Validation of Numerical Spray Modeling with HPLC Chemical Methods

Tyler O'Neil, Joseph Bindel, Kris Schumacher (MRIGlobal)
Amie Norton, Daniel Brabec, Mike Tilley, Deanna Scheff, Frank Arthur (USDA-ARS Manhattan, KS)

USDA Agricultural Research Service

Introduction

Figure 1. Vertical Flow Aerosol Exposure Chamber

Methoprene is a widely used aerosol insecticide in food facilities. The effectiveness of this applications is dependent on the droplet movement due to aerodynamics, gravity, and airflow patterns. Research is needed to determine the effects of droplet size, amount and distribution on the efficacy of the insecticides. Arthur et al. (2014) evaluated the effects of droplet size (2 µm vs 16 µm), concentration and exposure conditions on mortality of adult confused flour beetle (*Tribolium confusum*) in a vertical flow aerosol exposure chamber. Petri dishes served as exposure arenas inside the chamber and contained a layer of wheat flour in the bottom as a substrate for holding the deposition.

Objectives

- To model the airflow and insecticide droplet flow and deposition (as a function of droplet size) in the exposure chamber using computational fluid dynamics (CFD).
- To collect and measure spray chemical deposits using flour substrate in petri dishes.

Computational Fluid Dynamics Modeling (CFD)

ANSYS FLUENT (V. 21.1) CFD software was used to model the flow and deposition of droplets onto Petri dishes in the vertical exposure chamber. Flow conditions were scaled to a single-dish, axisymmetric model.

