5 Conclusion and future work

Determining CO_2 absorption in liquid phase of MEA-CO_2-H_2O system by an analytical technique is useful in many aspects. It saves time and gives access to online monitoring of the system. The accuracy of laboratory methods is based on the skill of the analyst, demand time, labour and resource. Offline laboratory methods cannot be used for process automation. Eventhough, these traditional methods are still used to control the process parameters in CO_2 plants due to the non-availability of in-situ analysis methods.

In this paper, we present the development of Labview/Matlab based software platform which is connected to iC Raman software in Raman RXN2 Analyzer. The platform provides concentration profiles of different chemical species present in an MEA-CO_2-H_2O system. These concentration values are calculated indirectly from measurements from Raman analyzer. The calculation is based on partial least square regression method. PLS and data pretreatment algorithms were written as matlab scripts.

If a calibration and validation data set is available, this system can be easily modified to another amine based CO_2 capture system without extensive effort. For instance, there are other amines which have the ability to absorb CO_2 and Raman instrument can be used to determine the total CO_2 absorbed and the concentration of other chemical species. If the user needs to use this GUI for such amines, he can input new calibration and validation data set into PLS script and change the preprocessing script in Matlab accordingly. The developed system can also be used to monitor how the reaction between an amine and CO_2 evolves with time in a batch reaction.

It is also recommended to take the use of the data to perform other chemometric analysis such as principle component analysis, outlier detection and multivariate curve resolution to better understand the chemical system. The plots related to these analysis can be implemented in the developed GUI similar to the concentration plots.

References

Andersson, M. (2009). A comparison of nine PLS1 algorithms. *Journal of Chemometrics*, *23*(10), 518-529. doi:https://doi.org/10.1002/cem.1248

Eigenvector Research, I. (29 March 2013). Advanced preprocessing: Noise, offset, and baseline filtering.

Eigenvector Research, I. (2018a). PLS toolbox. Retrieved from http://www.eigenvector.com/software/pls_toolbox.htm

Eigenvector Research, I. (2018b). PLS_Toolbox 8.2.1 software Manson, WA USA 98831. Retrieved from http://www.eigenvector.com

IEA. (2017). CO2 emissions from fuel combustion: Overview Retrieved from http://www.iea.org/publications/freepublications/publication/CO2EmissionsFromFuelCombustion2017Overview.pdf

Jinadasa, M. H. W. N., Jens, K.-J., Øi, L. E., & Halstensen, M. (2017). Raman Spectroscopy as an Online Monitoring Tool for CO2 Capture Process: Demonstration Using a Laboratory Rig. *Energy Procedia*, *114*, 1179-1194. doi:https://doi.org/10.1016/j.egypro.2017.03.1282

Kaiser. (2018). iC Raman™ 4.1 Software. Retrieved from http://www.kosi.com/na_en/products/raman-spectroscopy/raman-software/ic-raman-4.1.php

Li, H.-D., Xu, Q.-S., & Liang, Y.-Z. (2018). libPLS: An integrated library for partial least squares regression and linear discriminant analysis. *Chemometrics and Intelligent Laboratory Systems*, *176*, 34-43. doi:https://doi.org/10.1016/j.chemolab.2018.03.003

Li, T., & Keener, T. (2016). *A review: Desorption of CO2 from rich solutions in chemical absorption processes* (Vol. 51).