IH Mod 2.0 deterministic and probabilistic exposure models for industrial hygiene and consumer product applications *(in MS Excel)*

Thomas W. Armstrong, CIH, PhD, FAIHA

TWA8HR Occupational Hygiene Consulting, LLC, Branchburg, NJ, United States.
TWA8HR@gmail.com

Daniel Drolet, Retired, Longueuil, QC, Canada.
daniel.drolet@sympatico.ca

Introduction

IH Mod 2.0 is a suite of eleven mathematical models to estimate air concentrations of chemicals. It is freely available from the AIHA Exposure Assessment Strategies Committee web page.

This version contains the models from the first edition of IH Mod, as either deterministic or using Monte Carlo Simulation (directly in MS Excel) for probabilistic modeling with parameter variability/uncertainty. ***Note: it works ONLY with MS Excel due to extensive reliance on Excel functions and MS VBA. It does NOT require a new high end PC.***

Today, we will briefly look at the tool's contents and illustrate its use for selected scenario. We will tread lightly on parameter values and data sources.

IH Mod 2.0's main use is for occupational task inhalation exposure assessment,
but is also relevant to consumer product inhalation exposures.

Scenario for this talk. Use of a high volatility solvent (1-Bromopropane) in a dry cleaning operation

Specific tasks

- Addition of 5 gallons of the solvent through the front door of a 3rd generation (dry to dry cycle) dry cleaning machine
- Removal of clothes at end of dry cleaning cycle and exposure to residual solvent vapor from the dry cleaning machine

Blando 2010, *Journal of the Air & Waste Management Association, 60:9, 1049-1056*,

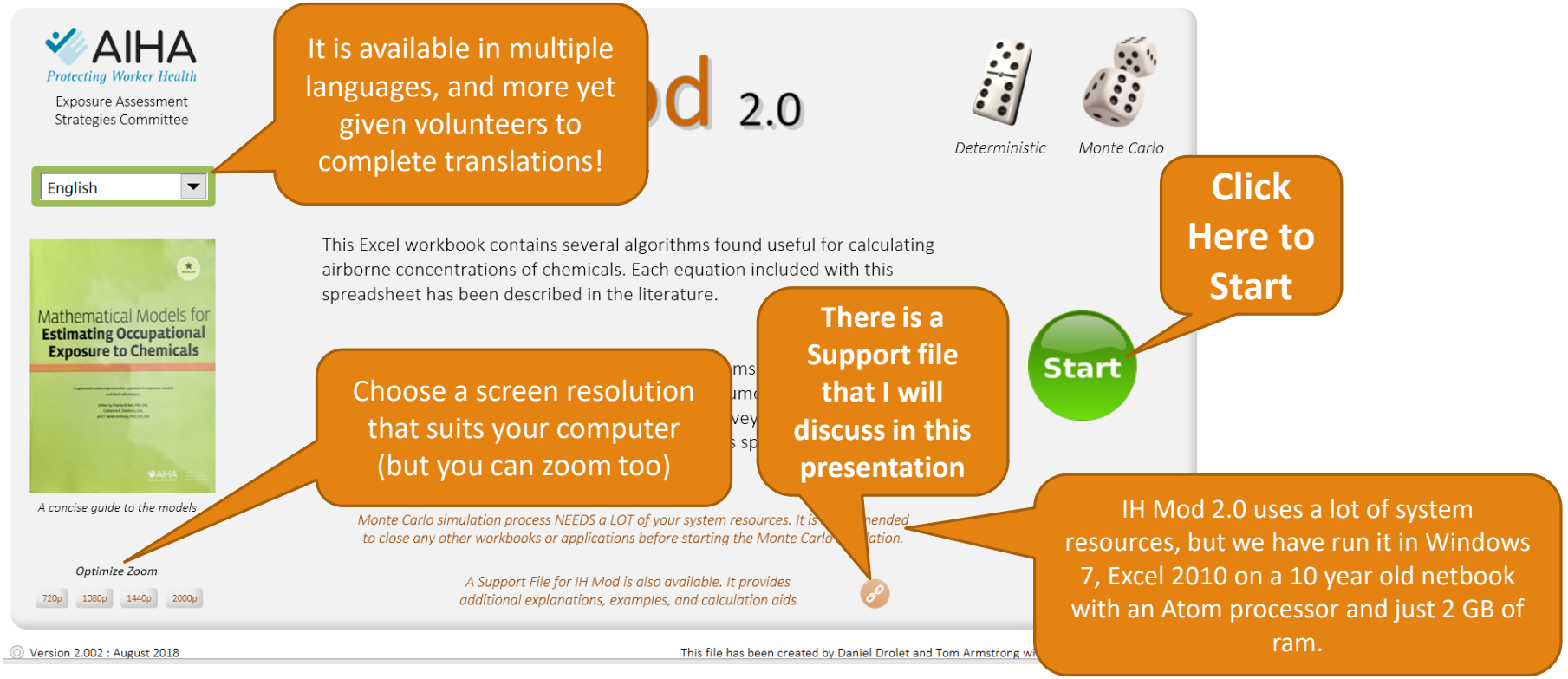
- Shop A volume 280 m^3
- Number of solvent additions and load/unload cycles

Ventilation rate not specified in the Blando report

- Assume Air Changes per Hour from *US EPA EPA Document# 740-R1-5001 February 2016*
- Other determinants derived from the same EPA document

Evaluate near field operator exposures, for tasks and full shift average

What is in IH Mod 2.0?



