Evaluation of the Accuracy of Select Mathematical Models to Predict Airborne Concentrations from Small Indoor Spills

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Agenda

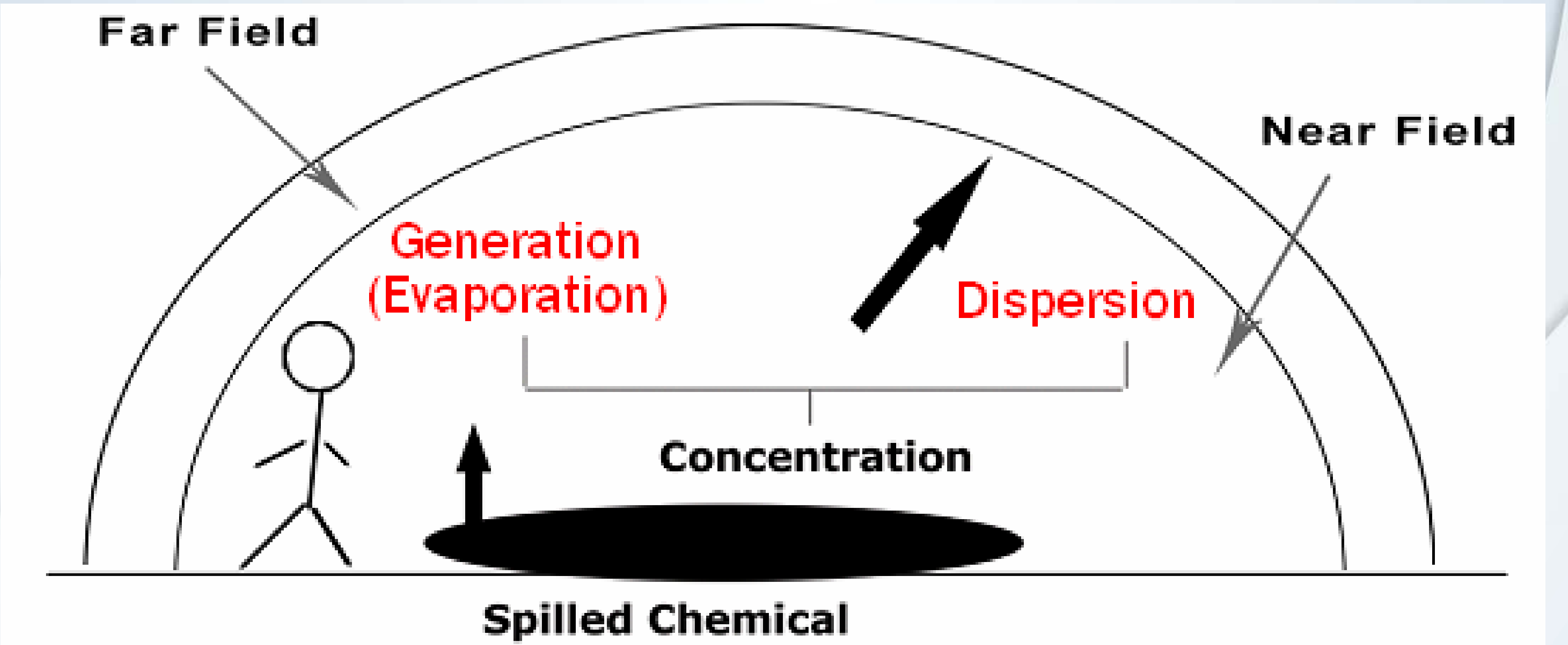
1. Background on Mathematical Models
2. Experimental Design
3. Results & Evaluation of Models

1. Background

1. Background on Mathematical Models

A Brief Introduction…

- A number of models available to predict exposures
- Generally broken into two components:



1. Background on Mathematical Models

Generation Rate Models

Hummel et al (1996)

$$\text{Evaporation Rate (g/sec/cm}^2\text{)} = \frac{\left(8.79 \times 10^{-5} (\mathrm{MW_A})^{0.823} (VP) \times \left(\frac{1}{MW_A} + \frac{1}{29}\right)^{0.25}\right)}{\mathrm{T}^{0.05}} \sqrt{\frac{V_X}{\Delta xp}}$$

Nielsen et al (1995)

$$R_{ii} = 0.662 D_{i,Air}^{2/3} v^{-1/6} V^{1/2} \left[\frac{\left(L^{3/4} - L_o^{3/4}\right)^{2/3}}{L - L_o}\right] \frac{\ln \frac{M^s}{M^\infty}}{\frac{M^s}{M^\infty} - 1} \frac{P}{\rho_{lm,Air}} \frac{\rho_{ii}}{RT}$$

Lennert et al (1997)

$$R_{ii} = 1.1 \times 10^{-6} V^{0.62} \rho_{ii}^{1.02} \left[\frac{\left(L^{3/4} - L_o^{3/4}\right)^{2/3}}{L - L_o}\right]^{0.86}$$

1. Background on Mathematical Models

Dispersion Models

Model	Theory	Limitation
The Well-Mixed Room	Exposure levels equal at all sources within a room	Underestimates exposure level near source
Two-Zone	Two distinct areas – the near-field & far field	Assumes air perfectly mixed within each zone
Eddy Diffusion	Complex concentration gradients around source	Requires experimental derivation of “diffusion coefficient” term

Others include Computational Fluid Dynamic Simulations, etc

1. Background on Mathematical Models

Dispersion Model

- Nicas (1996) – a two-zone model

$$C_{N,t} = \frac{G}{Q} + \frac{G}{\beta} + G\left[\frac{\beta \times Q + \lambda_2 \times V_N(\beta + Q)}{\beta \times Q \times V_N(\lambda_1 - \lambda_2)}\right]e^{\lambda_1 t} - G\left[\frac{\beta \times Q + \lambda_1 \times V_N(\beta + Q)}{\beta \times Q \times V_N(\lambda_1 - \lambda_2)}\right]e^{\lambda_2 t}$$

$$\lambda_1 = 0.5\left[-\left(\frac{\beta \times V_F + V_N(\beta + Q)}{V_N \times V_F}\right) + \sqrt{\left(\frac{\beta \times V_F + V_N(\beta + Q)}{V_N \times V_F}\right)^2 - 4\left(\frac{\beta \times Q}{V_N \times V_F}\right)}\right]$$

$$\lambda_2 = 0.5\left[-\left(\frac{\beta \times V_F + V_N(\beta + Q)}{V_N \times V_F}\right) - \sqrt{\left(\frac{\beta \times V_F + V_N(\beta + Q)}{V_N \times V_F}\right)^2 - 4\left(\frac{\beta \times Q}{V_N \times V_F}\right)}\right]$$

