Selecting, Calibrating, and Developing Models

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Yuma Pacific-Southwest Section

40th Annual Meeting

January 23, 2015

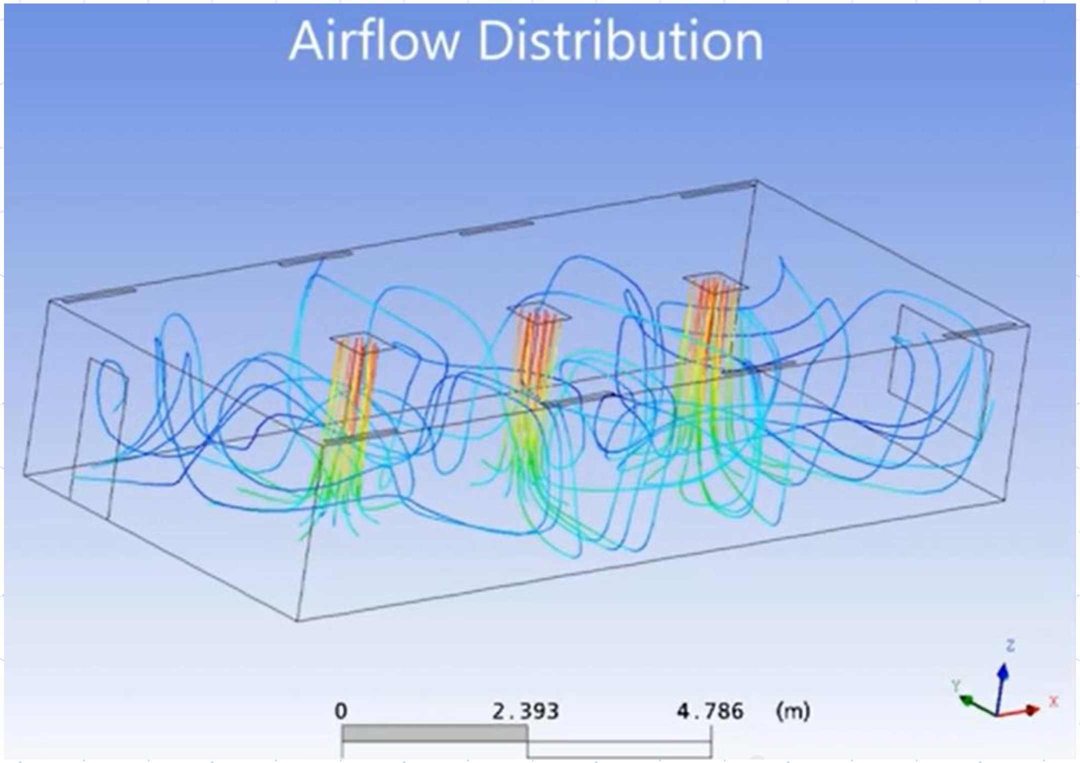
Exposure Assessment Solutions Inc.

Examples of Models
(for predicting occupational exposures)

- Statistical Models
  - e.g., x = f(GM, GSD)
- Empirical Models
  - e.g., x = f(plant, job, task, substance, year, other determinants)
  - e.g., x = f(NF & FF intrinsic emissions, handling, local controls, general ventilation, passive emissions, etc.)
    - Cherrie's Structured Subjective Assessment model
- Expert Systems
  - Advanced REACH Tool (Tier 2)
  - Stoffenmanager (Tier 1)
  - Targeted Risk Assessment (Tier 1)
  - UK COSSH Essentials (Tier ?)

Physical-Chemical Models

- Computational Fluid Dynamics (CFD)