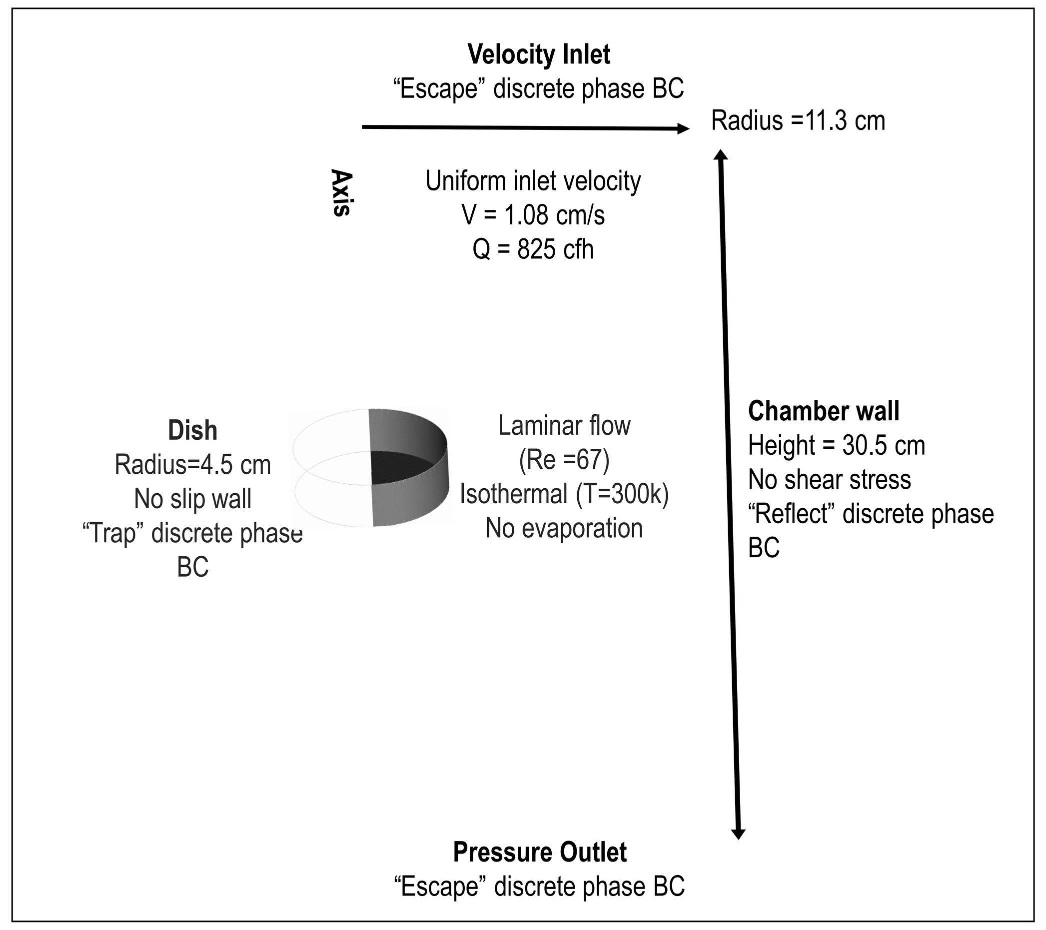


Figure 2. 2-D axisymmetric model domain and assumptions

Predicted Airflow and Spray Drop Trajectories

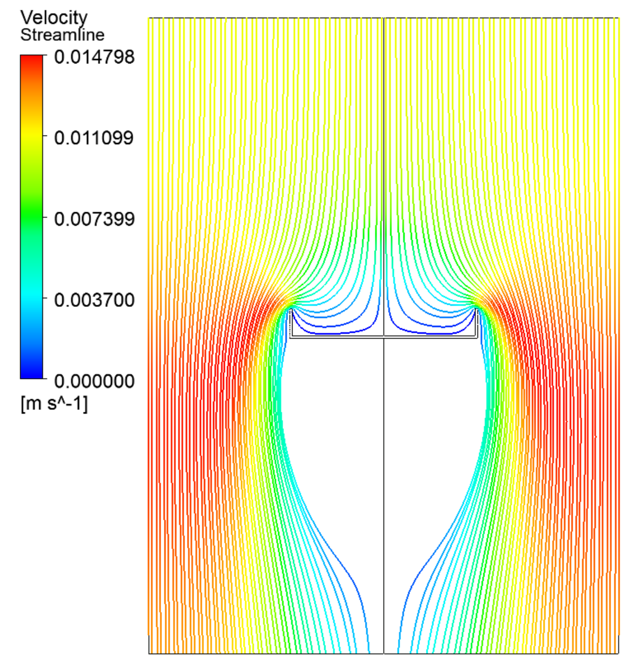


Figure 3. Airflow streamlines around petri dishes

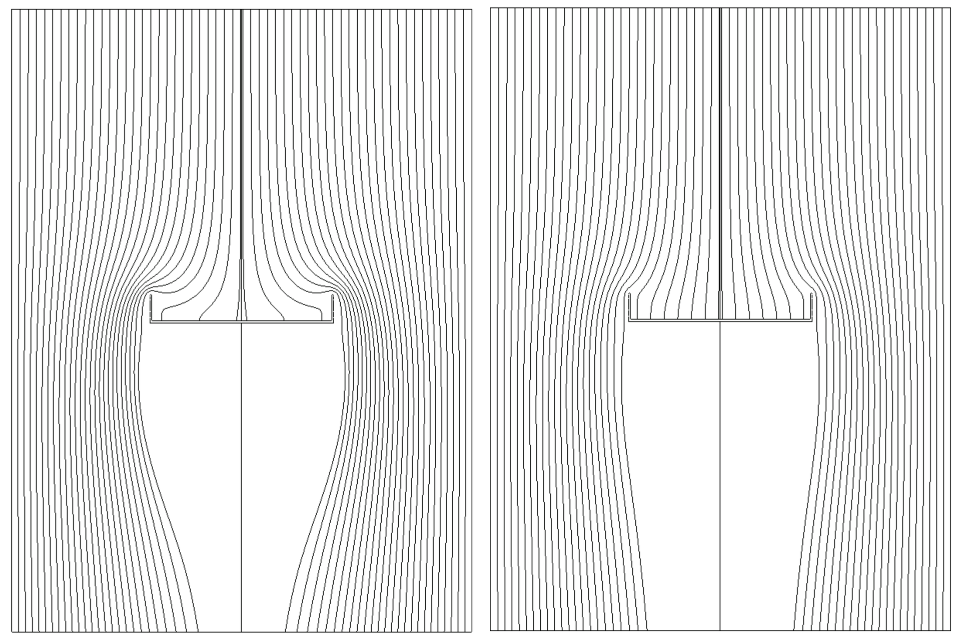


Figure 4. 4 µm drops (left) vs 16 µm drops (right) Predicted Trajectories

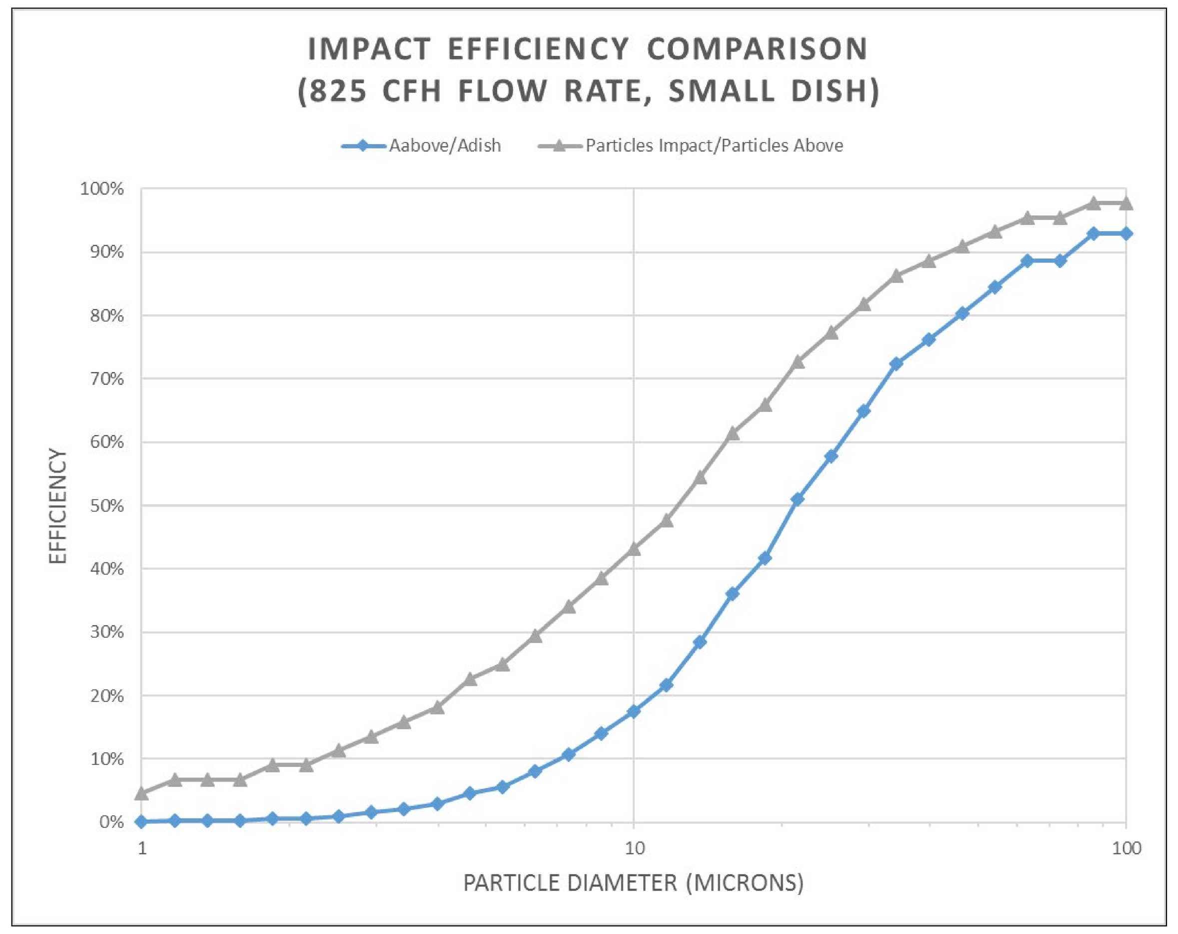


Figure 5. Comparison of impact efficiency methods

Spray droplets of various sizes (from 1 to 100 µm) were modeled. The model positioned droplets at the inlet uniformly. Droplet trajectories were calculated for each drop size with the petri dishes, located at the center of the simulated chamber. The impact efficiency was determined for each drop size.

Spray Distributions vs Impact Eff. >> Weighted Eff.

