Based on the patented technology of Encoded Photometric Infrared (EP-IR) Spectroscopy\(^1\), Aspectrics, Inc developed the Multicomponent™ 5000 and 5500 analyzers (MC5000 and MC5500).

Aspectrics EP-IR technology combines the advantages of both dispersive IR and FT-IR resulting in a unique design that is well suited for integration into process monitoring systems (autonomous sentries). The Multicomponent™ (MC) systems are designed and built for the rigorous demands of industrial applications.

\(^{1}\) US Patent 6,995,840 and others issued to Aspectrics Inc. Inventor Dr. Tom Hagler (CTO Aspectrics Inc.)
General Principle

The EP-IR system contains the encoder-spectrograph, as well as a real-time embedded micro-processor for signal analysis, data treatment, and Chemometrics (quantitative) analysis in a single small-footprint enclosure.

![Diagram showing EP-IR operation](image)

*Figure 1 Basic Schematic of EP-IR operation*

![Aspectrics Multicomponent™ 5000 system](image)

*Figure 2: Aspectrics Multicomponent™ 5000 system*

![Inside view of Aspectrics Multicomponent™ 5000 system](image)

*Figure 3 Aspectrics Multicomponent™ 5000 system. Inside view including Spectrograph and on-board computer for (1) real-time signal treatment into analytical results; (2) web server for remote diagnostic and maintenance; and (3) OPC Server for communication of analytical results and instrument data.*

Operation Principle

An infrared polychromatic beam is emitted from an external source (e.g. glow bar) onto the sample. Then it is either transmitted or reflected by means of appropriate transfer optics into the spectrograph and is focused through the entrance window (CaF2) of the EP-IR spectrograph.

The incoming focused beam is transferred directly onto the fixed holographic grating (which together with the detector determines the encoded wavelength range). The dispersed radiation (2.5 to 5.0 µm, 2000-4000cm⁻¹) is then projected through a slot aperture onto a spinning encoder disk as shown in Figure 4.
The encoder disk features 256 or 128 concentric modulator tracks located in an annular region to evenly cover the entire wavelength region dispersed by the fixed grating.

The composite reflected beam is imaged on a single element detector that generates a signal that forms a Discrete Interferogram, hence preserving multiplexing advantage. The intensity contribution for each region of wavelengths corresponding to the bandwidth of each photometric channel is obtained by applying a Fourier Transform to this interferogram.

The MC5000's encoder disk consists of 128 or 256 extremely accurate “halftone representations” of smooth orthogonal sinusoidal functions referred to as tracks.

These tracks are made of deposited metal formed via micro lithographic procedure and serve as the same purpose as optical bandpass filters to define the center wavelength and bandwidth of the encoded radiation of the photometric channel.

---

2 Standard all purpose disks are available in 256 and 128 “tracks” or channels. Covering the wavelength range defined by the grating in equal widths per channel. These disks allow the collection of continuous spectra in the selected wavelength range.
With the design it is possible to approximate an orthogonal sine wave for each encoded spectral component (see figure above). The orthogonal encoded beams are collected and focused onto a single-channel detector using a patented optical design (US Patent 6,995,840 and others pending) to produce a discrete interferogram.

The center wavelength and width are defined by the radial position and width of each track. The system runs at an acquisition frequency of 100 scans (rotation) per second, which is much faster than FT-IR and gives the EP-IR technology an enhanced Felgett or multiplex advantage as compared to dispersive IR spectrographs.
Due to the aligned fixed holographic grating and selection of matching thermal expansion coefficient materials for the disk and grating, the wavelength accuracy is determined and fixed after the factory wavelength calibration.

The onboard processor performs a discrete Fourier Transform without the need for apodization or zero filling, yielding a traditional emission spectrum which can be referenced to an internally stored spectrum and thus transformed to either transmission or absorbance spectrum.

The resulting spectrum can then be processed in real-time with the onboard Chemometrics engine which applies externally (via Chemobuilder™ PC software) created PCR calibration data parameters for the measurement of up to 64 compounds (up to 8 chemicals per each of 8 sets of principal components). The real-time output is up to 64 concentration values for up to 64 compounds measured within this spectrum. It shall be noted that, for very wide ranges of concentrations for which significant non-linear behavior is expected, several PCR calibration models optimized for several ranges of concentrations can be programmed into the on-board Chemometrics engine.