Source: http://www.c-ih.com/exposure-science/exposure-modeling/

Well-mixed Room Models

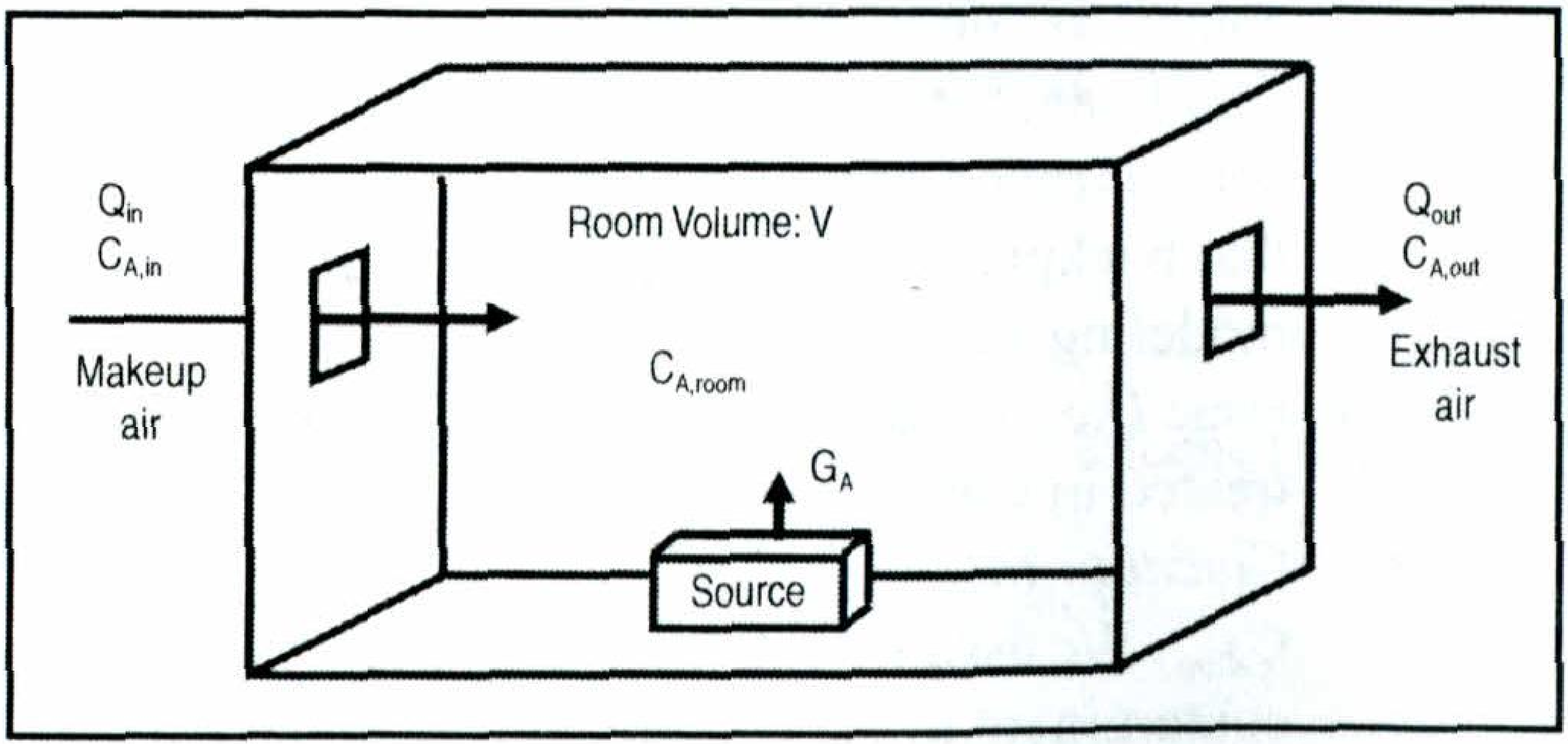
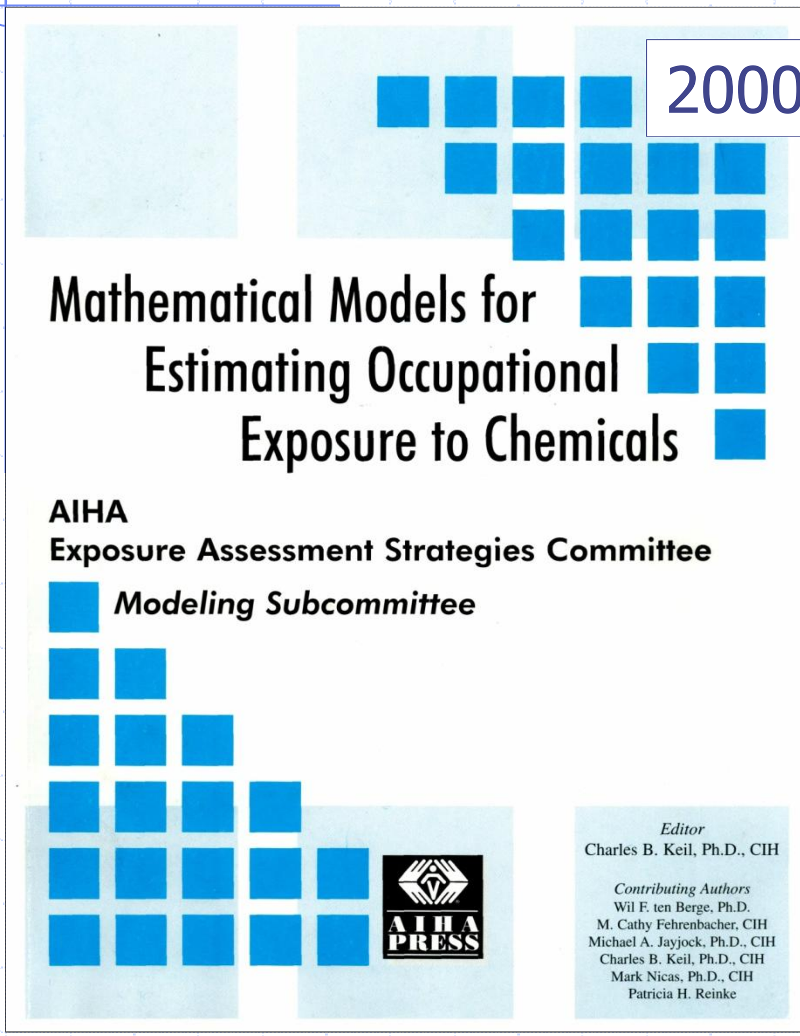


Figure 4.1 — Conceptual Model of the Well Mixed Box.

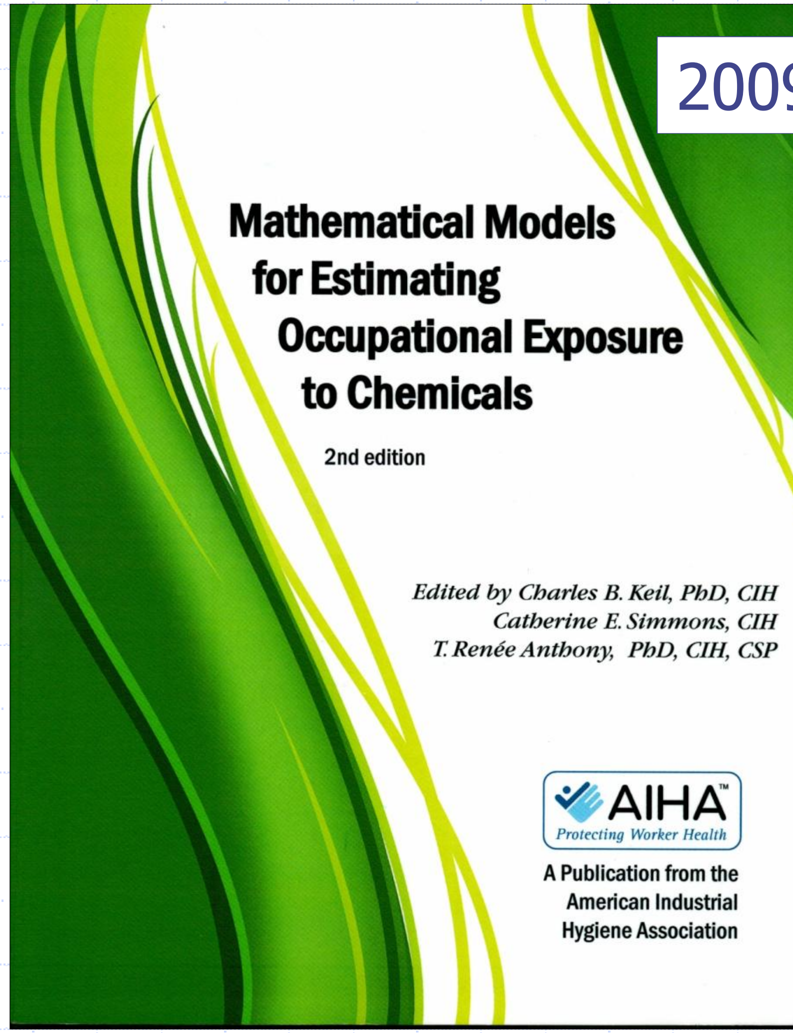
Source: AIHA (2009) Mathematical Models …

