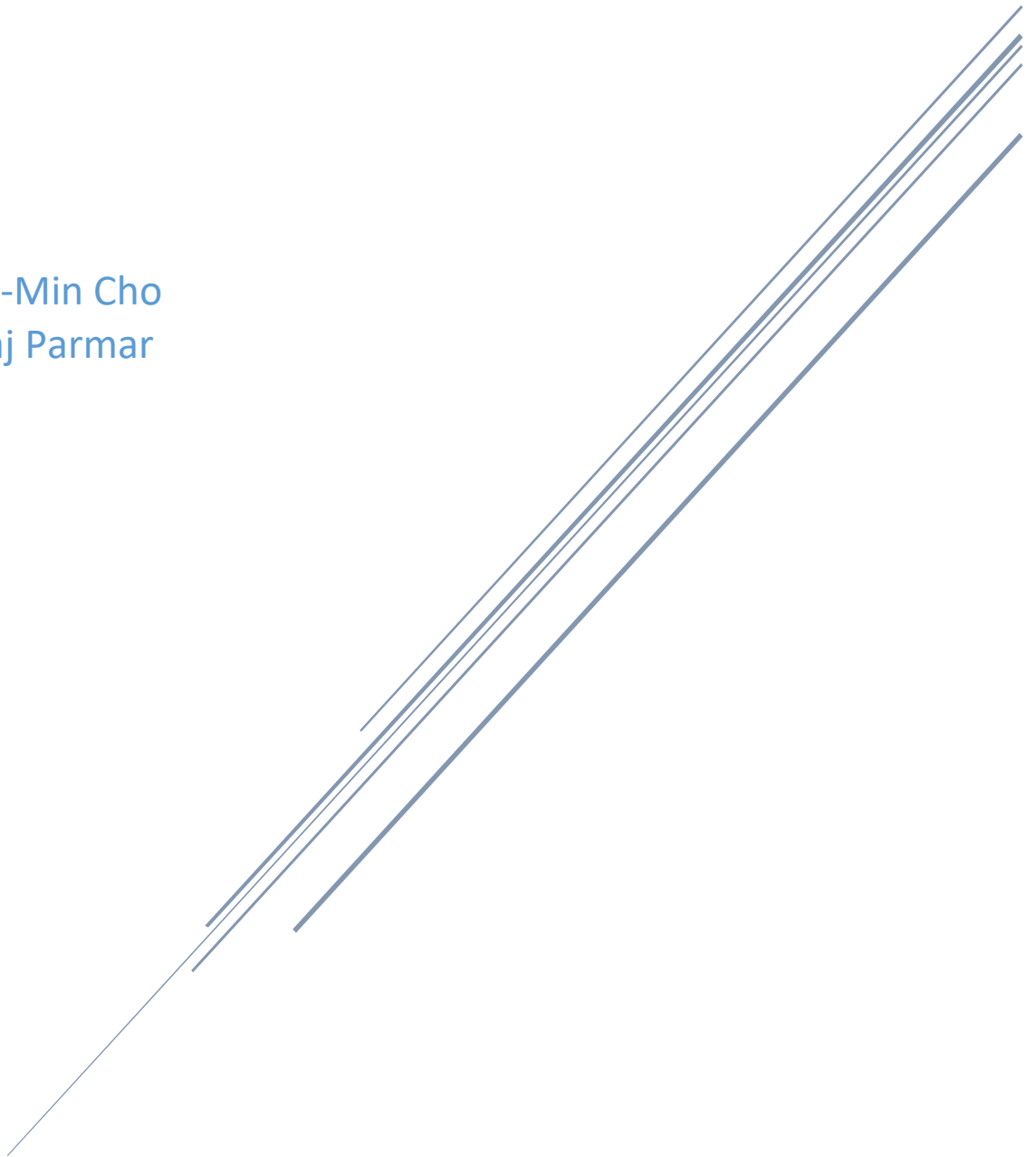


CFD SIMULATIONS IN ANSYS

For Microfluidic Applications

Hyeong-Min Cho
Harshraj Parmar



PREFACE

This handbook serves as a guide towards performing Computational Fluid Dynamics analysis in the multi-functional software ANSYS Inc. The literature covers both the underlying theory of a simulation and the procedure to bring out correct and reliable results. Theoretical concepts are connected with the solution procedure in order to enable moving beyond pushing buttons and start thinking from the solver's point of view. Efforts have been made to connect the two distinct domains without adding further complications. The recent advancements in Microfluidic Fuel Cells have led to increased dependency on simulations to obtain results and so the present book serves as a foundation for further extensive research.

I cultivated my interest in CFD analysis after an introductory course on Fluid Mechanics in the 4th Semester of my Bachelor's Degree. Since then I have been involved in the analysis of various types of flow i.e. Turbulent, Steady and Unsteady. Most of my analysis till now were confined to two dimensions and so the present problem served as a good opportunity for exploring my understanding of the solver and the theoretical concepts. The concepts were essentially the same but the main difference was involved in meshing the geometry.

The CFD analysis is laid out in seven phases which are organised in a sequential manner and are further divided into their respective defining steps. The presented approach applies in general to any simulation and is considered to be optimal in reducing errors and ensuring correct results. First, the underlying theory and motive is explained and meaningful hand calculations are carried out for cross-checking. Next, a step-by-step layout is made to help in adjusting the solver settings and to obtain results of our interest. The results are analysed and the errors from expected and analytical results are extracted. Finally, future possibilities for simulations are suggested and new problems are exposed to be solved for in an efficient manner. This literature is built upon grounds provided by articles in *Journal of Heat and Mass Transfer* [1], *Royal Society of Chemistry* [2] and *Biotechnology and Bioengineering* [3]. It is hoped that this book will present a good introduction to FLUENT solver in ANSYS and also enable further research oriented on simulations at the microscale.

I am highly grateful to everyone who has contributed either directly or indirectly towards the development of this book. In particular, I would like to thank Hon. Prof. Ahn for allowing me to work during the summers in the Micro-Electro Mechanical Systems Lab. I wish to thank my mentor, Mr. Hyeong-Min Cho for his immense help and experienced inputs in guiding the path for this assignment. Not to be left; Mr. Cheon-Ho Lee for his guidance in meshing the geometry for smaller microchannel heights and all the current lab members Mr. Tae-Seong Choi, Mr. Myeong-Hun Kim, Mr. Do-Gyun Jung and Mr. Yang Guitao. Finally, I would like to thank the Dept. Of Mechanical Engineering, IIT Guwahati for allowing me to undergo the internship despite it not being a part of my curriculum.

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Ansan, South Korea

Harshraj Parmar

Parmar Harsharajsinh Birendrasinh

B. Tech 4th Semester,

Mechanical Engineering,

Indian Institute of Technology, Guwahati.

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2. D. Vigolo, A. Sahu, H A. Stone, *Flow dependant performance of microfluidic microbial fuel cells*, Royal Society of Chemistry, 2014.
3. Z Li, Y Zhang, P R. LeDuc, K B. Gregory, *Microbial Electricity Generation via Microfluidic Flow Control*, Biotechnology and Bioengineering, 2011.

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For Bruno

1 PROBLEM OUTLINE

1.1 INTRODUCTION

Microbial fuel cells serve as an important technology for electricity production from a large variety of organic matter and thus are said to be the most close-to nature cells. They are mostly used in waste water treatment where they not only help in the purification process but also produce electricity. The main problem faced by MFCs is that they have low power output and so cannot be used in practical devices.

In order to overcome the limitation of low power output a lot more research has been carried out recently on the integration of Microbial fuel cells with the micro-scale. This has led to an enhancement in the power density of these cells and thus has widened the scope for their utilization. The performance of the cell is affected by many parameters like the flow conditions, electron transfer at the anode and the cathode, internal resistance and cell geometry. Most of the research has been carried out in the fields other than the effect of flow conditions on the performance. The main objective of this report is to study the effect of varying cell geometry on the shear stress experienced by the electrodes through ANSYS simulations.

Previous studies have laid certain foundations for further work to be carried out in this field. Vigolo et al. [1] reported that the growth and structure of the biofilm depend largely on the shear stress near the electrode surface. They checked the performance of the MFC for a range of flow rates and proposed an optimal value for maximum voltage output. The shear stress plays a role of stimulant for the bacteria and thus influences the output characteristics of the MFC. Additionally, at high flow rates the supply of nutrients to bacteria also increases and hence we observe a combined effect of the two parameters on the output. Pham et al. [2] observed the effect of high shear enrichment of MFCs for different strains of bacteria on their performance. The variation in the DNA, ATP amounts and the uniformity and thickness of biofilm layer were discussed in detail. This paper focused on the time dependant biological properties of bacteria in the MFC and thus provided a broader overview for our analysis.

Most of the prior research have been carried out using a fixed MFC geometry and variable flow rates to measure the shear stress. In the present analysis we intend to observe the effect of varying geometry on the flow rates to maintain a constant shear stress over the electrode.

1.2 ANALYSIS LAYOUT

The bacterial strain is stimulated the most in the presence of an optimal shear stress at a particular flow rate. This enhanced stimulation leads to maximum voltage and power output for a particular MFC configuration. Thus we can conclude that as far as the shear stress is concerned the bacteria prefers a particular value for working regardless of the flow conditions and the MFC geometry. The analysis can be laid out in the following steps:

- An experiment with a 55 μm channel height and variable flow rates was carried out. The optimal flow rate was found out to be 40 $\mu\text{L}/\text{min}$ and this gave us an initial analysis condition for our simulations in ANSYS Inc.
- The computational analysis of the flow was carried out in the software and the corresponding shear stress over the electrode was obtained.
- Flow analysis for different channel heights were carried out and the flow rates were tweaked in order to get the required shear stress value.
- 15 μm , 35 μm , 75 μm , 95 μm and 115 μm were the heights for our analysis.

The flow rate exhibits a positive relation with the current density and so higher the flow rate, higher is the current density. Thus the effort here is to combine the benefits of higher current density and optimal environment for bacteria. But there is an upper limit to the flow rate which is defined by fuel efficiency optimization as high flow rate decreases the efficiency. Present analysis is a fluid flow analysis which does not include the electro-chemical reactions that determine the output characteristics of the MFC. Experiments are thus required to be carried out after the simulations in order to determine which cell geometry results in the most favourable output.

References

1. D. Vigolo, A. Sahu, H A. Stone, *Flow dependant performance of microfluidic microbial fuel cells*, Royal Society of Chemistry, 2014.
2. H.T Pham, N. Boon, P. Aelterman, *High shear enrichment improves the performance of the anodophilic microbial consortium in a microbial fuel cell*, Microbial Biotechnology, 2008.

2 SIMULATION PROCEDURE

2.1 PROS AND CONS

Computational analysis is becoming more and more important nowadays due to the increasing number of variables and the time factor involved in physical testing. Also due to increasing computational abilities of computers, CFD serves as a good option for analysis. Physical testing in our case results in the production of different PDMS moulds and setup procedure for each channel height. This results in a lot of time and is not feasible from a research perspective. Simulations offer a comparatively shorter and easy method to get the appropriate results. Secondly, a large flexibility of the operating conditions and MFC geometry can be incorporated in the simulations with a lot of ease than in the experiments.

On the other hand, the results of simulations need to be verified and cannot be relied on without cross-checking. This implies looking for experimental data or solving the problem in a simplified manner and comparing the results. Usually, the experimental data for μ MFCs are hard to find which leaves us with hand calculations. Fluid flow analysis is carried out in 3D and so the Continuity and Navier-Stokes equation's solutions are beyond the scope of this context. This leaves us with approximate solutions to the velocity distributions in a 3D laminar channel flow. Secondly, the results rely hugely on the mesh and the boundary conditions provided by the user to the solver. Thus refinements and repeated observations are needed in order to assume a solution to be correct. These topics would be covered in detail later in the text.

2.2 PROCEDURE

The solution procedure is divide into seven major steps which serve as important phases that lead to an acceptable solution:

1. Pre-Analysis
2. Geometry
3. Meshing
4. Model Setup
5. Numerical Solution
6. Numerical Results
7. Verification and Validation

Finally, special techniques for meshing problematic cases and future analysis perspectives are discussed in detail. Possible modifications in the μ MFCs to increase their performance are also laid out.

3 PRE-ANALYSIS

Pre-Analysis involves deriving the approximate solutions for the flow with the help of a simplified model. The physical problem is solved with the help of certain assumptions which render the problem within the domain of appropriate solutions.

3.1 MATHEMATICAL MODEL

- The analysis is three-dimensional and so we have **three components of velocity and pressure to be found** out in our solution.
- The **flow is assumed to be steady** i.e. the partial derivatives of all variables with respect to time are zero.
- Analysis is done in the **fully developed** region i.e. the partial derivatives of the velocity components in the stream-wise direction are zero.
- Fluid is assumed to be of **constant density** and **constant viscosity** and is assumed to be an **incompressible flow**.
- Gravity is neglected in our analysis, signifying that there are **no body forces acting** on the fluid and is assumed to be **Newtonian fluid**.
- With the given channel dimensions and the possible velocity magnitudes that can be encountered, the Reynolds number is calculated. It turns out to be less than 4 and so we are safely in the **laminar flow domain**.

3.2 DOMAIN

- The domain is the 3D geometry of the channel created using Soliworks/AutoCAD or any other designing software.