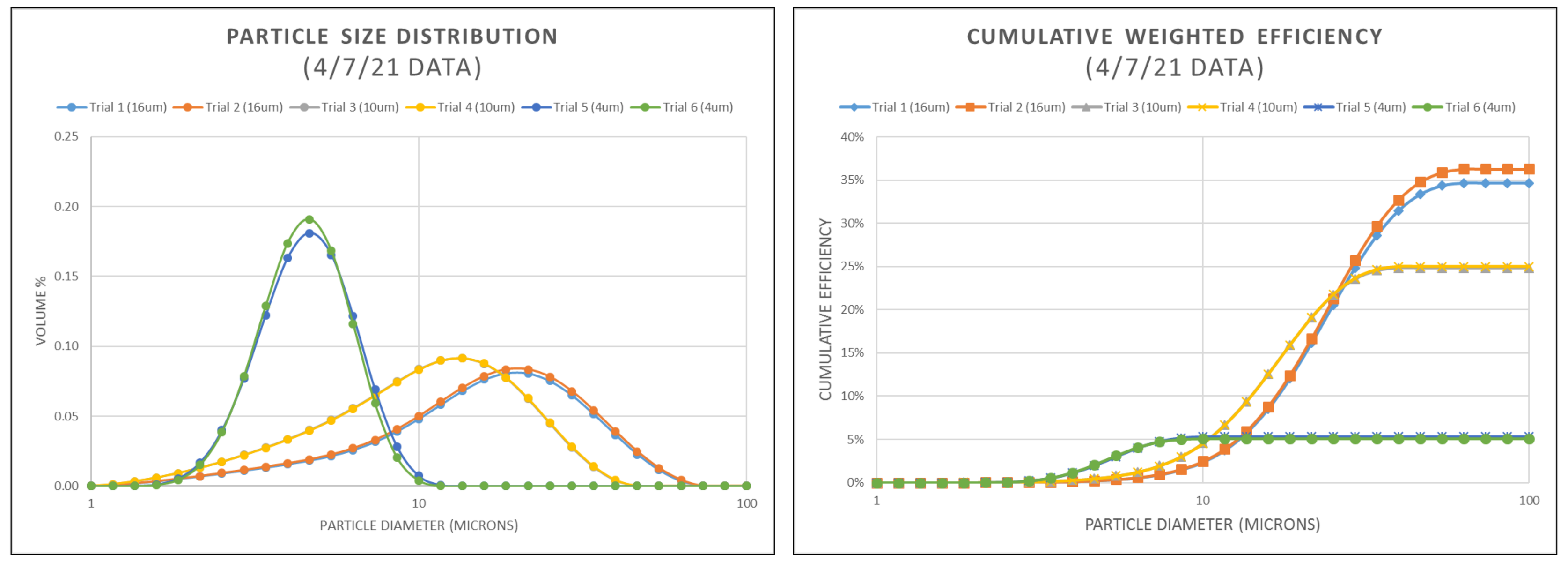


Figure 6. Spray Size Distribution (left), Cumulative Weighted Spray Efficiency (right)

HPLC Methoprene Standards and Calibrations

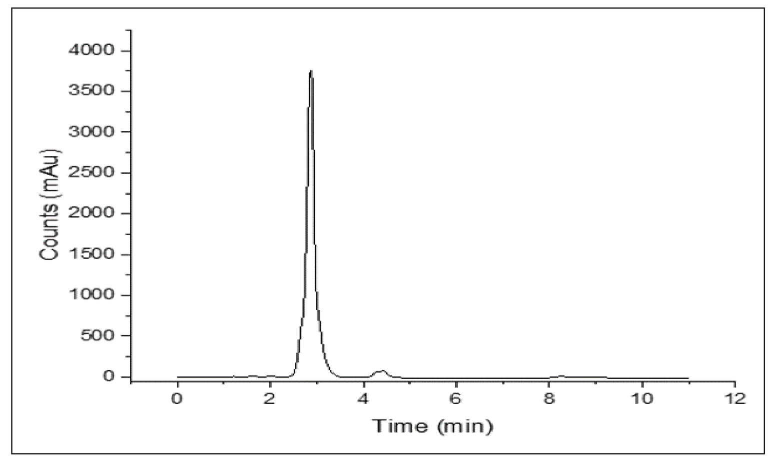


Figure.7 HPLC peak of methoprene at 20.6 ppm ($^{\mu g}/_{mL}$).

