Estimation of Point Source Emissions from Oil Refineries

Don Chmielewski
Vasilios Manousiouthakis

Bruce Tilton
Brad Felix

UCLA
Simulation Sciences

1998 AIChE Annual Meeting
Leak Detection in Above Ground Storage Tanks

Total Losses = Total Mass In - Total Mass Out
Estimation/Detection in the Chemical Process Industry

Data Reconciliation:

- Plant Model: Steady State
- Time Scale: Days
- Algorithm: Weighted Least Squares to Fit Mass/Energy/Component Balances

\[
\min \sum \frac{(y_i - \hat{y}_i)^2}{\sigma_i^2}
\]
\[
s.t. \quad f(\hat{y}) = 0 \quad g(\hat{y}) \leq 0
\]

Mass Balance Only $\Rightarrow$ DR Equivalent to MLE, Bayesian or MMSE.

- Fault Detection: Gross Error Detection to find Measurement Outliers
- Commonly Used in Industry
Estimation/Detection in the Chemical Process Industry

**Dynamic Data Reconciliation:**

- Plant Model: Dynamic
- Time Scale: Minutes
- Algorithm: Extended KF or Modified Weighted Least Squares to Fit Dynamic Mass/Energy/Component Balances
- Mass Balance Only $\Rightarrow$ DDR Equivalent to KF.
- Fault Detection: Extensions of Gross Error Detection (Largest Difficulty)
- Algorithm Still in the Development Stages
### Loss Sources

<table>
<thead>
<tr>
<th>Real Losses</th>
<th>Apparent Losses</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Fired Fuel</td>
<td>• Slops/Recycles</td>
</tr>
<tr>
<td>• Flares</td>
<td>• Metering Errors</td>
</tr>
<tr>
<td>• Evaporation</td>
<td>• Line Fills</td>
</tr>
<tr>
<td>• Leakage to Water</td>
<td>• Storage Tank Vapor</td>
</tr>
<tr>
<td>• Leakage to Ground</td>
<td>• Density Errors</td>
</tr>
</tbody>
</table>
Existing Methods to Estimate Losses

Real Losses (Emission Monitoring)

- Emission Models (EPA/API)
- Bag and Sniff Tests (Small Equipment)
- Tracer Tests (Large Equipment)
- Continuous Emission Monitoring Systems (CEMS)
- Off-Line Inspections

Apparent Losses

- Careful Tracking/Bookkeeping of Plant Operations
- Data Reconciliation
EPA Rules

Allowable Methods for Materials Accounting:

- Direct Measurements
- Business Records
- Mass Balances
- Engineering Calculations
Loss Accounting

Definition:

Employ All Data Sources to Identifying the Location of All Material Received into the Plant.

Loss Accounting Activities:

(1) Collect Relevant Data
(2) Extract Loss Information from Each Source
(3) Integrate Loss Information from Different Sources
(4) Interpret Results
Data Sources

Direct:
- Field Tests
- Emission Models

Indirect:
- Records of Plant Operations (DCS)
- Receipts, Inventory and Shipment Data
Example #1: Losses from an Isolated Tank

Mass Balance gives the amount of Lost Material

\[ L = m_{in} - m_{out} - (m_{close} - m_{open}) \]

Loss Measurement

\[
L^+ = m_{in}^+ - m_{out}^+ - (m_{close}^+ - m_{open}^+) \\
= L + n_{in} - n_{out} - (n_{close} - n_{open}) = L + n
\]

\((*)^+\) is a measurement: \((*)^+ = (*) + n_*\), and \(n_*\) is random error.
Loss Measurement Accuracy

Standard Deviation of $L^+$:

$$\sigma = \sqrt{\sigma_{in}^2 + \sigma_{out}^2 + \sigma_{open}^2 + \sigma_{close}^2}$$

Typical Loss Rates vs. Loss Measurement Accuracy:

<table>
<thead>
<tr>
<th>Tank Diameter</th>
<th>10 (m)</th>
<th>30 (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed Roof Tank</td>
<td>36.0 (gal/day)</td>
<td>348.0</td>
</tr>
<tr>
<td>Internal Floating Roof</td>
<td>2.7</td>
<td>12.3</td>
</tr>
<tr>
<td>External Floating Roof</td>
<td>11.0</td>
<td>33.0</td>
</tr>
<tr>
<td>EFR with secondary seal</td>
<td>0.5</td>
<td>1.6</td>
</tr>
<tr>
<td>Lower Bound on $\sigma$</td>
<td>± 47</td>
<td>± 425</td>
</tr>
</tbody>
</table>
Estimation of Loss Rates
from Indirect Data Sources

Does there exist enough accuracy in the measurement equipment to infer loss rates with a sufficient amount of accuracy?
Raw Loss Measurements
Moving Average Estimation

\[ \hat{L}_{k}^{(av)} = \frac{1}{k} \sum_{i=1}^{k} L_i^+ = \hat{L}_{k-1}^{(av)} + \frac{1}{k} (L_k^+ - \hat{L}_{k-1}^{(av)}) \]

- Weights Each Loss Measurement Equally

\[ \sigma_k \approx c_0 + c_1 \sqrt{\left| m_k^{(in)} \right| + \left| m_k^{(out)} \right|} \]

