

the concentration of the molecule itself within a sample through the Beer-Lambert law. Infrared (IR) instead is a vibrational spectroscopy technique based on the absorption of light in the region between 780 nm and 1 mm. IR spectroscopy is more common since most compounds can absorb radiation in the IR while not all molecules contain chromophores that can be excited by UV/Vis light. For crystallization processes attenuated total reflectance probes (ATR) are used in order to analyse only the liquid phase, with negligible interference from the suspended particles. The presence of an ATR crystal positioned at the end of the *in situ* probe determines a depth of penetration of the light beam between 0.5 and 2 μm . Both ATR-FTIR and ATR-UV/Vis have been used for monitoring the solute concentration during batch and continuous crystallization processes.⁷⁻¹⁰

9.2.3 Raman Spectroscopy

Raman spectroscopy is a form of vibrational spectroscopy based on the inelastic scattering of monochromatic laser light. It is complementary to infrared spectroscopy but, while IR bands are generated from a change in the dipole moment of molecules, Raman bands arise from a change in their polarizability. This form of spectroscopy does not require sample preparation and can be used to analyse gaseous, solid and liquid samples. Raman spectra can be used to determine the crystal structure (*e.g.*, polymorphism) of a solid sample or to analyse the solvent composition and measure solute concentration.¹¹

9.2.4 Imaging and Particle Vision Measurement (PVM)

Imaging instruments provide real-time information of the crystals' size and shape. Additionally, agglomeration, breakage and polymorphic transformation can be detected using imaging techniques. The low cost of high speed cameras and their reduced size make these sensors the preferred choice for on-line monitoring of continuous plug-flow and oscillatory baffled crystallizers.^{12,13} *In situ* particle vision and measurement (PVM) probes can be used to collect and analyse images of the slurry in mixed suspension mixed product removal (MSMPR) crystallizers. Quantitative information, such as size and shape distributions, can be extracted from the recorded images and used for on-line feedback control.

9.3 Data Analysis and Management

PAT instruments are designed to provide on-line measurements of quality attributes to ensure the final product quality. The simultaneous use of several measurement technologies generates a large amount of complex data that need to be managed and analysed in order to extract relevant information.