AIHA Exposure Assessment Strategies Committee

2000

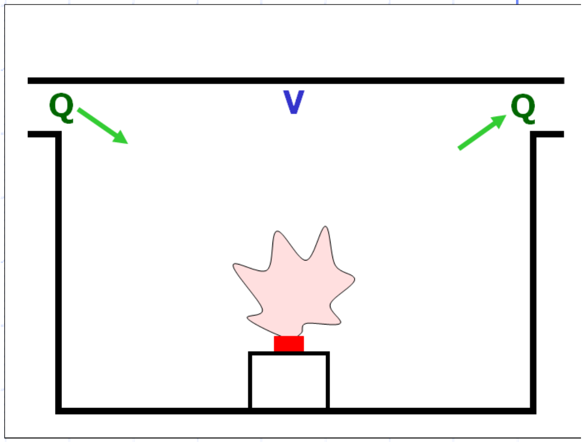


2009

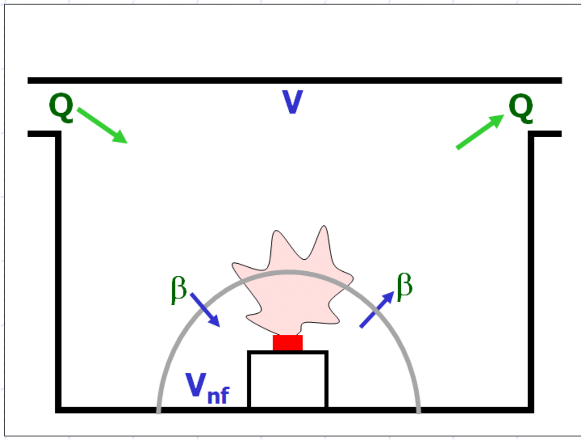


Well-mixed Room Models

- 1Box model
  - Continuous emissions (need G)
    - Steady State (SS)
    - Transient
  - Decreasing Emissions (need M,α)
    - Transient



- 2Box model
  - Continuous emissions (need G)
    - Steady State (SS)
    - Transient
  - Decreasing Emissions (need M,α)
    - Transient



