A New Measurement Model for an Unscented Kalman Filter for Effective Rise Time Reduction of Fourier Transform Infrared Spectroscopy Measurements

David Wilson, Casey Allen
Motivation: High-speed comprehensive emissions data needed for transient/instantaneous emissions models

Instantaneous and integrated emissions can be sensitive to speed-load history

(Rakopoulos et al., 2009), (Hagena et al., 2011)

Toxicity and environmental impact of engine exhaust depends strongly on the species distribution (e.g., benzene and 1,3-butadiene highly toxic)
Fourier Transform Infrared Spectroscopy

Intensity

Optical Path Difference

Fourier Transform

Transmittance

Wavenumber

Absorbed regions

Chemical Composition
Transient Exhaust Measurements with FTIR

FTIR measurements characterize historic emissions

Estimate with Bayesian Methods
Bayesian Model-Based Data Processing

Bayesian Processor

Model-based algorithm for filtering measurement data to predict most probable states.

State Prediction  Measurement  Gain/Update

Based on physical model  \( \hat{Z}_{in}(t_k) \)  Calculates new state distribution

\( p \)  \( Z_{in}(t_k) \)
Bayesian Model-Based Data Processing

State Transition Model

\[
\begin{bmatrix}
Z_{in}(t_k) \\
Z(t_k) \\
\dot{m}(t_k)
\end{bmatrix} =
\begin{bmatrix}
Z_{in}(t_{k-1}) \\
Z(t_{k-1}) \\
\dot{m}(t_{k-1})
\end{bmatrix}
\left(1 - e^{-\frac{\Delta t}{\tau(t_{k-1})}}\right) +
\begin{bmatrix}
Z_{in}(t_{k-1}) \\
Z(t_{k-1}) \\
\dot{m}(t_{k-1})
\end{bmatrix} e^{-\frac{\Delta t}{\tau(t_{k-1})}}
\]

Measurement Model

FTIR

\[
\begin{bmatrix}
Z \cdot \frac{MW_{mix}}{MW}
\end{bmatrix}
\]

Flow Meter

\[
\begin{bmatrix}
\frac{Z}{\dot{m}}
\end{bmatrix}
\]
Measurement Bias

Step change in propylene composition

FTIR measurements alternate between gradual and significant rise

Probable Cause

1) Alternation between forward and backward scan
2) Fourier transforming a transient signal
Consider a linearly changing signal at some wavenumber. The intensity calculated by FT is heavily weighted by the intensity at centerburst location.
Fourier Transform of Transient IR Band

\[ I(x) = A(x) \int_{-\infty}^{\infty} \Pi_{\nu_1, \nu_2}(\nu) \cos(2\pi \nu x) \, d\nu \]

\[ F(\nu, x) = A(x) \Pi_{\nu_1, \nu_2}(\nu) \]

\[ A(x) = \beta + \gamma x \]

\[ I(x) = A(x) \frac{\sin(2\pi \nu_2 x) - \sin(2\pi \nu_1 x)}{2\pi x} \]
Fourier Transform of Transient IR Band cont..

\[ \hat{F}(\nu) = 2 \int_0^\infty D(x)(\beta + \gamma x) \frac{\sin(2\pi \nu_2 x) - \sin(2\pi \nu_1 x)}{2\pi x} \cos(2\pi \nu x) dx \]

Apodization Function

\[ = \int_0^\infty D(x)(\beta + \gamma x) \cos(2\pi \nu x) dx \times 2 \int_0^\infty \frac{\sin(2\pi \nu_2 x) - \sin(2\pi \nu_1 x)}{2\pi x} \cos(2\pi \nu x) dx \]

\[ = \int_0^\delta D(x)(\beta + \gamma x) \cos(2\pi \nu x) dx \times \frac{1}{2} \left[ \Pi_{\nu_1,\nu_2}(\nu) + \Pi_{-\nu_2,-\nu_1}(\nu) \right] \]

