Gas Analysis and Toxicity Assessment of Combustion Products of Aircraft Materials

Louise C. Speitel
Fire Safety Branch ATO-P, AJP-6320
FAA W.J. Hughes Technical Center
Atlantic City International Airport, NJ  08405

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OUTLINE OF TALK

- FAA Gas Analysis Instrumentation
- Requirements for Toxicity Assessment of Combustion Gases
- The FAA Toxicity Model
- FTIR Method
- FTIR Results: Response Times, Gas Histories, Toxicity
TGA WITH EVOLVED GAS MONITORING
TGA-DTA WITH EVOLVED GAS MONITORING
GAS CHROMATOGRAPH WITH MASS SPECTOMETER (GC-MS) WITH PYROPROBE
FOURIER TRANSFORM INFRARED SPECTROMETER (FTIR) WITH PYROPROBE
ION CHROMATOGRAPH WITH ELECTROCHEMICAL & AMPEROMETRIC DETECTORS

GASES:
- HCN
- HF
- HCl
- HBr
- HI
- I₂
- H₂S
- SOₓ
- NOₓ
PROCESS ANALYZERS:

GASES:
CO
CO2
O2
Halo-carbons
THC
Water
FTIR PROCESS ANALYTICAL SYSTEM

GASES:

CO
CO₂
HCN
NH₃
NO
NO₂
SO₂
HF
HCl
HBr
COF₂
H₂S
... etc.
REQUIREMENTS FOR TOXICITY ASSESSMENT OF COMBUSTION GASES

• Combustion conditions of test must match fire to be modeled
• Quick time to full response for gas measurements
• Operational simplicity: fire test, gas analysis and toxicity calculations
• Estimate of the reliability of each gas measurement as a function of time
• Valid toxicity model
FAA TOXICITY MODEL: FED₁ & FEDₐ

For a constant concentration of a toxic gas:

The effect is predicted to occur when \( \text{FED}_{\text{Effect}} = 1 \)

Incapacitation & Lethality Models

\[
\text{FED}_{\text{Effect}} = \frac{\text{dose received at time } t}{\text{effective Ct dose to cause effect}} = \frac{C_t}{C_t \text{ effect}} = \frac{t}{t \text{ effect}}
\]

If the concentration varies with time:

\[
\text{FED}_{\text{Effect}} = \int_o^t \frac{dt}{t_{\text{Effect}}}
\]
\[ FED_I = FED_{I\ Gases} + FED_{I\ Heat} \]

\[ = FED_{I\ CO} + FED_{I\ HCN} + FED_{I\ HCl} + FED_{I\ HF} + FED_{I\ HBr} + \]

\[ FED_{I\ Acrolein} + FED_{I\ CO_2} + FED_{I\ NO_2} + FED_{I\ LowO_2} + FED_{I\ Heat} \]

\[ V_{CO_2} = \exp \left( 0.2496 \times C_{CO_2} + 1.9086 \right) \]

\[ \text{where} \quad C_{CO_2} = \% \ CO_2 \]

\[ \frac{6.8}{6.8} \]
FAA TOXICITY MODEL

\[ F ED_1 = \frac{1}{3.4250} \int \left( V_{CO_2} \times C_{CO} \right) dt \]
\[ + \int \frac{\left( V_{CO_2} \times C_{HCN} - 63 \right)}{564} dt \]
\[ + \int \frac{\left( 3 + \left[ \frac{3.36 \times 10^{-5}}{V_{CO_2} \times C_{HCl} - 300} \right] \right)}{dt} \]
\[ + \int \frac{\left( 3.0 + \left[ \frac{1.53 \times 10^{-5}}{V_{CO_2} \times C_{HF} - 136} \right] \right)}{dt} \]
\[ + \int \frac{\left( 3 + \left[ \frac{3.36 \times 10^{-5}}{V_{CO_2} \times C_{HBr} - 300} \right] \right)}{dt} \]
\[ + \int \frac{\left( 1.50 + \left[ \frac{4.0 \times 10^{2}}{V_{CO_2} \times C_{Acrolein} + 500} \right] \right)}{dt} \]
\[ + \int \frac{\left( V_{CO_2} \times C_{NO_2} - 290 \right)}{1.14 \times 10^{4}} dt \]
\[ + \int \frac{dt}{\exp \left( 6.1623 - 0.5189 \times C_{CO_2} \right)} \]
\[ + \int \frac{dt}{2193.8 - 311.6 \times C_{CO_2}} \]
\[ + \int \frac{dt}{\exp \left( 8.55 - 0.511 \left( 20.9 - \% O_2 \right) \right)} \]
\[ + \frac{1}{4.1 \times 10^{-8}} \int T^{3.61} dt \]

