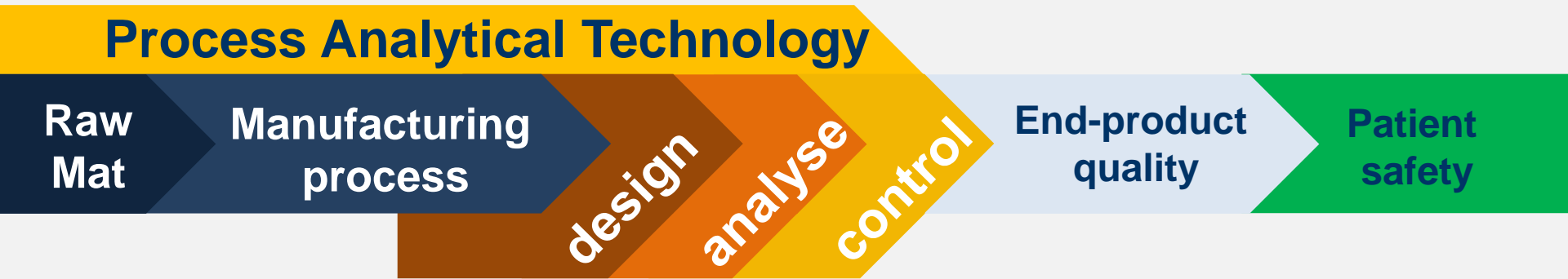


Spectroscopy & Predictive Analytics

Gledson Emidio



Quality by design

Quality should be built
not just tested

PAT Tools

Raman

VIS

NIR

FLUORESCENCE

CALORIMETRY

DIELECTRIC

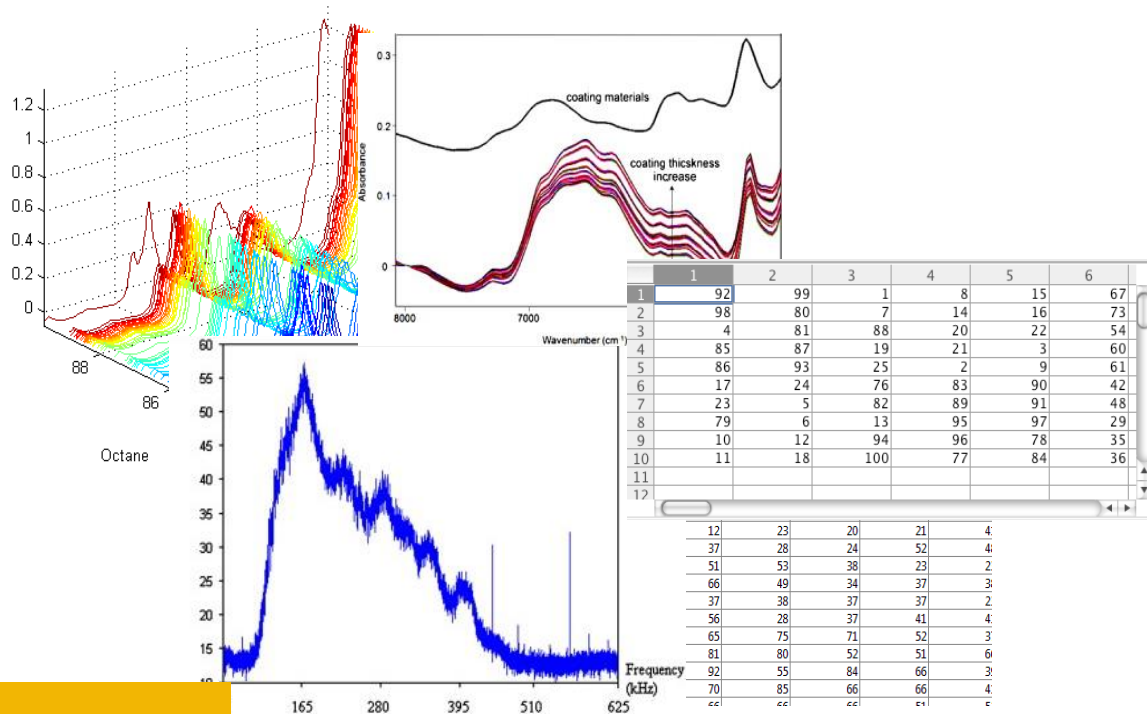
NMR

IMPEDANCE

VIDEO MICROSCOPY

ACCOUSTICS

SENSORS



PAT Tools

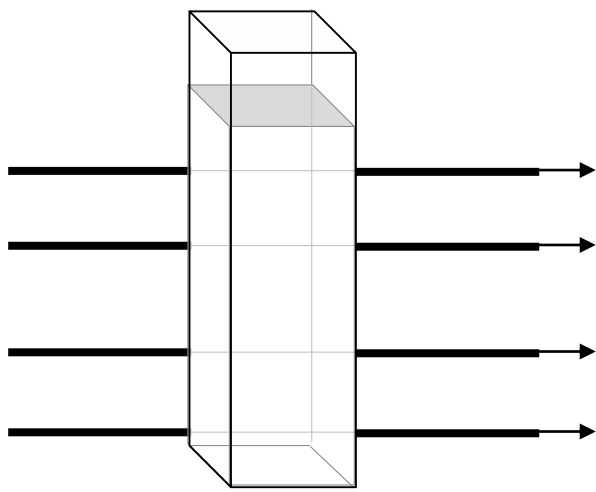
