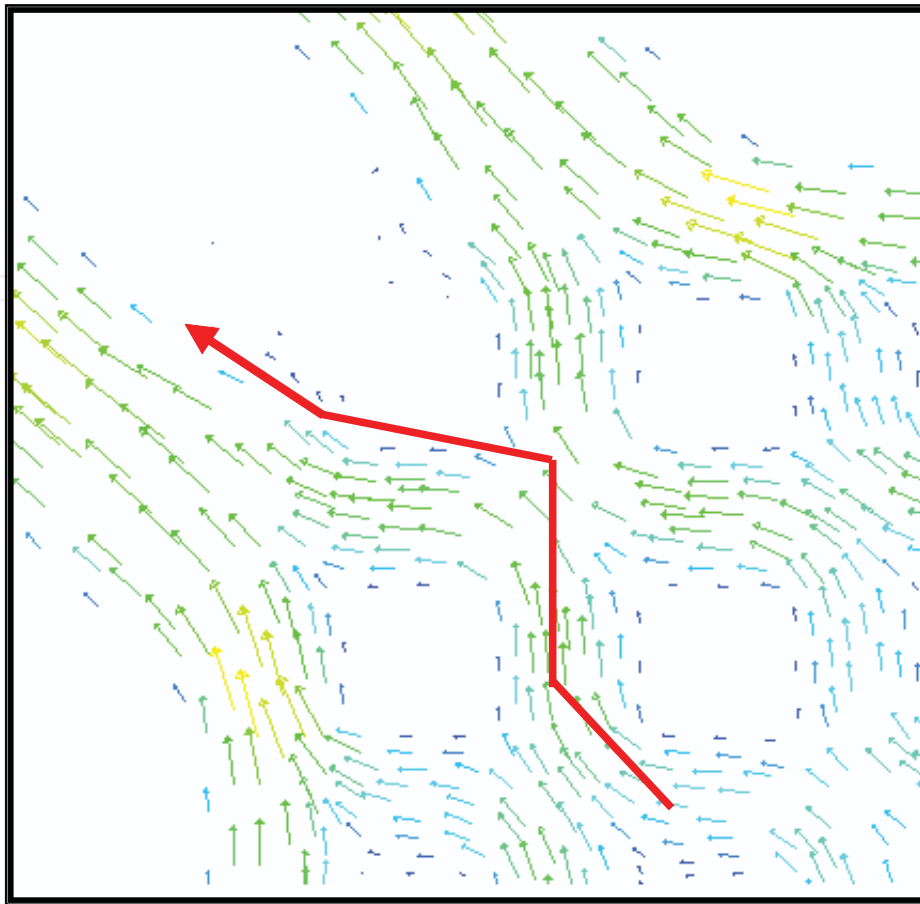


Fig. 5. Flow of cross strip in outlet

7.3 Assumptions of heat transfer analysis

In real estate, total area of MEA surface does not participate in chemical reaction uniformly for this reason that MEA has not a good efficiency and safety of the membrane. In analysis of thermal conductivity in the steel body of the cell that tried simplifying about reaction in the cell membrane that is given below:

- The total membrane surface response to in reaction.
- The total membrane area reacts in uniformly.
- There are similar rates of heat generation.
- The existence of gas bubbles in channels is apart.

Thus, flow is considered as single-phase and slow regimen for fluid motion. Heat generation is simulated by the MEA with a generation temperature area that total area generates heat with a constant rate. There for analysis done with these assumptions and use the energy equation in the calculations.

7.4 Energy equation

The energy equation is defined by below form:

$$\frac{\partial}{\partial t}(\rho v) + \nabla \cdot (v(\rho E + p)) = \nabla \cdot \left(k_{eff} \nabla T - \sum_j h_j J_j + (\tau_{eff} \cdot v) \right) + S_h \quad (2)$$

So that k_{eff} is effective conductivity equal to $k + k_t$ that k_t is thermal conductivity turbulence and that is defined accord to the turbulence model. J_j is the gush of components influence. Three term of Right side of the above equation shows energy transfer due to conduction, different influence and viscous waste regularity.

