

Inline Trace Water Detection Using NIR Absorbance



The Kemtrak DCP007-NIR photometric process analyzer can accurately monitor dissolved water in a wide range of liquid samples at trace concentration levels. It is a practical inline replacement for Karl Fischer titration, offering continuous real-time results with no reagents, no sample handling, and no maintenance requirements.

Unlike Karl Fischer titration, inline NIR measurement eliminates sample extraction, handling errors, and reagent costs – while providing a continuous output signal directly from the process stream.

MEASUREMENT PRINCIPLES

Water is detected in the near-infrared (NIR) via its hydroxyl (O-H) group absorption. Two spectral regions are used depending on the concentration range required:

Region	Absorption type	Typical use case
1400 nm	First overtone of O-H stretch (water and ethanol)	Full-range monitoring: 0-100% water
1900 nm	Combination of O-H stretch + H-O-H bending (water-specific)	Trace detection; water < 5%

The 1400nm region represents the first overtone of the O-H stretch in water as shown in Figure 1 and is ideal for 0 -100% water mixture monitoring. For trace detection, the 1900nm region represents a combination of O-H stretch and H-O-H bending which is specific for the water molecule and has approximately five times greater absorption than the 1400nm region, making it the preferred choice for trace analysis.

The H-O-H bending mode at ~1900 nm is unique to water (not shared by most organic solvents). This distinguishes it from the 1400 nm O-H overtone, which is also present in alcohols such as ethanol.

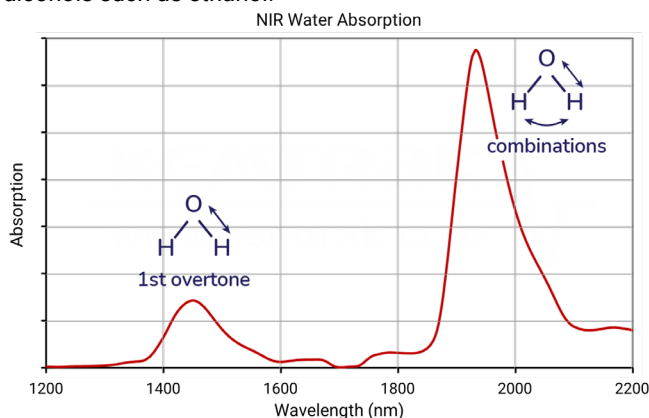


Figure 1: NIR absorption spectra of water

A reference wavelength (placed where absorption is minimal, typically below ~1300 nm) is used to compensate for changes in sample clarity caused by undissolved particulates, suspended matter, or cell window fouling.

APPLICATION FACTORS

Background Absorption and Optical Path Length

Absorbance from a sample's non-water components is defined as background absorption. As shown in Figure 1, water absorbs intensely in the 1900 nm region, whereas ethanol does not. The combined absorbance of this background and the water (at its maximum expected concentration) dictate the maximum Optical Path Length (OPL) allowable to keep the DCP007-NIR within its linear operating range.

In trace water analysis, background absorption is a critical variable. While a longer OPL enhances water content measurement resolution, it also increases total absorbance. Selecting an OPL involves a trade-off: while a longer path length improves resolution, it also increases total absorbance. For peak performance, the OPL should be maximized only to the point where the maximum water signal stays below 2 A and the non-water background remains under 1 A.

Per Figure 2, background absorbance varies between different matrices and must be taken into account when determining OPL for any specific application; absorbance is additive and total absorbance must not exceed the analyzer measurement capability.



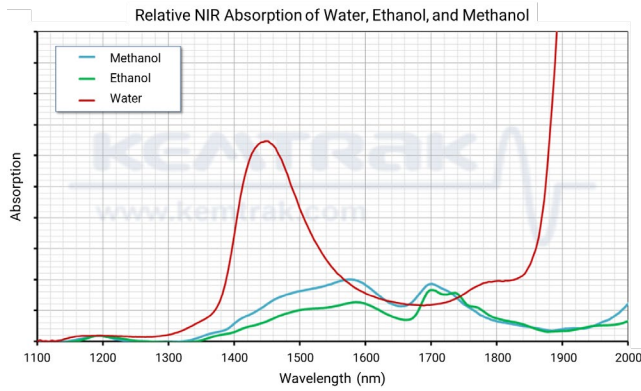


Figure 2: relative NIR absorption spectra of water, methanol, ethanol

Some typical background absorbances (at 1cm OPL) in the NIR are:

Solvent	Application Interest	Approx. Absorbance (1930 nm, 1 cm)
Acetone	Solvent purity, chemical synthesis	~ 0.00 – 0.05 AU
Acetonitrile	HPLC mobile phase, battery electrolytes	~ 0.00 – 0.05 AU
Tetrahydrofuran (THF)	Polymerization, Grignard reactions	~ 0.05 – 0.10 AU
Dichloromethane	Extraction purity	~ 0.00 – 0.01 AU
Chloroform	Pharmaceutical intermediates	~ 0.00 – 0.01 AU
Ethanol (Absolute)	Pharmaceutical manufacturing	~ 0.10 – 0.20 AU
Methanol	Chemical feedstock, fuel cells	~ 0.15 – 0.25 AU
Hexane / Alkanes	Hydrocarbon processing, extraction	~ 0.00 – 0.02 AU
Toluene / Aromatics	Moisture-sensitive organic synthesis	~ 0.01 – 0.05 AU

Water has a theoretical absorbance of 55 AU in a 1cm OPL at around 1930nm. In order to keep the DCP007-NIR within its measurement limits, the following approx. measurement ranges and resolution are possible with different OPL:

Optical Pathlength	Approx. Max Water Concentration (% v/v / ppm)	Measurement Detection Limit/Resolution
5 mm	6% / 60,000 ppm	+/- 40 ppm
1 cm	3% / 30,000 ppm	+/- 20 ppm
2 cm	1.5% / 15,000 ppm	+/- 10 ppm
5 cm	0.75% / 7,500 ppm	+/- 4 ppm
10 cm	0.35% / 3,500 ppm	+/- 2 ppm
20 cm	0.2% / 2,000 ppm	+/- 1 ppm

The OPL is factory set during manufacture.