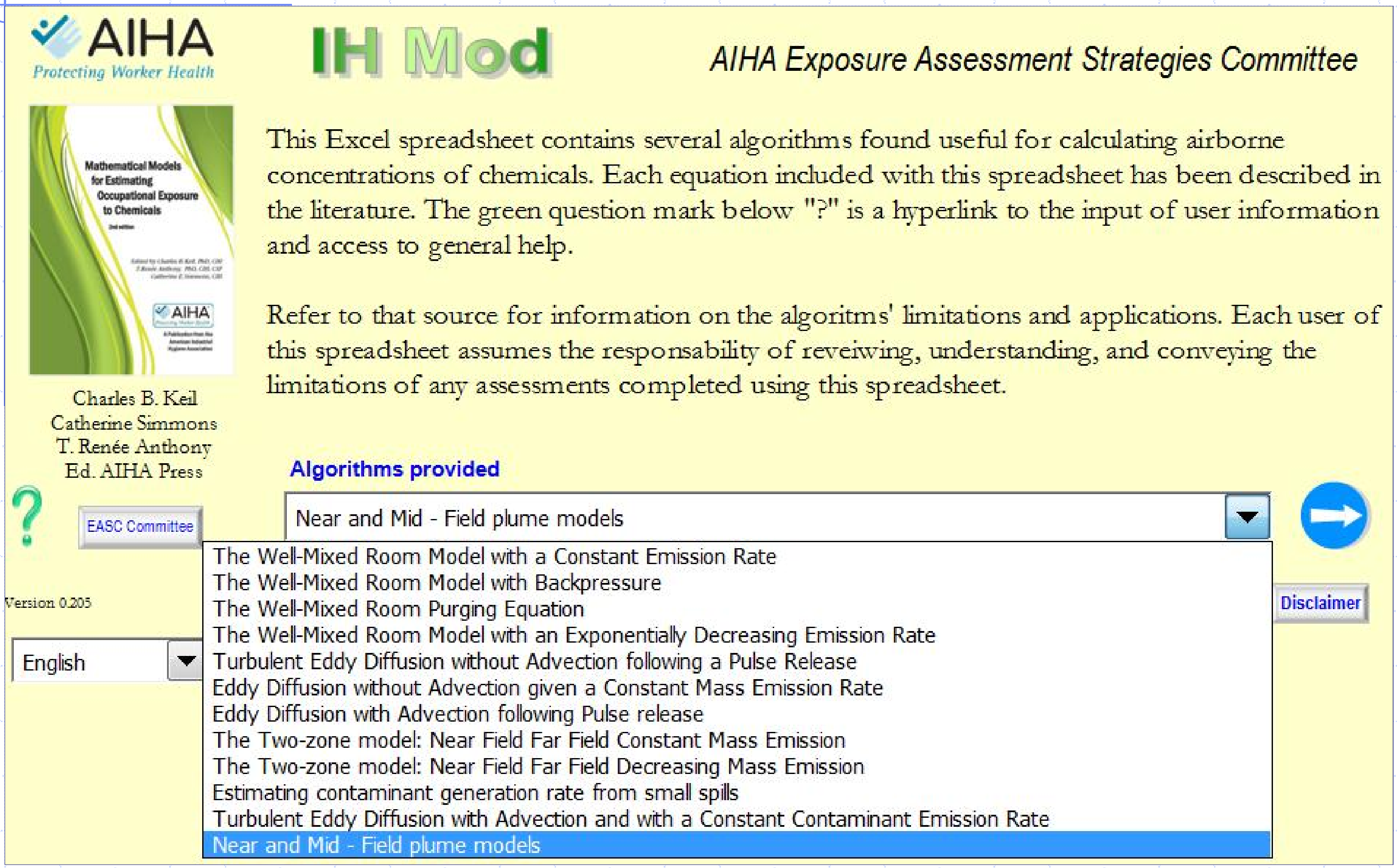
Advantages

- Quick and cheap
- Suitable for triage, identifying exposure scenarios …
  - that require immediate evaluation
  - that pose little or no risk.
- Can be applied retrospectively
- Can be used to …
  - identify critical exposure determinants
  - predict the effect of changes to the production level, process, controls, and general work environment
- **"Validated" models can be applied globally**

- Accuracy
  - *It is said* that estimates can be within ½ and 2x of the true concentration.
- Disadvantages
  - Model calibration procedures or guidelines are lacking.
  - Estimation of model parameters can be an issue, e.g.,
    - Generation rate (G)
    - Near field volume (V_{NF})
    - Near field flowrate (β)

- 1Box and 2Box models are deterministic.
- Probabilistic modeling is available, but easy implementation is lacking.
- **Model selection is *limited (up until now ?)***
- Limited software options

Tools for Modeling



IHMod

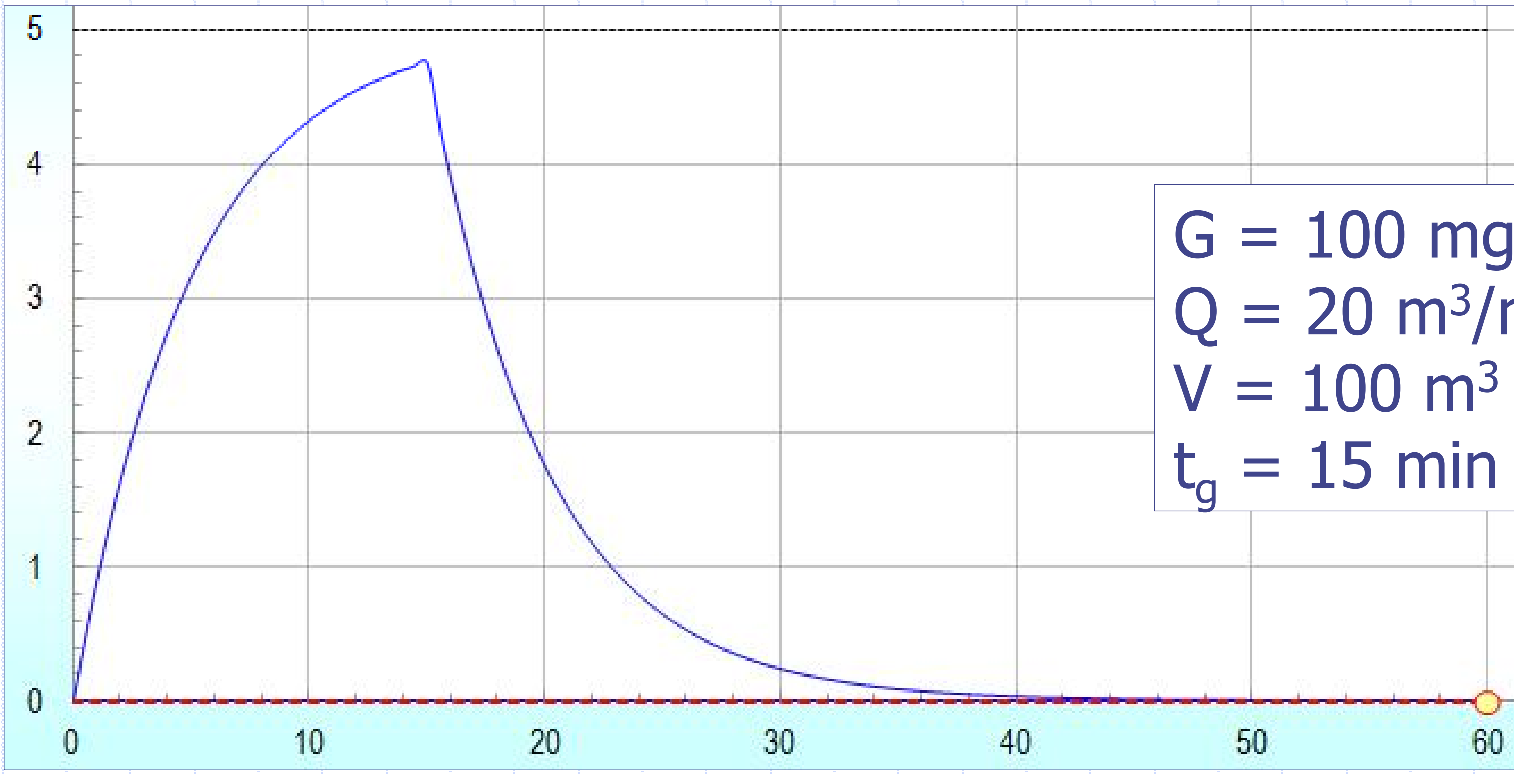
- 1Box CE Model (continuous emissions)

G>0

$$C(t) = \frac{G}{Q}\left[1 - \exp\left(\frac{-Q \cdot t}{V}\right)\right]$$

G=0

$$C(t) = C_0\left[\exp\left(\frac{-Q \cdot t}{V}\right)\right]$$



G = 100 mg/min

Q = 20 m^3/min

V = 100 m^3

t_g = 15 min

TEAS: Tasked-based Exposure Assessment Simulator (beta)