Note: Here we cannot use symmetry or any other simplifications as there is diffusive mixing of anolyte and catholyte involved. So the domain is just the geometry we have created.

3.3 GOVERNING EQUATIONS

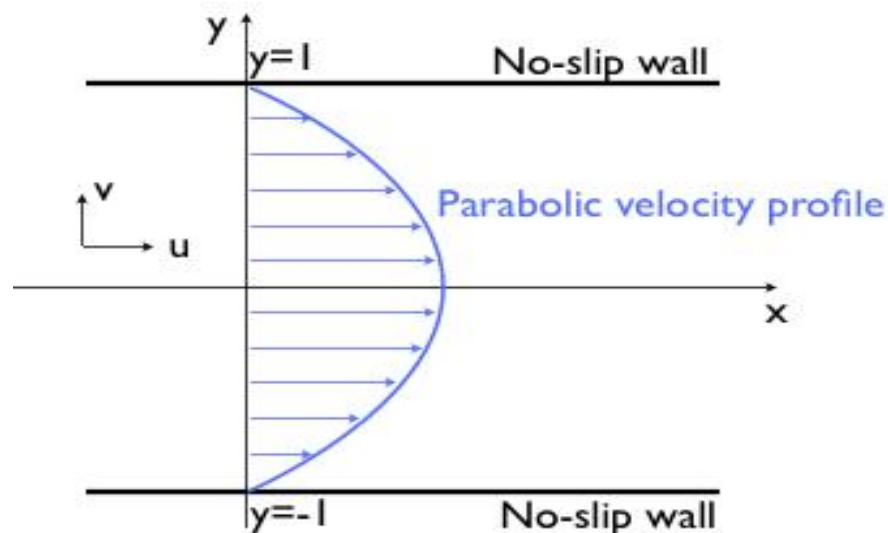
- Since this is only a fluid flow analysis of the μ MFC, the governing equations are the fluid conservation equations.
- **Mass conservation** under the assumptions taken can be written as:
Gradient. Velocity=0
This is a scalar as gradient decreases the order of a tensor.
- **Navier-Stokes equation** which is the conservation of momentum.
This has three components and is a vectorial equation.
- **Conservation of Energy** which is satisfied in most cases.

3.4 BOUNDARY CONDITIONS

- The boundary conditions define the path for our solution and so it is important to define them properly with proper physical meaning.
- The two inlets are set to uniform velocity inlet type conditions and the velocity is determined by the area and flow rate at inlets.
- The outlet is set to Outflow condition which is appropriate for our case and it will basically set the constant pressure condition at the outlet.
- The boundaries of the 3D channel are set to Wall boundary condition indicating that the velocity at that surface is zero.

3.5 HAND CALCULATIONS

- The hand calculations are based on two types of analysis and both of them are approximate. Unfortunately, the degree of approximation cannot be known as no resources pertaining to that were found.
 1. Poiseuille Flow Analogy:
 - The flow through 3D channel is approximated by that through a 2D channel with both walls fixed and an applied pressure gradient.
 - This approximation is valid only for the case where the channel dimensions are such that $H \ll W \ll L$.



Plane Poiseuille Flow

- On solving for this case we find the shear stress using the constitutional relations and the formulation for strains.

$$\sigma_s \simeq 6 \mu Q / (WH^2)$$

- Here μ is the dynamic viscosity, Q is the flow rate, W is the channel width and H is the channel height.
- On substituting the values of known variables we get the shear stress as:

$$\text{Shear Stress} = 1.615 \text{ Pa}$$

Note: The shear stress exhibits a linear relationship with the flow rate for constant viscosity and channel dimensions.

- So since we have the shear stress value for $55\mu\text{m}$ height channel and hence we can find the approximate flow rates for other heights using the above formulae.

2. 3D Channel Flow Approximate Solution:

- The velocity profile is the most important parameter to be found from the analysis and with it we can find the shear stress distribution over the electrode.
- As the analysis for 3D channel flow is beyond the scope of our analysis, the results were adopted from the article of Kundu et al [1]. They had compared four approximate models for the velocity distribution with exact analytical solution.
- Plots of velocity versus aspect ratio were made and compared for all the solutions proposed. In our range of aspect ratio, the most appropriate solution was Integral Ritz 1.

Integral Ritz1 (IR1) :

$$U(X, Y) = \frac{9(1 - X^2)(1 - Y^2)}{4(3 + 26A^2)} \left[\frac{(2 + 25A^2)}{(1 + A^2)} + 5X^2 \right]$$

- This formula was used in order to compare the profile dependency on the channel height at a constant width. The model results were compared with the expected results from this velocity profile.

Note: For this case also the shear stress follows a linear relation with the flow rate and hence for both the analysis this holds true.

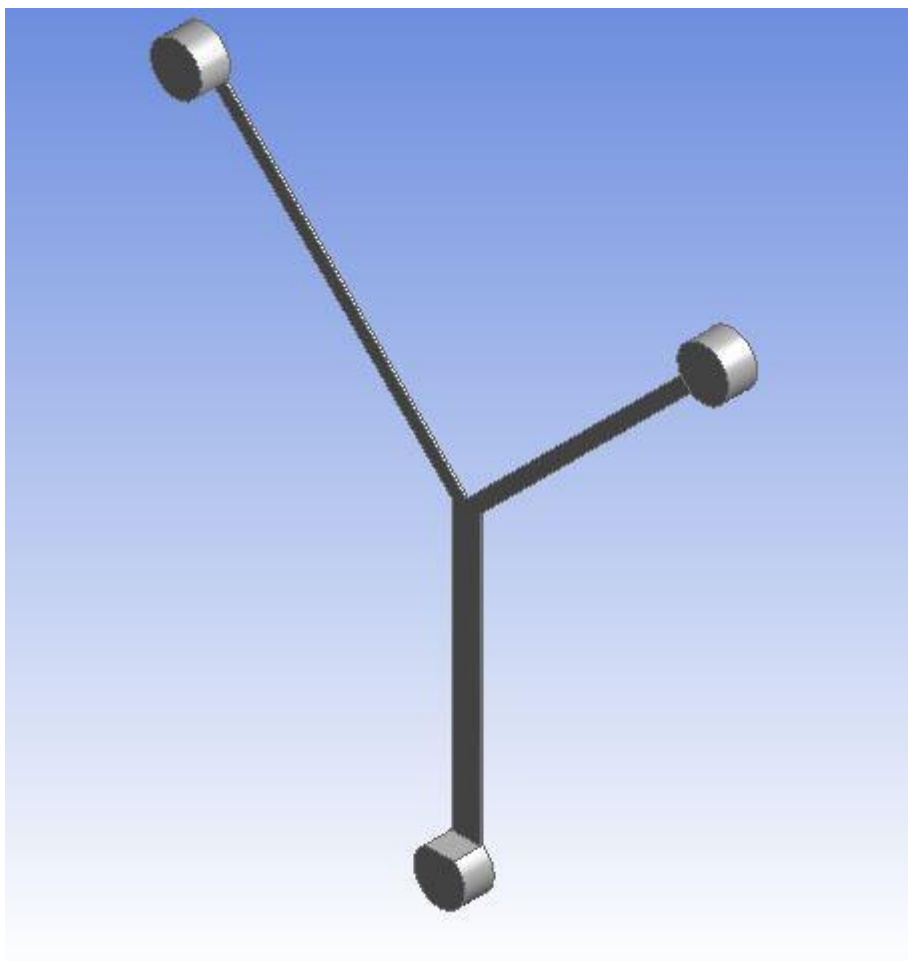
References

1. B. Kundu, S. Simlandi, P K. Das, *Analytical techniques for analysis of fully developed laminar flow through rectangular channels*, Heat and Mass Transfer, 2011.

4 GEOMETRY

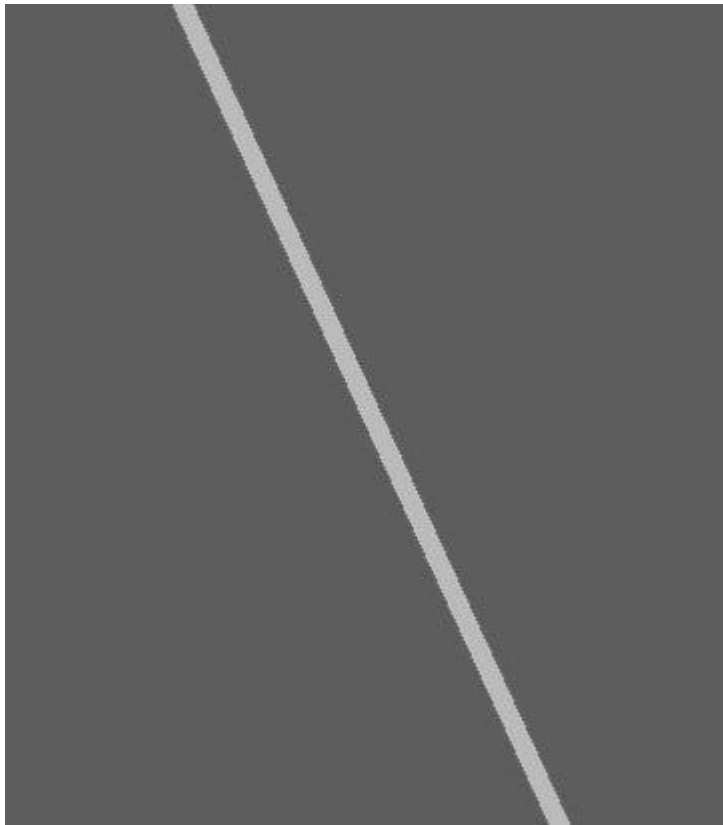
- Start a new fluent project and firstly ensure that the analysis type is set to 3D in the properties of Geometry.
- The geometry for the problem can be made in Design Modeller or in any other CAD software with proper dimensions.

Note: The heights of the inlets and outlets are arbitrary for the analysis but are very important for the solution procedure and convergence. The phenomenon of back-flow is controlled by that.



Channel Geometry for 55 μ m height

- The sketch of the channel is made first and then it is extruded up to the channel height. Thereafter the electrodes are cut extruded from the channel in order to realize them in the geometry.
- Basically our geometry represents the fluid domain i.e. the volume through which fluid can flow.



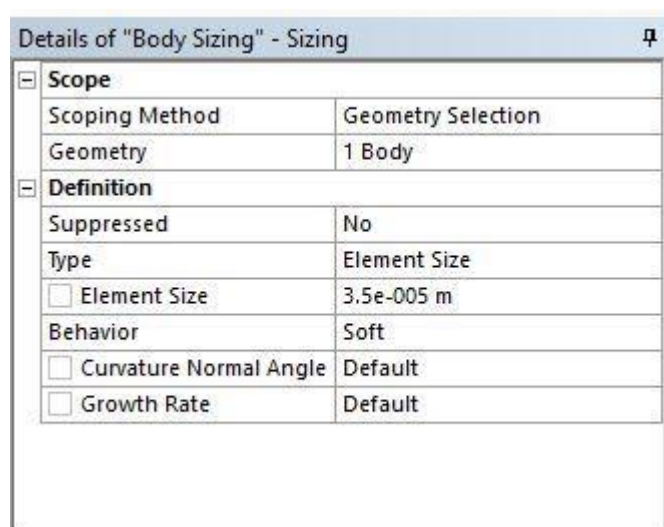
Cut-Extrude for realizing electrodes

- Once the body of the MFC is made, we need to set the domain type in the Modeller. Click on the body created and in the properties window specify the domain type as FLUID.
- After the sketching is completed we move on towards the most important step of the analysis which is Meshing.

5 MESHING

5.1 MESH SIZING

- Three sizing were introduced in the meshing step, on the channel body, electrode face and the outlet. The element size was defined by analysing the height of the channel and the outlet.
 - I. Firstly, if we consider the body sizing then the element size was given as $3.5E-05m$ as the channel height was $5.5E-05m$ and so could fit three or more tetrahedrons roughly. This would ensure proper element density for acceptable results.
 - In the behaviour setting of the body sizing, leave it to soft as the mesher may result in irregular mesh if we turn this setting to hard. Its recommended to keep it to soft for 3D meshes.



Body sizing settings

- II. Next we move on towards the electrode face sizing, this is done in order to get accurate velocity gradients near the electrode thereby increasing the accuracy of the calculated shear stress.
 - The element size is set to $1E-05m$ which ensures proper refinement near the electrodes to get precise gradients.

Note: As a general rule of thumb, refine the mesh near the areas of your interest, where you have to find the required quantity. Here we wanted the shear stress on the electrode and so we refined the mesh near it.

Details of "Electrode sizing" - Sizing	
Scope	
Scoping Method	Geometry Selection
Geometry	2 Faces
Definition	
Suppressed	No
Type	Element Size
<input type="checkbox"/> Element Size	1.e-005 m
Behavior	Soft
<input type="checkbox"/> Curvature Normal Angle	Default
<input type="checkbox"/> Growth Rate	Default

Electrode Sizing settings

- III. The outlet sizing is essential for proper accuracy and convergence of the solution. Refinement is needed at the outlet so that the solver can extract the velocity and pressure properly.
- Face sizing is introduced on the top and side faces of the outlet. The element size is set to $2E-05m$ so as to get enough refinement.