Combination Generation & Dispersion Model

- Keil and Nicas (2003) – a two-zone model

1. Background on Mathematical Models

Generation Rate Models

- Hummel et al (1996)
- Nielsen et al (1995)
- Lennert et al (1995)

Dispersion Models

- Nicas (1996)

Combination Generation & Dispersion Model

- Keil and Nicas (2003)

2. Experimental Design

2. Experimental Design

Selection of Chemicals to Evaluate

- Selected most common chemicals in our hospital laboratories:
  - Isopropanol
  - Ethanol
  - Methanol
  - Acetone
  - Acetic Acid
  - Xylene

2. Experimental Design

Quantitative Assessment

- Needed to select methods to quantitatively evaluate both generation and dispersion models over time
- Conducted simulated spills of these substances

2. Experimental Design

Quantitative Assessment

- Required:
  - Dedicated area to allow for multiple trials under set conditions
  - Segregated, negative pressure room
  - Environmental conditions approximating normal conditions
  - Visual access to room to allow researcher to exit room following spill

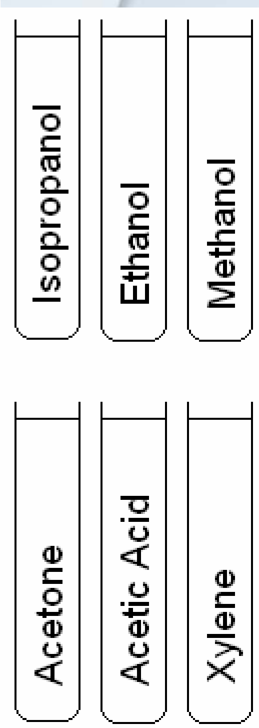
2. Experimental Design

Quantitative Assessment

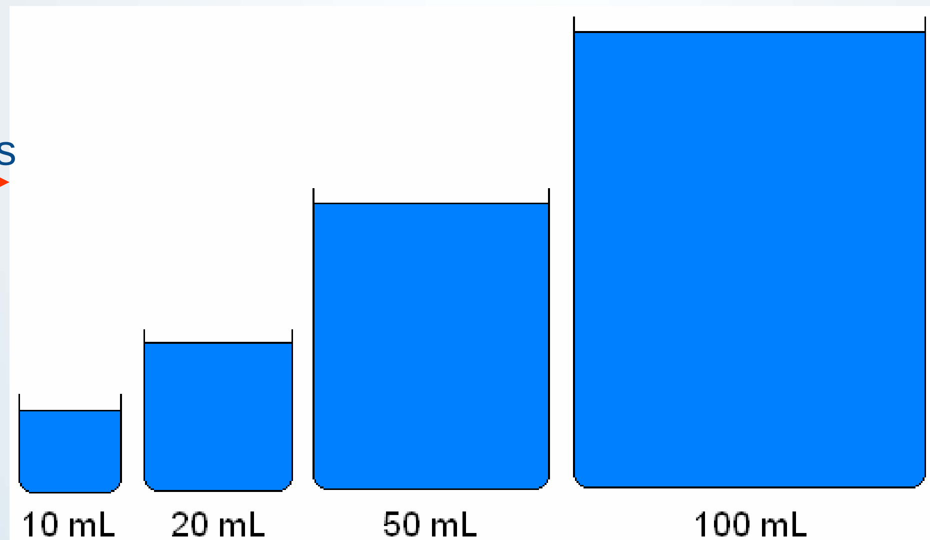
Ethylene Oxide Room in the Sterile Processing Department at Surrey Memorial Hospital