The data from the Multicomponent™ is sent as a TCP/IP data stream using a dedicated port and is also available via the built in OPC DA V2 compliant server.

The external sampling device and source assembly can be manufactured by the OEM or SI for the specific application in terms of material, heating capability, source power and type, or one of the optimized Aspectrics I-Cells can be utilized. Either one is connected directly to the Multicomponent™ analyzer. The integrated Aspectrics multipass gas cell accessories with powerful 11W focused IR source can be configured for optical path lengths from 1.0 to 3.2 m and can be heated up to 190°C. They are designed to be directly attached to the EP-IR for maximum throughput.

*Figure 4 Aspectrics Multicomponent™ 5000 with I-CELL*
Wavelength Range

Due to the EP-IR encoder disk all-reflective design, the wavelength range can be changed simply by selecting an appropriate grating–detector combination.

The modulation using the encoder disk can be used for all wavelength ranges from UV or NIR to MIR range. The technology can also be used for Raman spectroscopy and other applications. Refer to the patents for details. (US-Patent number 6-995-840)

![Figure 7 Electromagnetic Radiation](image)

The optical grating will follow the 2x free-spectral-range rule which limits the available range for an individual grating.

Current production units are equipped with a grating which disperses the light in the 2.50 to 5.00 microns range (2000-4000 cm⁻¹) and from 2.85 to 5.50 microns (1818-3600 cm⁻¹). (All spectral ranges value nominal).

The high performance detector being used in the systems is a double stage Thermo Electric Cooled (TEC) Lead Selenide (PbSe) detector which can operate at 1 MHz acquisition frequency.

Other detectors may be used, as long as they have a suitable acquisition capacity of 1 MHz.
Visible Species in the Mid-IR Range

As an example (non extensive) the following figure shows common gases which can readily be measured using the Multicomponent™ 5000 system. The Mid-IR range from 2.5 to 5.0 microns (nominal) is ideal for gas analysis since it offers resolved peaks for most of the gases.

Other chemical species can be observed in the MC5000 EP-IR Spectrometer spectral range. As pertaining to combustion emissions analysis, they are:

Figure 8 Chemical species (combustion) detectable in the MC5000 wavelength range
Encoder Disk Capabilities – Custom Design

The Multicomponent™ 5000 and 5500 are equipped with "standard" encoder disks which cover the entire wavelength region of the grating.

It is possible to customize the disk design to optimize it for a specific application. With this disk and the same optics as before the analyzer will have improved performance in terms of S/N and thus better analytical performance for the given application than the "general purpose" encoder disk based system. For an identified application (e.g. compounds absorption bands and background bands to be used) Aspectrics, Inc. creates the proprietary design of the encoder disk. This disk then can be used in all analyzers to be deployed in the field for this application. This process is also applicable for low volume sales since the cost of the disk is the same as for a "standard" disk.

Combined with the embedded Chemometrics method developed using the encoder disk the system becomes or is transformed to an optimized intelligent sensor, for a specific application. This approach is particularly suited for larger volume applications segments to obtain maximum performance and ease of production and calibration.

Refer to US Patent 6,995,840 for details on the creation of such a custom disk.
Embedded Chemometrics and Software

As previously stated the Multicomponent™ series includes a built in Chemometrics engine, which allows the system to function as a networked answer box.

Using the Aspectrics Command Center™ software suite provided with all instruments the system can be calibrated using an external PC computer.

The software suite contains command and data control software called Aspectrics Commander™, which enables the user to acquire data simultaneously from multiple systems using a program based approach including the control of an external gas blender. The data acquired is automatically tagged with the desired compound and concentration information of the substances being measured and also contains relevant instrument data, including temperature, pressure readings from internal sensors or external sensors.

Chemobuilder™ is then used to perform an automated or scripted PCR based calibration with the obtained data files, creating a modular calibration data structure for all calibrated compounds. This quantitative method (or “calibration”) is then uploaded via TCP/IP to the Multicomponent™ Analyzer with which the calibration spectra (learning set) were collected.