S_h is including heat of the chemical reaction or other heat source that is defined. With simplify the above equations have:

$$E = h - \frac{p}{\rho} + \frac{v^2}{2} \quad (3)$$

So that h is defined as the sensible enthalpy for ideal gas and that is in the following form:

$$h = \sum_j Y_j h_j \quad (4)$$

For incompressible fluid we have:

$$h = \sum_j Y_j h_j + \frac{p}{\rho} \quad (5)$$

Y_j is mass fraction of the samples j and

$$h_j = \int_{T_{ref}}^T c_{p,j} dT \quad (6)$$

So that is $T_{ref} = 298.15^\circ K$. Thermal analysis is applied by using of energy formula for cross strip flow field for the incompressible fluid that is presented in equation (3). Results are reported in continue. For analysis, thermal characteristics are given in Table (1).

MATERIAL	METHANOL SOLUTION	STEEL-316
Density (Kg/m ³)	785	8030
Specific heat capacity (j/Kg.k)	2534	502.48
Heat transfer coefficient (W/m.k)	0.2022	16.27

Table 1. Thermal characteristics

After analyzing with the different mass flows (\dot{m}), highest temperature with consideration by conduction heat transfer from the wall with displacement transfer coefficient $10W/m^2K$ for air are listed in Table (2). Cell temperature is $300^\circ K$ in normal state. The number of iterations to converge to solutions in Figure (6) is given. Heat transfer contour in tangent membrane on the page in Figure (7) is shown.

In this analysis, show the effects of the temperature distribution around heat generation membrane with contours that is specified more clearly with red lines that high light in

figure. The contour dispersals are to output side. This term of view performance is also acceptable. That is Because of temperature generation and high transfer rate of mass flow in micro channel that because the temperature contours aggregation in outlet gate and temperature dispersal in outlet is more that seems quite reasonable.