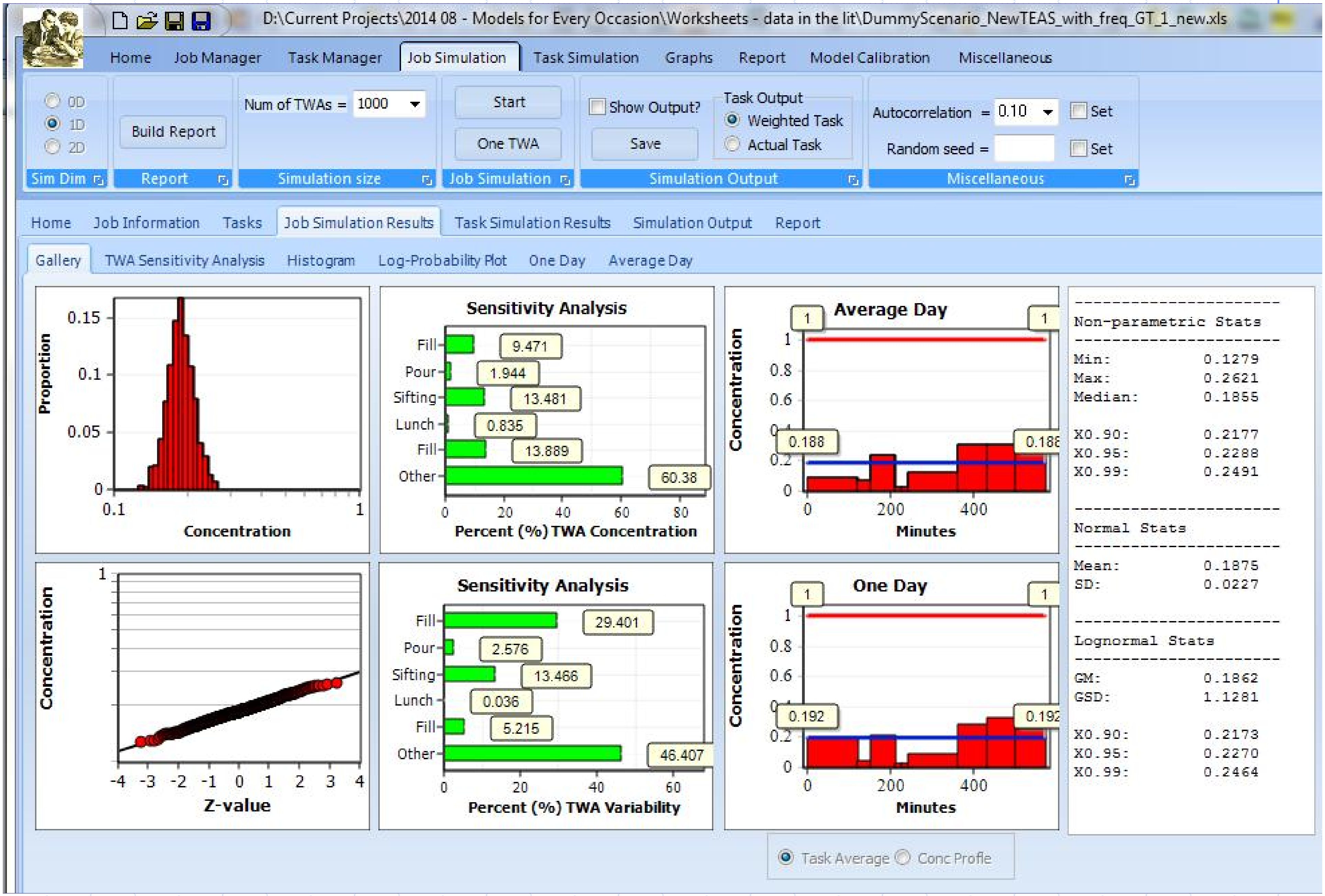
D:\Current Projects\2014 08 - Models for Every Occasion\Worksheets - data in the lit\DummyScenario NewTEAS with freq GT 1 new.xls

Home | Job Manager | Task Manager | Job Simulation | Task Simulation | Graphs | Report | Model Cal

0D / 1D / 2D — Sim Dim | Add, Delete, Cut, Copy, Paste, Insert, Clone, Paste Before, Paste After — Clipboard | Contract, Expand — Task Nodes | 480 min — Duration | All, 1Box, 2…, Statistical, Expert Sy… — Generic Models

Home | Job Information | Tasks | Job Simulation Results | Task Simulation Results | Simulation Output | Report

Index	Name	Desc	Freq	Duration	Task Model	Variable	Units	Var Model	P1Name	P1	P2Nam	P2	P3Nam	P3	Comments
1	Fill	filling	1	120	1Box										dd
1						G	mg/min	Normal	Mean =	0.833	SD =	0.0833			
1						Q	m^3/min	Uniform	Min =	0.06	Max =	9			
1						V	m^3	Constant	K =	100					
1						tq	min	Constant	K =	40					
2	Pour	pouring	1	30	Lognormal										dd
2						GM	mg/m^3	Lognormal	GM =	0.05	GSD =	2			
2						GSD		Triangular	Mode =	1.5	Min =	1.25	Max =	2	
3	Sifting	sifting	1	60	Triangular										dd
3						Mode	mg/m^3	Triangular	Mode =	0.25	Min =	0.15	Max =	0.3	
3						Min	mg/m^3	Triangular	Mode =	0.05	Min =	0.025	Max =	0.1	
3						Max	mg/m^3	Uniform	Mode =	0.5	Min =	0.35	Max =	1	
4	Lunch	backgr	2	15	Constant										dd
4						K	mg/m^3	Uniform	Min =	0.01	Max =	0.05			
5	Fill	filling	1	120	1BoxSS										dd
5						G	mg/min	Normal	Mean =	0.833	SD =	0.0833			
5						Q	m^3/min	Uniform	Min =	5	Max =	9			
6	Other	misc	3	70	2Box										dd
6						G	mg/min	Uniform	Min =	5	Max =	10			
6						Q	m^3/min	Triangular	Mode =	30	Min =	20	Max =	40	
6						V	m^3	Constant	K =	100					
6						Vnf	m^3	Triangular	Mode =	8	Min =	4	Max =	16	
6						ß	m^3/min	Uniform	Min =	5	Max =	10			
6						tq	min	Constant	K =	30					
6						ta	min	Constant	K =	0					
6						tb	min	Constant	K =	15					

