

TAC 2011 report prepared by D. Kumar Khamar

Thermal Analysis and Calorimetry (TAC) 2011 conference was held at the School of Pharmacy in Queen's University, Belfast from 18-20th April. This meeting is held annually by the Thermal Methods group (TMG) of The Royal Society of Chemistry. Taking place just before Easter every year it attracts people from a wide range of disciplines; crystallization, polymer science, catalysis, agricultural, food science, ionic liquids etc.

Upon arriving to Belfast in the morning, I went straight to the conference venue using public transport without much trouble. This year, on the first day an intensive short course; "Thermal Analysis Techniques An Overview" was organized. This workshop covered different aspects of Differential Scanning Calorimetry (DSC), Thermo Gravimetry Analysis (TGA), Thermo Mechanical Analysis (TMA), Dynamic Mechanical Analysis (DMA) and evolved gas analysis. In the morning session, Nicole Hunter (Thermo Fisher Scientific) and Paul Gabott (PETA solutions and Thermal Instruments Ltd) gave a detailed overview of principles, different types of DSC and TGA instruments, hyphenation options with these techniques, various factors affecting analysis and discussed scope and application of these thermal techniques in various fields. Followed by this, Ted Charsley (University of Huddersfield) gave a comprehensive talk on calibration of DSC and TG equipment. He showed potential errors involved in calibrating DSC at single heating rate when calibrant and sample may have significantly different heating rate dependencies and suggested use of stepwise isothermal heating for calibration. In the afternoon session, Simon Gaisford (University of London) gave an interesting talk about the application of DSC in polymorphic phase transformations where he discussed the importance of separating kinetic and thermodynamic events by using different heating rates. He also showed usefulness of isothermal calorimetry with humidity modifier to quantify amorphous content. Ian Pristely (Syngenta) gave a final talk in the workshop about industrial use of thermal analysis to study thermal instability in materials and in turn determining safe methods for the screening, handling and processing of potentially explosive materials. In his talk, he discussed handling of up to 400kg sample for calorimetry which was quite fascinating for everybody in the conference. After finishing the workshop, I then went to my bed and breakfast accommodation where I spent most of the time watching a John Travolta movie in a communal room before retiring to bed.

The actual conference started on the second morning with the presentations divided into four sessions: stability and ageing for first two sessions, polymer processing in the afternoon and pharmaceuticals as the last session. Duncan Price (Edwards Vacuum) talked about controlling combustion chemistry to reduce hazardous material out into environment and echoed the notion in the morning session that "dilution is not a solution to pollution." In the polymer session, Sam Gnaniah (National Physical Laboratory) gave an interesting talk about an international interlaboratory exercise as part of VAMAS (www.vamas.org) Technical Work Area, which will assess glass transition (T_g) determination by DMA. He outlined the lack of precision in determining T_g with alternate methods - thermal methods and DMA and need for standardization.

There were plenty of opportunities for networking and poster viewing during the afternoon tea session. Like the oral presentations, the content of posters varied from different fields and I particularly liked the cocrystal study using Thermally Stimulated Current (TSC) spectroscopy. In the pharmaceutical session, I enjoyed Paul Matejtschuk's (National Institute

for Biological Standards) talk about using thermal techniques over non-thermal methods for the residual moisture detection in the lyophilized biological material. His data showed a better sensitivity, even in low masses by TGA with evolved gas analysis over gravimetry, NIR and Karl Fisher method and he also discussed measures to improve repeatability by TGA in such cases; by reducing helium flow rate and appropriate pan selection. The first day of the conference was ended with an appealing reminder of wine reception before the conference dinner which was organized in the evening.

The second day of the conference was divided into three sessions. First session included pharmaceutical presentations in which Cameron Alexander (University of Nottingham) set the scene with discussions on new and emerging materials for targeted delivery systems and analytical constraints with them. I was the second speaker in the morning and felt bit nervous in discussing a detailed thermal analysis of theophylline in front of expert calorimetrists. The audience was great and patient until I used "any questions" phrase at the end! I received a number of questions and the answers were well received.

The second session was kept for manufacturer's scientific presentations each comprising 15 minutes and it was decided that this session would not have question-answer time at the end of each presentation. Rather delegates were encouraged to inquire any question in the lunch time. Tim Mann (Perkin Elmer) talked about application of TGA-GCMS for complex organic systems and recent advances in transfer lines which can enable TGA-IR-GCMS. This could be very useful for pharmaceuticals as it allows faster, efficient and simultaneous characterization of small quantity of material. I was impressed by some of the applications of Flash DSC shown by Lester Troughton (Mettler Toledo). This DSC can be used to heat material over 2 million K/min heating rate and can be used to study polymorphic transformation, glassy and amorphous state along with number of other applications. John Davies (Optas) emphasized using organic solvent in Dynamic Vapour Sorption (DVS) to get additional information out of DVS study especially in case of amorphous characterization. Long lunch time in a manufacturer's exhibition area provided boost for the delegates to discuss and inquire various instruments with the representatives of various instrument manufacturing companies. I was also impressed by the option of using high pressure with a Setaram DSC instrument. The final session included presentations on ionic liquids and catalysis.

In the end, the prizes were announced; £100 for oral presentation, £50 for poster presentation. These two prizes were decided by committee and one people's choice award was reserved for one of the manufacturer representative for which each delegate voted for one speaker from manufacturer's scientific presentations. I am very happy to say that I received a prize for oral presentation in this conference. The group from Agri-food and & Biosciences institute, Belfast received a prize for their poster presentation on seaweed characterization work. People's choice award was given to Tim Mann from Perkin Elmer. He received a pack of wine bottles. He seemed happy but lamented that he has to pay to carry those bottles back to England as he did not have any checked-in luggage. Finally, the closing remarks were given by Ian Priestley. He thanked the host - Vicky Kett (Queen's University, Belfast), representatives of different companies, all the delegates and announced TAC 2012 at University of Nottingham.

The conference ended at 3pm and gave me plenty of time to think about both conference and workshop before I went to the airport. In those 3 days I had great opportunity to discuss and present my work with experts in thermal analysis, which I did. I received valuable feedback

from number of delegates including the most fruitful discussions with Simon Gaisford, Ian Priestley and John Davies. Importantly, I could realize the vast potential of these techniques in a wide range of subjects apart from my work. It was still early to go to the airport. So, I took a break from science and felt relaxed after watching historical and magnificent photo exhibition of the Titanic at city hall, Belfast. I was amazed to see the scale of shipping industry 100 years ago in that lively city.

I would like to say a big thank you to BACG. I am very grateful to BACG for providing me such a great opportunity at this juncture where I would not have made it to Belfast without a financial help from BACG. I am also thankful to my supervisor Dr Linda Seton for her help in registration of this conference and raising my resources to attend it.