Details of "Outlet sizing" - Sizing	
Scope	
Scoping Method	Geometry Selection
Geometry	3 Faces
Definition	
Suppressed	No
Type	Element Size
<input type="checkbox"/> Element Size	2.e-005 m
Behavior	Soft
<input type="checkbox"/> Curvature Normal Angle	Default
<input type="checkbox"/> Growth Rate	Default

Outlet sizing settings

Note: The element size for the sizing introduced will differ from case to case. Also the height of the outlet may change with different channels; the adopted element sizes and outlet heights have been mentioned in [\[1\]](#).

5.2 ADVANCED SIZING FUNCTION

- Advanced sizing function is a pre-defined meshing option available in ANSYS which helps in introducing refinement at the edges and sharp corners.
- There are four settings available: proximity, curvature, proximity and curvature, fixed. Each settings result in refinement in specific areas of the channel.
- For our analysis, we used the *Proximity and Curvature* setting with the min and max size set to their default.
- Also the *Relevance Center* and *Smoothing* setting affects the number of elements in the mesh severely. We set the *Smoothing to Medium* and the *Relevance Center to Coarse*.

Sizing	
Use Advanced Size Function	On: Proximity and Curvat...
Relevance Center	Coarse
Initial Size Seed	Active Assembly
Smoothing	Medium
Transition	Slow
Span Angle Center	Fine
<input type="checkbox"/> Curvature Normal Angle	Default (18.0 °)
<input type="checkbox"/> Proximity Accuracy	0.5
<input type="checkbox"/> Num Cells Across Gap	Default (3)
<input type="checkbox"/> Min Size	Default (1.0305e-005 m)
<input type="checkbox"/> Proximity Min Size	Default (1.0305e-005 m)
<input type="checkbox"/> Max Face Size	Default (1.0305e-003 m)
<input type="checkbox"/> Max Size	Default (2.0611e-003 m)
<input type="checkbox"/> Growth Rate	Default (1.20)
Minimum Edge Length	2.e-007 m

Advanced sizing settings

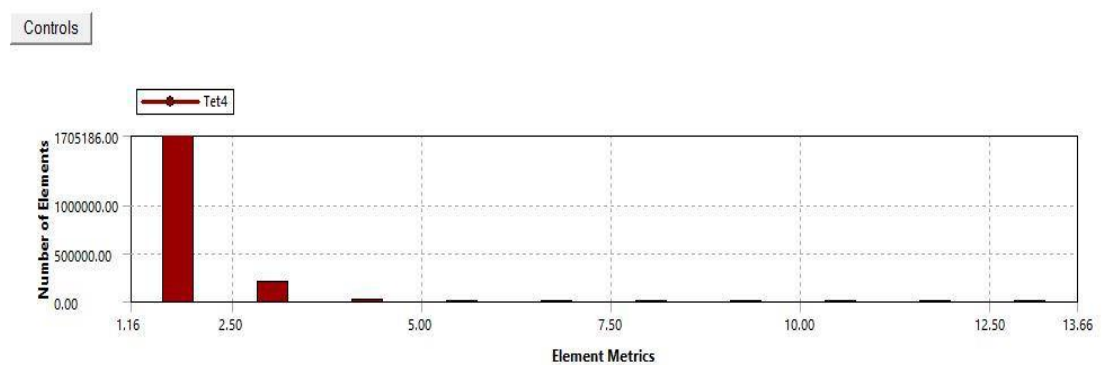
Note: For smaller channels it is recommended to set the relevance center to *Fine* and the smoothing to *High*. This will allow us to get proper refinement near the electrodes which is not possible by sizing.

- Meshing the channel side walls for small heights is very tough in the sense that only two layers of tetrahedron array are obtained.
- This can be solved by decreasing the *min size* in the settings tab. But this increases the number of elements to a very large amount (roughly 1,00,00,000) which is not in our computational domain.
- So another method needs to be adopted in order to solve the problem which will be discussed later.
- For further information on advanced sizing functions please refer to the website:
https://www.sharcnet.ca/Software/Ansys/16.2.3/en-us/help/wb_msh/msh_msh_ASF_Intro.html

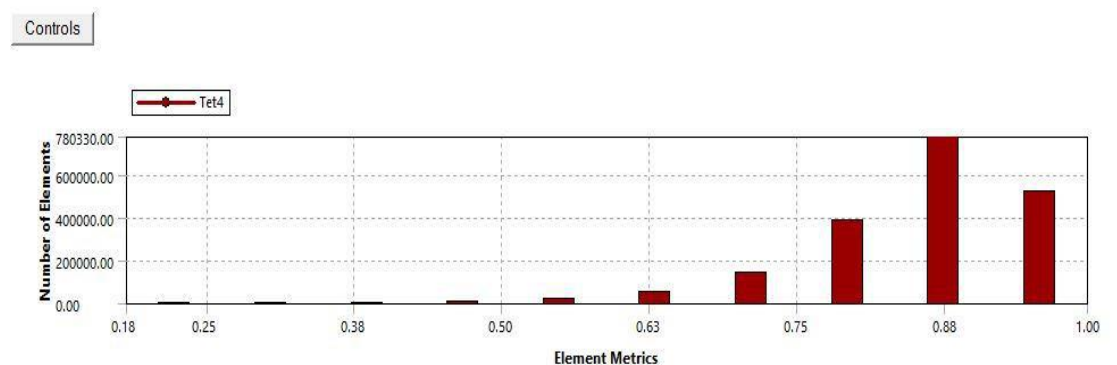
5.3 QUALITY ANALYSIS

- I. The mesh quality can be analysed using the *Mesh Metric* settings in the *Statistics option* of the tree. There are two types of checks that are very important for ensuring proper mesh.

a) Aspect Ratio: The aspect ratio signifies the ratio of height to width of the channel. High aspect ratio is not desirable and the solver will show an error message during the start-up. Usually a ratio of 1 to 100 is favourable.



b) Orthogonality: This represents the angle between the sides of the elements and is often the most important parameter to look for. Orthogonality close to one represents a rectangular element and usually between 0.6-1 is good for a mesh.



- II. The refinement of a mesh determines the accuracy and computational time involved for a solution. So it is very important to check using varying sizes so as to determine the proper refinement.
- With adequate number of checks by step refining the mesh, we conclude that the number of elements in the range of 14,00,000-19,00,000 is favourable to get near-mesh independent solutions.

- III. If you get errors in meshing something like, “*Given element size does not lie in the allowed range*” then change the *min size* in the advanced sizing functions settings.

5.4 NAMED SELECTIONS

- In the FLUENT solver we cannot click on a boundary and give the associated boundary condition. We need to make a named selection in the mesher and then use it.
- We made five named selections, two for the inlets, one for outlet, electrode surface and channel wall boundary.
- The named selections are made by selecting the required faces or bodies and selecting the *Create Named Selection* option. The names can be given as desired.
- Named selections conclude our meshing step and next we move on to FLUENT to start the solution set-up.

References

1. <https://drive.google.com/file/d/0Bwwl5g9eZz24ODl5UF9VOEtIVVU/view?usp=sharing> – Sizing used in the meshes.

6 SETUP

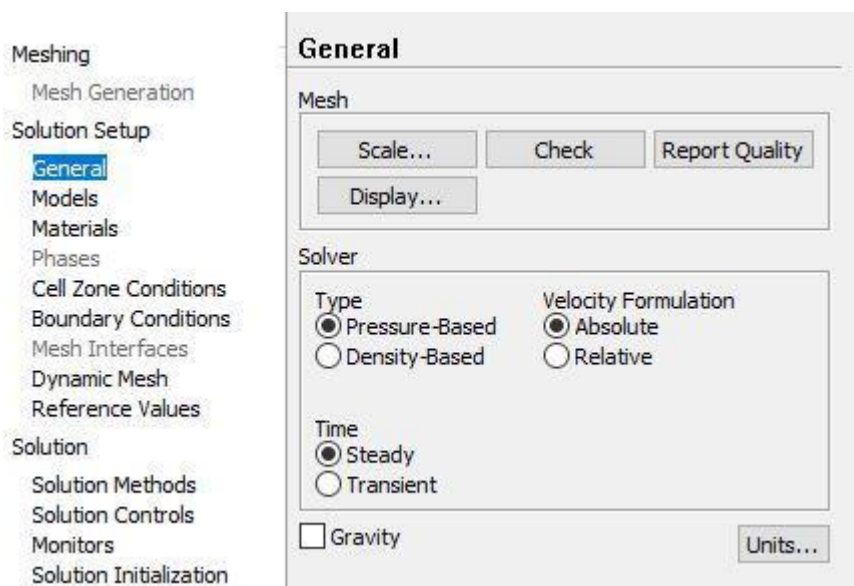
6.1 START-UP

- I. Double-clicking on fluent opens up the launcher window, select the **“Double Precision”** option in the window and this gives increased precision for each number. Although it takes up more memory and performance out of the system.
- II. In the FLUENT solver click on **“Check”** option, this checks the mesh that we have made and gives a warning if there is any problem with it.

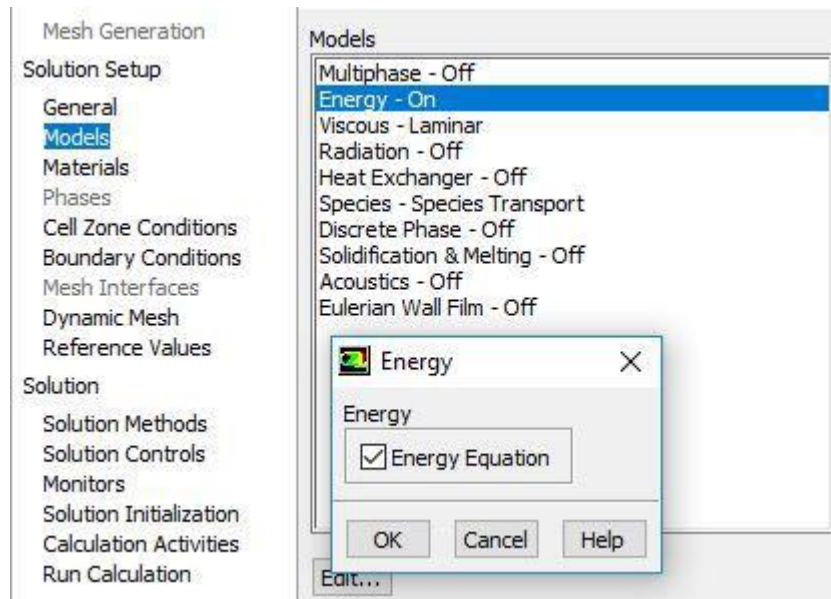
Note: This step is necessary as the mesh may contain high aspect ratio elements that would be solvable by the solver.

6.2 DEFINING THE GOVERNING EQUATIONS

- I. In the **“General”** tab the settings available are solver type and its time dependency. We used the **“Pressure based”** and **“Steady”** solution settings as per the pre-analysis and the problem specification.



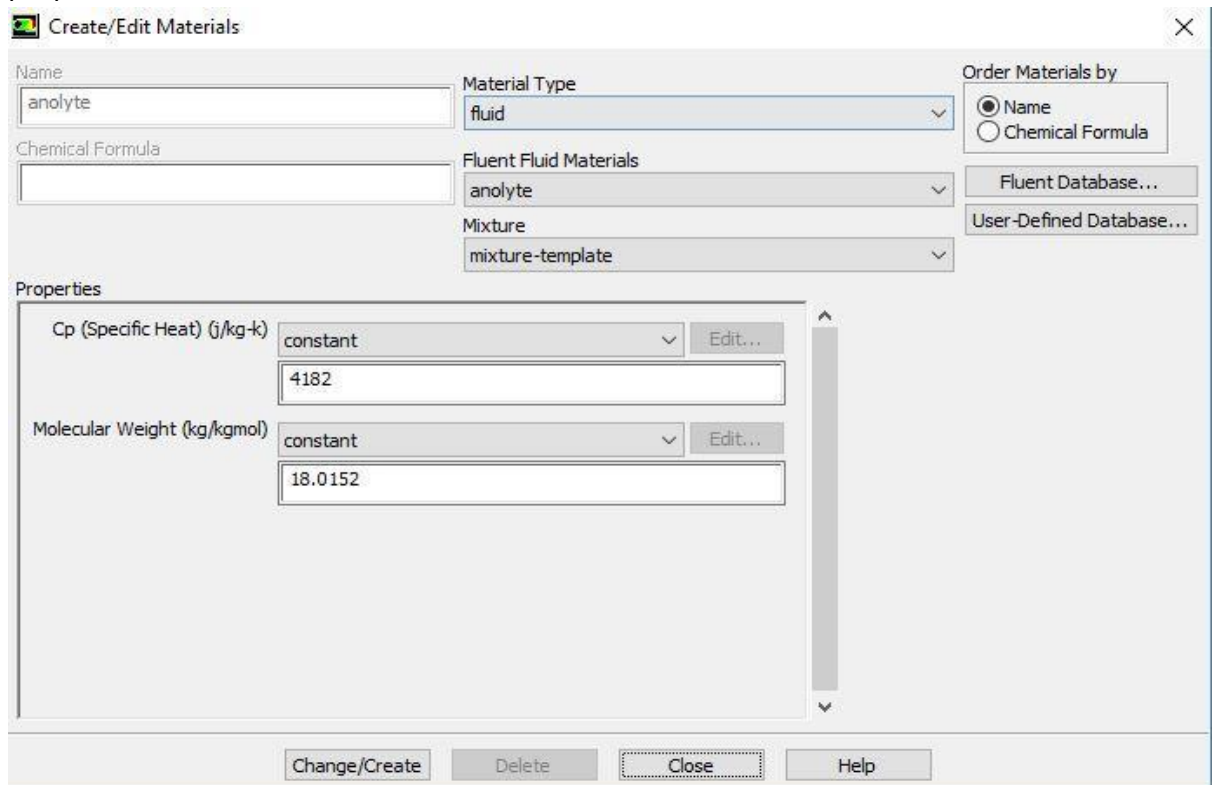
- II. Next we move on to **“Models”**, where there are most of the settings related to the equations to be accounted for.
 - Double click on **“Energy”** and select the energy equation in order to enable the conservation of energy equations.