Assume resolution is half the bandwidth

\[ \frac{1}{\delta} = \frac{1}{2}(\nu_2 - \nu_1) \]

True spectrum of steady, uniform, unit band

\[ \hat{F}(\nu) = \frac{\beta}{2\pi} Si(2\pi) + \frac{\gamma \delta}{8\pi^2} \]
**Modified Measurement Model**

\[
\hat{F}(v) = \frac{\beta}{2\pi} Si(2\pi) + \frac{\gamma \delta}{8\pi^2}
\]

\[
\begin{align*}
\beta & \propto Z_0 \\
\gamma \delta & \propto Z_\delta - Z_0 = \Delta Z \\
\hat{F}(v) & \propto \hat{y} \text{ (measured composition)}
\end{align*}
\]

\[
\hat{y} = \left[ Z_0 + \frac{\Delta Z}{4\pi Si(2\pi)} \right] \cdot \frac{MW_{mix}}{MW}
\]

**Forward Scan**

\[
\hat{y}(t_k) = \left[ Z(t_{k-1}) + \frac{Z(t_k) - Z(t_{k-1})}{4\pi Si(2\pi)} \right] \cdot \frac{MW_{mix}}{MW}
\]

**Backward Scan**

\[
\hat{y}(t_k) = \left[ Z(t_k) - \frac{Z(t_k) - Z(t_{k-1})}{4\pi Si(2\pi)} \right] \cdot \frac{MW_{mix}}{MW}
\]
Results
Summary

- Bayesian model for processing FTIR data was created
- FTIR measurements of transient composition were shown to be biased
- A new measurement model was created to account for bias
- The modified measurement model was shown to improve inlet composition estimations

Future Work
- Validate for wider range of inlet composition profiles
- Apply to engine studies
Small corrections for forward scan

**Reason**

Measurement is a weak function of current composition

\[
\hat{y}(t) = \left[ z(t - 1) + \frac{z(t) - z(t - 1)}{4\pi Si(2\pi)} \right] \cdot \frac{MW_{mix}}{MW}
\]

Covariance between \( \hat{y} \) and \( Z_{in}(t)/Z(t) \) small, yielding small \( K(t) \) and \( e(t) \)

\[
e(t) = y(t) - \hat{y}(t|t - 1)
\]

\[
\hat{x}(t|t) = \hat{x}(t|t - 1) + K(t)e(t)
\]

**Diagram**

- Actual Inlet Z
- Estimated Inlet Z
- Estimated Gas Cell Z
- Measured Gas Cell Z

Here, \( Z \) represents the concentration, \( y(t) \) the actual measurement, \( \hat{y}(t) \) the estimated measurement, \( e(t) \) the error, and \( K(t) \) the Kalman gain.
Bayesian Processing Algorithms

**Prediction**

\[ \hat{X}(t_k|t_{k-1}) = A\hat{X}(t_{k-1}|t_{k-1}) \]
\[ \tilde{P}(t_k|t_{k-1}) = A\tilde{P}(t_{k-1}|t_{k-1})A' + R_{ww}(t_{k-1}) \]

**State**

**State Error Covariance**

**Innovation**

\[ e(t_k) = y(t_k) - CX(t_{k-1}|t_{k-1}) \]
\[ R_{ee}(t_k) = C\tilde{P}(t_k|t_{k-1})C' + R_{vv}(t_{k-1}) \]

**Innovation Covariance**

**Gain**

\[ K(t_k) = \tilde{P}(t_k|t_{k-1})C'R_{ee}(t_k)^{-1} \]

**State Update**

\[ \hat{X}(t_k|t_k) = \hat{X}(t_k|t_{k-1}) + K(t_k)e(t_k) \]
\[ \tilde{P}(t_k|t_k) = [I - K(t_k)C]\tilde{P}(t_k|t_{k-1}) \]

**Covariance Update**

**Initial prediction of current state, utilizing state transition model**

**Forward Time Step**

- Initial prediction of current state, utilizing state transition model
- Difference between measurement prediction, actual measurement
- Correction of state, covariance estimates