when \( V_{CO_2} \times C_{CO} > 0.01\% \)
when \( V_{CO_2} \times C_{HCN} > 63 \) ppm
when \( V_{CO_2} \times C_{CHCl} > 300 \) ppm
when \( V_{CO_2} \times C_{CHF} > 136 \) ppm
when \( V_{CO_2} \times C_{CHBr} > 300 \) ppm
when \( V_{CO_2} \times C_{Acrolein} > 300 \) ppm
when \( V_{CO_2} \times C_{NO_2} > 290 \) ppm
when \( C_{CO_2} > 7.0\% \)
when \( 5.5 \leq C_{CO_2} \leq 7.0\% \)
when \( \% O_2 < 11\% \)
when \( T > 50°C \)

See http://www.fire.tc.faa.gov

FAA FTIR SYSTEM AND METHOD

- Extractive FTIR analytical system to analyze rapidly changing moist fire gas concentrations as a function of time for 20 gases
- Short system response times
- Quantitative evaluation over wide dynamic range
- Estimate of reliability of each gas measurement over time
- 20+ gas method with low residuals
DYNAMIC FTIR SYSTEM RESPONSE WITH GAS INTRODUCED AT HEATED SAMPLE LINE INLET
FTIR CALIBRATION SPECTRA OF SIXTEEN GASES
AT 170 DEGREES C: FULL-SCALE

- H_2O, 3%
- Phosgene
- SO_2
- COF_2
- NO
- HF
- HCN
- HCl
- HBr
- NO_2
- C_2H_2
- CO
- CH_4
- C_2H_6
- C_2H_4
- CO_2

Wavenumbers (cm^{-1})
FTIR SPECTRA OF MIXED PLASTIC SPECIMENS

Nonflaming

1.2
1.0
0.8
0.6
0.4
0.2
0.0

Absorbance

4500  4000  3500  3000  2500  2000  1500  1000

Wavenumbers (cm\(^{-1}\))

H\(_2\)O

HCl + Unknown gases

CO\(_2\)

H\(_2\)O

CO

C\(_2\)H\(_4\)

Flaming
FIRE GAS HISTORIES FOR DUPLICATE NONFLAMING TESTS OF MIXED PLASTIC SPECIMEN

![Graph showing concentrations over time for various gases including HCL, CO, CO2, ethylene, methane, and HCN.](image)
FIRE GAS HISTORIES FOR DUPLICATE FLAMING TESTS OF MIXED PLASTIC SPECIMEN

- Concentration H₂O, CO₂, HCl, CO
- Concentration All Other Gases

Graph showing concentrations over time:
- Water
- CO₂
- HCl
- CO
- Acetylene
- NO
- Ethylene
- HCN

Time (seconds) and Concentration (parts per thousand/parts per million)
OBJECTIVES

TOXICITY ASSESSMENT OF MATERIALS IN FIRE

• Develop software that calculates toxicity histories and mass balance histories for a cone calorimeter-FTIR test.
• The FAA models for incapacitation and lethality form the basis for the calculations. (FAA Report DOT/FAA/AR-95-5).
TOXICITY HISTORIES OF FLAMING MIXED PLASTIC SPECIMEN
TOXICITY HISTORIES OF NONFLAMING MIXED PLASTIC SPECIMEN
MASS BALANCE (KG) OF FLAMING MIXED PLASTIC SPECIMEN
MASS BALANCE (KG) OF NONFLAMING MIXED PLASTIC SPECIMEN
FED₁ OF FLAMING MIXED PLASTIC SPECIMEN
FED_{TOTAL} OF FLAMING AND NONFLAMING MIXED PLASTIC SPECIMEN

FLAMING

NONFLAMING