From that point onward the system predicts automatically and in real time the concentrations of the compounds for which the system is calibrated. Moreover, calibration limits can be set when developing the method using Chemobuilder™ and are applied automatically to the real-time predicted data stream. Lastly, predicted analytical data are available via OPC DA Server or thru the TCP/IP data stream.

Chemobuilder™ was designed to enable the non-spectroscopist to generate with a single click a complex calibration for routine operation. In the expert mode an experienced Spectroscopist or Chemometrician can fine tune and optimize the calibration method by having access – amongst other diagnostics – to reference spectra, variance spectra and individual principal components for consideration and analysis. Once finalized the procedure can be saved in a script and applied to other systems, thus enabling the volume production of the finished analyzer.
Application examples
The following 2 sections illustrate some application examples. More application notes can be found on the Aspectrics website at www.aspectrics.com

Chemometrics Resolution

Example 1

A traditionally difficult application is the development of a quantitative method for the simultaneous measurement of spectrally overlapping and/or morphologically similar compounds. An example is the development of a method for the simultaneous measurement of 4 Hydrocarbon homolog’s without observing statistically significant cross sensitivities between the 4 compounds. These 4 hydrocarbon homologs are n-butane, iso-butane (2-methylpropane), n-pentane and iso-pentane (2-methylbutane), labeled nC4, iC4, nC5 & iC5, respectively.

The 4 homolog’s show little discernable difference in their absorbance spectra when superimposed:

![Overlaid Spectra of 4 HC homolog's](image)

*Figure 11 Overlaid Spectra of 4 HC homolog’s (nC4, iC4, nC5, iC5), each at the same concentration.*

Using the standard 256 channel encoder disk on an MC5000, measurements of the single gases were made using the program mode in the software which supports the Environics™ gas blender series 4000. Each gas was passed through the measurement cell which was mounted on the Aspectrics Mid-IR Development Bench³.

The data file was then treated with Chemobuilder™ and a calibration data structure for all 4 (four) compounds were created and uploaded on the instrument. Another automatic blender run was initiated using the program feature of the Aspectrics Commander™ software, which passed the same gasses through the measurement cell in different sequences and as mixture.

³ The MID-IR Development bench enables the use of standard FT-IR accessories with the Multicomponent™ series analyzer. It contains a IR source, opening for accessories using the Mattson Galaxy 3.5” standard and a optics block to focus the signal into the Multicomponent™ system.
The Proof:

Blender Profile:

<table>
<thead>
<tr>
<th>Step #</th>
<th>Gas</th>
<th>Step #</th>
<th>Gas</th>
<th>Step #</th>
<th>Gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>N2</td>
<td>7</td>
<td>N2</td>
<td>13</td>
<td>nC5</td>
</tr>
<tr>
<td>2</td>
<td>nC4</td>
<td>8</td>
<td>iC5</td>
<td>14</td>
<td>N2</td>
</tr>
<tr>
<td>3</td>
<td>N2</td>
<td>9</td>
<td>N2</td>
<td>15</td>
<td>nC4</td>
</tr>
<tr>
<td>4</td>
<td>iC4</td>
<td>10</td>
<td>iC4</td>
<td>16</td>
<td>iC5</td>
</tr>
<tr>
<td>5</td>
<td>N2</td>
<td>11</td>
<td>iC5</td>
<td>17</td>
<td>iC4</td>
</tr>
<tr>
<td>6</td>
<td>nC5</td>
<td>12</td>
<td>nC4</td>
<td>18</td>
<td>nC5</td>
</tr>
</tbody>
</table>

4 HCs - Chemobuilder Model

Figure 12 Run sequence and predicted Chemometrics output

As can be seen by the following evaluation of the above data the model did not yield any false positives and also satisfies the VDI and TUEV requirements for cross sensitivity.

