

## Flow Commander™ Software

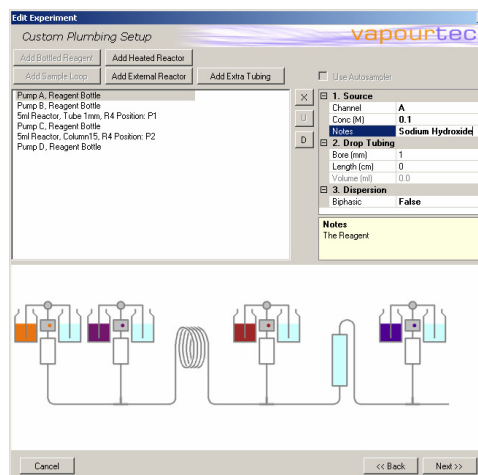
The Vapourtec R Series flow chemistry system can be used in a standalone mode, with a simple to use interface and clear, easily visible displays. But it is with the addition of the Flow Commander™ software that the chemist is able to get the full benefit out of the system.

What exactly can this software do ?

### Setting up the Experiment and Planning Reactions

First of all, Flow Commander allows you to specify your experimental setup and then define the details of each specific reaction you wish to carry out using that setup (ratios of the reagents, reactor temperatures and residence times, how much product to collect etc).

Flow commander will take the residence times, reagent concentrations and stoichimetric ratios you specify, and calculate flow rates. It will then handle all the details of calculating time delays based on pipe lengths and reactor volumes.



Specifying the experimental setup

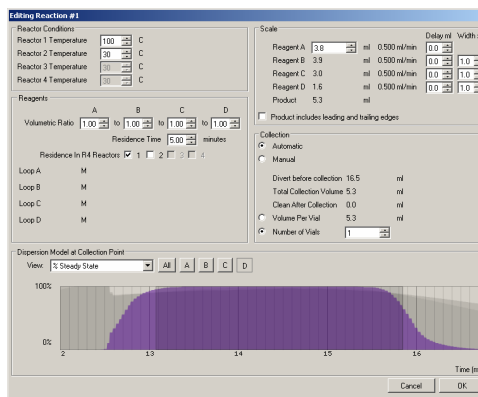
### Collection and Dispersion

Flow Commander™ also calculates the dispersion that will occur as reagents proceed through each of the tubes and reactors specified in your experimental setup. It is therefore able to say exactly how much of the leading and trailing ends of your finished product stream should be collected.

This can be visualised (see right) so that you can see exactly which part of the “peak” each vial corresponds to.

For each reaction, you can define either the amount of product you want to collect or the amount of reagent you want to consume (e.g. “I only have 10 mls of reagent A – what is the most good product I can make ?”).

You can choose collect the product from a reaction in any number of vials.



Defining an individual reaction  
(Dispersion graph shown at bottom)

## Fully Automate Any Number of Reactions

Flow Commander™ can not only calculate all the details of *one* reaction - it allows you to define a sequence of reactions (**limited only by the number of collection sites on your fraction collector**) and then run these reactions completely unattended, whether you are there or not. This allows you to optimise reactions by exploring a wide multi dimensional workspace, varying reaction temperature, residence time, concentration and reagent ratios.

And as you add reactions to the queue, the software calculates the total of each reagent that will be consumed by the whole series, so that you know how much of each to load before starting the sequence.

Flow Commander 1.6

File Experiment Logs Setup Tools Help

Charts Experiment

Edit Experiment Clear Run Stop Emergency Stop Add Add From Current Edit Delete Up Down Prime Autosampler

Experiment

Collection

Solvent Usage: 63.7 ml est.  
 Reagent A Usage: 14.6 ml  
 Reagent B Usage: 13.5 ml  
 Reagent C Usage: 11.3 ml  
 Reagent D Usage: 6.3 ml

#	Reagents A : B : C : D	Res Time (Reactors)	Temperature	Collection (FC sites)	Notes
<input checked="" type="checkbox"/>	1.00 : 1.00 : 1.00 : 1.00	5.0 min (1)	100 C, 30 C	5.27 ml (1)	
<input checked="" type="checkbox"/>	1.00 : 1.00 : 1.00 : 1.00	10.0 min (1)	100 C, 30 C	5.02 ml (2)	
<input checked="" type="checkbox"/>	1.00 : 1.00 : 1.00 : 1.00	10.0 min (1)	150 C, 30 C	5.02 ml (3)	
<input checked="" type="checkbox"/>	1.50 : 1.00 : 1.00 : 1.00	10.0 min (1)	150 C, 30 C	5.15 ml (4)	

Reactions in this Experiment

Action

- 1: Set flow of all pumps to zero, reset reagent and sample loop valves, power off
- 2: # Initialise Fraction Collector
- 3: Initialise Fraction Collector
- 4: Switch Collection Valve to Collect
- 5: Set Reactor 1 to OFF
- 6: Set Reactor 2 to OFF
- 7: Set Reactor 3 to OFF
- 8: Set Reactor 4 to OFF
- 9: Set System pressure limit to 15.0 bar

Connection: COM1 Not Connected

System I Pump A Pump B  
 bar bar bar  
 set limit  
 Power  
 air air

System II Pump C Pump D  
 bar bar bar  
 bar bar  
 air air

Pump Speed set  
 Pump A: ..... Pump B: .....  
 Pump C: ..... Pump D: .....

Reactor Temperature set  
 20/0 20/0 20/0 20/0

Valve Control I Valve Control II

Heater Key 1 2 3 4 Pressure  
 System I  
 Pump A  
 Pump B  
 System II

**Main Experiment Display showing queued sequence of reactions and the target fraction collector positions of each product**

Once you have a sequence of reactions lined up, you can start them and leave the system to run. Because the Vapourtec system can detect blockages, leaks or air in the system, it runs safely unattended.

## Remote operation

Once the R Series system is running under Flow Commander™ control, the PC becomes the system's user interface. You can therefore observe and interact with the system from elsewhere (perhaps back in your office, using Remote Desktop Connection, or from offsite using GotoMyPC® or LogMeIn®). You might prefer to design your sequence of experiments while sat at your desk in a quiet office, rather than in the lab, for example. You can even make changes to the running sequence (i.e. disable reactions that have yet to be done if you decide they might not be worthwhile). It is also possible, if necessary, to locate the actual PC running Flow Commander™ remote from the R Series system and connect the two via a LAN.

## Saving, Logging, Sharing and Reporting

Flow Commander™ allows you to save a given experimental setup and reactions, then re-use the information later. This information can be shared with others who also have a Vapourtec system, allowing them to instantly repeat proven reactions. During any reaction, key information can be logged and saved, then presented later (and charted) in a report. If (for example) a UV Detector is used, the report will show the UV trace for each vial that was collected.

Files can of course be put into an electronic lab note book system if required.

## Scale Up

When it is time to scale up a proven reaction, things couldn't be simpler. Simply change to a bigger reactor, and tell Flow Commander™ the new reactor details. All the key independent parameters (time, temperature, stoichiometric ratios) remain the same, and the flow rates are automatically recalculated. You can now decide how much product you want to make.

## In Summary

The Flow Commander™ software turns the R Series into an fully integrated optimisation platform. It enables the integration of a fraction collector, UV sensor, and even an autosampler. Up to 4 separate pumped reagent channels can be precisely controlled, enabling maximum productivity, flexibility and reagent efficiency, while keeping a solid documentary record of everything that goes on.

In short, Flow Commander™ enables R Series owners to get the very best out of their investment by making the best of their time and reagents.