Multivariate Data Analysis

Design of experiments | denoising

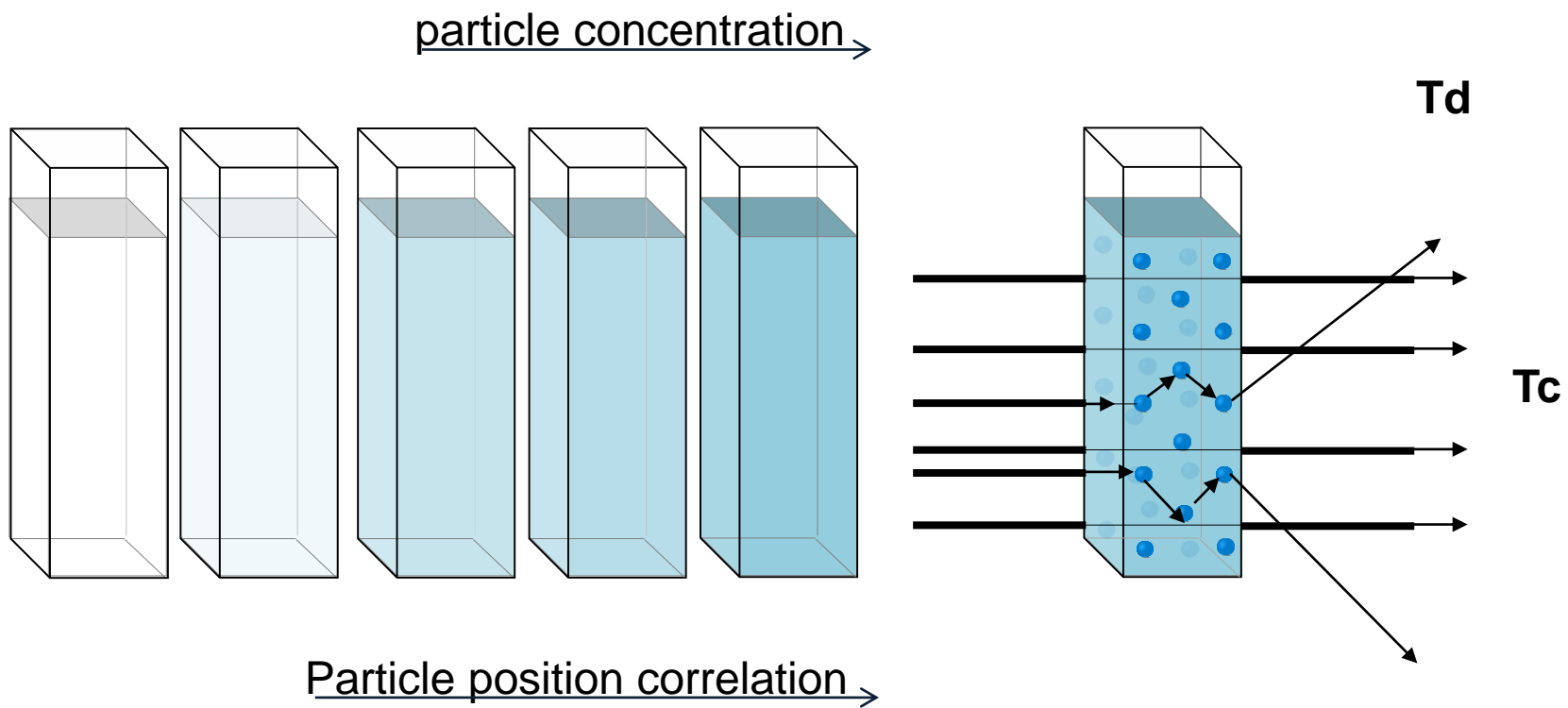
Scatter correction | Variable selection

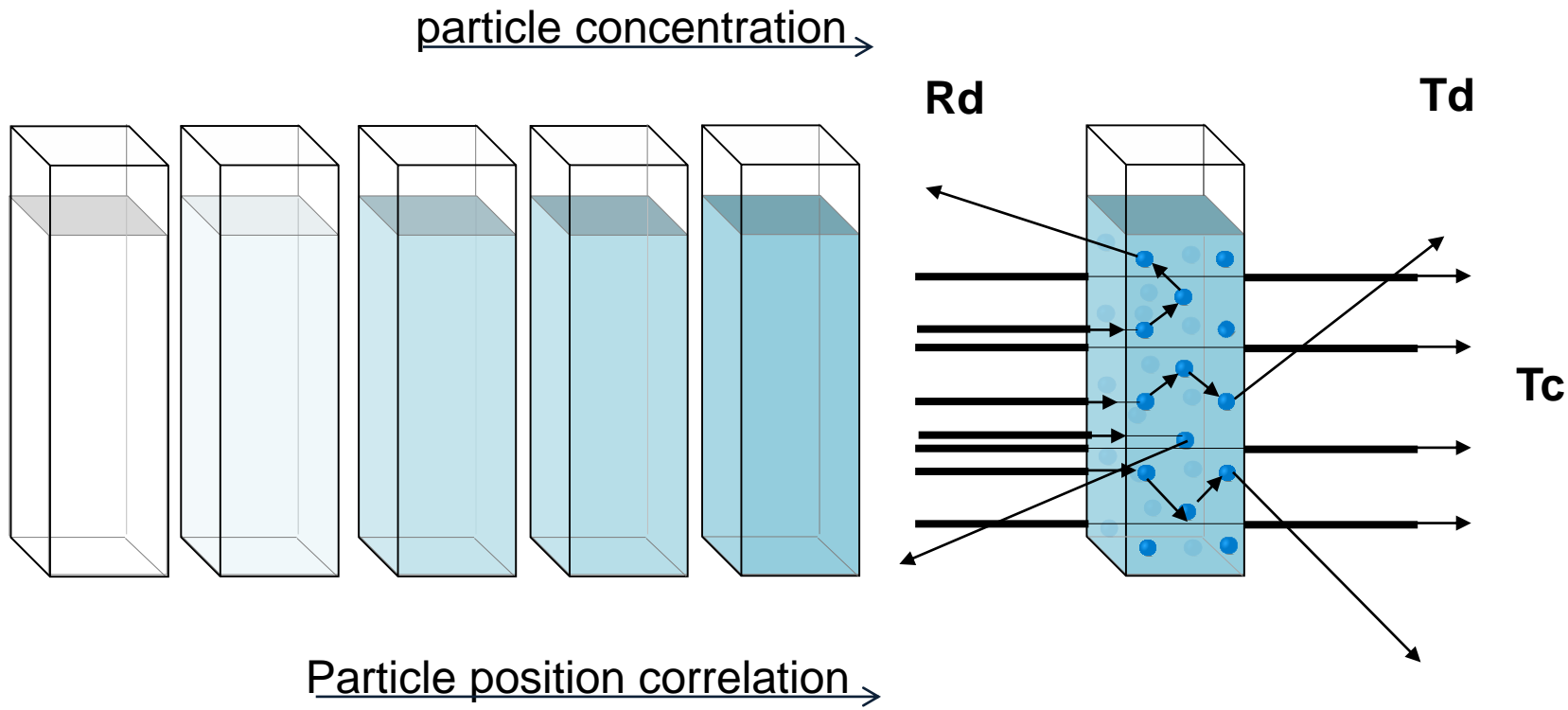
Sample selection | Predictive models

Classification models

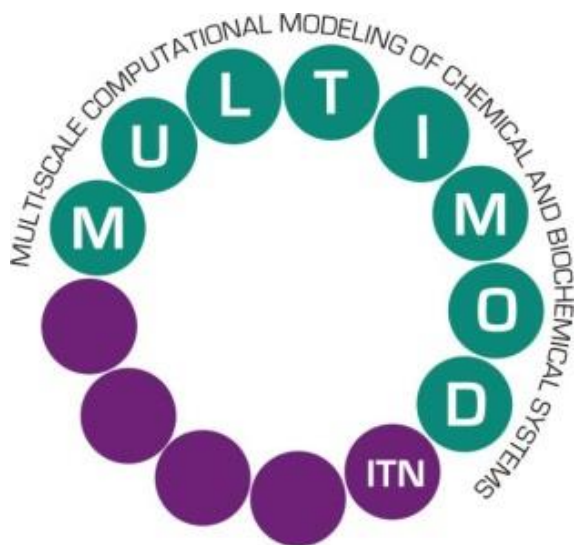


Tc





Light Scattering



ITN-initial training Networks

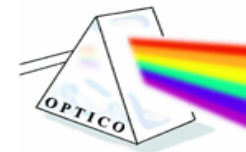
- equipping young researchers with the knowledge and skills required for Europe's knowledge-based economy
- offering decisive training and transfer of knowledge opportunities.
- SusChem report 'Vision for 2025 and Beyond' as 'the urgent need to train the next generation of individuals able to work across the boundaries of chemistry, biology, chemical and biochemical engineering'.