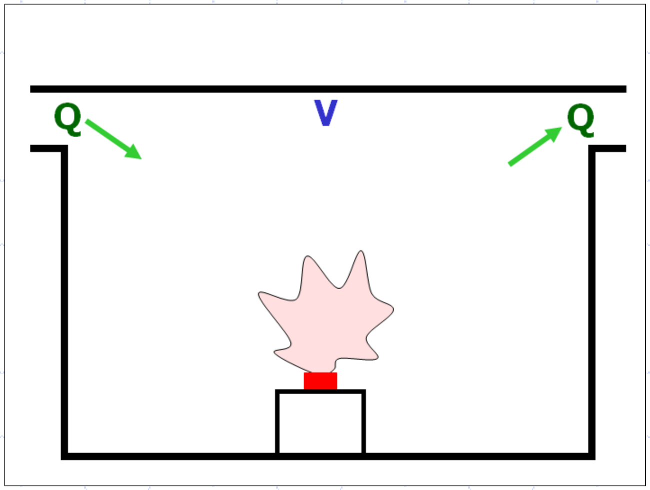

D:\Current Projects\2014 08 - Models for Every Occasion\Worksheets - data in the lit\DummyScenario_NewTEAS_with_freq_GT_1_new.xls
Home
Job Manager
Task Manager
Job Simulation
Task Simulation
Graphs
Report
Model Calibration
Miscellaneous
0D
1D
2D
Build Report
Num of TWAs = 1000
Start
One TWA
Show Output?
Save
Task Output
Weighted Task
Actual Task
Autocorrelation = 0.10
Set
Random seed =
Set
Sim Dim
Report
Simulation size
Job Simulation
Simulation Output
Miscellaneous
Home
Job Information
Tasks
Job Simulation Results
Task Simulation Results
Simulation Output
Report
Gallery
TWA Sensitivity Analysis
Histogram
Log-Probability Plot
One Day
Average Day
Proportion
Concentration
Sensitivity Analysis
Fill
Pour
Sifting
Lunch
Other
9.471
1.944
13.481
0.835
13.889
60.38
Percent (%) TWA Concentration
Average Day
Concentration
Minutes
0.188
Non-parametric Stats
Min: 0.1279
Max: 0.2621
Median: 0.1855
X0.90: 0.2177
X0.95: 0.2288
X0.99: 0.2491
Normal Stats
Mean: 0.1875
SD: 0.0227
Lognormal Stats
GM: 0.1862
GSD: 1.1281
X0.90: 0.2173
X0.95: 0.2270
X0.99: 0.2464
Z-value
29.401
2.576
13.466
0.036
5.215
46.407
Percent (%) TWA Variability
One Day
0.192
Task Average
Conc Profile

Selecting a Model

Exposure Assessment Solutions Inc.

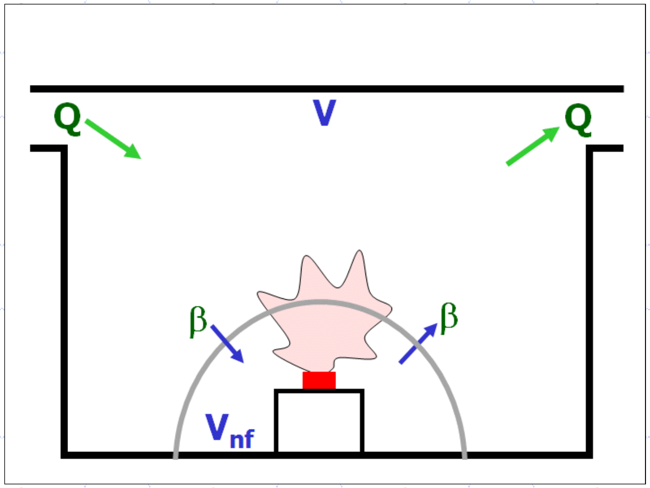
Standard 1Box and 2Box Models

(CE=continuous emissions; DE=decreasing emissions)



$$\bar{c} = \frac{G}{Q}$$

1Box:
CE SS
CE Transient
DE Transient



$$\bar{c}_F = \frac{G}{Q}$$

$$\bar{c}_N = \bar{c}_F + \frac{G}{\beta}$$

2Box:
CE SS
CE Transient
DE Transient

In preparation:

Models for Nearly Every Occasion: Part I - One Box Models

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Gary H. Ganser, Department of Mathematics, West Virginia University, Morgantown, West Virginia