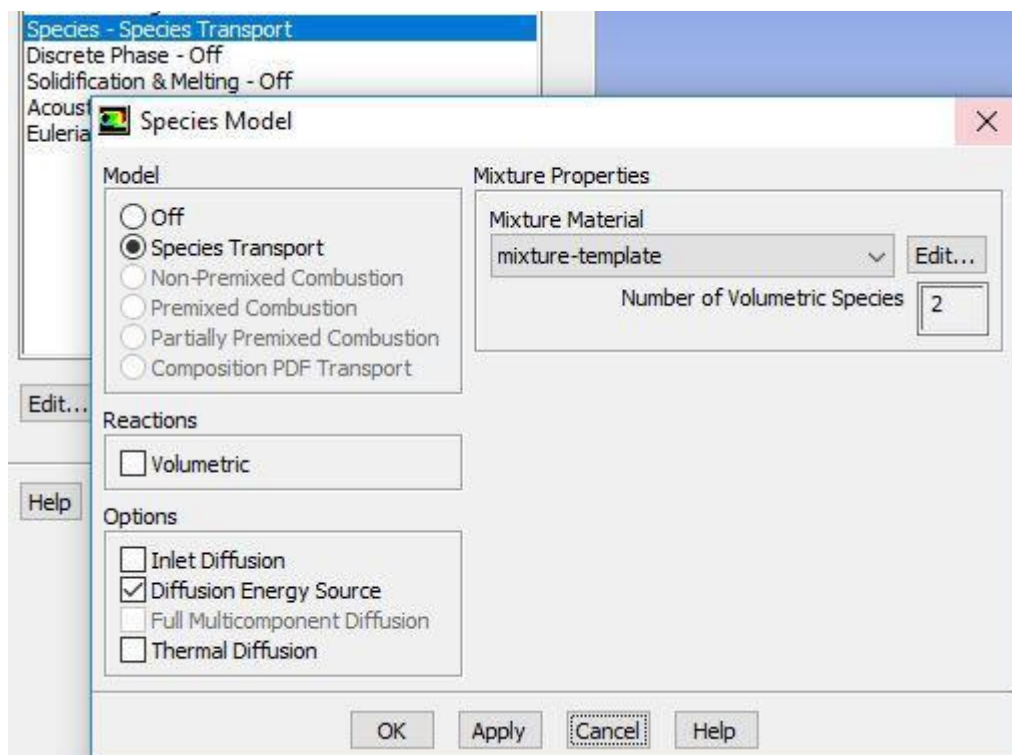
- The Viscous setting is set to Laminar by default and so check if it is in that setting or not.

Note: Before we move on to the settings for species transport we need to define the materials for our catholyte and anolyte. Then we will incorporate them inside the mixture.

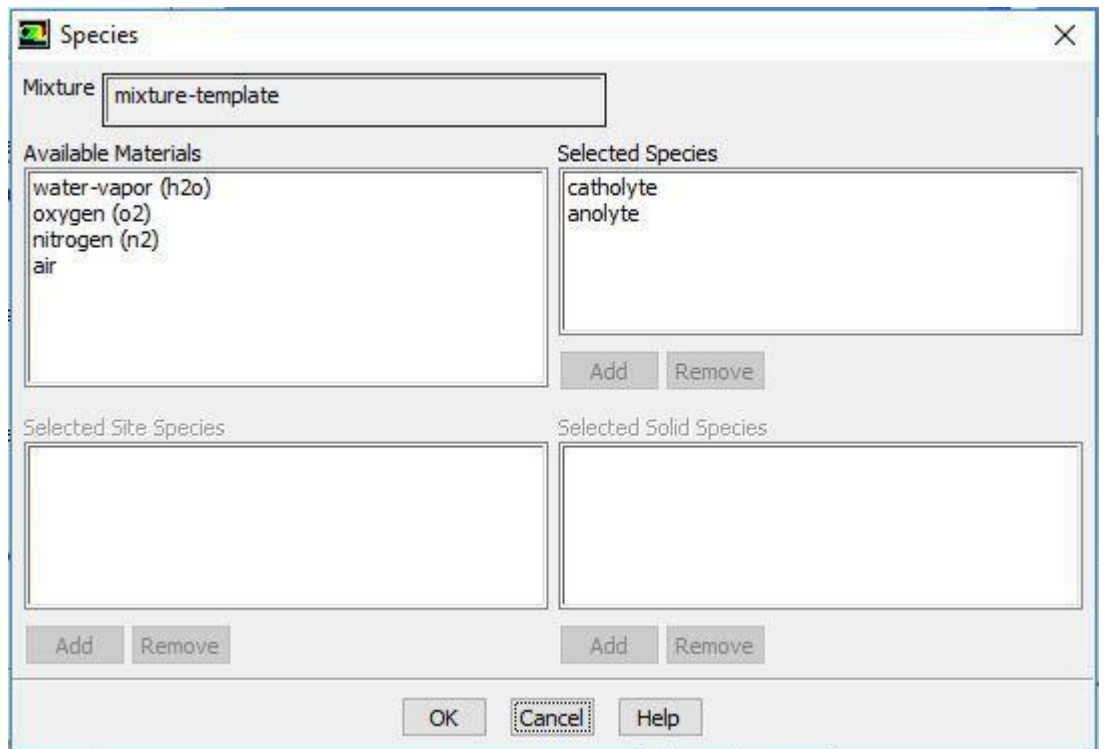
- III. Click on **“Materials”** and in the create material window give the name and the other properties of the fluid.



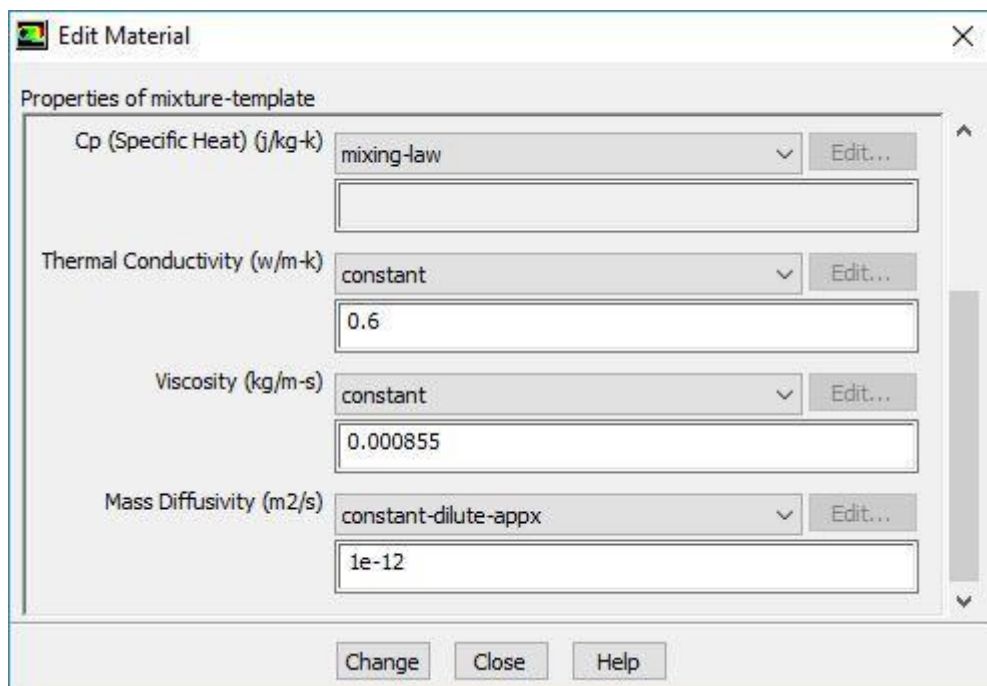
- Similarly do for the Catholyte fluid with the properties given in [1].
- II. Returning to the **“Models”** we now create the mixture of anolyte and catholyte defined earlier.
- Double click on the **“Species”** option to open the window as shown



- Ensure that the **“Mixture Template”** is selected for the materials and click on **“Apply”**, ignore any warning dialog box by clicking OK.
- Now again go to the Species window and click **“Edit”** option in the material tab.
- In the **“Edit Material Window”** under the Mixture Species option click on Edit. Add the anolyte and catholyte to the **“Selected Species”** and click OK to create the mixture.



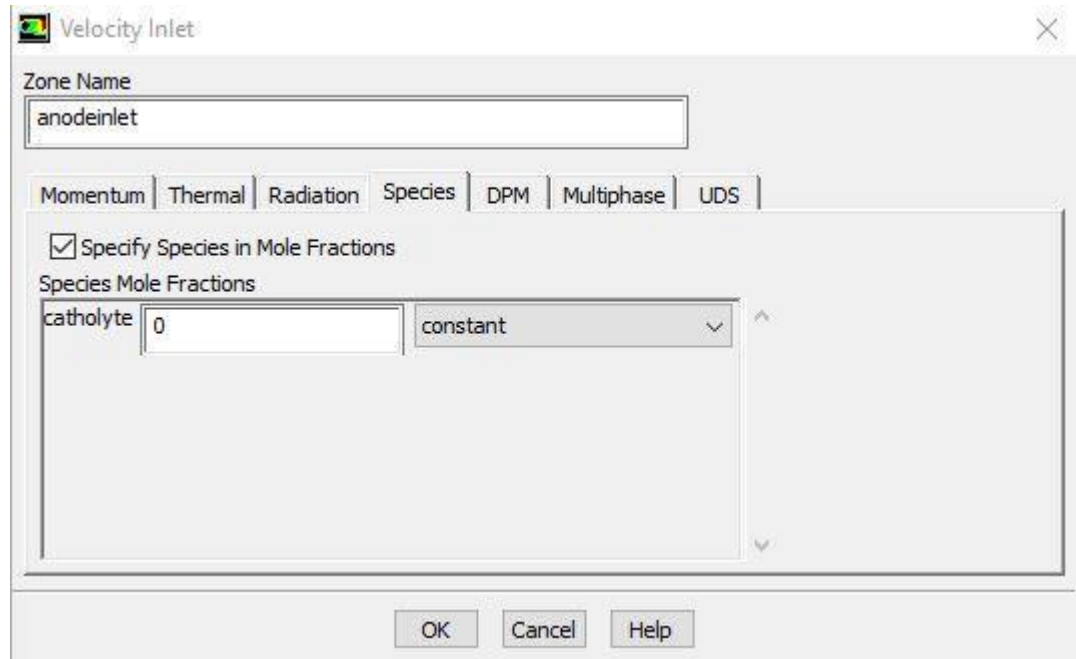
- In the Edit Material window input the properties of the mixture as given,



- This completes the defining process of governing equations and next we move on towards defining the boundary conditions.

6.3 DEFINING BOUNDARY CONDITIONS

- I. The inlets are set to **“Velocity”** type condition and the velocity is set to the desired value by clicking on the Edit option.
 - In the species tab, check the **“Specify Species in Mole fractions”** and for the anolyte inlet set the mole fraction of catholyte to zero.



- Similarly set the same for the cathode inlet side.
- II. The outlet boundary condition is set to **“Outflow”** which suits the best for our mixed analysis.
 - III. The named selection of channel wall boundary and electrode surface are set to **“Wall”** conditions.
 - This completes our definition of the mathematical model and we next move on to the numerical solution procedure.

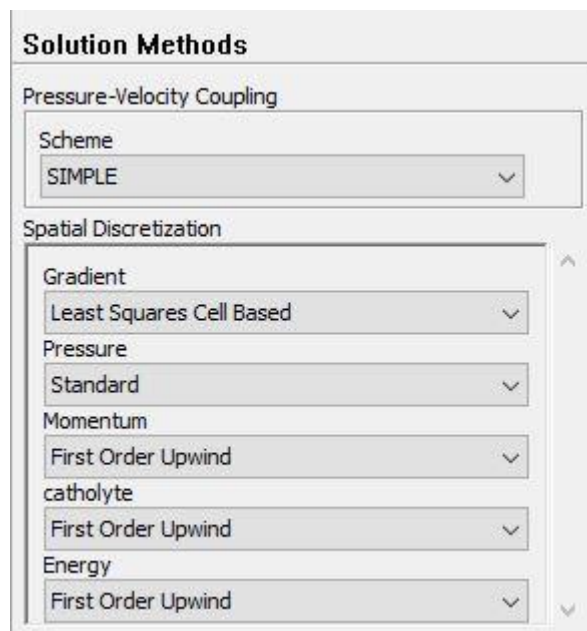
References

1. <https://drive.google.com/file/d/0Bwwl5g9eZz24cEhEYjEzQ0lQNG8/view?usp=sharing> – Fluid Properties.