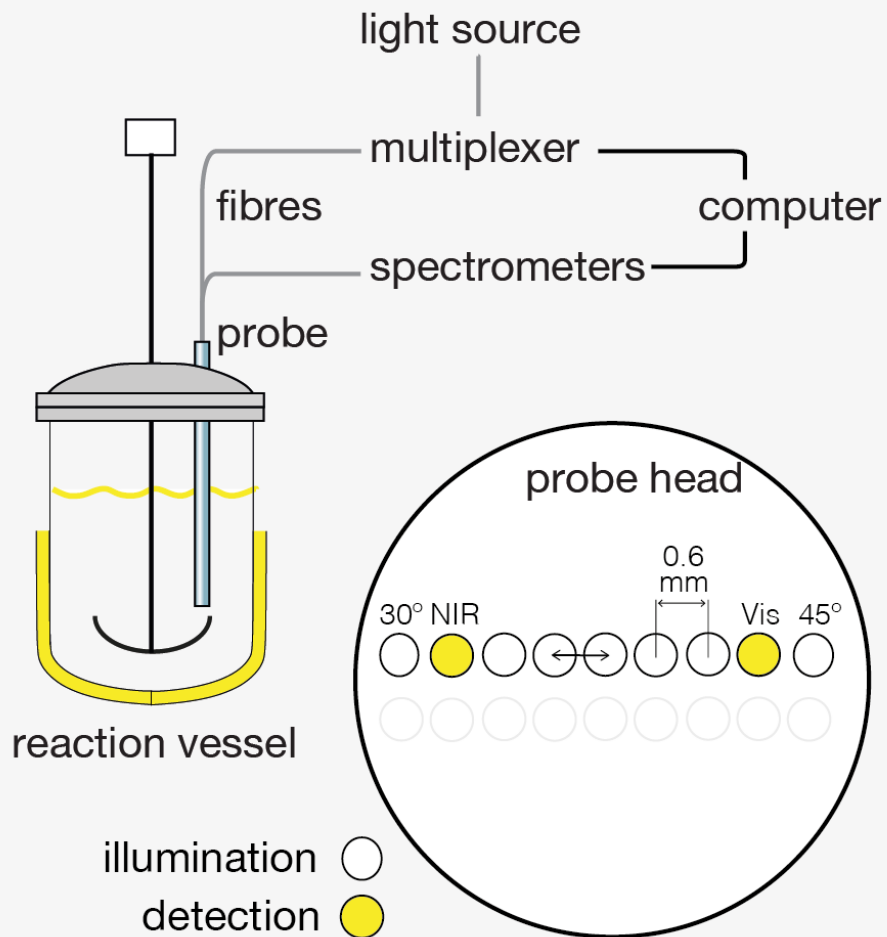
University of Strathclyde campus



Suspension polymerisation reactions



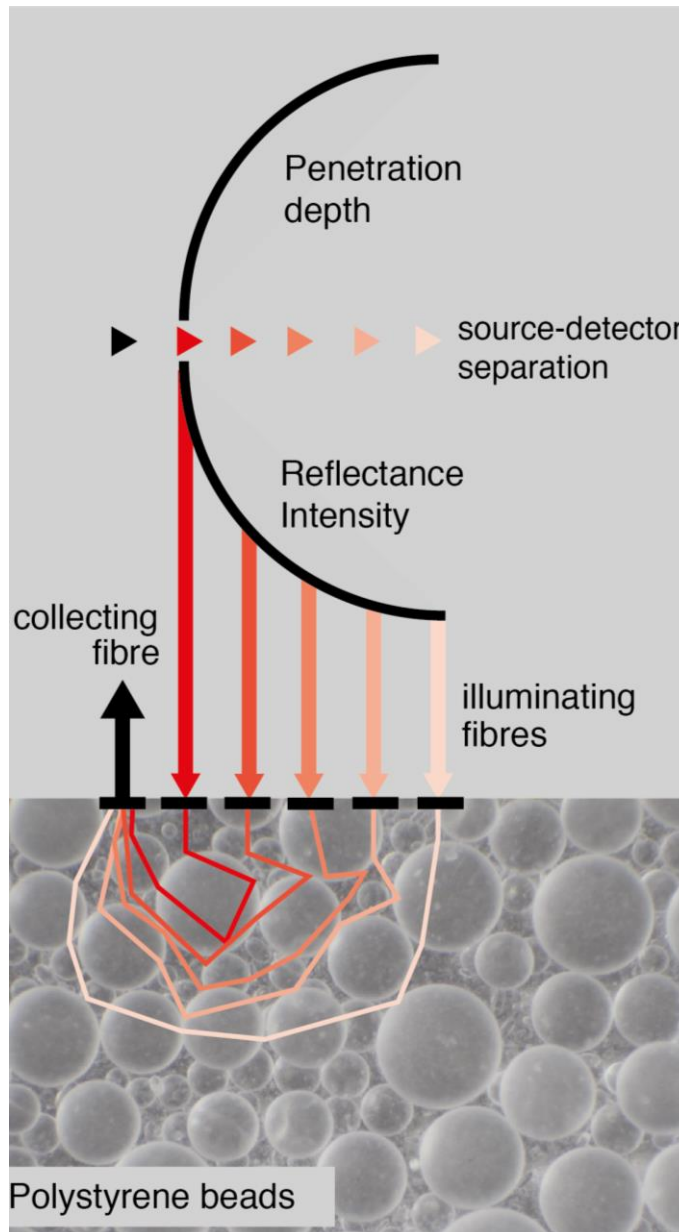
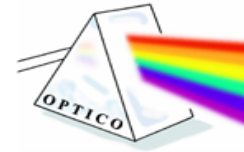
Experimental system