- Will Not Track Time-Varying Loss Rates
Optimal Estimation

Choose $\hat{L}_k(\cdot)$ to minimize the mean squared error

$$E \left[ \left( L_k - \hat{L}_k(L_k^+) \right)^2 \right]$$

where

$$L_{k+1} = L_k + d_k$$

$$L_k^+ = L_k + n_k$$

Solution:

$$\hat{L}_{k+1} = \hat{L}_k + \frac{P_k}{\sigma_k^2}(\hat{L}_k - L_k^+)$$

$$P_k = \frac{P_{k-1} + \sigma_{dk-1}^2}{1 + P_{k-1}(\sigma_{dk-1}^2 + \sigma_k^2)}$$
Filtered Loss Measurements

![Graph showing Actual Loss Rate, LTI Filter (averaging), and Optimal Filtering over time (days), with loss rate in gallons/day.](image)
Generalization to the Network Case

Generalization will allow for

- Exploitation of Additional Correlations
- Simultaneous Estimation of Apparent Losses
- Operation Dependent Loss Mechanisms
Example 2: A Simple Tank Network

Additional Correlation due to Mass Flow Interconnections

\[ L_k^{(1)+} = m_k^{(op1)+} - m_k^{(cl1)+} = L_k^{(1)} + n_k^{(op1)} - n_k^{(cl1)} - n_k^{(1)} \]

\[ L_k^{(2)+} = m_k^{(op2)+} - m_k^{(cl2)+} = L_k^{(2)} + n_k^{(op2)} - n_k^{(cl2)} - n_k^{(2)} \]

\[ L_k^{(3)+} = m_k^{(1)+} + m_k^{(2)+} = L_k^{(3)} + n_k^{(1)} + n_k^{(2)} - n_k^{(3)} \]

\( n_k^{(1)} \) and \( n_k^{(2)} \) are present in multiple measurements \( L_k^{(i)+} \).
Apparent Losses

- Network Case with a Single Day of Measurements is Equivalent to Data Reconciliation.

- Removal of Apparent Losses will Improve the Estimation of Real Losses.

- Data Reconciliation will Force all Balances to Close.

- Real and Apparent Losses can be Estimated Simultaneously.
Meter Bias

Errors in Mass Flow Measurements:

\[ m_k^{(in)} + = \underbrace{m_k^{(in)}}_{\text{True Value}} + \underbrace{b_0 m_k^{(in)}}_{\text{Systematic Error}} + \underbrace{n_k^{(in)}}_{\text{Random Error}} \]

Resulting Loss Measurement:

\[ L_k^+ = L_k + b_0 m_k^{(in)} + n_k \]
Generalized Model of Loss Rates

\[
\begin{bmatrix}
\L_{k+1} \\
\b_{k+1} \\
\a_{k+1}
\end{bmatrix} = \begin{bmatrix}
I & 0 & 0 \\
0 & I & 0 \\
0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\L_{k} \\
\b_{k} \\
\a_{k}
\end{bmatrix} + \begin{bmatrix}
\nabla(L) \\
\nabla(b) \\
\nabla(a)
\end{bmatrix}
\]

(Time-Evolution of Loss Rates)

\[
\y^+_k = C_k \begin{bmatrix}
\L_{k} \\
\b_{k} \\
\a_{k}
\end{bmatrix} + G\n_k
\]

(Indirect Measurements)

Compactly written as

\[
x_{k+1} = A x_k + d_k 
\]

\[
y^+_k = C_k x_k + G\n_k
\]

\[
E[d_k d'_k] = \Sigma^{(d)}_k 
\]

\[
E[\n_k \n'_k] = \Sigma_k
\]
Optimal Loss Estimation  
(Kalman Filtering)

\[\hat{x}_{k+1} = A\hat{x}_k + P_kC_k\Sigma_k^{-1}(y_k^+-C_kA\hat{x}_k)\]

\[P_k = (I + H_{k-1}C_k\Sigma_k^{-1}C_k)^{-1}H_{k-1}\]

\[H_{k-1} = AP_{k-1}A' + G\Sigma^{(d)}_{k-1}G'\]

where

\[\hat{x}_k = \begin{bmatrix} \hat{L}_k \\ \hat{b}_k \\ \hat{a}_k \end{bmatrix} \]
Example 3: Network with Meter Bias

- **Crude Pool**: $m_1$, $m_2$
- **Gas Oil**: $m_5$
- **Jet Fuel Pool**: $m_3$, $m_4$
- **Waste Oil Tank**: $m_6$
Estimates With No Bias Present

- Actual Loss
- Optimal Filter without Bias Detection
- Optimal Filter with Bias Detection

Loss Rate at Jet Tank #1 (gallons/day)

Time (days)
Estimates With 0.5 % Bias
Integration with Direct Measurements

- Estimates must be Combined with the Results of Field Tests

- Integration Scheme should Weight the Accuracy of the Estimates vs. the Accuracy of the Direct Measurements

- Uncertainty of Direct Measurements will Increase as the Time Since Last Test Increases
Interpretation of Results

- Graphical Approaches

- Statistical Quality Control Methods (Automated Rules)
Conclusions

- Loss Accounting can Provide Higher Quality Information that the Usual Emission Monitoring Activity.

- The Quality of a Leak Detection and Repair (LDAR) Program can be Improved, in turn Reducing Maintenance and Environmental Compliance Costs.

- Indirect Measurements can Provide Sufficiently Accurate Estimates of Plant Losses.
Acknowledgments

Financial Support provided by:

The National Science Foundation
award number: GER 95-54570

and

Simulation Sciences Inc.