7 NUMERICAL SOLUTION

7.1 SOLUTION METHOD

- Convergence of a solution is always an important aspect of a simulation and so here we have adopted a stepped solution procedure in order to achieve it.
- The first-order solutions are easy to converge but are approximate and often give misleading results. Second-order on the other hand result in higher accuracy but are harder to converge.
- This technique seems to provide a hybrid solution with nearly the same accuracy as the second order.
 - I. Firstly, the momentum, catholyte and energy are set to first-order in the solution controls option. The pressure is left at standard setting.

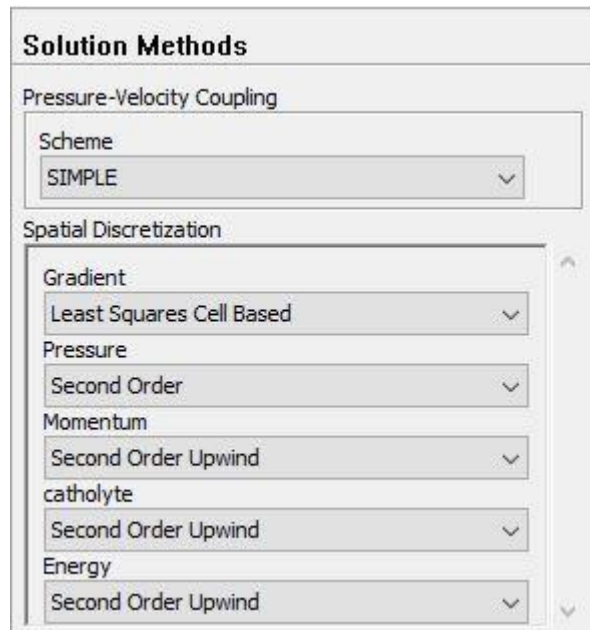


- II. Residuals monitors are limited to $1E-03$ for all of the variables so as to attain a better initial guess value for the second order solution to follow.
- III. The initialization used here is ***“Hybrid Initialization”*** as this enables proper initial conditions for the solution.

Note: The initialization affects the convergence i.e. a good initial value can lead to uniform and relatively easy convergence.

- IV. It is better to click on the ***“Check case option”***, this shows up if there are any incorrect settings in the Solution Methods tab.
- V. Run the iterations till convergence to our set limit of $1E-03$ for the residuals.

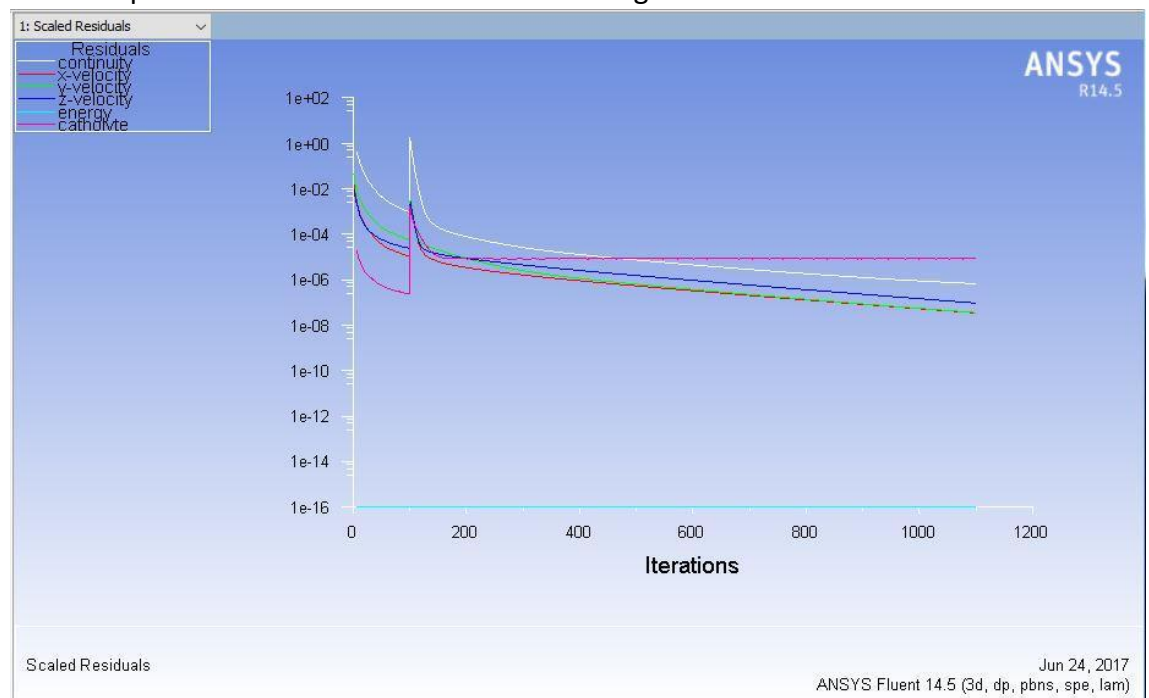
- VI. Now go to Solution Methods tab and change the settings for pressure and others to second order.



- VII. Change the limits for the residuals in the Monitors tab to $1E-05$ for *Catholyte* and $1E-06$ for the other residuals.
- VIII. Run the Calculation once again and allow it to run until 1000 iterations for proper convergence and results.

Note: The solution may take 3-6 hours to converge depending on the number of elements in the mesh and the computational ability of the system.

- IX. The final plot of the residuals will look something like



Note: The convergence limit for catholyte residuals is usually recommended at $1E-05$ and we can have correct results at that level.

- X. A close observation at the convergence is required as fluctuating residuals can lead to misleading results.
- XI. In our analysis the residuals of catholyte were fluctuating a bit for the first order solution phase whereas in the second order solution they became relatively stable.
- XII. The continuity and momentum residuals showed a continuously decreasing nature throughout the solution which is a good sign.

7.2 TROUBLESHOOTING

1. Backflow Problems:

- Backflow occurs when the flow going out is not defined properly by the solver. This usually occurs due to poor meshing at the outlet resulting in insufficient cells to define the flow.
- One of the important reasons why backflow occurs at the outlet is attributed to ***“The flow not becoming fully developed before going out of the channel”***.
- The easiest way to prevent this is to ***“Increase the height of the outlet”*** as this will provide the flow enough room for becoming fully developed.
- This measure needs to be complemented by ***“Mesh Refinement at the outlet”*** so as to maintain sufficient number of cells in order to realize the flow.
- It is feasible to have backflow occurring at 1-3 faces at the outlet, but in order to assure a correct solution it is recommended to completely remove any backflow occurring.

Note: This might affect the number of elements in the mesh and requires balancing in order to remain in the computationally feasible range.

2. Catholyte convergence (Species convergence):

- On solving for different heights and meshes of the microchannel, we observed that the *Convergence of catholyte is the most frequently encountered problem* in the analysis.
- The ***“Species residuals tend to attain a steady state”*** for all the cases that we analysed. Although it is not possible to influence the nature of convergence for the species residuals, we can alter their steady state values.
- The steady state values can be brought down by ***“Global refinement of the mesh by changing the body sizing”*** as this enables to resolve the mass fraction

of the species properly throughout the body and hence decrease the imbalance.

- Another method which results in a more pronounced effect is “**Use Fine Relevance Center in the Advanced Sizing Function**” as this will not only improve the overall element density but will also refine the mesh at the corners leading to better refinement of the mixing.
- Lastly, take a look at the mesh and “**Analyse the regions where refinement is necessary**” and apply sizing for them. This was typically the case for 15µm height where the element density at the channel sides was too low.
- In our analysis we performed the above given steps and were able to reduce the species residuals till $6.5E-06$ - $9E-06$ which is below the recommended limit of $1E-05$.

Note: The case for 15µm requires a special meshing method and thus will be discussed in the later part of this analysis.

- For further information, please refer to some online CFD discussion forums and websites like:
 - I. https://www.sharcnet.ca/Software/Ansys/16.2.3/en-us/help/ai_sinfo/flu_intro.html
 - II. <https://www.cfd-online.com/Forums/fluent/90281-convergence.html>
 - III. <https://www.computationalfluidynamics.com.au/convergence-and-mesh-independent-study/>
 - IV. <http://willem.engen.nl/uni/fluent/documents/external/guide-suc-fluent-sim.html>
 - V. <http://www.engr.uconn.edu/~barbertj/CFD%20Training/Fluent/4%20Solver%20Settings.pdf>

8 NUMERICAL RESULTS

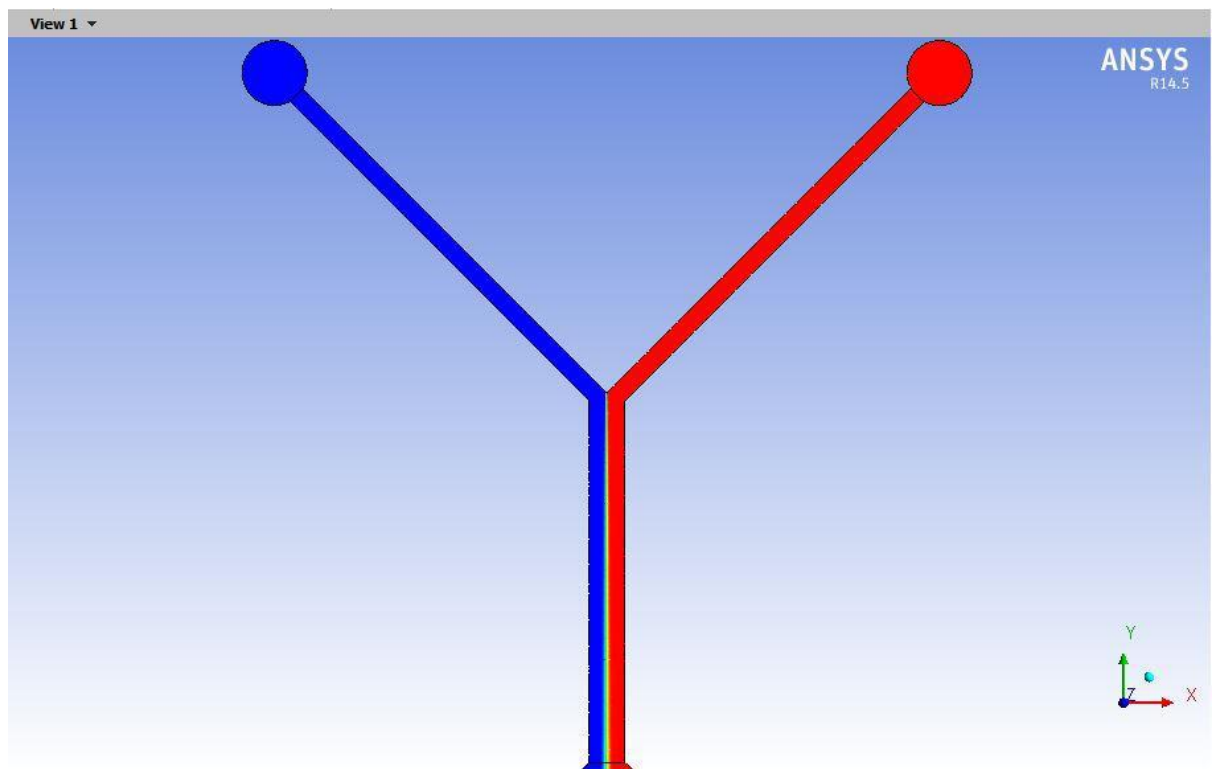
8.1 DEFINING THE POSITIONS

- CFD Post allows us to make contours, vectors, streamlines and plots of various variables calculated. These graphics require a domain to be plotted up onto.
- **Contours and Vectors require a plane** on which they can be plotted and so click on *Locations and select Plane* from the dropdown list. Give the appropriate coordinates to generate the plane.
- **Plots require a line** in order to generate a graph and so click on *Locations and select Line* from the dropdown list, and give the coordinates of two points

