

# Vapourtec R Series and METTLER TOLEDO FlowIR<sup>™</sup> Integration

#### November 2011.

As a result of a collaboration between Vapourtec and METTLER TOLEDO, users of the Vapourtec R Series and the FlowIR<sup>™</sup> can now enjoy tighter integration.



Vapourtec R Series

The FlowIR<sup>™</sup> is a in-situ FTIR system which enables a chemist to see the exact chemical composition of the output of their continuous flow reactor system in real time providing structural information across a wide range of functional groups/chemistry. (More information at the end of this article)

As a result of this new integration:

- Data from the FlowIR<sup>™</sup> can be displayed in real time and logged by the Vapourtec FlowCommander<sup>™</sup> software, along with other reaction data,
- Collection of reaction product peaks can be triggered automatically based on the values detected by the FlowIR<sup>™</sup> in the output product stream



### How It Works

The setup is straightforward. A special software component ("SpreadMon") from Vapourtec is run on the same PC used for the METTLER TOLEDO iC IR<sup>™</sup> software. This component extracts the specified data, and sends it through the LAN to the FlowCommander software.

Up to 8 different data sets can be sent to FlowCommander™

In the FlowCommander<sup>™</sup> software, these trends are displayed on a single chart along with the other reaction data charts (flow, temperature, pressure, reactor power consumption), and the predicted concentrations from the dispersion algorithm.



The trend data can be saved and viewed offline in the FlowCommander<sup>™</sup> software away from the lab, or extracted to a spreadsheet for further analysis alongside other reaction parameters.



## **Triggering Product Collection**

In March 2011, Vapourtec announced the facility to automatically trigger the collection of product peaks in real time based on the output of a UV detector placed in the product stream. http://www.vapourtec.co.uk/newsletter/archive/mar11

This same facility can now be used to define triggering criteria for capturing product output based on FlowIR<sup>™</sup> data.

etector Triggered Collection		
0.30 AU		
0 AU 0 Node: Whole Peak	Expected Peak AU: 0.30	20
Trigger Conditions	End Conditions	
Level Above 0.05 🚔 AU	Level Margin 0.01 🜩 AU	
Slope Above 2.0 * AU/ml	Slope Margin 0.1 C AU/ml	
Collection starts when the LIV/Vis level is	above 0.05 AU, and the slope is above 2.0 A	
	below 0.04 AU, and the slope is below 1.9 AU	
	v at 0.20 ml/min through 90cm is 212 seconds.	
ovivis Detector to conscion rom dela	at 0.20 minimin through socin is 212 seconds.	- OK

Note that, as with UV triggering, it is possible to define different criteria for each reaction in a queue. For example, it would be possible to add the same reaction to the queue twice and collect product in each case according to different collection criteria.

# FAQ

- Q When is this facility available ?
- A January 2012
- Q What do I need to use this ?
- A The latest version of FlowCommander<sup>™</sup> software (running on PC or touchscreen) and a METTLER TOLEDO FlowIR<sup>™</sup> system.
- Q How is the FlowIR<sup>™</sup> system connected to the Vapourtec system ?
- A The Vapourtec touchscreen (or PC) and the METTLER TOLEDO PC must be connected via a LAN.
- Q How I define the IR data I want to use ?
- A Configuration of the trends (up to 8) to be monitored by the FlowCommander<sup>™</sup> software is done within the iC IR<sup>™</sup> software. "SpreadMon" extracts the data, and FlowCommander<sup>™</sup> then displays the data and can be configured to collect product based on one of the datasets.



#### More about the FlowIR<sup>™</sup>



The FlowIR<sup>™</sup> in-situ FTIR system from METTLER TOLEDO enables a chemist to see the exact chemical composition of the output of their continuous flow reactor system in real time providing structural information across a wide range of functional groups/chemistry.

The small footprint (equivalent to a Knauer micro HPLC pump) allows the unit to be positioned virtually anywhere, maximizing it's flexibility and minimizing it's impact on the limited space available. The interchangeable FlowIR<sup>™</sup> Sensors allow the user to quickly and easily swap sensor types to meet the application needs. No liquid nitrogen for detector cooling and lack of instrument purge also make this system the least complicated to use for synthetic chemists, while maintaining the high level performance expected by traditional ReactIR<sup>™</sup> technology. Some of the key benefits that the FlowIR<sup>™</sup> can bring to flow chemistry are;

- Sub millimolar sensitivity covers wide range of chemistry concentrations
- Versatile software allowing real time monitoring of starting material, product and intermediates
- Greatly assists in reaction understanding and optimization
- Covers full spectral region with swappable diamond and silicon sensors
- Allows stoichiometric reaction control (minimizes excess of expensive materials and reduces workup)
- Detect process upsets instantly (improve product quality and loss of product)

For more details see <a href="http://www.mt.com/flowir">http://www.mt.com/flowir</a>