Vis and NIR

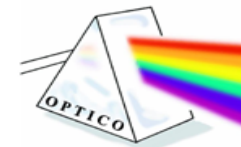
**Spatially and angularly resolved
diffuse reflectance spectroscopy**

Suspension polymerisation reactions

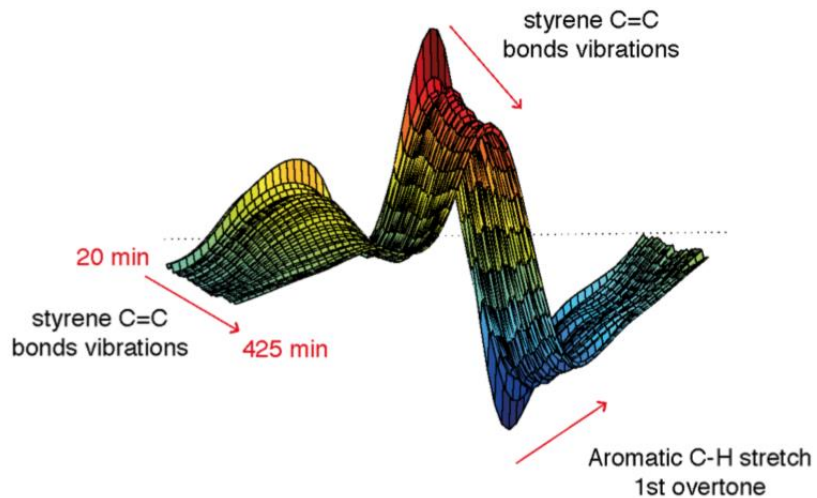


Vis and NIR
Spatially and angularly resolved
diffuse reflectance spectroscopy

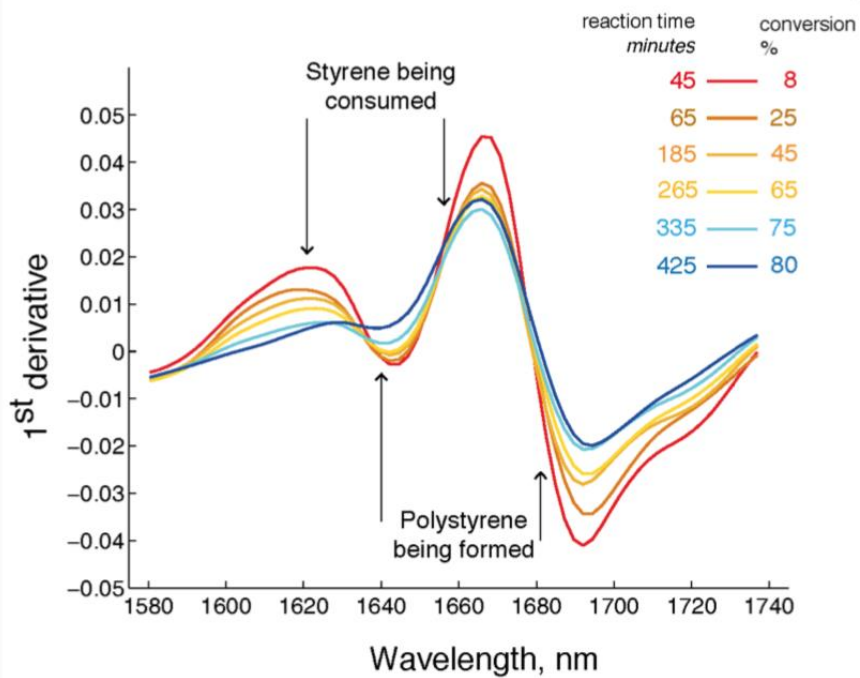
Reaction evolution



a)