2. Experimental Design

Quantitative Assessment

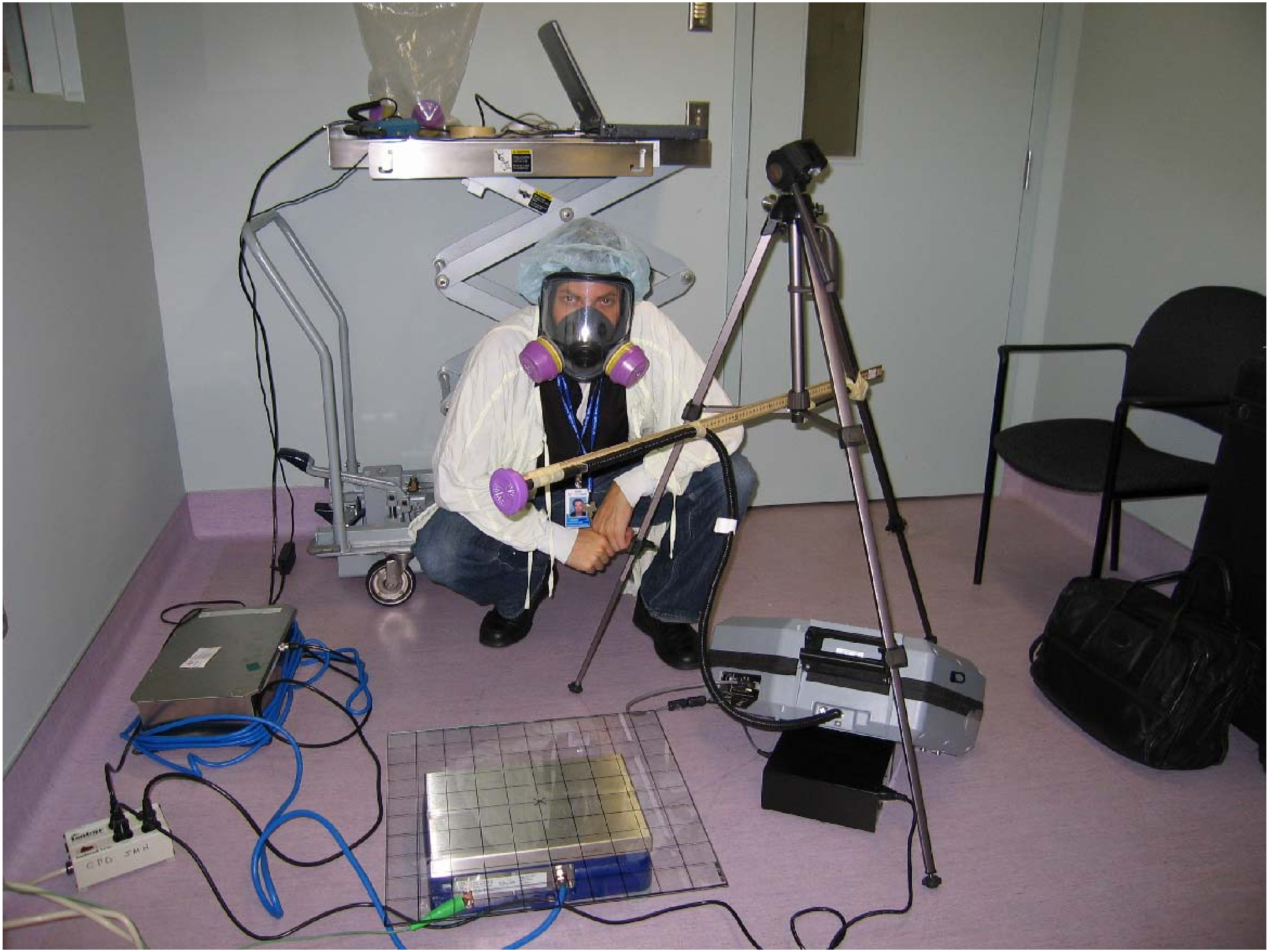


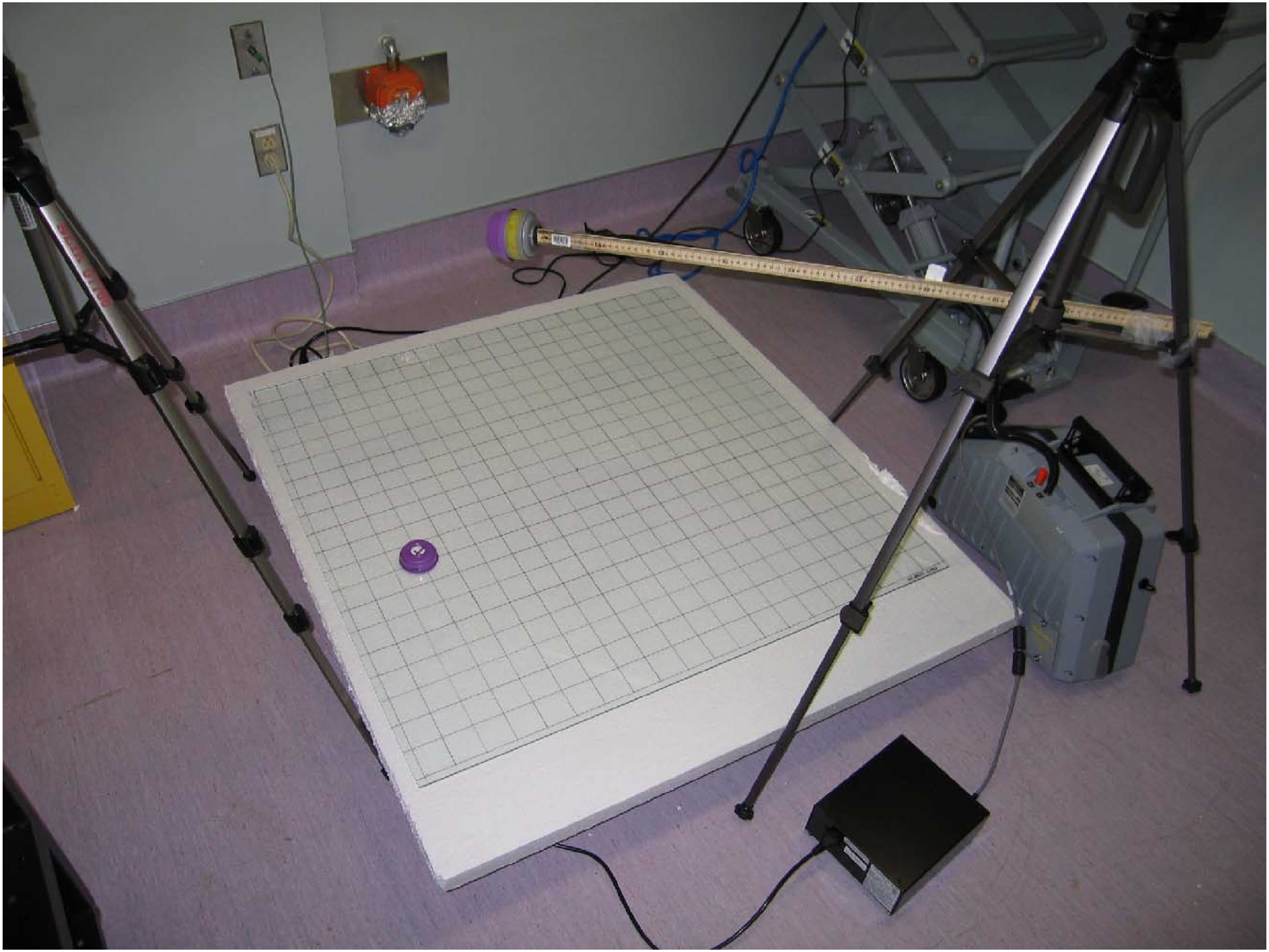
x 4 volumes



x 8 replicates **192 Total Trials**

Each trial ran for a total of 30 minutes, or until substance evaporated and level in room reached background