Simultaneous Analysis of nC4, iC4, nC5, iC5

Cross Sensitivity Study

Criteria / Calculation Methods: TUV 4201 & MCERTS 323

Maximum Allowed Cross Sensitivity (TUV 4201) < ± 4%

<table>
<thead>
<tr>
<th>Interferent</th>
<th>Cross sensitivity of chemical to interferent</th>
</tr>
</thead>
<tbody>
<tr>
<td>nC4 100 ppm</td>
<td>iC4 -0.5% PASS nC5 0.5% PASS iC5 0.6% PASS</td>
</tr>
<tr>
<td>iC4 100 ppm</td>
<td>nC4 0.5% PASS nC5 -0.4% PASS iC5 0.3% PASS</td>
</tr>
<tr>
<td>nC5 100 ppm</td>
<td>nC4 -0.6% PASS iC4 -0.1% PASS iC5 -0.3% PASS</td>
</tr>
<tr>
<td>iC5 100 ppm</td>
<td>nC4 -0.5% PASS iC4 -0.5% PASS nC5 0.6% PASS</td>
</tr>
</tbody>
</table>
**Example 2**

Simultaneous measurement of spectrally overlapping compounds CH₄, C₃H₈ and NO₂ (overtone info) using an MC5500 A 128 channel EP-IR spectrometer.

This experiment is a practical example of the Chemometrics (i.e. analytical) resolution of an MC5500 analyzer using a standard 128 photometric channel encoder disk. Data were collected at room temperature and pressure under a flow rate of 4 liter/minute. The gas sampling accessory utilized was an Aspectrics 2.0 meter path length multipass I-Cell. Integration time for each spectrum measured was 5.12 second (corresponding to a set boxcar average on EP-IR signal of 512.)

<table>
<thead>
<tr>
<th>Compound</th>
<th>Calibration Results (in mixture)</th>
<th>Validation Results (in mixture; independent set of data)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>R²</td>
<td>SEC (ppm)</td>
</tr>
<tr>
<td>CH₄</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0-100 ppm</td>
<td>0.9999</td>
<td>0.41</td>
</tr>
<tr>
<td>C₃H₈</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0-641 ppm</td>
<td>1.0000</td>
<td>0.19</td>
</tr>
<tr>
<td>NO₂</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0-256 ppm</td>
<td>0.9998</td>
<td>1.31</td>
</tr>
</tbody>
</table>

*Note: Gas Blender Precision of 1% rel.*
Long Term Stability Measurement n-Pentane

A n-Pentane single gas calibration was developed using a 128 channel system. Data was collected at room temperature using a standard 5-meter pathlength multipass gas cell.

Once the EP-IR spectrometer was calibrated, various concentrations of n-pentane were injected in the gas cell over a period of 17 hours without re-referencing (re-zeroing) the instrument. Resulting analytical results for the prediction of n-pentane were saved and evaluated for stability of instrumental response as a function of time.

After three validation runs were performed, we had:

n-Pentane long-term stability
n-Pentane long-term stability
Zoom on +14 to +17 Hrs Time Frame

The results (without any re-reference measurement) over 17h (see figure 13) are:

<table>
<thead>
<tr>
<th>Repeatability Run 1</th>
<th>n</th>
<th>σ (ppb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ppb level</td>
<td>7998</td>
<td>17</td>
</tr>
<tr>
<td>100 ppb level</td>
<td>N/A</td>
<td></td>
</tr>
<tr>
<td>250 ppb level</td>
<td>5365</td>
<td>17</td>
</tr>
<tr>
<td>500 ppb level</td>
<td>656</td>
<td>11</td>
</tr>
<tr>
<td>1,000 ppb level</td>
<td>788</td>
<td>13</td>
</tr>
<tr>
<td><strong>Weighted Average σ</strong></td>
<td><strong>15009</strong></td>
<td><strong>16</strong></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Repeatability Run 2</th>
<th>n</th>
<th>σ (ppb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ppb level</td>
<td>7998</td>
<td>12</td>
</tr>
<tr>
<td>100 ppb level</td>
<td>N/A</td>
<td></td>
</tr>
<tr>
<td>250 ppb level</td>
<td>5797</td>
<td>22</td>
</tr>
<tr>
<td>500 ppb level</td>
<td>1288</td>
<td>25</td>
</tr>
<tr>
<td>1,000 ppb level</td>
<td>788</td>
<td>27</td>
</tr>
<tr>
<td><strong>Weighted Average σ</strong></td>
<td><strong>15871</strong></td>
<td><strong>17</strong></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Repeatability Run 3</th>
<th>n</th>
<th>σ (ppb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ppb level</td>
<td>7998</td>
<td>10</td>
</tr>
<tr>
<td>100 ppb level</td>
<td>5365</td>
<td>17</td>
</tr>
<tr>
<td>250 ppb level</td>
<td>N/A</td>
<td></td>
</tr>
<tr>
<td>500 ppb level</td>
<td>1720</td>
<td>17</td>
</tr>
<tr>
<td>1,000 ppb level</td>
<td>788</td>
<td>15</td>
</tr>
<tr>
<td><strong>Weighted Average σ</strong></td>
<td><strong>15871</strong></td>
<td><strong>13</strong></td>
</tr>
</tbody>
</table>

