CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

From the results it can be concluded that the gas chromatography behavior of CFC compounds can be described by means of general physico-chemical properties, like boiling point and topological descriptors, like connectivity index (χ) on non-polar stationary phases, since these interactions are non-specific. For the more polar columns, a specific parameter, like dipole moment, is required. The everage error of the models with BP as one of the parameters on the three columns is about 20 index units (i.u.) and is about 46 i.u. for the models without BP. The agreement between predicted and measured retention indices is satisfactory.

The three approaches of analysis have advantages and disadvantages. PCA is a good method to use to study the behavior or background of the system from the score and loading plots, but it is not suitable for prediction. PLS can also make one understand the system and seems to be the best method for predicting the retention indices or the missing data in the data matrix but only if there are some data of the products. Therefore PLS cannot be used for recognition of unknown products. Stepwise regression analysis can provide several models based on purposes and data available. It can be used for both prediction and recognition. It gives a good prediction result but is less accurate than PLS. So in the case of prediction, if one does not have the PLS program in hand, combination of PCA and regression analysis will be sufficient to obtain a good model and to understand the behavior of the system.

6.2 Recommendations

1. The models obtained from this study can give the prediction results with a defined percentage of certainty only for the CFC compounds with one and two carbon atoms. Additional work can be done to modify the models for basic predictions of CFCs with higher carbon atoms by examining other families of CFCs and try to relate all the data with number of carbons (nC) as one of the parameters.

2. Additional work can be done to improve the global equation in function of the McReynolds polarity scale by investigation of the retention indices of these compounds on other columns of different polarity.