CPD SMN



2. Experimental Design

Additional Parameters Measured

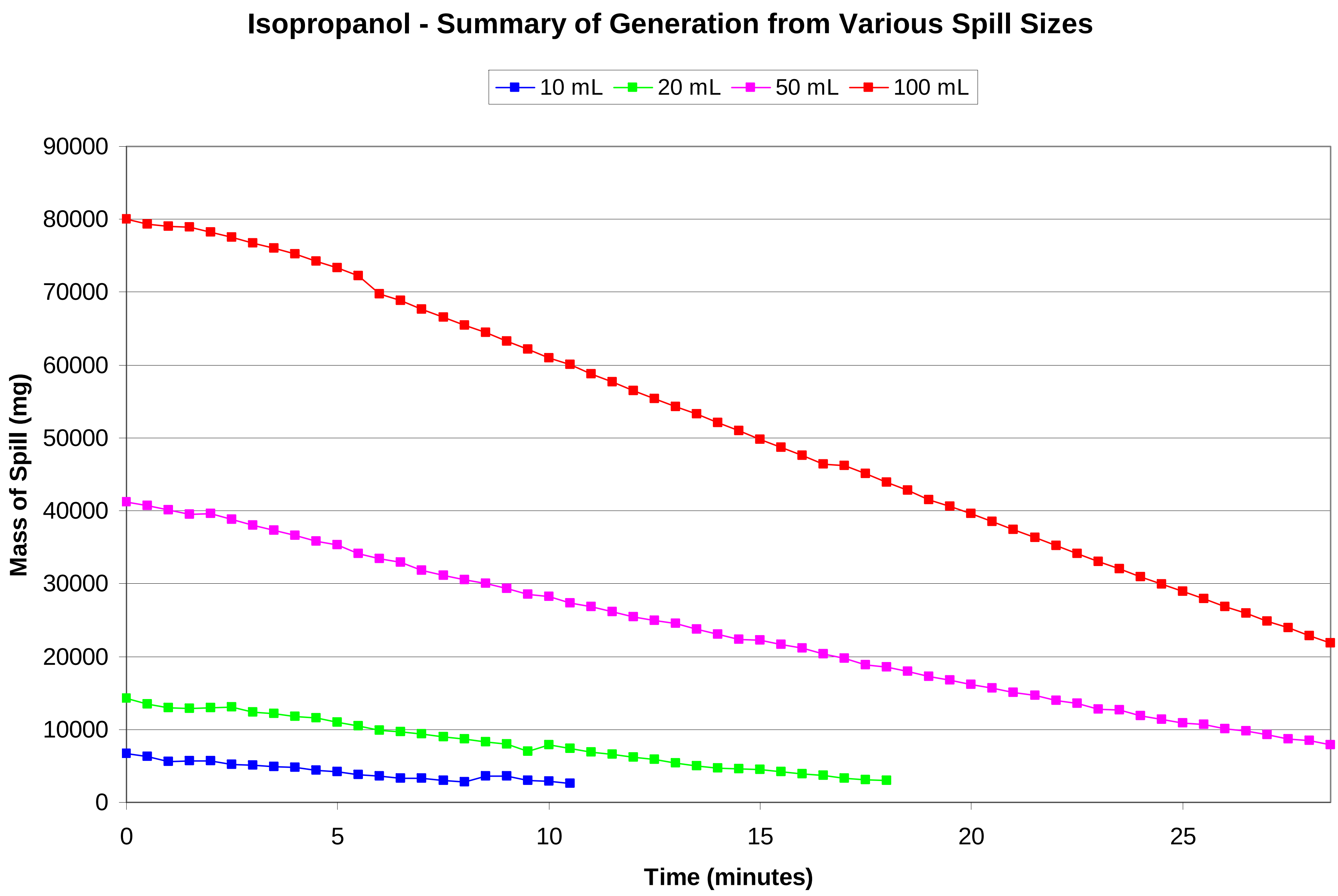
- Room temperature and humidity
- Room ventilation rate
- Spill volume
- Spill surface area
- Air velocity at spill surface
- Direction of airflow
- Pool length along airflow

3. Results & Evaluation of Models

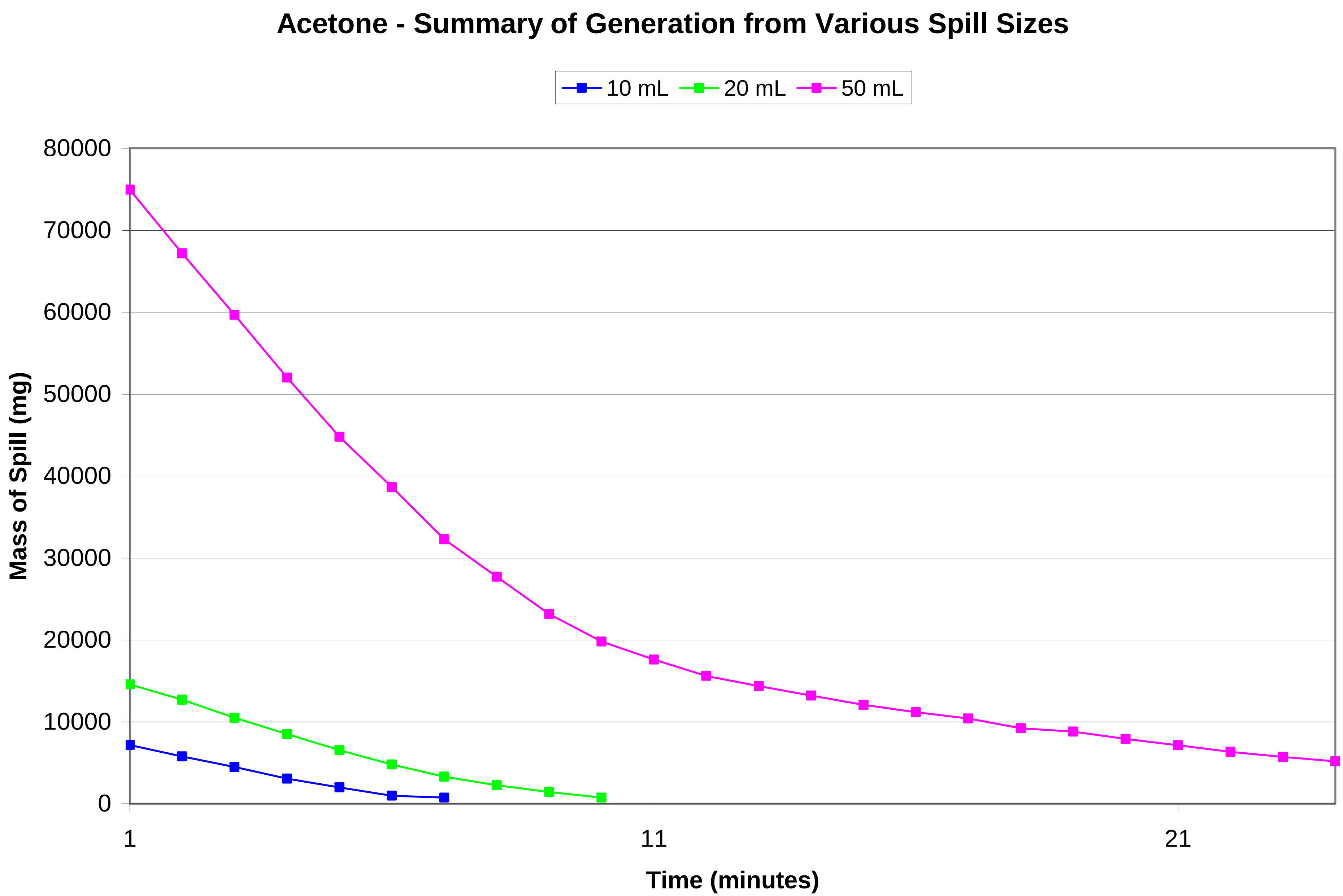
3. Results & Evaluation of Models

Generation Rate

- Data from scale plotted over time



Isopropanol - Summary of Generation from Various Spill Sizes
10 mL
20 mL
50 mL
100 mL
Mass of Spill (mg)
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
0
5
10
15
20
25
Time (minutes)



Acetone - Summary of Generation from Various Spill Sizes
10 mL
20 mL
50 mL
Mass of Spill (mg)
80000
70000
60000
50000
40000
30000
20000
10000
0
1
11
21
Time (minutes)