8.2 CONTOURS, VECTORS AND PLOTS

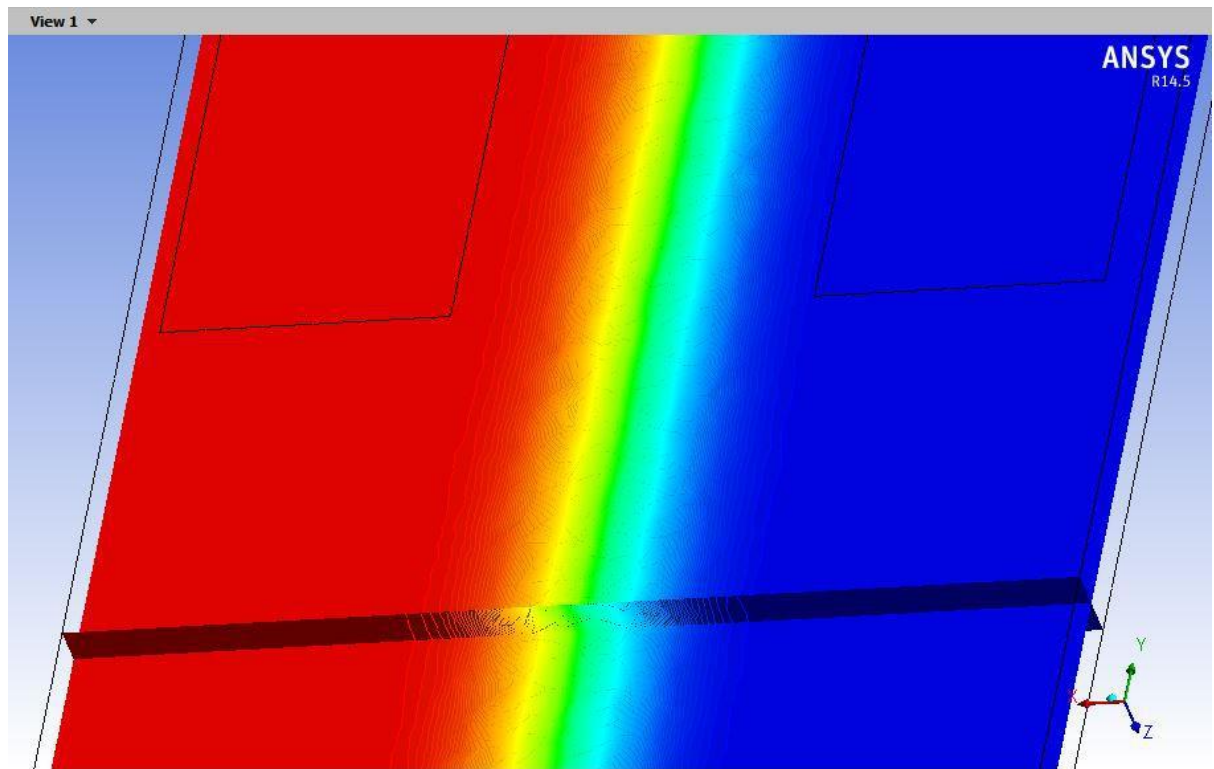
- The present results are of the 55 μ m height channel and they are as follows:

1. Mass Transport



- The contours of Mass Transport were plotted on the center plane and five other vertical planes of the channel.

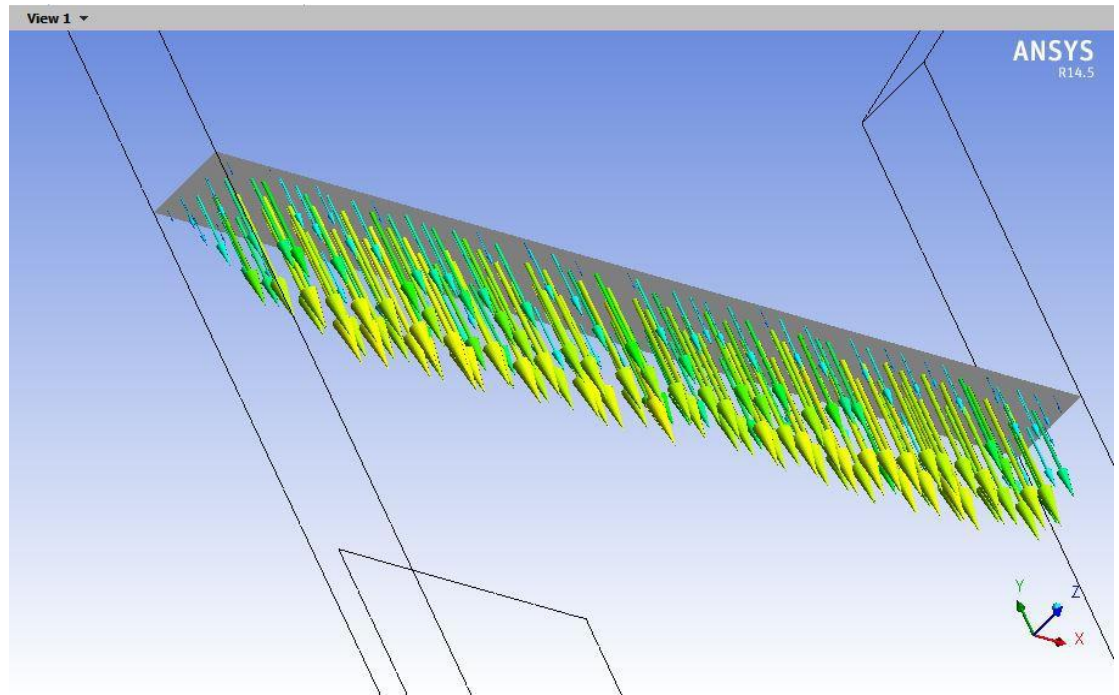
- There is an evident tapering of the diffusion layer between the catholyte and anolyte. This is consistent with experimental observations that suggest a downstream tapering.
- Another observation was made from the contours; the diffusion layer was away from the electrodes throughout the downstream length.
- This is essential as diffusion results in loss of reactants in their pure functional form and thus decreases the power output of the MFC. The given figure is the diffusion layer at the bottom part of the electrode:



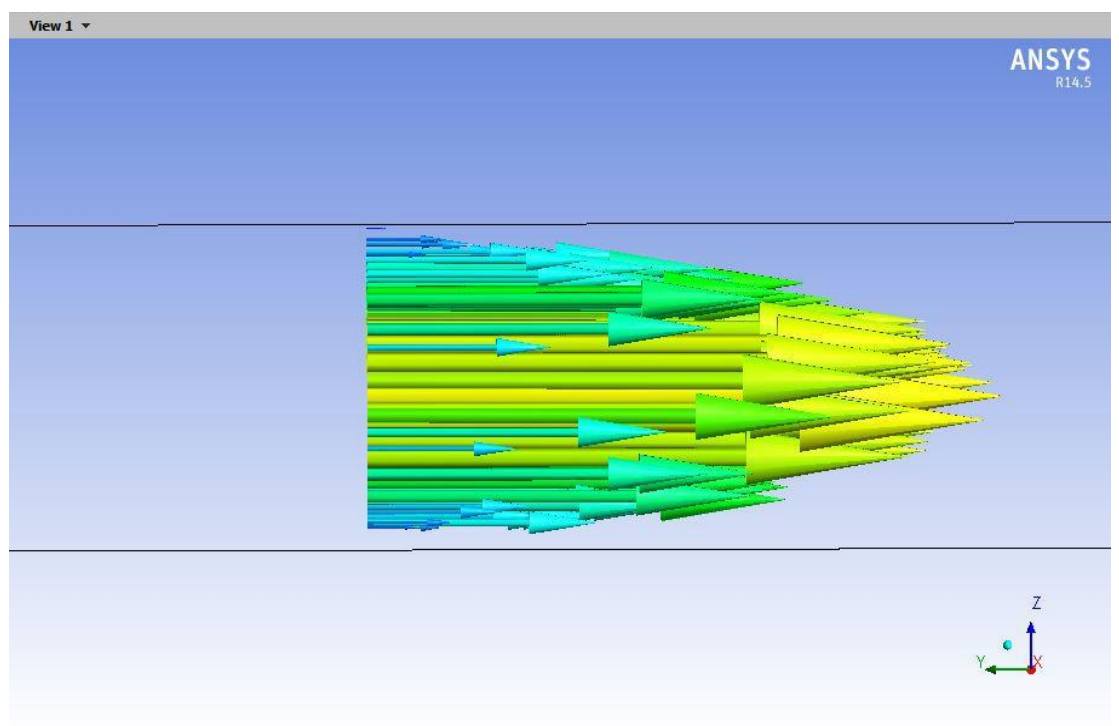
- From the figure above it is ensured that the diffusive mixing does not reach electrodes throughout the length and the power output is maintained.

2. Velocity Vectors

- The velocity vectors help us in visualizing the profile across a particular plane and make meaningful conclusions.
- The velocity vectors were plotted on four planes equally spaced along the length of the channel and their profile was observed and compared to analytical ones.



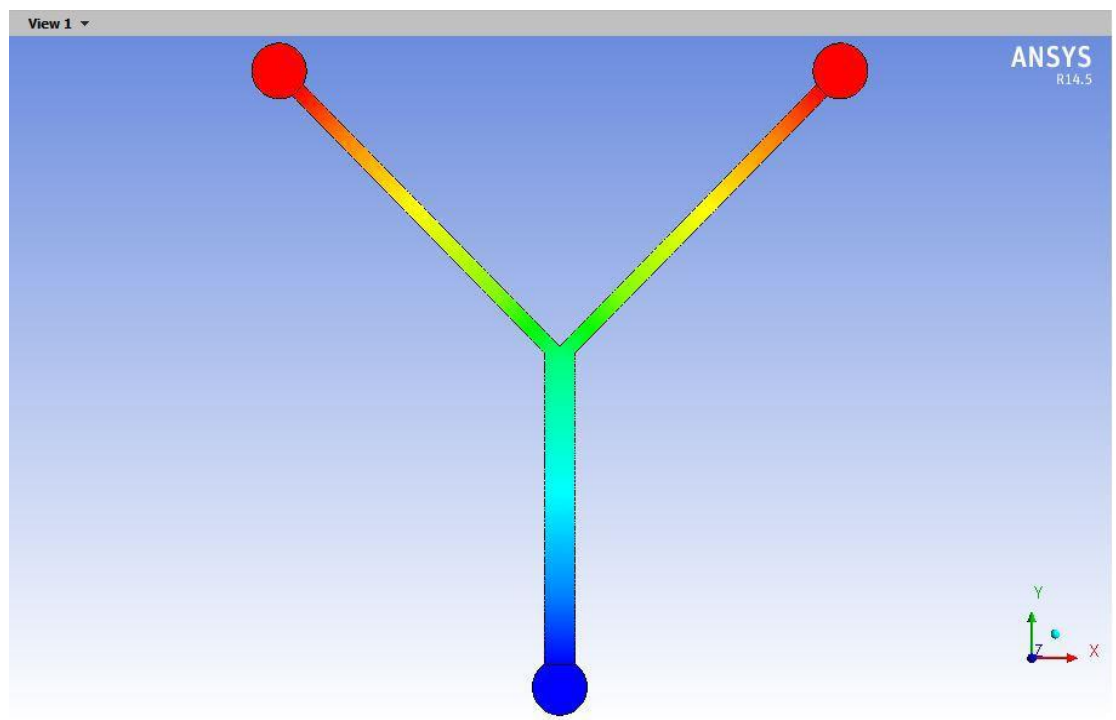
- This shows that the velocity is approximately constant across the center line of the plane. The number of vectors have been set to 100 though which may be increased to get a better view.
- Another important visualization is to see the profile from $-X$ axis and compare its nature to the Plane-Poiseuille flow profile.



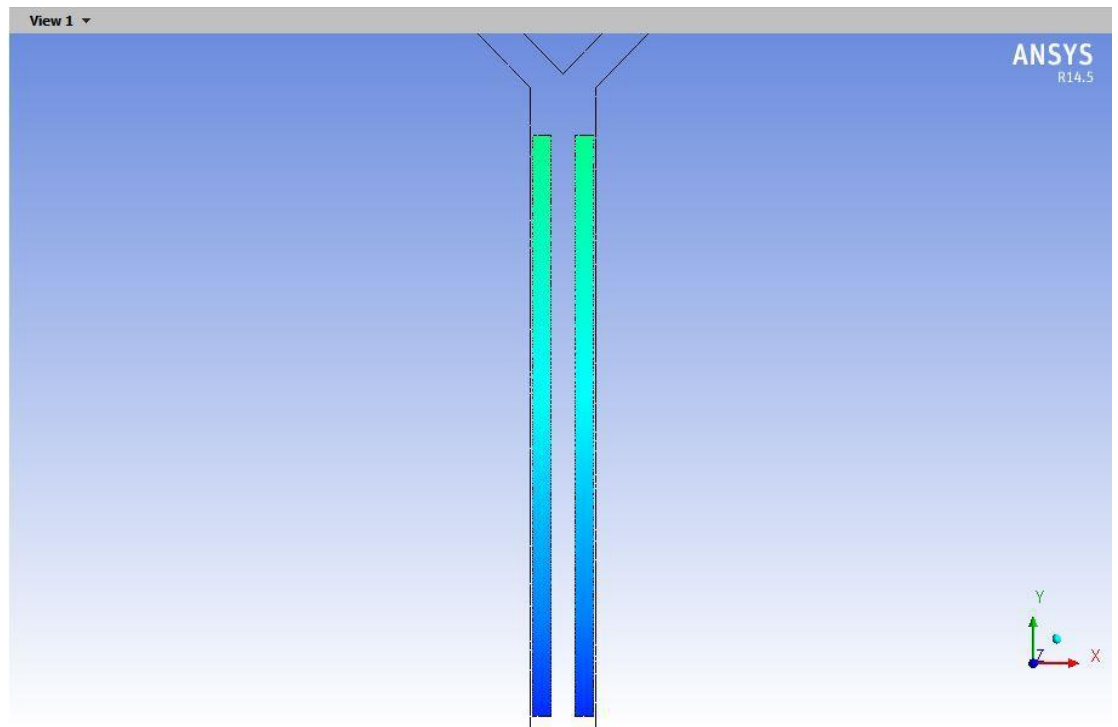
- As we can see, the velocity profile is mostly parabolic and thus is compatible with our expectations from the plane-poiseuille flow analogy profile.
- The maximum velocity occurs at the center of the channel and is consistent with the approximate analysis conclusions.