As shown; EP-IR technology with “traditional” accessories such as a SPECAC 5 m gas cell and the Aspectrics Mid-IR Development Bench shows minimal drift and excellent long term stability. The bias of the above described measurement was 17 ppb after 17 h. The original calibration accuracy (SEP) was 21 ppb. For more details refer to the Long term stability application note on the Aspectrics web site www.aspectrics.com.
**Typical Detection Limits in the Gas Phase**

**Protocol:**
- **Instrument:**
  - EP-IR MC5000A\(^4\) (128 channels; 2.50-5.00 µm nominal range)
- **Gas Cell:**
  - I-Cell 3.2 meter pathlength
- **Environmental:**
  - Room temperature and pressure
- **Data Collect:**
  - 1 minute integration (6000 scan boxcar average)
- **Experimental:**
  - Data collected at concentrations of 0, 1% rel., 5% rel., 10% rel., 50% rel. and 100% relative of maximum concentration range.
  - 2 independent sets of data were collected for each gas.

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Range (ppm)</th>
<th>LOQs (All Results in ppm; 60-second integration; 3.2 meter pathlength)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Precision @ &quot;0&quot; Method (1\sigma) (2\sigma) (3\sigma) VDI 4201-4203 Method (1\sigma) (2\sigma) (3\sigma)</td>
</tr>
<tr>
<td>Acetylene</td>
<td>0-100</td>
<td>0.070 ± 0.140 ± 0.210 0.111 ± 0.222 ± 0.333</td>
</tr>
<tr>
<td>Ethylene</td>
<td>0-100</td>
<td>0.163 ± 0.326 ± 0.489 0.161 ± 0.322 ± 0.483</td>
</tr>
<tr>
<td>Methane</td>
<td>0-25</td>
<td>0.065 ± 0.129 ± 0.194 0.076 ± 0.152 ± 0.228</td>
</tr>
<tr>
<td>CO</td>
<td>0-50</td>
<td>0.173 ± 0.347 ± 0.520 0.225 ± 0.451 ± 0.676</td>
</tr>
<tr>
<td>Ethane</td>
<td>0-100</td>
<td>0.034 ± 0.069 ± 0.103 0.070 ± 0.141 ± 0.211</td>
</tr>
<tr>
<td>Propylene</td>
<td>0-100</td>
<td>0.067 ± 0.134 ± 0.201 0.215 ± 0.429 ± 0.644</td>
</tr>
<tr>
<td>(iC_5)</td>
<td>0-10</td>
<td>0.008 ± 0.016 ± 0.024 0.017 ± 0.033 ± 0.050</td>
</tr>
</tbody>
</table>

Precision @ "0" Method \(1\sigma\) is calculated as the standard deviation of predicted concentrations using the full range calibration model when the concentration in the chemical of interest is equal to zero.

VDI 4201-4203 Method \(1\sigma\) is calculated as the standard error of prediction (SEP) for the calibration covering a range of concentrations equal to 0-10% relative to the maximum concentration range.

**Wavelength Accuracy**

Although a laser is not part of the system, the EP-IR exhibits excellent wavelength accuracy due to the aligned fixed holographic grating and the encoder disk. The wavelength calibration is performed on each system leaving the factory, and uses certified high purity gases to obtain continuous multi spectra data which then is fitted to HiTran reference spectra. Using this approach each channel is characterized by a center wavelength and bandwidth which is stored with each file and on the embedded computer system. Wavelength Accuracy exceeds 0.1 cm\(^{-1}\) at 2000 cm\(^{-1}\) (256 channel system)

\(^4\) With dual stage TEC operating set at -35 deg C
Signal to Noise and P2P Performance