3. Results & Evaluation of Models

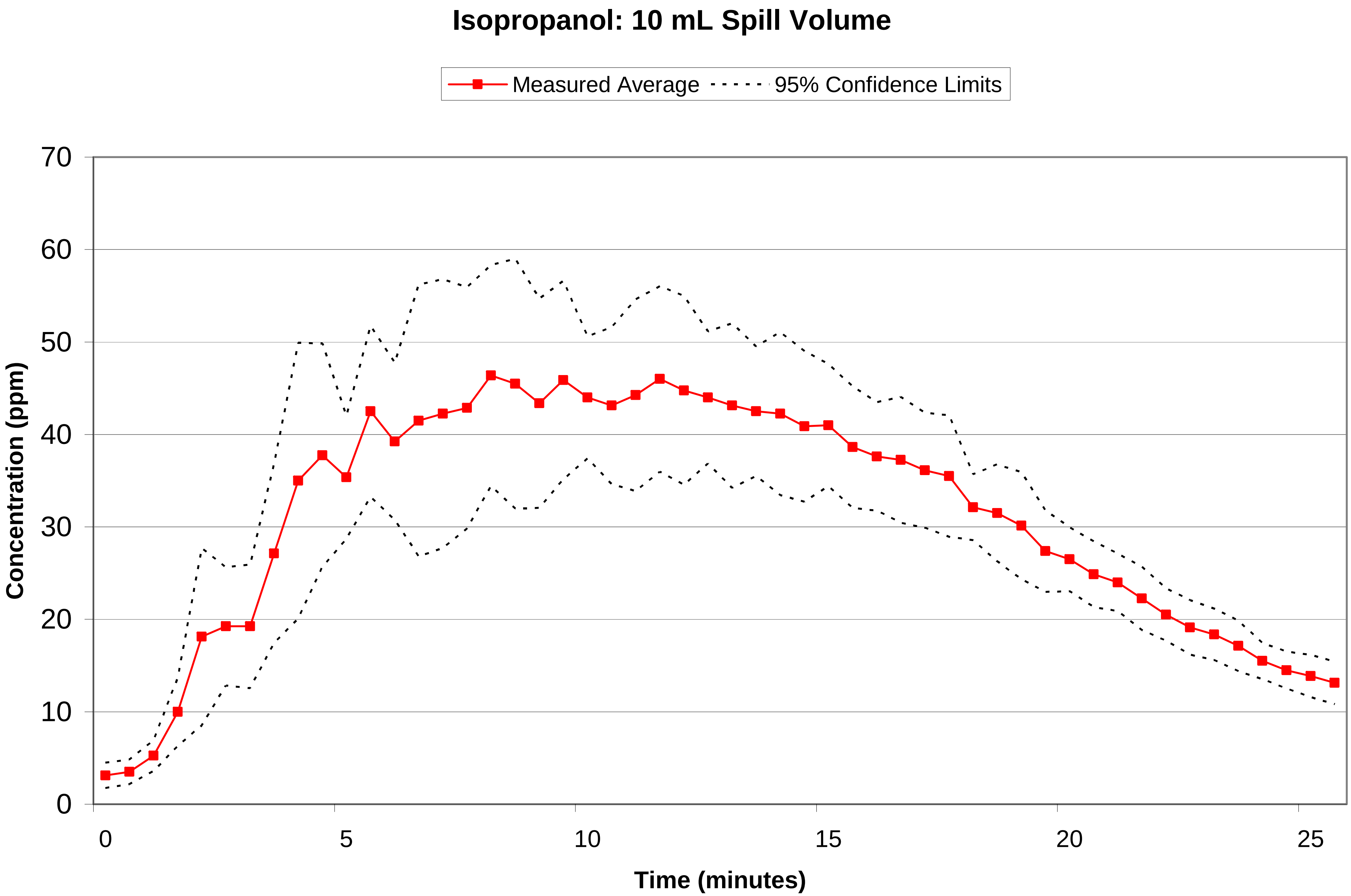
Generation Rate Models

- Hummel, Lennert, and Nielsen models assume constant generation rate over time
  - Models severely <u>underestimated</u> generation rate
  - On average 7x lower; ranged from 1.2x – 19x lower