Then, (after disclaimer) model selection, from eleven currently included

The user gets to choose which to Start

AIHA
Protecting Worker Health
Exposure Assessment Strategies Committee

IH Mod 2.0

To Help (explanation) screens for deterministic of MCS versions

Help DET

Help MCS

		Deterministic	Monte Carlo
1	*Well Mixed Box Room Model*	→	→
2	*Well-Mixed Room Model with Backpressure*	→	→
3	*Well-Mixed Room Purging Equation*	→	→
4	*Spill Model, Decreasing Emission*	→	→
5	*Turbulent Eddy Diffusion without Advection following a Pulse Release*	→	→
6	*Eddy Diffusion without Advection given a Constant Mass Emission Rate*	→	→
7	*Eddy Diffusion with Advection following Pulse release*	→	→
8a	*Two-Zone Model, Constant Emission*	→	→
8b	*Two-Zone Model, Decreasing Emission*	→	→
10	*Turbulent Eddy Diffusion with Advection and with a Constant Emission Rate*	→	→
11	*Near and Mid - Field plume models*	→	→

This file has been created by Daniel Drolet and Tom Armstrong with review by Michael Jayjock

The two zone constant generation model MCS version (not set up for the scenario yet)

Set the number of iterations.

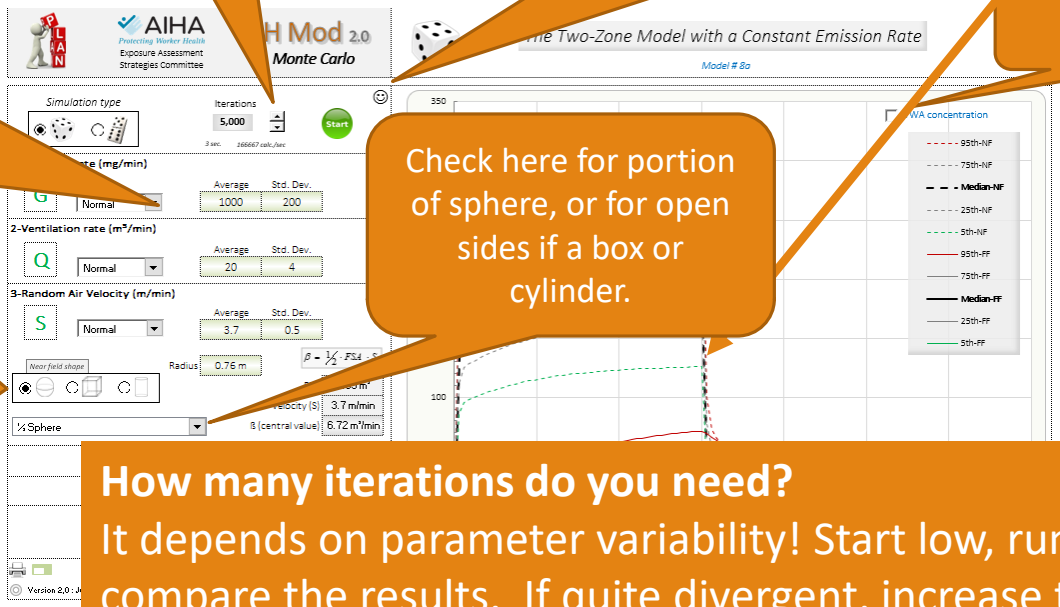
Choose the distribution type and set the parameters.
The normal distribution is truncated to avoid zero and negative values

Smile = good to go!
Frown = parameters, etc. not quite right!