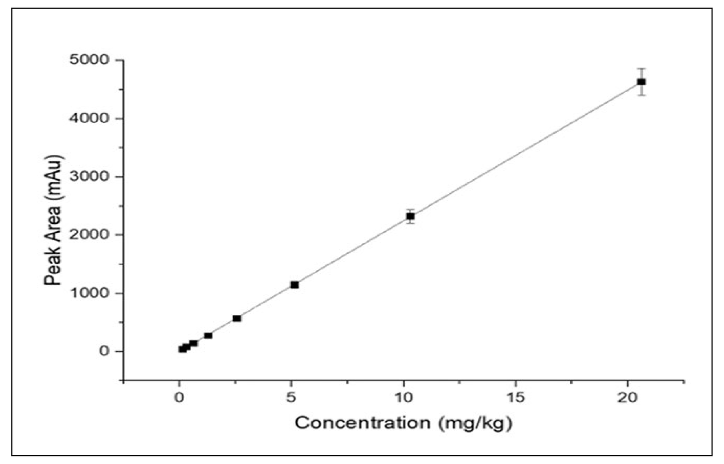
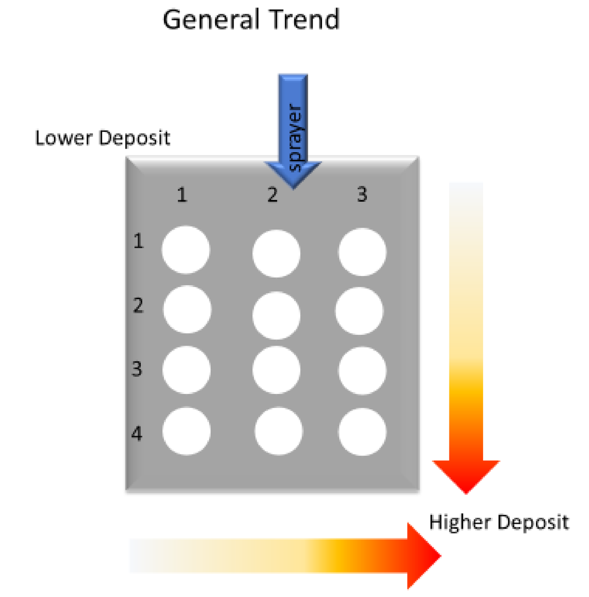


Figure.8 HPLC Calibration graph for methoprene standards (0.16– 20.6) ppm ($^{\mu g}/_{mL}$).

HPLC Chemistry Analysis of dishes with flour



Small Petri-dishes – ½ tsp flour

Drop Size= 16µm (Position)	1	2	3
1	1.73 ppm	1.63 ppm	1.96 ppm
2	1.65 ppm	1.74 ppm	2.35 ppm
3	1.92 ppm	2.88 ppm	3.06 ppm
4	2.51 ppm	2.77 ppm	2.90 ppm

Avg(16um) = 2.26 ppm

Drop Size= 10µm (Position)	1	2	3
1	1.02 ppm	1.48 ppm	1.53 ppm
2	1.20 ppm	1.59 ppm	1.74 ppm
3	1.27 ppm	1.54 ppm	1.51 ppm
4	1.23 ppm	1.54 ppm	1.32 ppm

Avg(10um) = 1.42 ppm

Drop Size= 4µm (Position)	1	2	3
1	0.30 ppm	0.31 ppm	0.38 ppm
2	0.29 ppm	0.44 ppm	0.34 ppm
3	0.31 ppm	0.36 ppm	0.38 ppm
4	0.29 ppm	0.49 ppm	0.42 ppm

Avg(4um) = 0.36 ppm

Chemical Results vs CFD Model

Theoretical maximum amount of methoprene for 10 min spray collected in small dish

Spray Rate in chamber = 1.8 mL/min
Vol of Spray in chamber = 1.8 mL/min * **10 min** = 18mL
Methoprene was 1% of the total spray.
Vol of Methoprene = 1% * 18mL = 0.18 mL
Density of Methoprene ~ 0.86 g/mL
Total weight = 0.18 mL * 0.86 g/mL = 0.155 g
Methoprene base was 33.6% active ingredient
Active Methoprene = 33.6% * 0.155 g = 0.052 g

%area of dish vs chamber = 62 cm2 / 6075 cm2 ~ 1%

Est max weight per dish = 0.00052 g = **520 µg**

Est chemical deposition eff. for 4 um spray and 10 min treatment

Avg Methoprene Measured (4µm) ~ 0.36 ppm = 0.36 µg/mL
HPLC method dilution factor = 80
Weight collected in dish = 0.36 µg/mL* 80 = 28.8 µg
Est deposition eff = 28.8 µg / **520 µg >** 5.5%

Drop Size µm	CFD Prediction %	Chemical Recovery %
4	5	5.5
10	25	21.8
16	35	34.9

Conclusion

CFD results were validated with the HPLC chemical analysis. The chemistry results were in close agreement with the CFD model estimate for deposition into the petri dishes.

Acknowledgement

This research was partially supported by the USDA-NIFA Methyl Bromide Transitions Program (grant no. 2016-51102-25816).

The science you expect. **The people** you know.

816-753-7600 • www.MRIGlobal.org • info@MRIGlobal.org • Headquarters - 425 Dr. Martin Luther King, Jr. Blvd., Kansas City, MO 64110 | Missouri • Colorado • Maryland • Kansas