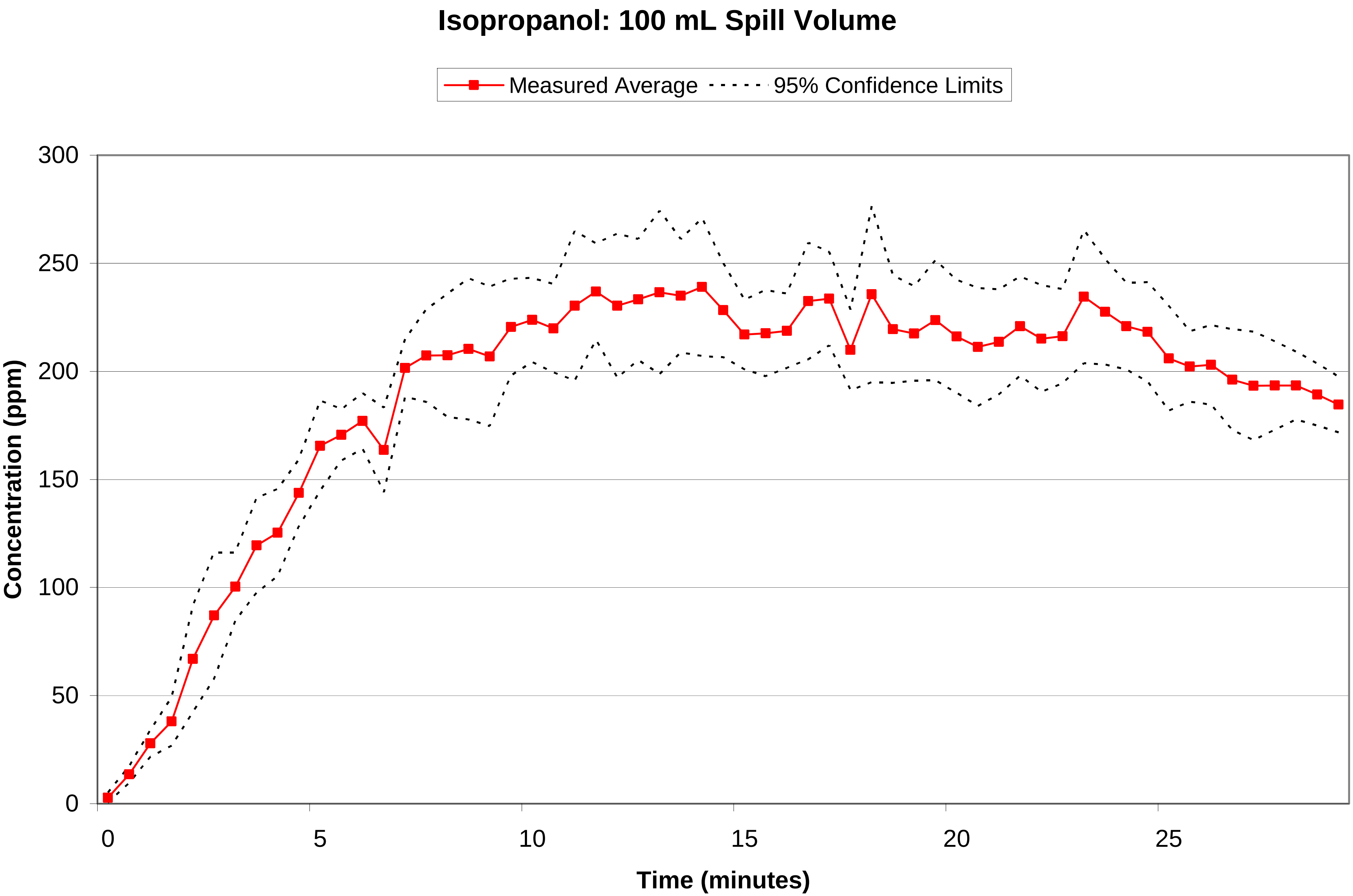
3. Results & Evaluation of Models

Dispersion Rate

- Data from Miran plotted over time



Isopropanol: 10 mL Spill Volume
Measured Average
95% Confidence Limits
Concentration (ppm)
0
10
20
30
40
50
60
70
0
5
10
15
20
25
Time (minutes)

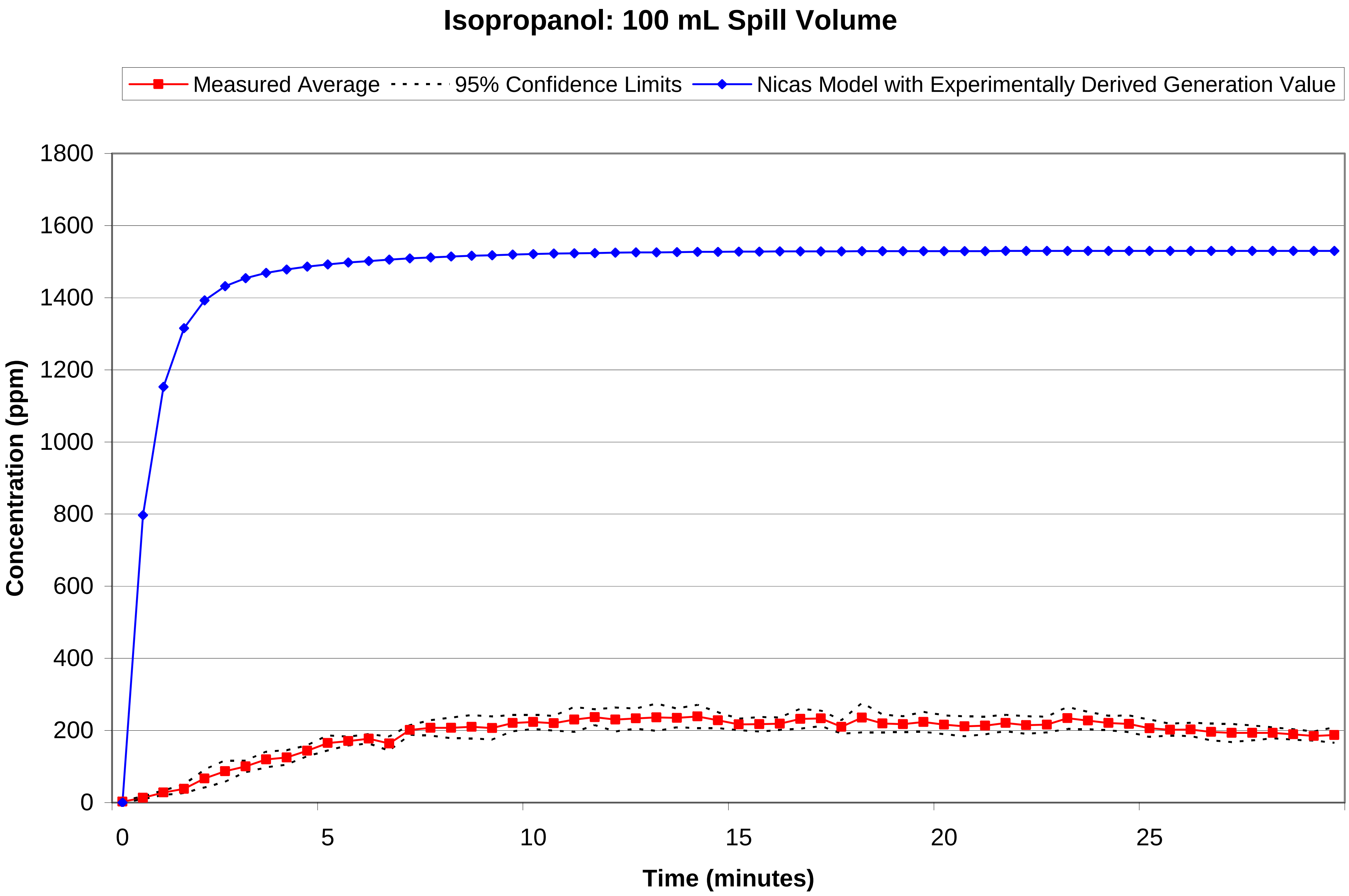


Isopropanol: 100 mL Spill Volume
Measured Average
95% Confidence Limits
Concentration (ppm)
300
250
200
150
100
50
0
0
5
10
15
20
25
Time (minutes)

3. Results & Evaluation of Models

Dispersion Rate Models

- Since generation rate models severely underpredicted, input experimentally-derived G values directly into Nicas dispersion model
- Found Nicas dispersion model to severely overpredict