Show graph for TWA or C vs T

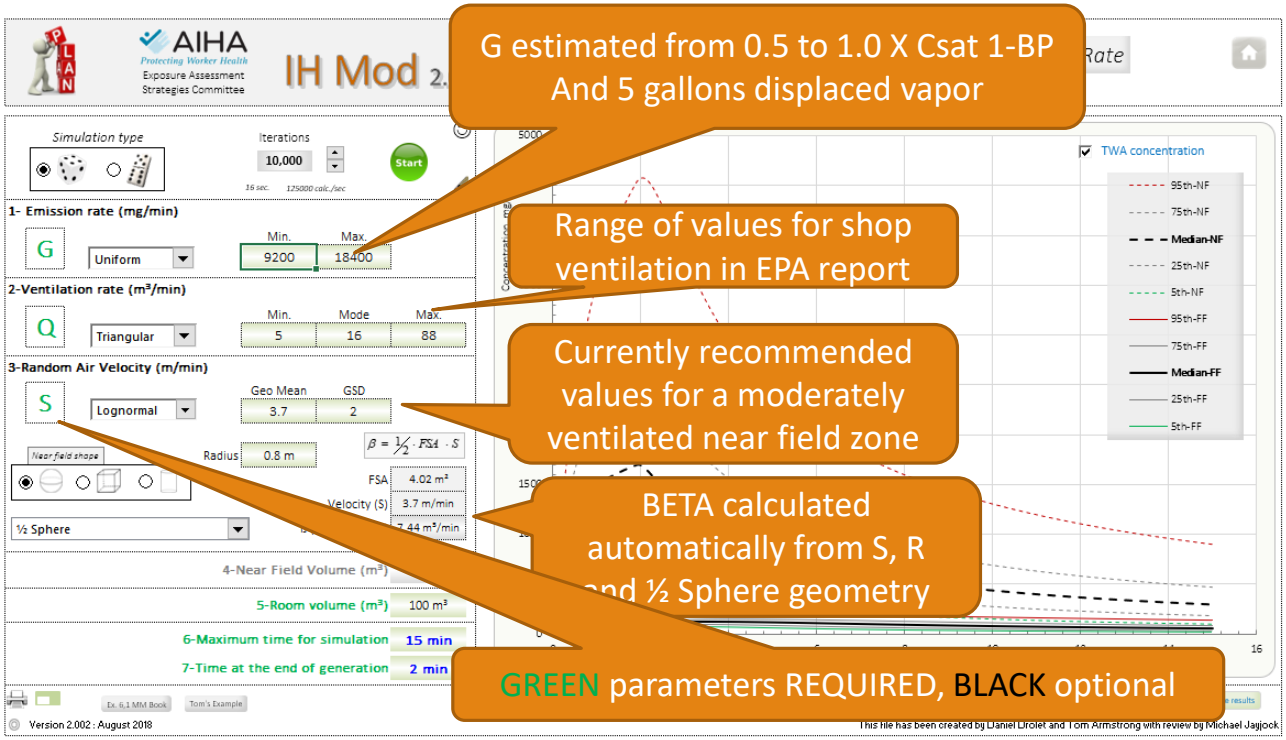
Check here for portion of sphere, or for open sides if a box or cylinder.

Here you define the Near Field shape and calculate Beta. Specify shape, S and FSA, then Beta is set up!
Room Volume adjusts too.



How many iterations do you need?
It depends on parameter variability! Start low, run twice and compare the results. If quite divergent, increase the iterations until you have satisfactory "stability" from run to run.

Modeling solvent addition to a "3rd generation" dry cleaning machine , *showing TWA to 15 minutes*



G estimated from 0.5 to 1.0 X Csat 1-BP And 5 gallons displaced vapor

Range of values for shop ventilation in EPA report

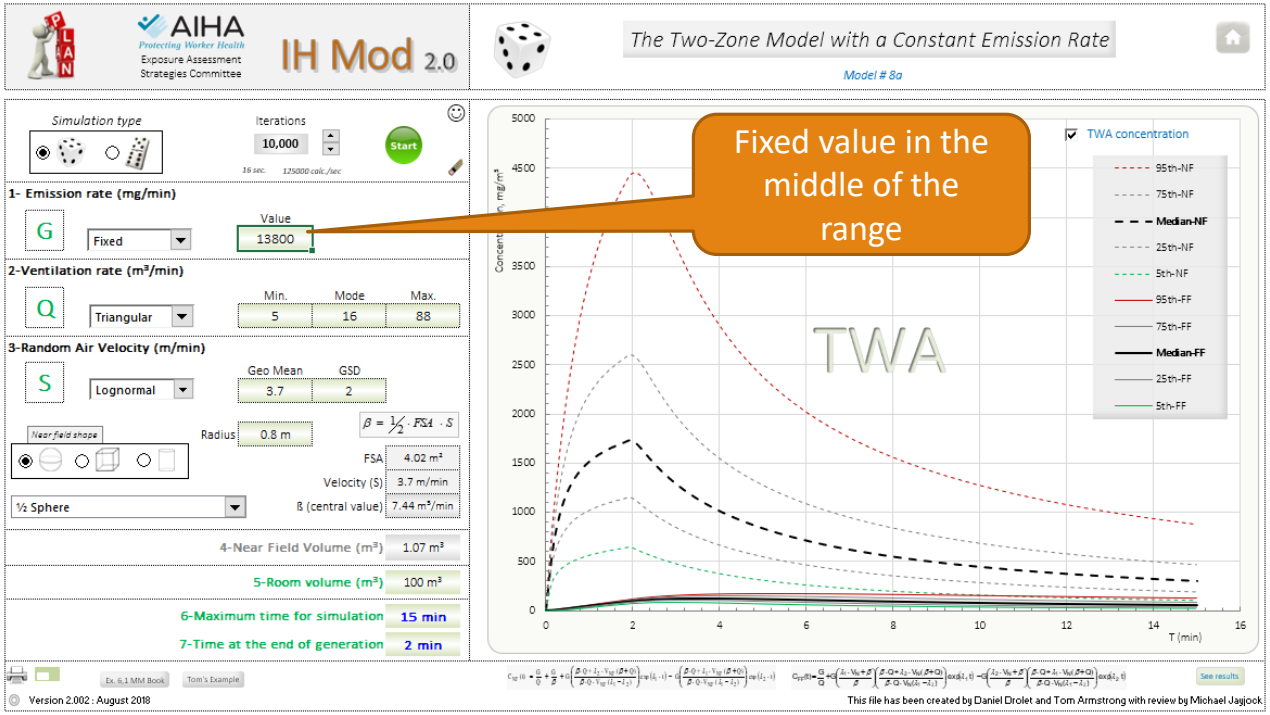
Currently recommended values for a moderately ventilated near field zone