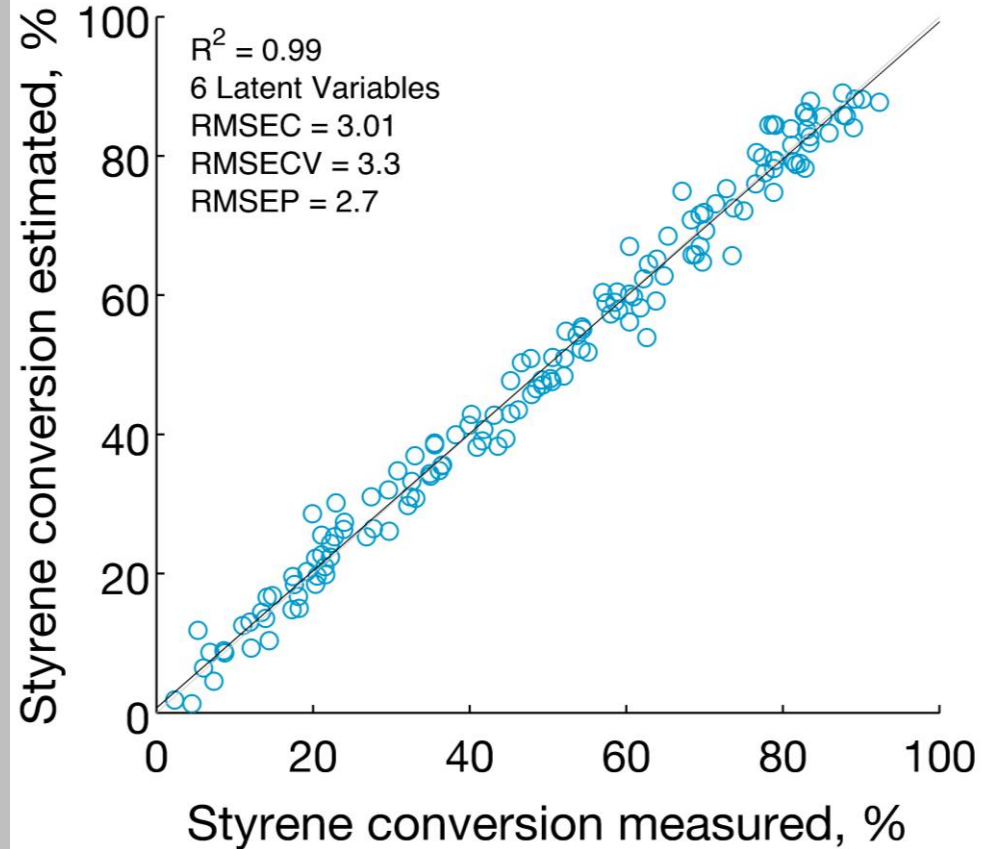
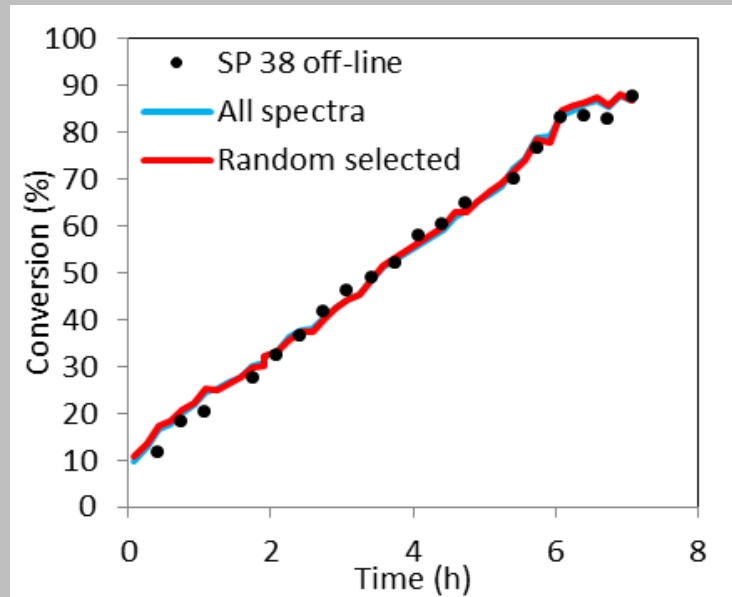
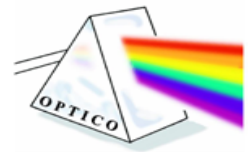


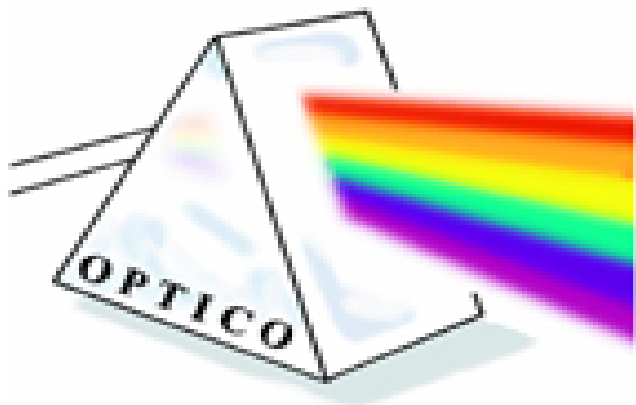
b)