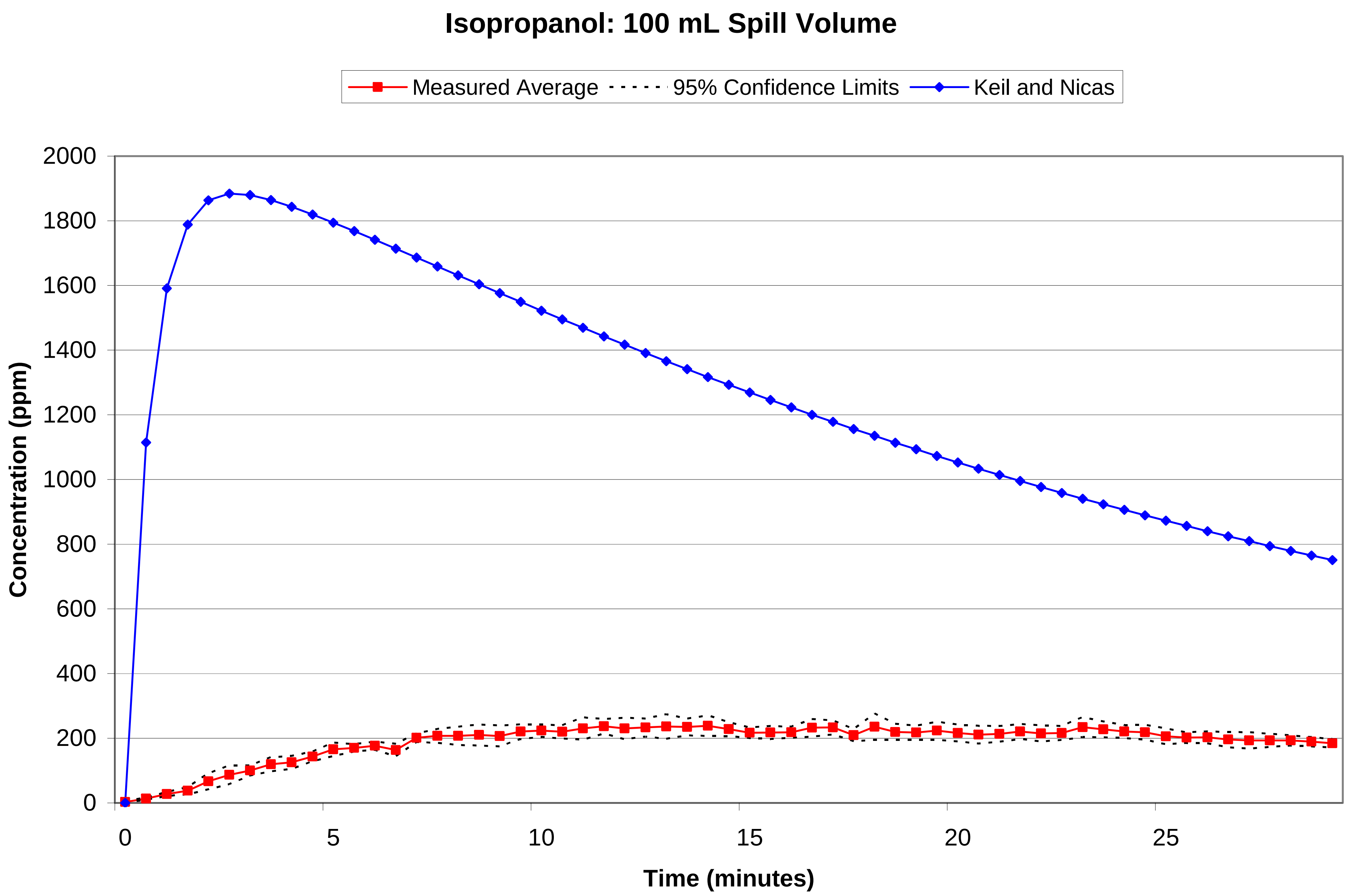


Isopropanol: 100 mL Spill Volume
Measured Average
95% Confidence Limits
Nicas Model with Experimentally Derived Generation Value
Concentration (ppm)
0
200
400
600
800
1000
1200
1400
1600
1800
0
5
10
15
20
25
Time (minutes)

3. Results & Evaluation of Models

Dispersion Rate Models – Keil and Nicas

- Keil and Nicas model incorporates both generation and dispersion components
  - Generation rate components derived from experimental data
- Severely overestimated



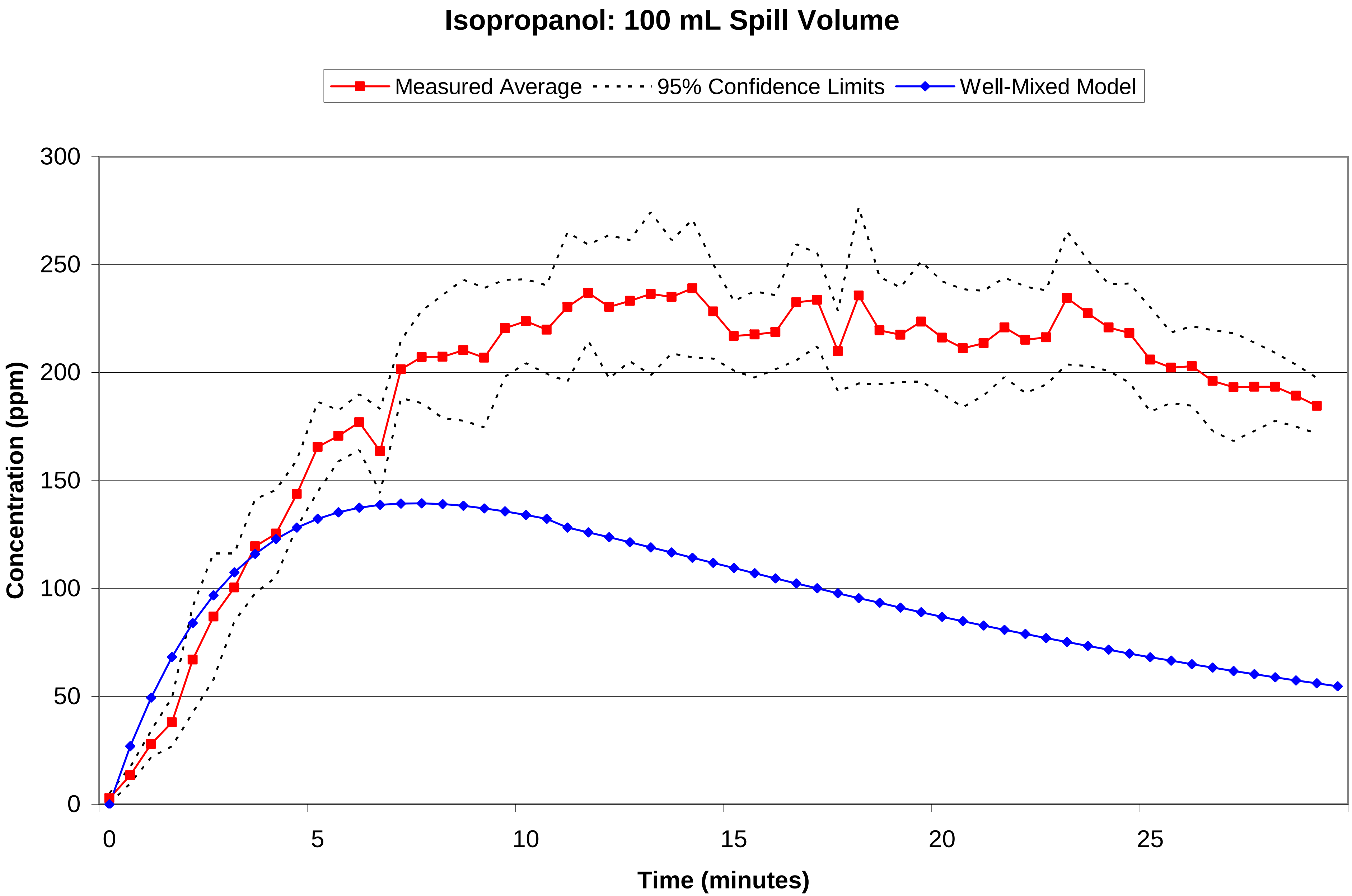
Isopropanol: 100 mL Spill Volume
Measured Average
95% Confidence Limits
Keil and Nicas
Concentration (ppm)
0
200
400
600
800
1000
1200
1400
1600
1800
2000
0
5
10
15
20
25
Time (minutes)