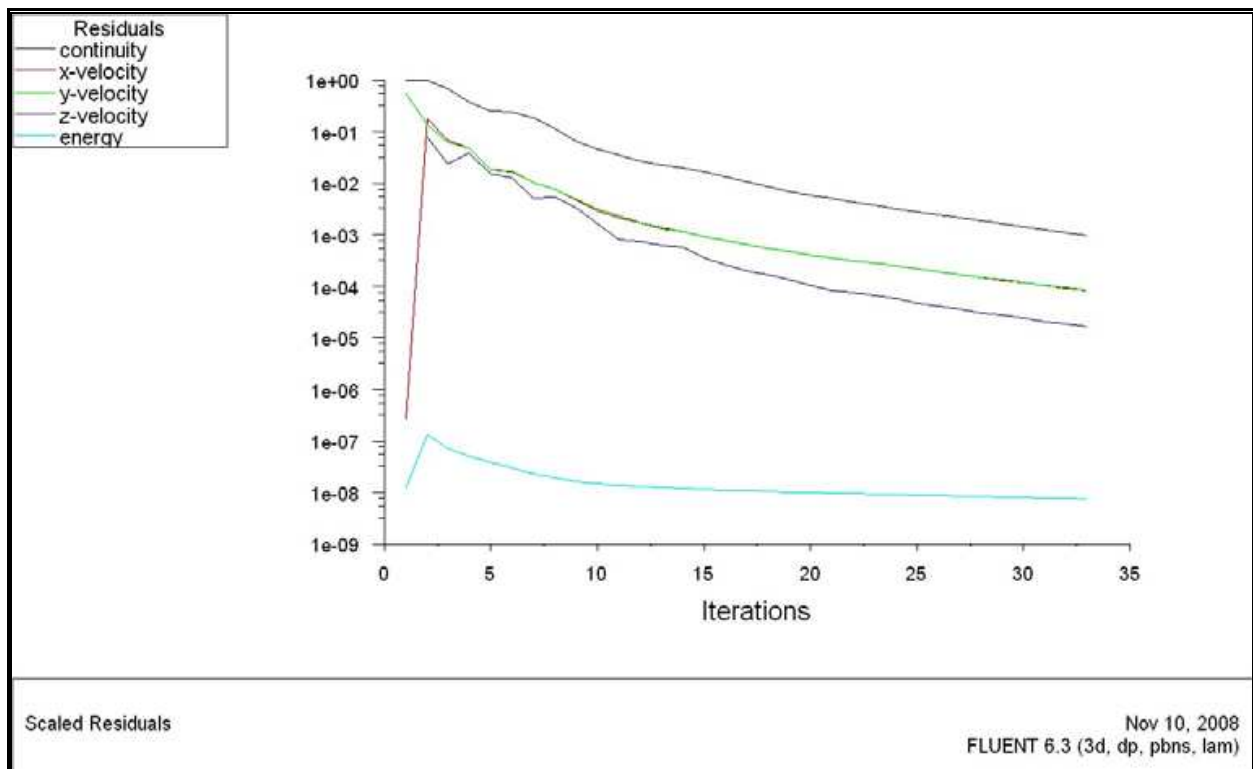


Fig. 6. Converge to solutions

$T_{\max}(K^{\circ})$	$\dot{m}(mLit/s)$
312.5	0.3
310.7	0.6
307.8	0.9

Table 2. Highest temperature generate with heat transfer

Figure (8) is shown heat transfer in cross section of steel plate of channel. Following this study, heat transfer existence in cross is the micro reactor. In this cross section is observed the temperature gradient contour is put away with a sharp slope relatively. But in comparison with heat transfer plate mode convention is small relatively. Because temperature displacement because of mass transfer of micro-channels compared to the dimensions of micro channels is more effective than heat-conduction in touch with the hot membrane. High speed of mass transfer in micro channels prevents conduction heat transfer.