Suspension polymerisation reactions

Predictive models for conversion

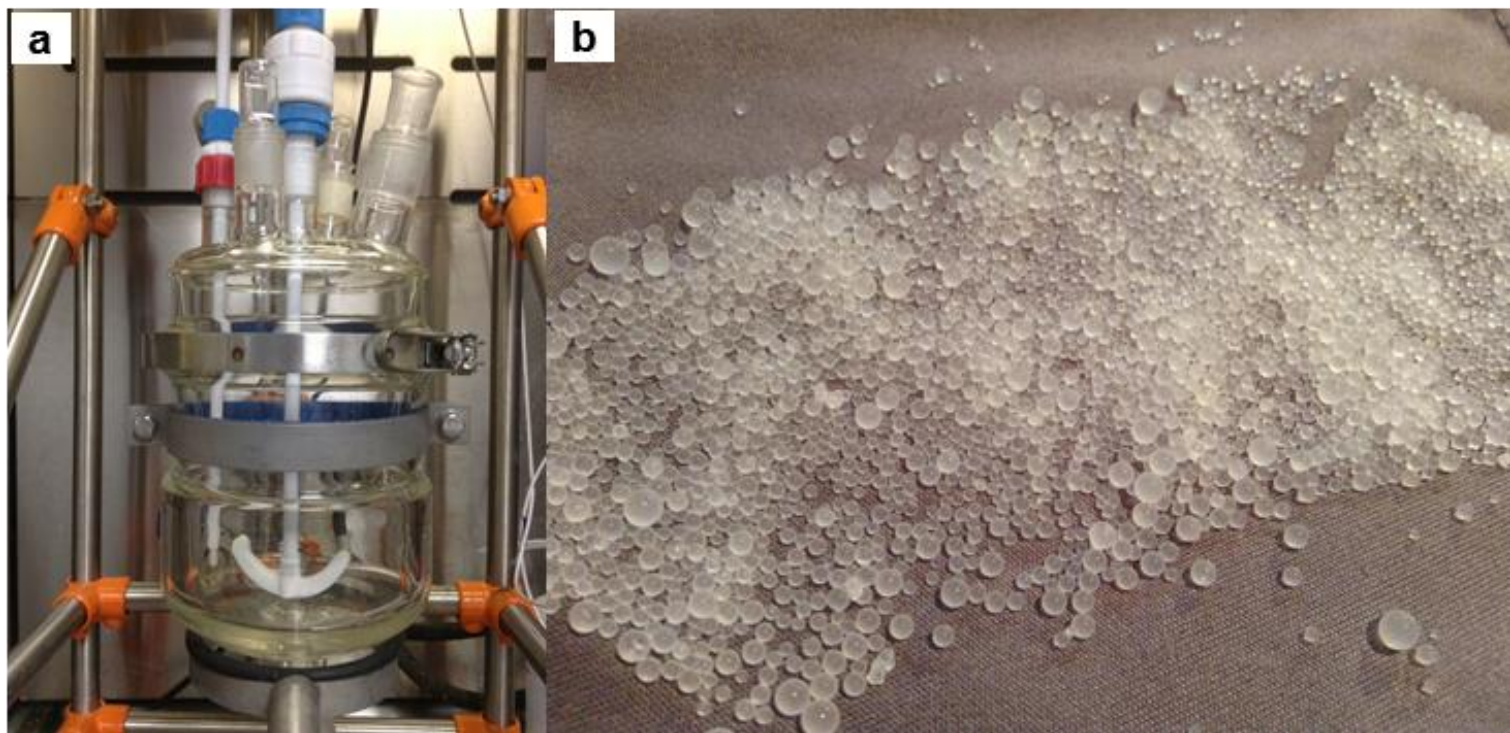




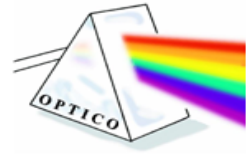
MODEL-BASED OPTIMIZATION &
CONTROL FOR PROCESS-
INTENSIFICATION IN CHEMICAL AND
BIOPHARMACEUTICAL SYSTEMS

Part. no.	Participant Legal Name	Country
1	Centre for Research and Technology Hellas (CERTH)/Chemical Process Engineering Research Institute (CPERI)	GREECE
2	Imperial College (ICL)	UK
3	RWTH Aachen (RWTH)	GERMANY
4	ETH Zurich (ETHZ)	SWITZERLAND
5	Technical University of Denmark (DTU)	DENMARK
6	Technical University of Delft (TUD)	NETHERLANDS
7	University of Gent (UGENT)	BELGIUM
8	University of Strathclyde (USTR)	UK
9	BASF (BASF)	GERMANY
10	ARKEMA (ARKEMA)	FRANCE
11	DSM (DSM)	NETHERLANDS
12	FIBRE PHOTONICS	UK
13	CHROMACON AG	SWITZERLAND

