CONCLUSIONS

Chitosan polymer can be applied to the membrane of proton exchange membrane fuel cell. The proton transfer mechanism is the important key to improve the performance of the cell. The determination of geometrical parameters of chitosan is the first step to study for this mechanism.

This thesis focuses on the simulation of chitosan oligomers for finding the best conformation of chitosan oligomers giving the lowest molecular energy. The results obtained from PM3, AM1 and *ab inito* F/6-31G* are good agreement with the reported X-ray crystallographical data. It can be concluded from the results that the model of chitosan oligomers can be used to determine the proton transfer mechanism for the membrane of PEM fuel cell.

Chitosan oliogomers was firstly studied. The extrapolation of chitosan polymer gives the energy gap. The near zero energy gap shows the good conducting property of polymer. The energy gap, in this research, is investigated by semiempirical AM1 and *ab initio* HF-6/31G*. The obtained energy gaps from extrapolation are 0.04 and 0.89 eV., respectively. Therefore, the chitosan polymer has high potential to be the conducting polymer because of its near zero energy gap.

The proton transfer mechanism is investigated based on proton hopping mechanism. The important key of this part is the water content. The study is varied into 3 water contents; 10, 35 and 90%. The results propose that the 35% water content is the best content for proton transfer in chitosan membrane because the amount of water is consistent. The distance between water and the active sites of chitosan oligomers of 35% water content is closer than that of 10%, thus, proton can transfer easily. In addition, the large amount of water in chitosan oligomers with 90% water content can induce the hopping of proton from water to water and cause flooding in the membrane which decreases the performance of the proton transfer.

The proton transfer mechanism will release an equivalent number of electrons. Thus, the electrical current is calculated by conversion of the electron charge per time in second. The result gives the current output from one chain of chitosan pentamer, in fact the membrane using for PEM fuel cell is the polymer, thus, the electron will release more than this result. Therefore, the current output must be greater than one chain of chitosan pentamer.

In the future, modifying of chitosan membrane by additional salt as a conducting part in the membrane should be studied for the improvement of conducting performance. In addition, the proton transfer in any polymers should be studied for comparison in the performance of each polymer and for investigation of making the membrane for the best performance of PEM fuel cell.