Interfacing of Off-line Data Analysis and Instrument Control for SGA/ACM

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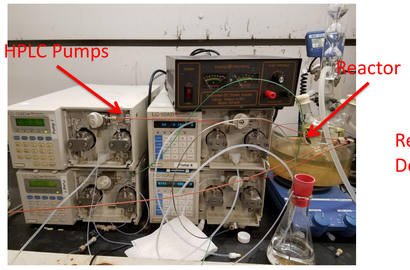
SMART SUMMER MATERIALS RESEARCH @ TULANE

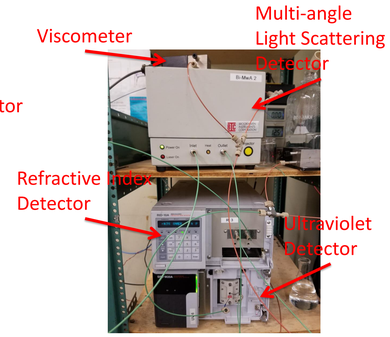
Abstract

The goal of this project is to development several programs that be capable of 1) analyzing data from either of the ACOMP or ACM systems to provide a user friendly interface to study the physical properties of different types polymer/ polymer reactions, 2) controlling instruments such as monomer feeding pump, SGA infusion multi head syringe pumps, to realize the polymerization reaction control or control/adjust stimuli conditions.

ACOMP and ACM

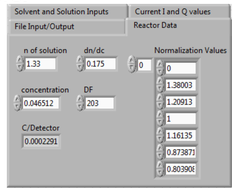
Automatic continuous online monitoring of Polymerization (ACOMP) and automatic continuous mixing (ACM) were used to preform our reactions. The ACOMP systems acquires the polymerization reaction information by Extracting a very small amount of sample from the reactor, after a serial of dilution/conditioning of the sample, the online product continuously enters a series of detectors. These detectors include a viscometer, multi-angle light scattering, ultra-violet, and refractive index detectors. The ACM system utilizes one pump that mixes the solution and solvent before pumping it through the detectors.



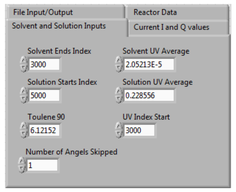


Data Analysis Program

A customized program which could conduct offline data analysis from results gathered from ACOMP and ACM has been successfully developed . To operate the program, the user needs to input basic reaction information. The program analyzes the Mw based on the Zimm equation and calculates extrapolated Mw by plotting MALS data kc/I(θ) vs Q^2, where q = (4πn/λ)sin(θ/2). This extrapolation of kc/I(0), which equals to 1/Mw + $2A_2$ could also provide as the second Viral coefficient. Considering the angular independency of the 90 degree LS signal, the program is be able to plot kc/I(90) vs c as well, and kc/I(0) vs c, where k is the optical constant, c is the concentration, I is the intensity of the scattered light, and Mw is the average molecular weight of the polymer. The ACOMP data analysis version can calculate the polymer information based on both the reaction information and Instrument's parameters.



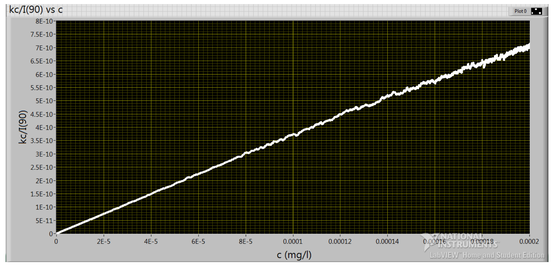
Instrument information input window

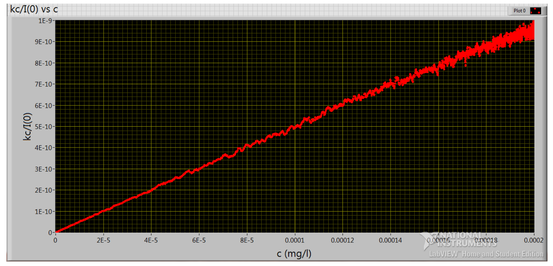


Polymerization reaction input window

ACOMP Data Analysis

Analysis results of the polymerization reaction of styrene sulfonate.