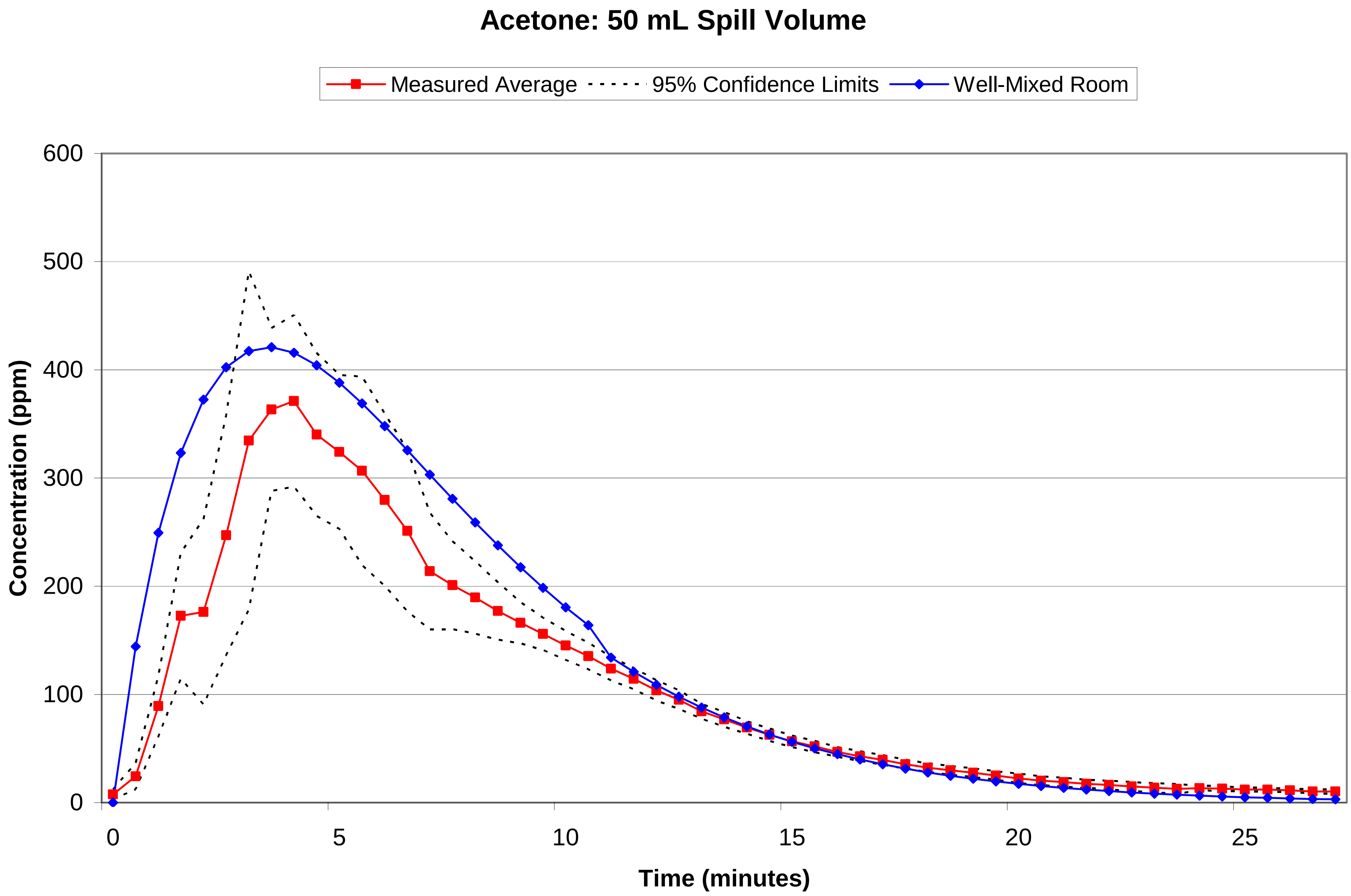
3. Results & Evaluation of Models

Other Models – Readdressed…

- Decided to try a simpler model e.g. Well-Mixed Room model

$$C_t = \frac{k \cdot L_o}{k \cdot V - Q}\left(e^{\frac{-Q}{V}t} - e^{-k \cdot t}\right)$$


Isopropanol: 100 mL Spill Volume
Measured Average
95% Confidence Limits
Well-Mixed Model
Concentration (ppm)
300
250
200
150
100
50
0
0
5
10
15
20
25
Time (minutes)



Acetone: 50 mL Spill Volume
Measured Average
95% Confidence Limits
Well-Mixed Room
Concentration (ppm)
0
100
200
300
400
500
600
0
5
10
15
20
25
Time (minutes)

3. Results & Evaluation of Models

Summary of Results

- Generation rate and dispersion models evaluated were poor predictors under conditions measured
- Correction factor possible for Keil and Nicas model
- Large number of quantitative results for a number of organics at different volumes

Acknowledgements

- WorkSafeBC Research Secretariat
- Fraser Health Workplace Health Management Team and Prevention Team
- Surrey Memorial Hospital Sterile Processing Department
- Royal Columbian Hospital Laboratory Department
- Graham Rhodes, MSc
- UBC SOEH
- Occupational Health & Safety Agency for Healthcare in BC
  - Dr. George Astrakianakis
  - Cris Barzan
  - Tanya Tang

Questions?