Traditional spectroscopic signal treatment expresses the performance as Peak to Peak (P2P) and Root Mean Square (RMS) of the background noise. The Signal to Noise (SNR)\(^5\) is the ratio of Signal to the RMS value.

\[ \text{SNR} = \frac{S}{\sqrt{N}} \]

\(^5\) Signal to Noise Ratio (SNR): Indicates the quality of the baseline of the sample’s infrared spectrum; mathematically, the SNR is a comparison of the size of the noise to the size of the signal. The SNR improves with the number of scans acquired because of the averaging nature of the data acquisition: after averaging each scan the signal increases in size while the noise diminishes. The dominant noise in FT-IR is the detector-limited noise, which varies as the square root of the number of scans (\(\sqrt{N}\) for N scans). Hence, combining these two factors, the SNR varies with the number of scans \(N\) as

\[ \frac{N}{\sqrt{N}} = \sqrt{N} \]

Acquiring a larger number of scans will improve the SNR or a cleaner baseline spectrum.
Reproduced in the next figure are the results of study performed with the Multicomponent™ 5000 system using the Aspectrics Mid-IR Development Bench in non-purged open beam configuration.

<table>
<thead>
<tr>
<th>Open Beam, Mid IR Development Bench</th>
<th>Multicomponent™ 5000A</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Integration</strong></td>
<td><strong>Max En</strong></td>
</tr>
<tr>
<td>1</td>
<td>7051</td>
</tr>
<tr>
<td>5</td>
<td>7046</td>
</tr>
<tr>
<td>10</td>
<td>7057</td>
</tr>
<tr>
<td>15</td>
<td>7123</td>
</tr>
<tr>
<td>30</td>
<td>7116</td>
</tr>
<tr>
<td>60</td>
<td>7062</td>
</tr>
</tbody>
</table>

Figure 16 P2P and RMS noise data for Multicomponent™ 5000

The following figures plot the standard deviation of each channel vs. the used boxcar average on a logarithmic scale to illustrate that the EP-IR technology follows the trend Sqrt 1/N.

The noise is normalized against the boxcar. Integration time would be the boxcar average divided by 100 seconds. (EP-IR scans at 100 scans per second).

The boxcar used by the Multicomponent™ 5000 system is a true boxcar averaging, where $n$ number of scans are kept in a bin to be averaged. Each new spectrum displaces the oldest one from the bin. The average is calculated for each spectrum acquired.

As in non-dispersive IR, noise is calculated for each channel, not a specific wavelength range.
Figure 17 Log Scale display of noise vs. boxcar average

Figure 18 Linear scaled display of Noise vs. Boxcar average
**Optical Resolution**

Each EP-IR channel provides an INTEGRATED intensity characterized by a center wavelength and bandwidth.

The channels from the standard 256 or 128 channel disks form a continuous spectrum of the range defined by the grating. The optical resolution limitation is a function of the grating and the number of channels which can be fitted on a given disk for the optical design of the instrument. Using the current image spot size the maximum number of usable unique harmonic channels is 144.

Using a proprietary sine and cosine encoding scheme (UA Application 20050286049) the number of usable channels is increased 256.

By using multivariate Chemometrics method (PCR or PLS) for the quantification it is possible to model the small absorbance differences and achieve application success where the naked eye is not able to discern a significant variation in signal. The Chemometrics resolution in EP-IR is much higher than what can be expected by calculation from traditional photometric spectroscopy factors.

**256 vs. 128 channels vs. Custom Disk Design**

Comparing the same sample in the same experimental setup using the two available general purpose encoder disks indicates that the intensity of the signal is increased when using the 128 channel disk. This derives from the fact that the radial width of the track on the disk is wider and more light is reflected from that track. See figure 19.