BETA calculated automatically from S, R and ½ Sphere geometry

GREEN parameters REQUIRED, BLACK optional

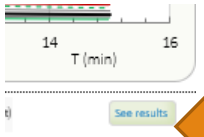
NEAR FIELD 15 Min TWA mg/m³	
5th	101
Median	294
75th	467
95th	899

The models are easy to rerun with different parameter choices Set G to fixed value, 13800 mg/min



NEAR FIELD	
15 Min TWA mg/m³	
5th	108
Median	299
95th	880

Summary results are available via a button on the lower right of the graph section



IH Mod 2.0

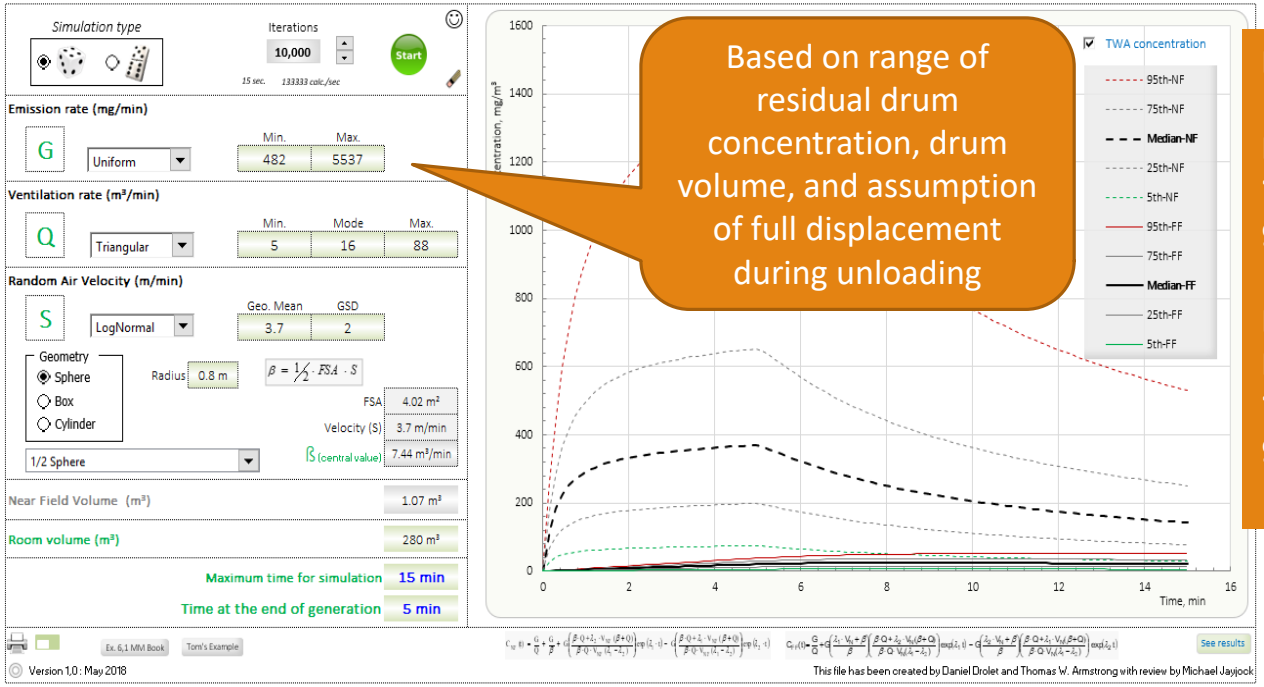
Probabilistic Results

Back to model

Values in blue refer to TWA Concentrations

	Time	Median-NF	5th-NF	25th-NF	75th-NF	95th-NF	Median-NF	5th-NF	25th-NF	75th-NF	95th-NF	Median-FF	5th-FF	25th-FF	75th-FF	95th-FF	Median-FF	5th-FF	25th-FF	75th-FF	95th-FF
	12.3	7.5872288	0.1407704	1.3327652	27.665602	76.688219	363.0142	131.6693	235.1906	567.0216	1057.163	7.0933886	0.1210332	1.1974332	26.46115	75.216586	65.1291	29.00129	43.86826	95.34186	139.2735
	12.45	7.2224654	0.1268839	1.2369936	26.786682	75.347719	358.7786	130.1034	232.4055	560.5902	1045.475	6.7472104	0.1090475	1.1118455	25.640181	73.918066	64.43408	28.65734	43.35926	94.51207	138.4955
85	12.6	6.8780677	0.1143673	1.1498828	25.9423	74.058193	354.6386	128.5741	229.6848	554.3002	1034.046	6.4192657	0.0982488	1.0332493	24.844874	72.636292	63.75155	28.32135	42.86131	93.69246	137.7207
86	12.75	6.549333	0.102946	1.0667915	25.134922	72.774295	350.5911	127.0802	227.0264	548.1472	1022.869	6.1066902	0.0884584	0.9599847	24.076655	71.367144	63.08126	27.99306	42.37408	92.88297	136.9491
87	12.9	6.2295753	0.092318	0.9896211	24.363686	71.493604	346.6329	125.6206	224.4283	542.1267	1011.933	5.8100836	0.0795637	0.8904089	23.332286	70.120171	62.42297	27.67222	41.89726	92.08354	136.1809
88	13.05	5.9251185	0.0830946	0.9184632	23.611795	70.253218	342.7612	124.194	221.8884	536.2344	1001.232	5.5277294	0.0716554	0.8256078	22.608648	68.894986	61.77644	27.35857	41.43053	91.29405	135.4163
89	13.2	5.6408392	0.074742	0.8536351	22.874126	69.034351	338.9733	122.7994	219.4049	530.4663	990.7584	5.2596537	0.0645334	0.7665704	21.90635	67.69512	61.14142	27.0519	40.97364	90.51442	134.6554
90	13.35	5.3595146	0.0672195	0.793268	22.171023	67.744921	335.2665	121.4357	216.9759	524.8186	980.5027	5.0039491	0.0580718	0.7119868	21.225867	66.52384	60.51767	26.75197	40.52628	89.74454	133.8984
91	13.5	5.1003656	0.060602	0.737201	21.475295	66.583168	331.6383	120.102	214.5996	519.2874	970.4596	4.7613781	0.0522536	0.6614209	20.566523	65.34325	59.90496	26.45856	40.08821	88.98435	133.1451