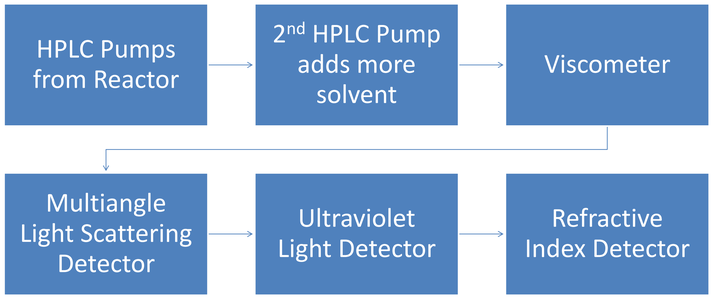




The off-line data analysis is comparable with that done by Matlab program, but such operation interface offers a more user friendly environment. Also it could be adapted to a supplementary subprogram of the SGA online DAQ/ Analysis interface, which could be utilized if the normalization factors are adjusted in the reaction process or certain angle(s) signal quality is bad.
Another feature of this homemade program is that data from MALS units from different manufacturers (5 angles or 7 angles).

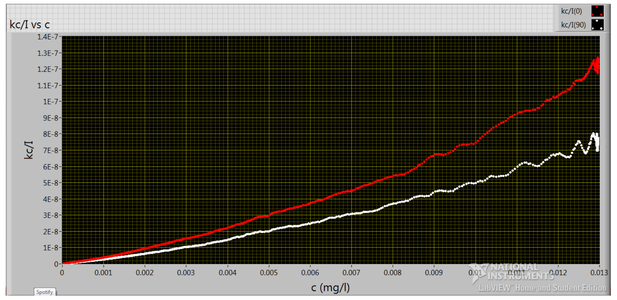
ACOMP System for Polysoap Reactions

The Sketch below is the configuration used for the specific reaction of poly-soap, the monomer concentration is about 3 mg/ml in MeOH, and after dilution the concentration is targeted at .03 mg/ml in order to get the best resolution and quality of signal.



ACM Data Analysis

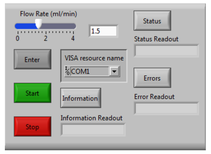
Analysis results of polystyrene sulfonate ACM test.

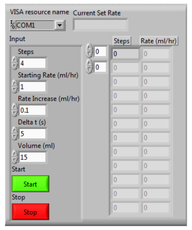


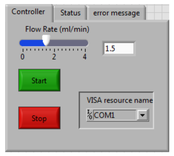
Besides ACOMP off-line data analysis capability, the home made program has certain versatility that can handle ACM characterization data, which simplify the data analysis.

Instrument Communication

Multiple applications of communicating with different pumps have been successfully developed. The programs are able to control the flow rate of the pumps as well as start and stop these pumps.
The programs can control a Nexus 6000 HP Syringe Pump and HPLC pump. The control of HPLC pump allows us composition control for copolymer semi-batch reactions to design molecules at specific molecular weights. While the syringe pump control improve the automation degree of the SGA system. Communication via different protocols have been done based on the type of instruments , such as RS232 serial communication with RTS/CTS flow control, and conventional USB serial communication.
The programs were developed based on LabVIEW 2015, and C language codes.







Conclusion

The offline data processing was successfully able to analyze data from polymer reactions and ACM . Data taken from the multi-angle light scattering detector and the ultra-violet light and RI detectors was used in the program. The program was able to accurately make Zimm plots and extrapolate further information about the polymer. The program calculated the molecular mass and concentration of the polymer for every data point.
The instrument control programs have be successfully developed via different communication protocols, which are ready to be utilized on SGA system

Acknowledgements

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