Models for Nearly Every Occasion: Part II - Two Box Models

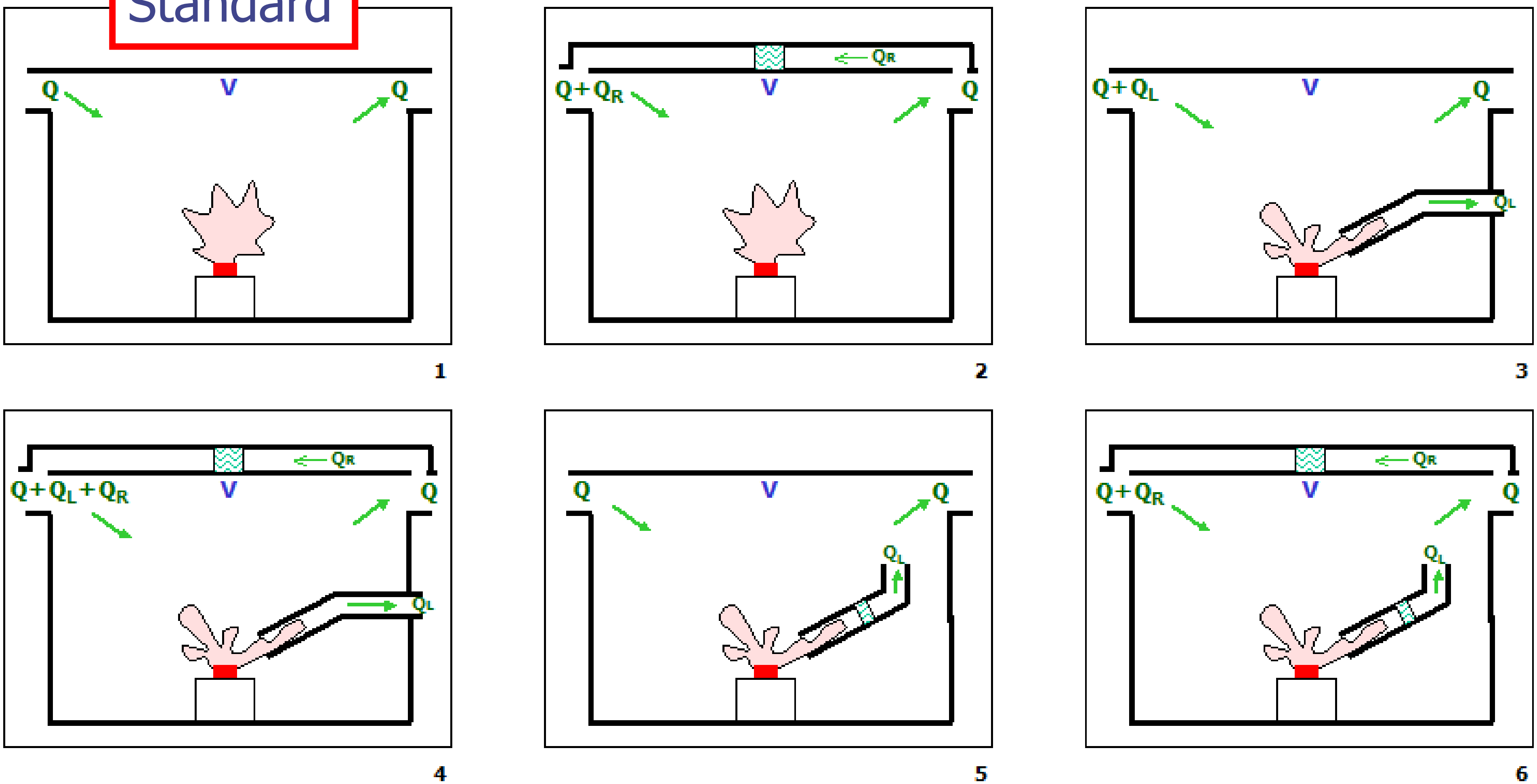
Gary H. Ganser, Department of Mathematics, West Virginia University, Morgantown, West Virginia
Paul Hewett, Exposure Assessment Solutions, Inc.; Morgantown, West Virginia

Models for Nearly Every Occasion: Part III - A Proposed Calibration Procedure

Paul Hewett, Exposure Assessment Solutions, Inc.; Morgantown, West Virginia
Gary H. Ganser, Department of Mathematics, West Virginia University, Morgantown, West Virginia

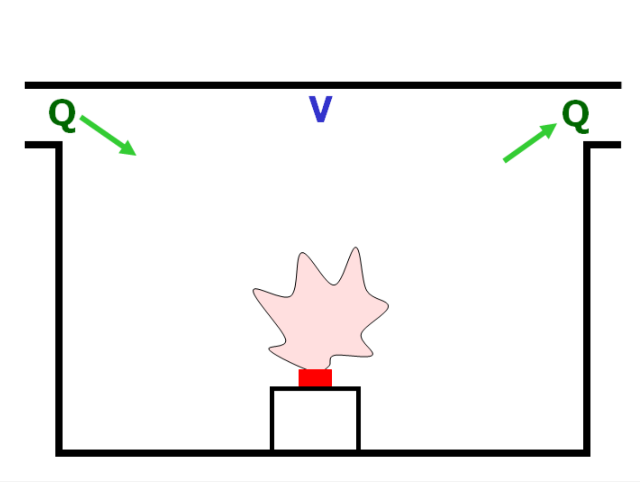
1Box Models

Standard



1Box Model (standard) (1Box.CE.Gv)

	SS	Transient
1	G	G
2	Q	Q
3	γ	V
4		t_g
5		
6		
7		
8		
9		
10		



$$\bar{c} = \frac{\gamma G}{Q}$$

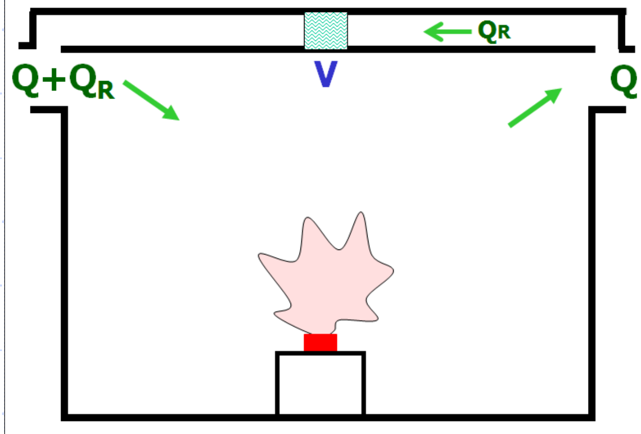
average G

where $\gamma = \frac{\sum t_g}{T}$

- t_g = generation time for each task
- T = sum of task times

Newish !!