92	13.65	4.8561985	0.0546359	0.6854892	20.794246	65.441337	328.0863	118.7971	212.2745	513.869	960.6224	4.5276001	0.0470133	0.6145541	19.927661	64.201516	59.30303	26.17148	39.65915	88.23373	132.3957
93	13.8	4.6181786	0.0492147	0.6357185	20.128489	64.319088	324.6082	117.5202	209.9988	508.5599	950.9848	4.3074113	0.0423067	0.571081	19.302427	63.085814	58.71168	25.89052	39.23885	87.49253	131.6504
94	13.95	4.3963821	0.0442922	0.5909676	19.499056	63.216085	321.2017	116.2705	207.7711	503.3572	941.5404	4.0986948	0.0380917	0.5304087	18.70275	61.993825	58.13069	25.6155	38.82705	86.76073	130.9094
95	14.1	4.1744512	0.0398474	0.5489442	18.890879	62.131996	317.8646	115.047	205.5898	498.2575	932.2835	3.9000923	0.0343061	0.4925467	18.121252	60.920739	57.55984	25.34622	38.42353	86.03821	130.1726
96	14.25	3.9740971	0.0358535	0.5097294	18.297201	60.95228	314.5949	113.849	203.4535	493.2579	923.2071	3.7111136	0.0308532	0.4573408	17.557727	59.866006	56.99892	25.08252	38.02805	85.32487	129.4403
97	14.4	3.7831281	0.0322958	0.4733555	17.728644	59.902095	311.3906	112.6756	201.3609	488.3556	914.3071	3.5312923	0.027726	0.4244614	17.011727	58.829339	56.44771	24.82422	37.64039	84.62061	128.7123
98	14.55	3.600655	0.0290983	0.4395618	17.177755	58.857527	308.2499	111.5262	199.3107	483.5476	905.578	3.3599755	0.024949	0.3940475	16.482227	57.810623	55.906	24.57117	37.26032	83.92532	127.9889
99	14.7	3.4272858	0.026214	0.40854	16.638515	57.842447	305.1709	110.3999	197.3016	478.8314	897.015	3.1963675	0.0224502	0.3657295	15.967401	56.808574	55.37358	24.3232	36.88765	83.23888	127.2699
100	14.85	3.2630527	0.023537	0.3792234	16.116837	56.844874	302.1518	109.2961	195.3324	474.2042	888.6133	3.0404958	0.0202267	0.3394668	15.470126	55.822712	54.85025	24.08017	36.52217	82.56119	126.5554
101	15	3.1072186	0.0211719	0.3524597	15.614629	55.864943	299.191	108.2142	193.4019	469.6637	880.3683	2.892226	0.0182248	0.3149106	14.988732	54.833634	54.33581	23.84193	36.16368	81.89215	125.8453

Dry cleaning machine unloading task exposure
Modified from App K, EPA Document# 740-R1-5001 February 2016



Based on range of residual drum concentration, drum volume, and assumption of full displacement during unloading

Near Field mg/m³	**15 min TWA**
5th	**31**
Median	**142**
75th	**251**
95th	**531**

Far Field mg/m³	15 min TWA
Median	**25**
75th	**45**
95th	**85**

What is the eight hour TWA?