Suspension polymerisation reactions



Suspension polymerisation reactions



techniques

RAMAN + **VIS** + **NIR**

↓
providing information
at low concentrations
of residual monomer
and of styrene conversion

↓
contain information on
particle size provided
repeatable measurements
can be made

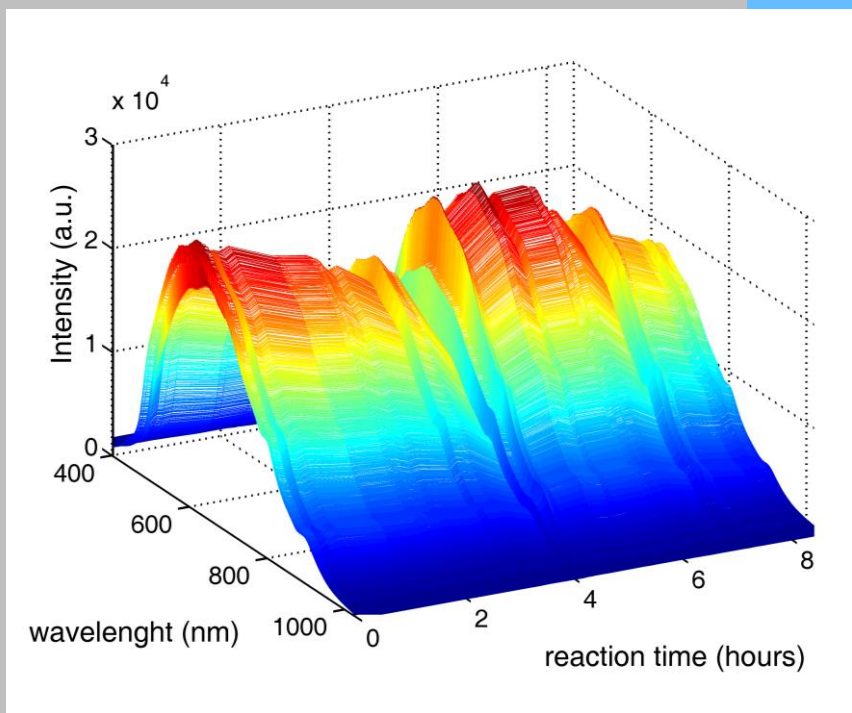
↓
providing information
of styrene conversion

Suspension polymerisation reactions

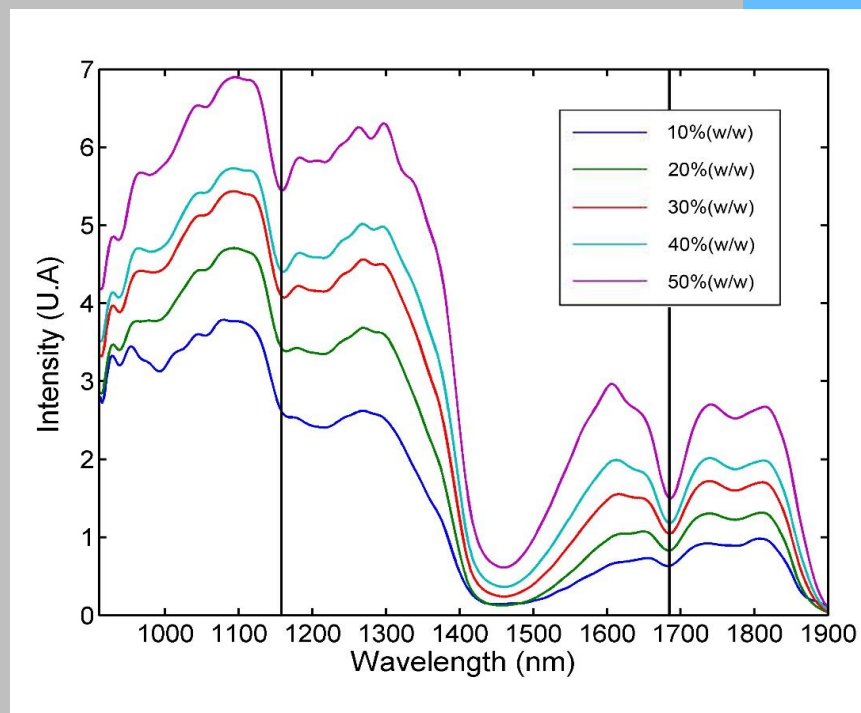
Vis and NIR spectra



VIS



NIR



LATIN
AMERICA
MCAA
RESEARCH
CONFERENCE



Thank you