3. Pressure contours

- The pressure gradients in the channel determine the velocity magnitudes and so they are important to plot and compare with our expected trends.



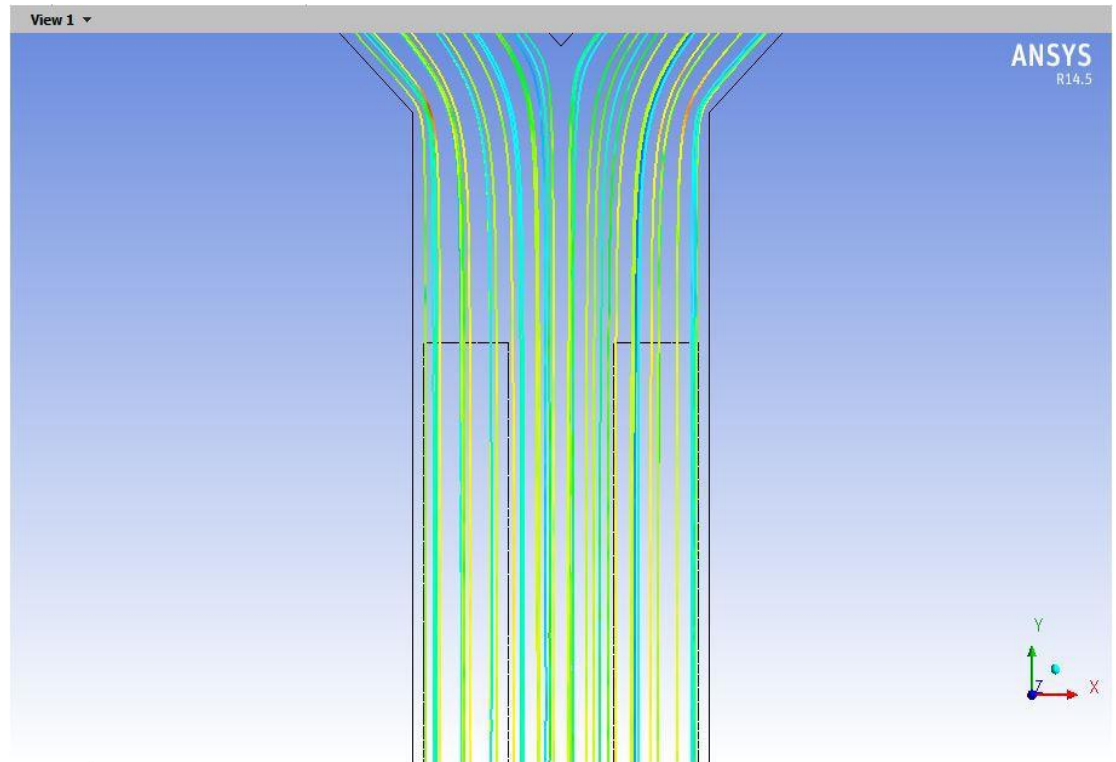
- The contour plot shows that the pressure decreases downstream of the flow. This is obvious as the flow can only occur if there is a pressure gradient across the channel.
- Another observation is that; the pressure remains the same at a cross section of the channel away from the intersection of the two inlet streams.
- The contour was plotted on the central plane and the pressure contour over the electrodes is shown as:



4. Streamlines / Pathlines

- The μ MFC utilizes laminar flow in order to separate the catholyte and the anolyte. This eliminates the need of a PEM and its associated losses and cautions.
- The laminar flow induced barrier can be visualized by plotting the Pathlines for the flow.

Note: Our analysis is a steady flow analysis which implies that the streamlines, streaklines and pathlines are the same.

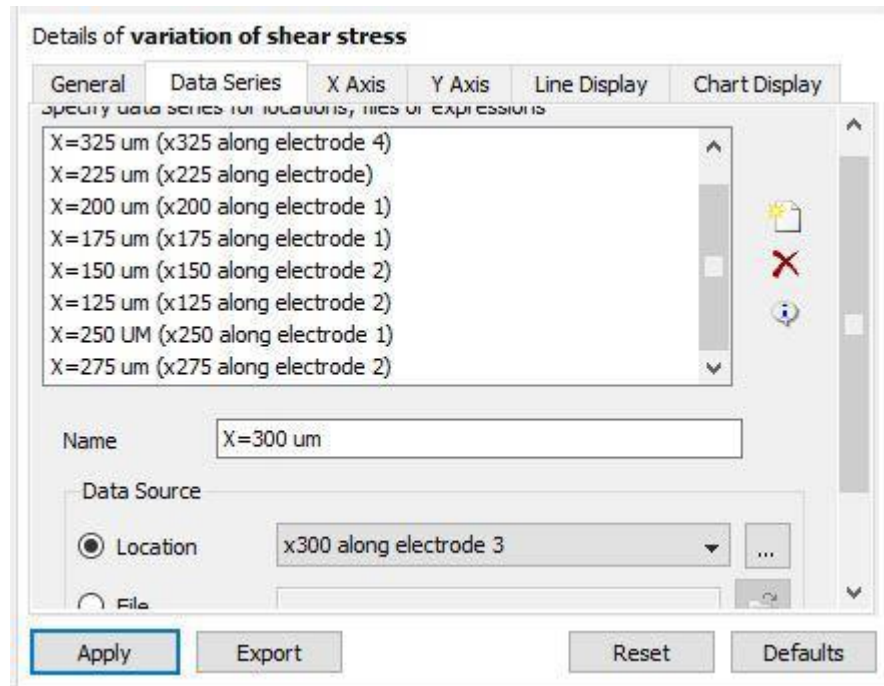


- We notice that the separation of the two fluids is maintained properly throughout the length of the channel and the only crossover is due to the diffusive mixing.

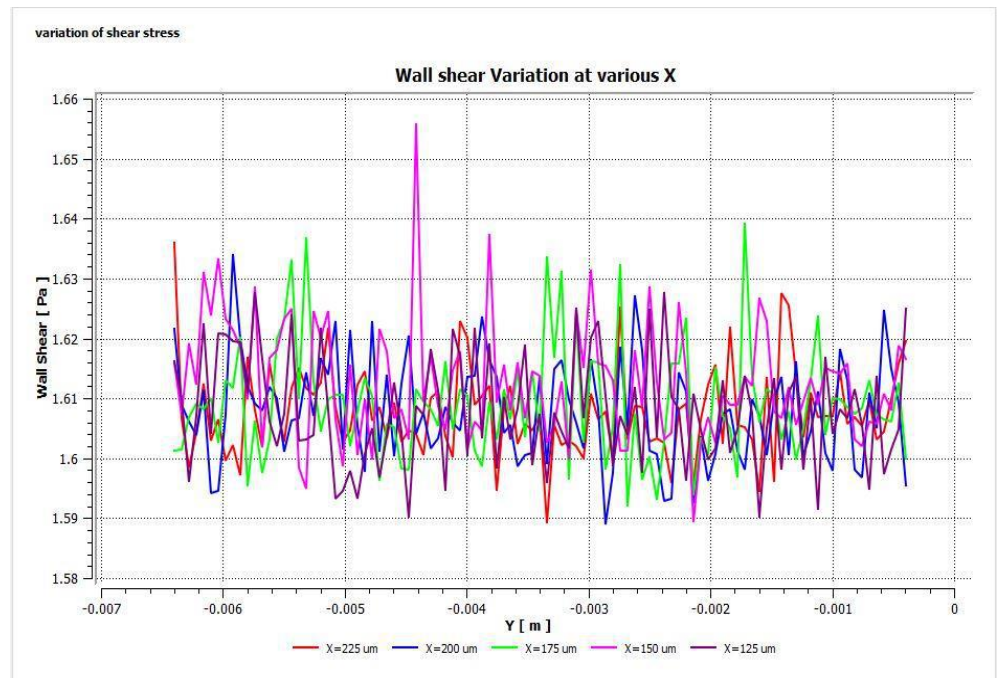
5. Wall Shear

- The wall shear over the electrodes is the most important variable in our analysis and its result defines the path ahead.
- Our previous results have helped in ascertaining that our setup and boundary conditions are correct. The flow properties match closely to that of our pre-analysis.
- We plotted the wall shear along streamwise lines on the electrode positioned at increasing distance from the center. The average of these values was taken to approximate the shear stress over the entire electrode.
- The shear stress was compared to our pre-analysis value but for this only half of the electrode was used (the one closer to the center). This was done in order to bring the channel case as close as possible to the plane-poiseuille flow.
- Near the corners of the channel the shear stress will decrease due to the low velocities at that locations.
 - i. Wall shear is averaged over the electrode and so we need to plot it with respect to Y distance at various X positions.

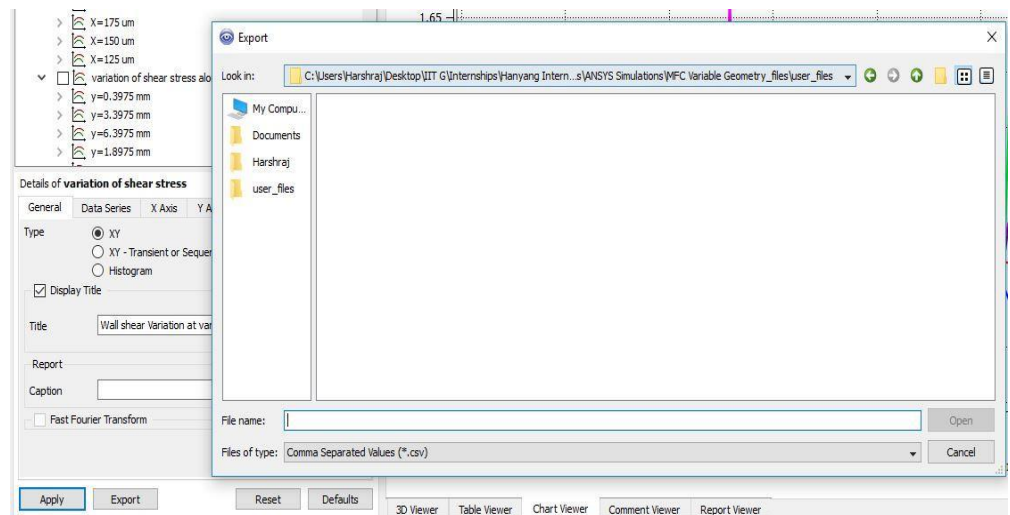
- ii. The lines required for the plots were created in the starting phase and so we will utilize them for our results.
- iii. **Click on the Chart** option from the toolbar on the top and name the chart as you like.
- iv. Now under the chart settings, In the *General* tab you can give the Title of the plot.
- v. In the *Data series* tab one can give locations for the plot to be made on and can add more than one plots to be made on the same graph.



- vi. The X-axis has the variable set to Y distance and the Y-axis has the variable as Wall Shear.
- vii. The wall shear variation is found to be quite irregular and we found the plot to be like:



- viii. Such plots were made after solving for different microchannel heights. Then the values were averaged to estimate the shear stress.
- ix. **Click on the Export** Option in order to create an excel file of the shear stress data. The averaging can be done on this excel file and so it is quite a handy option.



- The average shear stress from the plots for half electrode was
Shear Stress = 1.609 Pa
- Comparing this with our hand calculations we observe that the simulated stress is lower than the assumed case. This is expected as the assumed case

has infinitely long plates whereas here a channel is there which reduces the velocity.

- After this plots were extended to the other side of the electrode and the results were observed.
- The shear stress dropped drastically after 275 μ m distance from the center and this carried on till the end of the electrode where the shear stress was around 1.2 Pa.
- We noticed that the majority of the electrode had a more or less constant shear stress till 275 μ m and so the further analysis is based on the shear stress over half electrode as it constitutes the maximum shear region.
- All the plots and excel files for the shear stress are archived in a separate file on the system.

8.3 FINAL RESULTS

Height (μ m)	Shear Stress (Pa)	Error %	Proposed Q (μ L/min)
15	1.344	13.893 %*	3.592
35	1.537	2.132 %	16.995
55	1.609	-	40
75	1.67	0.519 %	72.25
95	1.709	2.17 %	112.969
115	1.734	5.07 %	162.391

**This case is addressed further in the special meshing techniques to reduce the large error involved in the shear stress.*

References

1. <https://drive.google.com/file/d/0Bwwl5g9eZz24Q0JwTzFNbmNqWEE/view?usp=sharing> – Results Report.

9 SPECIAL CASE

9.1 PROBLEM ASSOCIATED

- The large error in the 15 μ m case is due to the significantly low element density on the channel sidewalls which hampers proper refinement of the flow near the boundary.
- The species residuals for this case were at around $2.5E-05$ which is not favourable and leads to incorrect results.
- Thus efforts are made here in order to bring the catholyte residuals down to below $1E-05$ so that we can get reliable results.