**Comparison 128 vs. 256 channels MC 5000**

![Figure 19 Comparison of Emittance spectra of Polystyrene for 128 and 256 channels](image-url)
As expected for the Signal to Noise ratio, the 128 channel systems perform better than the 256 channel design as more signal (energy) is integrated due to the wider channels. FT-IR spectral energy is constant however there is noticeably less absorption at the lower resolution as band peaks can be missed or not integrated (Note H2O, polystyrene and CO2 bands)

![Figure 20 Overlaid FT-IR single beam intensity transmission spectra of a polystyrene sample at 1cm⁻¹ and 32cm⁻¹ optical resolution.](image)

**Conclusion**

The Aspectrics EP-IR platform was design and engineered in response to customer requests for improvements in real-time process monitoring. The following is a short list of those areas that customers identified as the most challenging, and how EP-IR addresses these challenges:

**Durability**

- EP-IR spectrometers contain only one **vibration insensitive** moving part, the spinning encoder disk, with a rated MTBF > 50,000 hours.
- EP-IR spectrometers contain no hygroscopic parts and can be operated “as is” in any non-condensing condition
- EP-IR spectrometers contain no consumables such as HeNe lasers

**Small Size**

- The total volume occupied by an EP-IR spectrometer is approximately 7.8 dm³ (0.275 cu ft.) with a foot print of less than 6 dm² (0.645 sq ft.)
- Each EP-IR spectrometer contains: a) a complete spectrograph with appropriate optics, encoder disk w/ spindle motor assembly and detector (upgradeable within the same form factor to a dual detector system); b) computer boards enabling (1) real-time signal treatment with delivery of analytical results; (2) remote maintenance and diagnostic using the built-in web server; and (3) real-time communication capabilities
using the built-in OPC server with the ability to add PC104 boards as needed for custom developments.

**Multi-component analytical performance**

- Scanning speed of 100 Hz enables faster access to low LODs by co-addition
- Access to information covering the entire spectral range (using default 128 or 256 channels encoder disk) enables the observation of the IR spectroscopic signature of all IR absorbing compounds present in the sample
- Built-in multivariate chemometrics methods (PCR) enable the development and the application of quantitative methods for the simultaneous measurement of multiple components in the matrix, even if the species are spectrally overlapping
- Custom encoder disks can enhance the analytical performance for only the spectral regions relevant to the analysis

**On-Board Computational Capabilities**

- EP-IR spectrometers contain an On-board Computer (no external PC required) for real-time processing capabilities, including:
  - The Chemometrics Engine, i.e. the capability to treat the IR signal in real time and output analytical results in real time.
  - OPC DA v2 Server to communicate both analytical results and instrumental / analytical parameters in real time to external means (local and/or remote) of data archiving, and
  - A Web server with Java applet enabling remote diagnostic and maintenance of both the spectrometer and the methods embedded therein

**Simplified Calibration, Validation and Calibration Maintenance**

- A complete chemometrics and instrument control software package is included with each EP-IR spectrometer
- Intuitive user interface and innovative approaches to the development of PCR-based quantitative methods enables almost anyone to quickly calibrate / validate new instruments or perform remote maintenance of existing instruments
- Calibration maintenance is as simple as implementing remote collection of new calibration spectral information, adding the information to the already existing learning set, and re-computing PCR models for all components of interest in the mixture

**Ease of integration**

- EP-IR spectrometers are packaged for the OEM and SI market.
- Post-dispersive optical configuration enables greater flexibility in spectroscopic sampling techniques. In addition, EP-IR optimized sampling accessories with built-in IR sources and optics transferred are available.
- On-board signal treatment (including computation of analytical results) and OPC and Web servers facilitate integration through TCP/IP communication
- Rugged design and construction facilitate integration process. Lack of consumables (lasers) in the instrument reduces the need for on-site regularly scheduled service
Multicomponent™ System Hardware

Figure 21 Outside view Housing

Figure 22 Multicomponent™ series front view

Figure 23 Multicomponent™ series back view
Figure 24 Multicomponent™ inside view

Figure 25 Inside view (schematic) with 2 detector grating modules
**Aspectrics, Inc. US and International Patents**

The following patents were issued. Log on to [www.uspo.gov](http://www.uspo.gov) to download the full text version.

- 6,271,917
- 6,897,952
- 6,388,794
- 6,762,833
- 6,982,788
- 6,999,165
- 6,995,840

The following International patents are applied for or have been awarded:

- EP: 10090276 (Europe)
- EP: 037164506 (Europe)
- JP: 2003-575391 (Japan)
- CN: 03810389.3 (PRC)
- Au: 2003-220156 (Australia)
- CA: 2478611 (Canada)