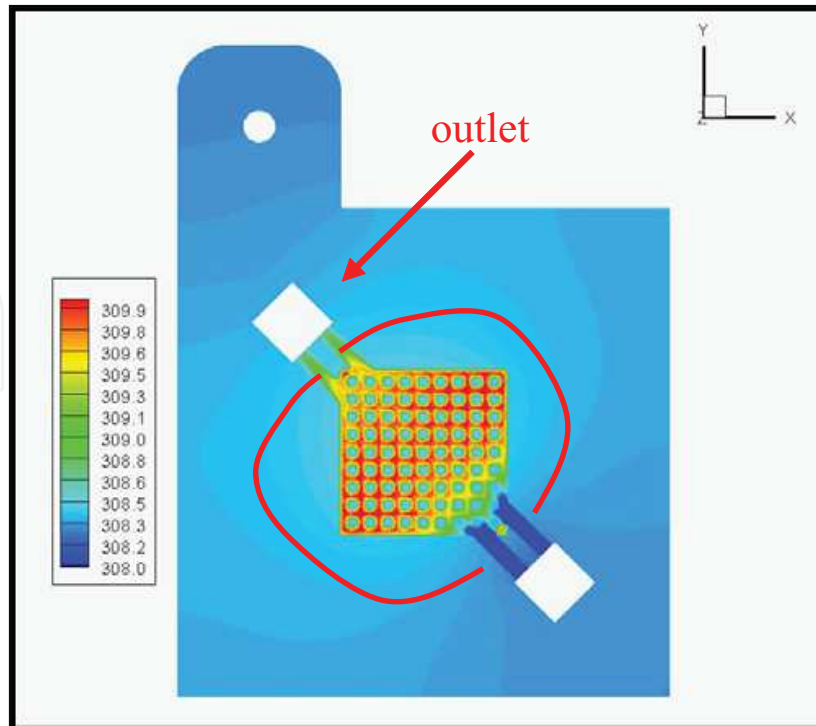


Fig. 7. Heat transfer for Steel plate

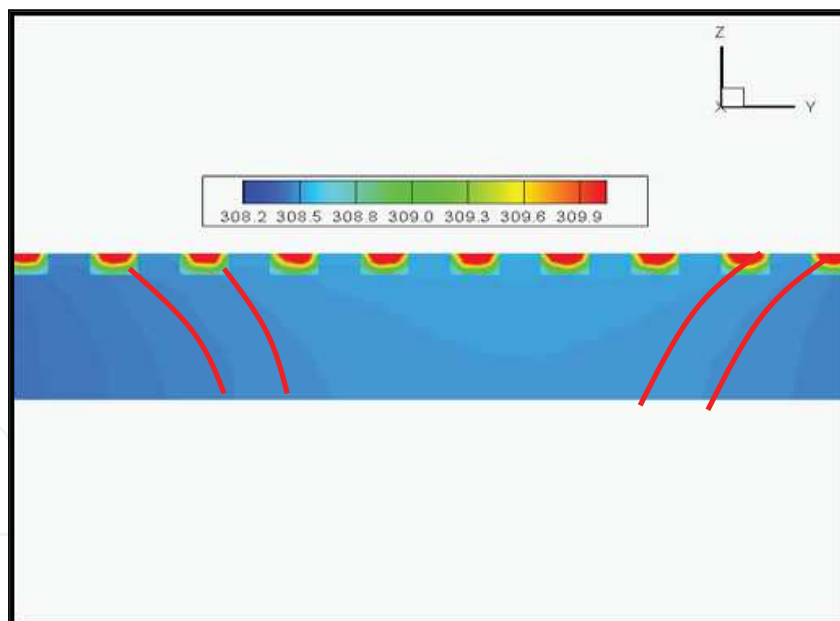


Fig. 8. Heat transfer of steel cross section plate

8. Conclusion

Performing the numerical simulation can be determined very uniform distribution cross strip flow field rather than parallel flow field. So with simulation can be determined distribution of methanol in the membranes. Because if we have good distribution, we have more uniform fuel distribution in the anode side and result in good performance in reaction.

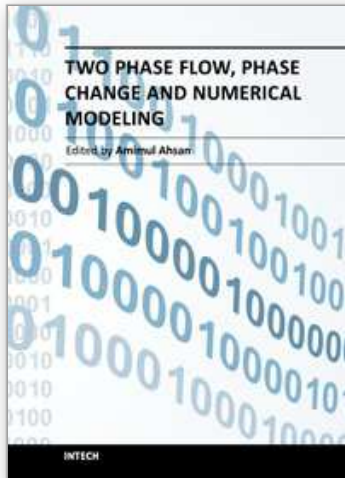
With simulation of heat transfer, is found heat distribution in the cell and can be show the small scale of the chemical reaction in steel surface areas that are more affected by temperature, even at very low temperatures different from doing the chemical reaction. Finally, the comparison between two kind of flow field and give the best distribution in cross strip flow field and good reaction other than parallel flow field.

9. Acknowledgment

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Two Phase Flow, Phase Change and Numerical Modeling

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The heat transfer and analysis on laser beam, evaporator coils, shell-and-tube condenser, two phase flow, nanofluids, complex fluids, and on phase change are significant issues in a design of wide range of industrial processes and devices. This book includes 25 advanced and revised contributions, and it covers mainly (1) numerical modeling of heat transfer, (2) two phase flow, (3) nanofluids, and (4) phase change. The first section introduces numerical modeling of heat transfer on particles in binary gas-solid fluidization bed, solidification phenomena, thermal approaches to laser damage, and temperature and velocity distribution. The second section covers density wave instability phenomena, gas and spray-water quenching, spray cooling, wettability effect, liquid film thickness, and thermosyphon loop. The third section includes nanofluids for heat transfer, nanofluids in minichannels, potential and engineering strategies on nanofluids, and heat transfer at nanoscale. The fourth section presents time-dependent melting and deformation processes of phase change material (PCM), thermal energy storage tanks using PCM, phase change in deep CO₂ injector, and thermal storage device of solar hot water system. The advanced idea and information described here will be fruitful for the readers to find a sustainable solution in an industrialized society.

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