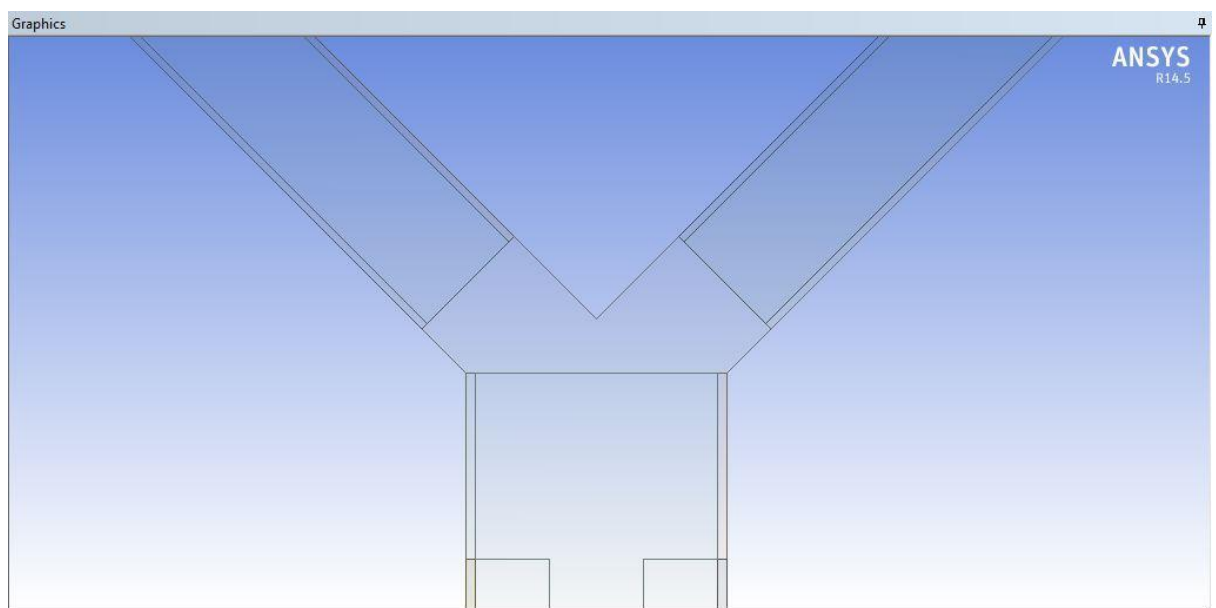
9.2 SOLUTIONS

- There are some solutions to this problem and they can be put together as:
 - I. Using *Fine Relevance Center* in the Advanced Sizing Function results in refinement at the corners and can help a bit in bringing the species residuals down.
 - This will only result in a small drop in residuals as the mesh is refined only at the corners and selected parts.
 - Also it does not rectify the underlying problem of having less tetrahedral layers at the channel walls and has the same number of layers as before.
 - II. Decreasing the *min size in the Advanced Sizing Function* will result in smaller tetrahedrons and hence will allow us to have more than two layers at the sidewalls.
 - This will result in a considerable decrease in the residuals and can lead to a correct solution

- But the number of elements after this operation reach an alarming value i.e. 1,00,00,000 elements. Solving for these many elements is not within the computational limits of our system.
 - This leaves us with the final method, which is economical in terms of number of elements and relatively easy to adopt.
- III. The main problem is associated with the side walls and so if we can independently mesh the walls and the rest of the body then we can reduce the number elements and still get enough layers.
- This is handled by slicing the geometry into parts and applying **Sweep Operation** on the sidewalls. The elements will be of hex type and so we can get 10-15 layers at the walls without increasing the number of elements drastically.
 - But here the main problem comes in defining the interfaces of the parts in FLUENT and usually it is not able to realise the boundary types effectively.

9.3 SWEEP METHOD

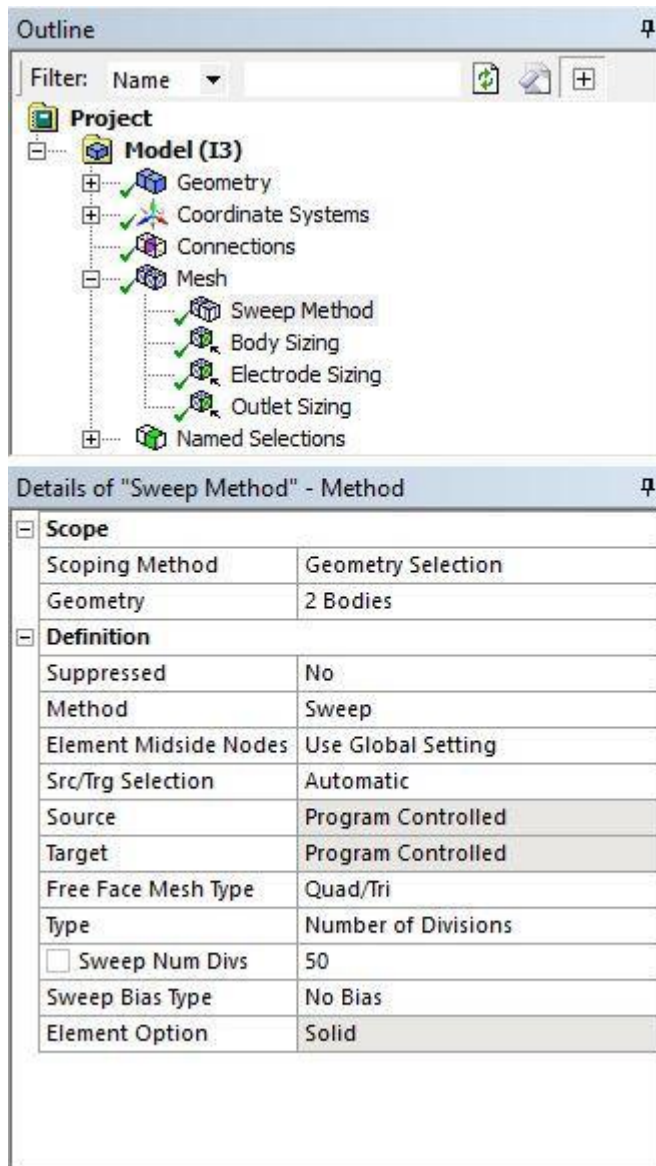
- The sweep method is mostly used in the problems where there are parts and meshing needs to be done by introducing different sizing in them.
- In our case we have a single microchannel body and so we need to slice it into parts to apply the sweep process.
- We sliced it in such a way that most of the wall area gets covered in the sweep and the rest of the parts were joined to form a single body.



- Then we used sweep operation on the wall parts and set the number of divisions to 10 in order to get sufficient refinement.
- For information on how to use the sweep process refer to these sources:

<https://www.youtube.com/watch?v=Uw-SK2y2w9M>

<https://www.youtube.com/watch?v=CQ7ISccRecQ>



Note: This example is for a different case, but it is enough to give an idea of how to manage the settings for the sweep operation.

- Before you use the sweep operation it is recommended to check the sweep able bodies in our geometry. This operation is performed in the Meshing module of ANSYS.
 - Right click on Mesh in the tree** and then under **Show -> Sweep able bodies**.
 - This shows the bodies that are available for the sweep operation.
 - Select the bodies onto which you wish to generate the refined mesh.

- iv.** Also the source and target matter in the sweep operation, automatic is mostly appropriate but if more characteristics are desired then manual selection is favourable.
- v.** The type of elements can be Tri, Quad or Quad/Tri depending on the requirements. Here in order to allow the largest freedom to the mesher Quad/Tri has been selected.
- vi.** Number of division are bounded by the refinement needed and the number of elements at the bottom and top respectively.
- vii.** The bias setting introduces a sizing gradient in the sweep. This is effective in capturing the boundary layer effects in turbulent problems and so is not much needed for our application.

9.4 COMPLICATIONS IN SWEEP OPERATION

- The slicing of the geometry in our case led to many parts and thus lead to many interfaces between the parts.
- FLUENT solver needs defined connections at these interfaces in order to connect them together. The connections were made in the mesher but they did not appear as is in the solver.
- Thus difficulties arose in assigning boundary conditions on so many interfaces which led to incorrect setup of the solution.
- The end effect was that the Hybrid Initialization did not work and so the problem was rendered to be quite difficult to solve because of improper initial conditions.
- Thus although this method results in good refinement at the walls it created problems in solving due to the large number of interfaces.

10 VERIFICATION

- Convergence is not the only measure of checking whether the solution is correct or not. There are further checks to be performed before we conclude a final solution.

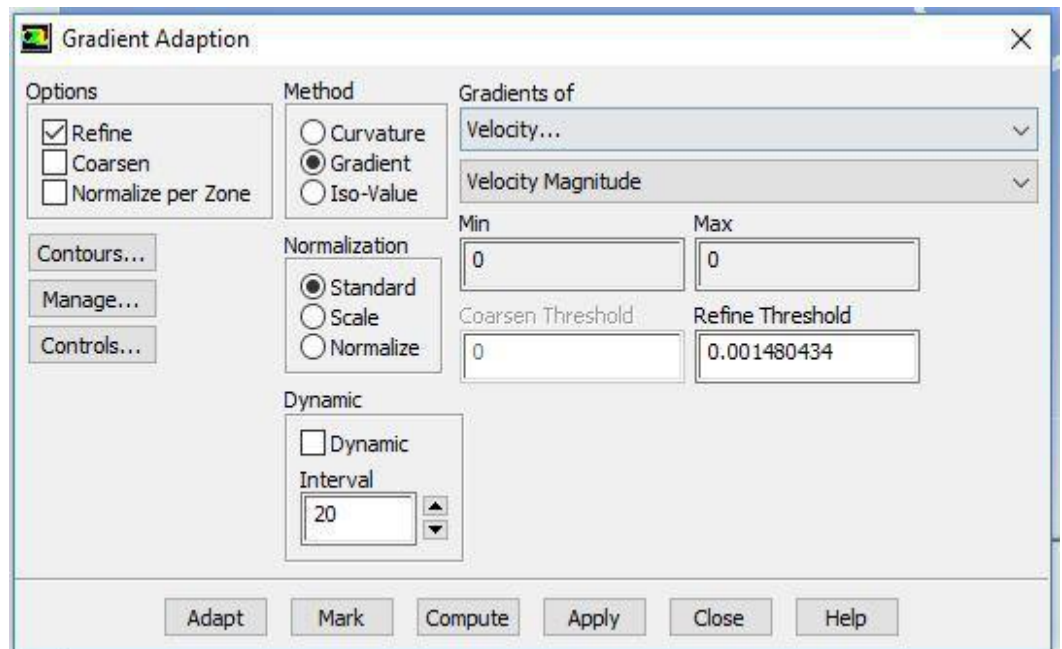
1. Mesh Independence Study

- The mesh size affects the solution of a problem and so iterative solution processes with refined meshes are needed in order to attain a mesh independent solution.
- Due to the involved time and memory restrictions the refinements were only carried out until 20,00,000 elements. Initial mesh sizes were around 15,00,000 elements.
- So further refinement resulted in the limiting number of elements. The shear stress value changed but changes were very small in comparison to the magnitude.
- Hence we concluded that the solution was mesh independent to a considerable extent.

2. Grid Adaption Studies

- ANSYS has an inbuilt mesh alteration program which refines the mesh at certain critical areas where the gradients in variables are high.
- This is called grid adaption and is extensively used in turbulent flows or in flows where abrupt changes are expected.
- Grid Adaption is usually done after the solution has been completed once and has been initialized again for the next process.
- For the procedure leading to grid adaption refer to the following source:
<https://www.youtube.com/watch?v=DPwK6W2e9RA>
 - i. Solve the problem once with a certain mesh and obtain the results.
 - ii. Next Open FLUENT by double clicking on Setup in the project home page.
 - iii. Grid Adaption requires the solution to be initialized and so go to Hybrid initialization and perform the same.

- iv. **Click on Adapt** option on the title bar and **select Gradient** from the dropdown list.
- v. Ensure that the following settings are maintained:



- vi. The variable in the Gradients of options defines the refinement that will be needed in the adaption process.
 - vii. **Click on Compute** to find the min and max values for the variable variations. Now we need to define the threshold for refinement.
 - viii. The Refine threshold is generally set to 1% of the maximum value in most of the cases.
 - ix. **Click Adapt** in order to change the mesh and to capture the gradients properly of the specified variable.
- The grid adaption was carried out for the velocity variable and around 2000 cells were introduced in the original mesh.
 - The shear stress in the grid adapted case was same as the original mesh till the fifth decimal place. Thus this ensured that the solution is correct and independent of any alterations in the mesh.
 - Though it was apparent as the number of cells in the refined mesh were only 2000 more than the original and hence one can expect the same result for both cases.

11 FUTURE POSSIBILITIES

1. Solution for 15 μ m case

- The sweep method allowed us to introduce extra layers at the walls but resulted in complex solution setup.
- The main reason behind failure of the setup was lack of knowledge on part meshing and solving. Though easy problems involving one or two interfaces can be dealt but such a complex problem was beyond our knowledge.
- Future possibilities of solving the part-sweep method still remain open for working on and they will surely result in closer solutions and less errors.

2. Tapered Electrode

- The diffusion width increases as we move downstream and so in order to maximize the contact with fresh fuel and oxidant in the MFC a tapered electrode design can be formulated.
- Thus it would be interesting to observe the shear stress over tapered electrodes and how they vary with the flow rates.

3. Embossed Electrodes

- Surface area available for the flow to occur affects the performance of the MFC. The higher the surface area the better is the performance.
- We propose an embossed electrode surface which not only increases the surface area but also results in higher shear stresses at the same flow rate as the normal ones.
- This results in lower flow rate for the optimal shear stress and hence higher fuel efficiency which is an important gain for a MFC.