Temperature Variation

The water absorption peak near 1940 nm shifts to shorter wavelengths (blue-shifts) as temperature increases, altering the measured absorbance signal. For highest accuracy,

samples should be measured at constant temperature.

When sample temperature varies by more than 10°C, it is recommended to feed a temperature signal into the Kemtrak DCP007, which applies an automatic correction to the reported concentration.

Solubility

Water has limited solubility in many organic solvents. When present above its solubility limit, water forms suspended droplets that create a turbid emulsion, which can interfere with NIR absorption measurements.

Solvent	Water solubility (approx.)	Implication
Hexane	~100 ppm	Emulsion risk above this concentration
Kerosene	~5 ppm	Turbidity likely even at very low water content (Figure 3)

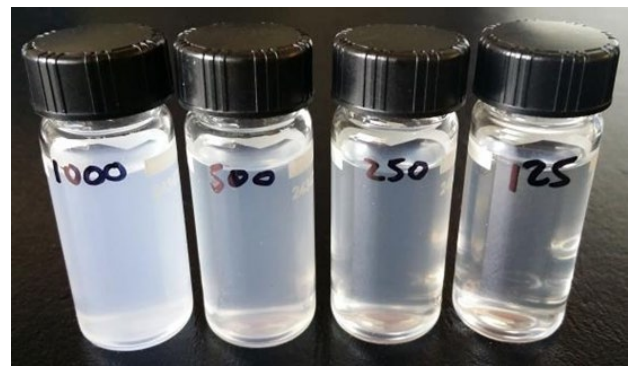


Figure 3: Water dispersed in kerosene at 1000, 500, 250 & 125 ppm concentration.

Results near or above the solubility threshold should be interpreted with care. The reference wavelength channel partially compensates for turbidity, but severe emulsification will degrade measurement accuracy.

Volatility and Handling

Volatility is a commonly overlooked source of error in offline laboratory testing. When samples contain volatile components – alcohols, ketones, or low-boiling solvents – preferential evaporation during sample collection and transport shifts the composition before measurement, meaning the result reflects a degraded sample rather than the actual process stream.

At trace water levels, atmospheric moisture is an additional concern. Anhydrous methanol, for example, is strongly hygroscopic, and even brief handling exposure can introduce significant water contamination.

Inline measurement eliminates these errors by analyzing the sample directly in the process stream – no extraction, no transport, no atmospheric exposure.

INSTRUMENT: KEMTRAK DCP007-NIR

The Kemtrak DCP007-NIR is a rugged inline photometric process analyzer designed for precise, continuous concentration monitoring. It uses solid-state LED light sources and fiber optics connected to an inline measurement cell, delivering accurate, drift-free measurements directly in the process stream without sample extraction.



Figure 4 DCP007-NIR Field Mounted Process Photometer Unit

Parameter	Value	Notes
Resolution	±20 ppm	1cm OPL
Photometric resolution	0.001 AU	
Measurement wavelengths	Up to 2 discrete	Factory configured
Recommended NIR region	~1930 nm	Low percent/trace water concentrations
Max total absorbance (Atotal)	≤ 3 AU	Exceeding causes non-linearity
Max background absorbance	≤ 1 AU	Water-free chemical background
Temperature compensation	External signal input	Required if $\Delta T > 10^{\circ}\text{C}$ or non-isosbestic operation
Light source and Detector	Long-life LED and InGaAs photodetector with multiple stage solid-state Peltier temperature regulation	Highly stable measurement with zero maintenance
Interface	Web-based	Configuration & data up/download



DCP007-NIR FEATURES

- **Real-time continuous measurement:** Immediate process feedback; no waiting for laboratory results
- **Inline, sealed measurement:** Eliminates volatility errors and sampling-related inaccuracies
- **Isosbestic point operation:** Minimizes temperature sensitivity without external compensation
- **External temperature input:** Enables accurate measurement when temperature varies $> 10^{\circ}\text{C}$
- **Reference wavelength compensation:** Corrects for window fouling and particulates automatically
- **Zero-maintenance LED light source:** No lamp replacements; long service intervals; low cost of ownership
- **No moving parts:** High reliability and minimal downtime in industrial environments
- **Automatic zeroing:** Drift-free measurements without manual baseline adjustment
- **Fiber optic connection to cell:** Electronics isolated from harsh process environments
- **Web-based interface:** Remote configuration, monitoring, and data export from any browser
- **Wide OPL / cell selection:** Adaptable to 0–100% range across alcohols, glycols, acids, caustics, and solvents
- **Outperforms other sensors:** Specific, linear response across full concentration range; unaffected by ionic contaminants

GET IN TOUCH

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