Via off to the Side calculations

Estimated 8 hour TWA from one solvent addition + fourteen unloads + remaining time at room background from far field values

Median = (293 * 15min + 151*14*15 Min +6.5*240 min)/480min = 78 mg/m³ = **15 ppm**

75th = (466*15 min + 262*14*15min + 12*240min)/480 min = 130 mg/m³ = **26 ppm**

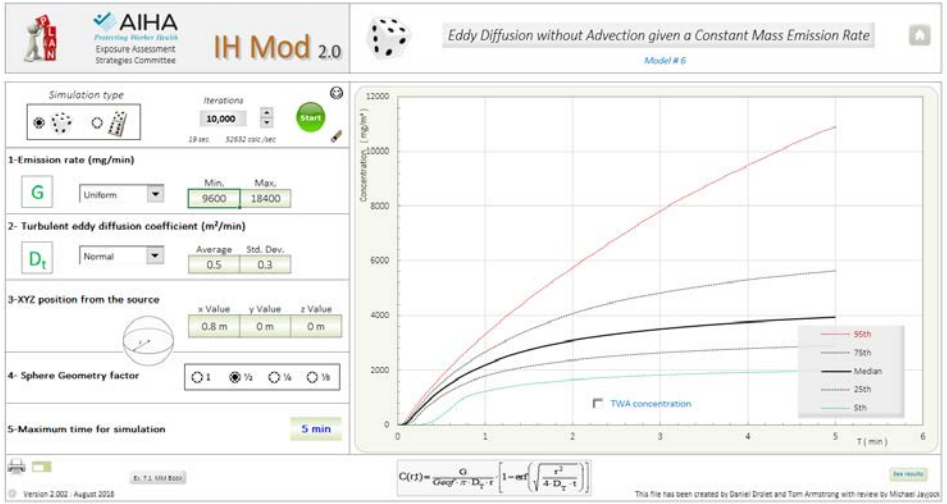
95th = (902*15 min + 565*14*15min +41*280min)/480min = 296 mg/m³ = **59 ppm**

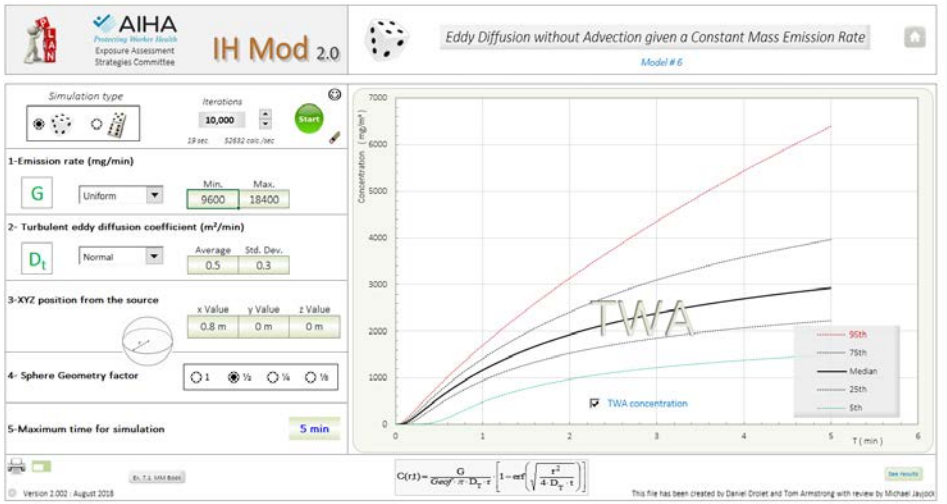
Available* measured 8 hr TWA **AM 32 ppm, 95th 82 ppm**

**Blando 2010*

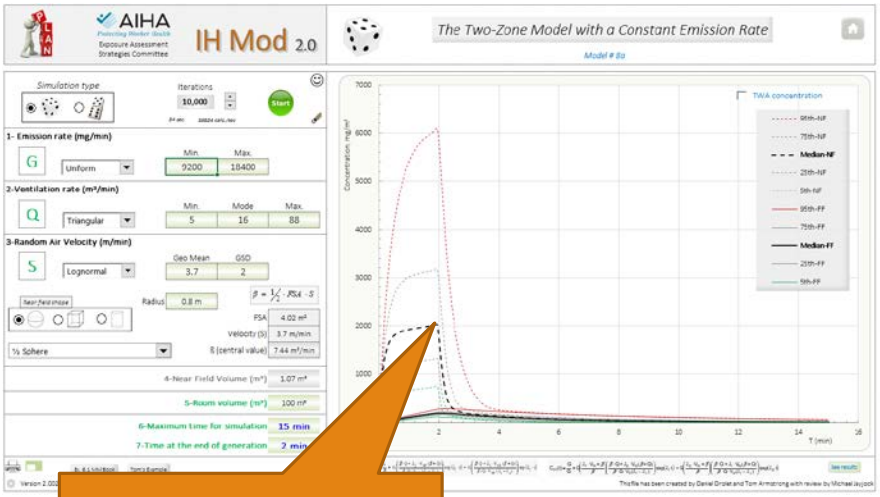
Let's quickly look at one other model, dry cleaning solvent addition, C_t & TWA

The D_T value of 0.5 is proving to be a reasonable "default" assumption for moderately ventilated spaces



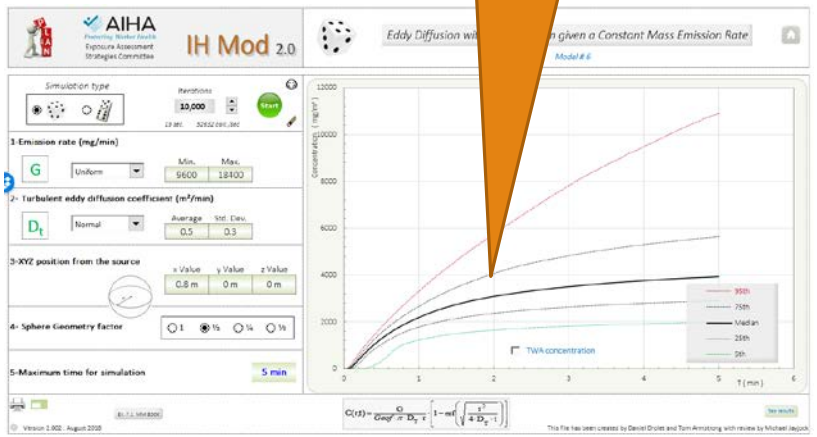


Comparison: 2 zone vs turbulent diffusion, solvent addition task, C_t curves

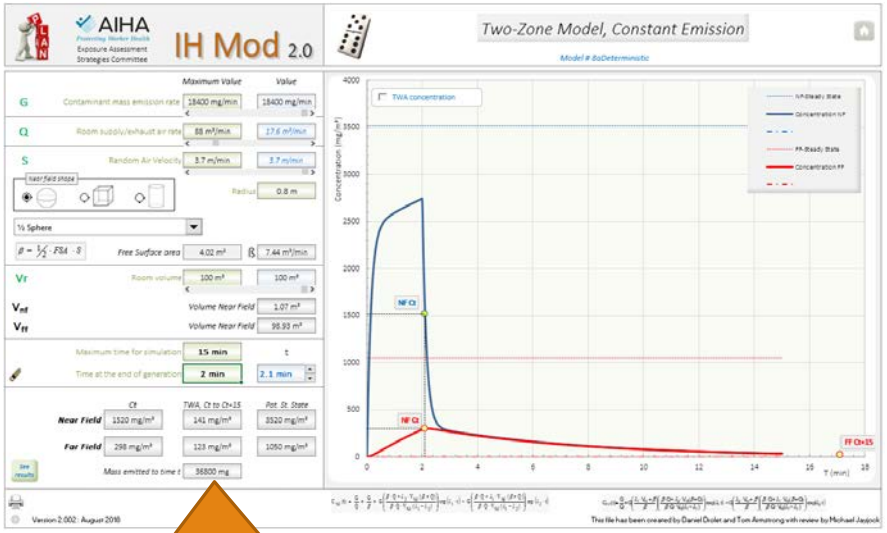


Median at 2 minutes
2000 mg/m³
TWA at 2 minutes
1700 mg/m³

Median at 2 minutes
3100 mg/m³
TWA at 2 minutes
1900 mg/m³

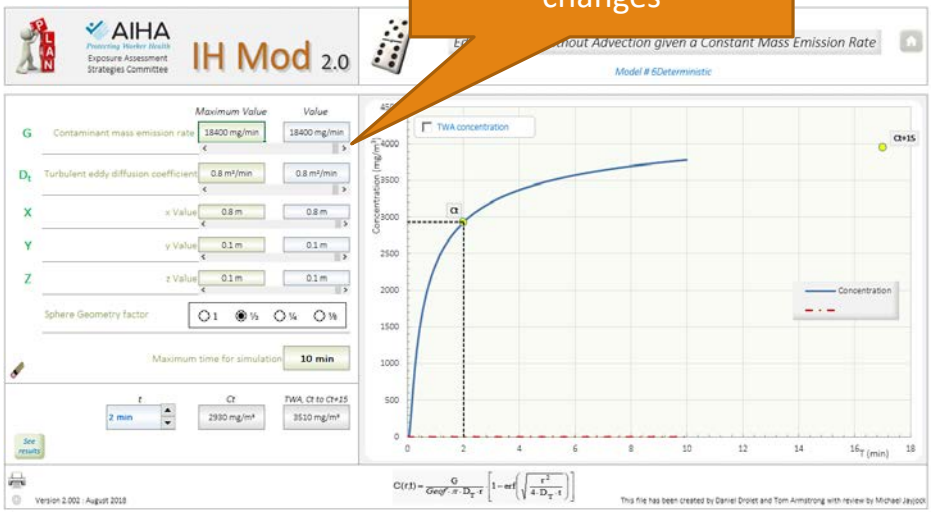


How are the deterministic models different?



Rough “mass balance” calculations in some of the models, mass emitted to time t

Data “sliders” to vary parameters and see changes



OK, but what about consumer exposures?

These can still be task based assessments

Usually consumers have lower frequency, duration and intensity of TASK exposure

Usually lower generation rates

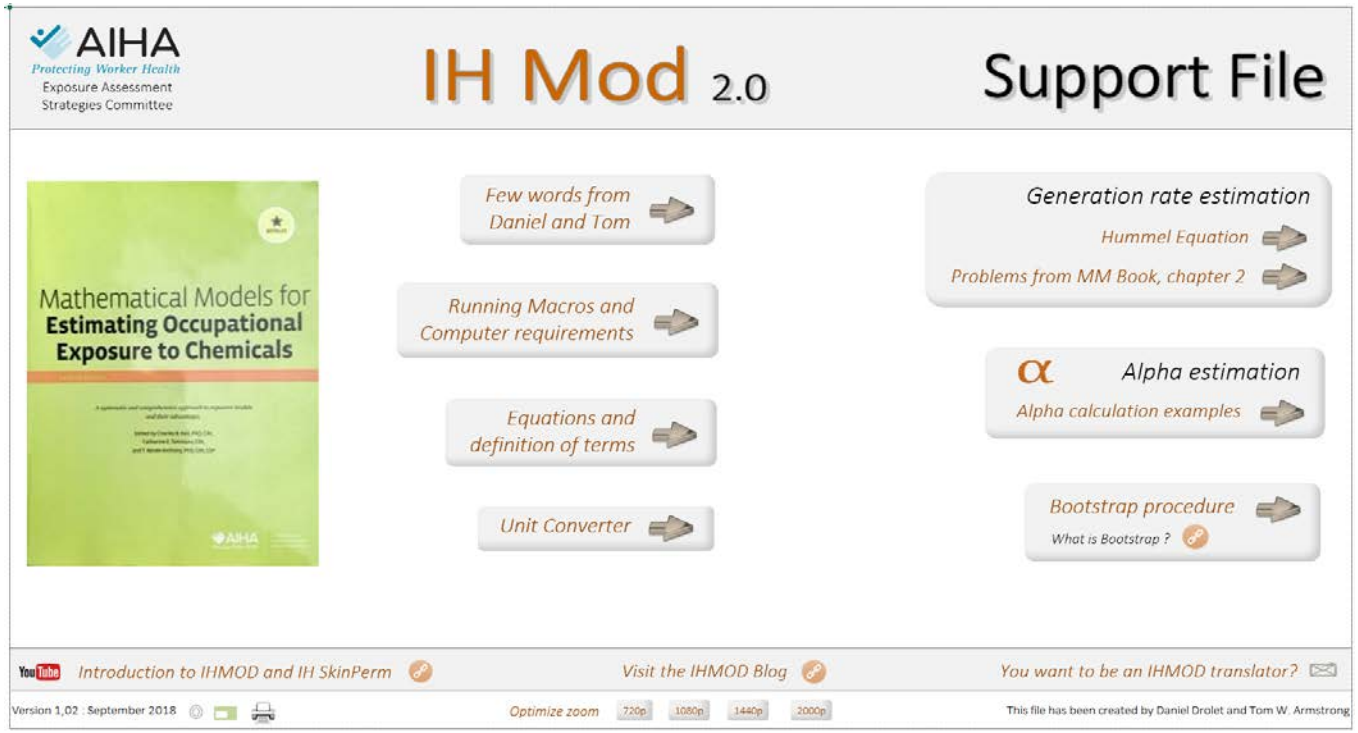
Chemicals can be similar or different formulations

Use may be with different room volumes, different ventilation rates

24 hour exposure duration (or more) can be relevant

We give additional guidance in a support file

http://bit.ly/eascaiha



We have been encouraging others to contribute to this file.

We expect expanded contents on parameter choices, sources, and more examples

What's in the future for IH Mod 2.0?

Further guidance in the support file for reasonable scenario and specific model default parameters

Further guidance on generation rate estimation

Further guidance on estimation of ventilation rates, near field random air velocity, turbulent diffusion values

Additional model equations? Provide a comparison to Saturated Vapor Concentration?

More examples for each model

Slight revamp of the MCS summary. AM? GSD? Other?

Maintenance

EVERYTHING in IH Mod 2.0 was done on a volunteer basis, and its long term future will depend on **additional volunteer contributions**

For periodic news about IH Mod 2.0, visit the IH Mod BLOG site www.IHMod.org

In summary

IH Mod 2.0 is freeware, openly available and provides transparent, easy to use approaches mathematical modeling and illustration of variability and uncertainty.

It provides for scenario definition and documentation of key exposure determinants

The user can select either deterministic or MCS versions of the multiple algorithms found useful for occupational or downstream user scenario evaluation

The AIHA EASC volunteers involved in developing these tools welcome collaboration on their further development and for translations of the multi-lingual tools

This tool illustrates the potential power of other MCS tools in MS Excel