1Box.CE.GvR



	SS	Transient
1	G	G
2	Q	Q
3	Q_R	Q_R
4	$\varepsilon_{R.F}$	$\varepsilon_{R.F}$
5	γ	V
6		t_g
7		
8		
9		
10		

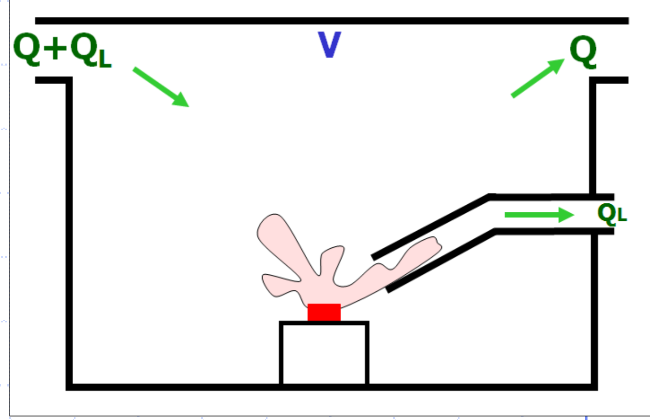
$$\bar{c} = \frac{\gamma G}{Q + Q_R \varepsilon_{R.F}}$$

- $\varepsilon_{R.F}$ = efficiency of the recirculation filter

New !!

1Box.CE.Lev.Gv

	SS	Transient
1	G	G
2	Q	Q
3	Q_L	Q_L
4	$\varepsilon_{L.F}$	$\varepsilon_{L.F}$
5	γ	V
6		t_g
7		
8		
9		
10		



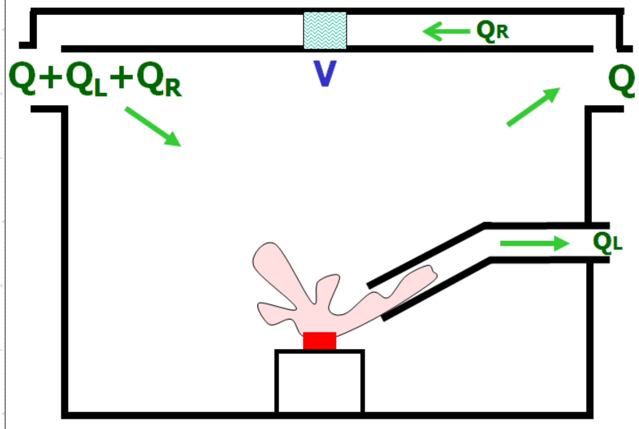
$$\bar{c} = \frac{\gamma G(1-\varepsilon_L)}{Q+Q_L}$$

- ε_L = LEV efficiency (fraction of G immediately captured by the LEV)

New !!

1Box.CE.Lev.GvR

	SS	Transient
1	G	G
2	Q	Q
3	Q_L	Q_L
4	$\varepsilon_{L.F}$	$\varepsilon_{L.F}$
5	Q_R	Q_R
6	$\varepsilon_{R.F}$	$\varepsilon_{R.F}$
7	γ	V
8		t_g
9		
10		

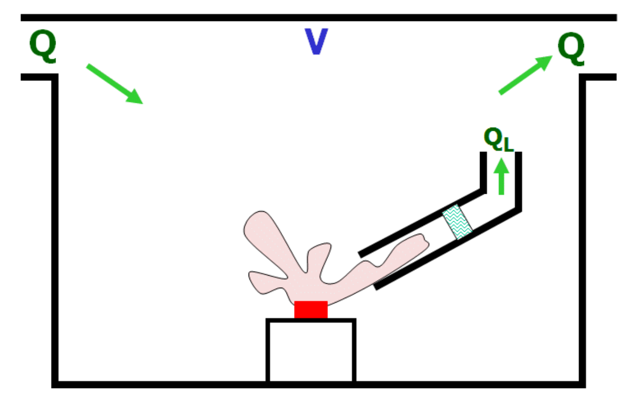


$$\bar{c} = \frac{\gamma G(1-\varepsilon_L)}{(Q+\varepsilon_{R.F}Q_R) + Q_L}$$

New !!

1Box.CE.LevR.Gv

	SS	Transient
1	G	G
2	Q	Q
3	Q_R	Q_R
4	ε_L	ε_L
5	$\varepsilon_{L.F}$	$\varepsilon_{L.F}$
6	γ	V
7		t_g
8		
9		
10		



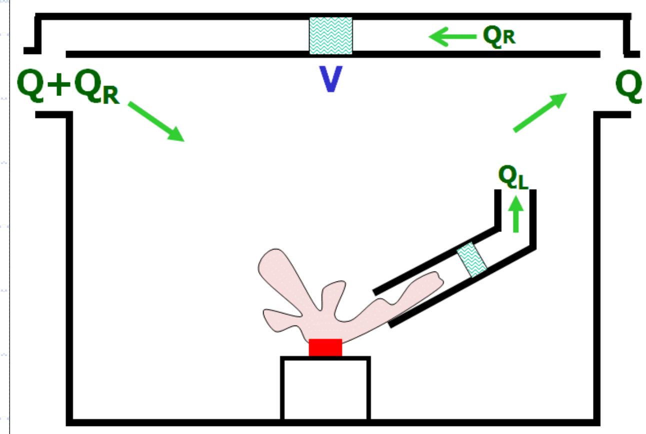
$$\bar{c} = \frac{\gamma G(1-\varepsilon_L \varepsilon_{L.F})}{Q + \varepsilon_{L.F} Q_L}$$

- $\varepsilon_{L.F}$ = efficiency of the LEV return filter

New !!

1Box.CE.LevR.GvR

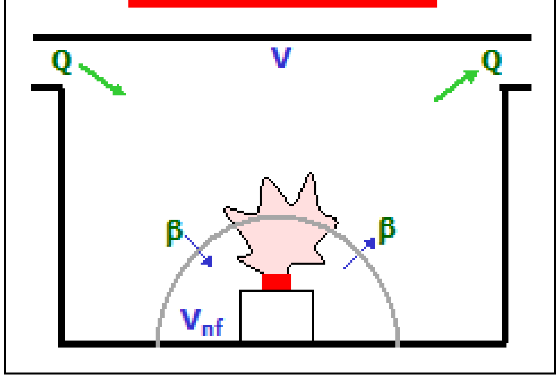
	SS	Transient
1	G	G
2	Q	Q
3	Q_R	Q_R
4	ε_L	ε_L
5	$\varepsilon_{L.F}$	$\varepsilon_{L.F}$
6	Q_R	Q_R
7	$\varepsilon_{R.F}$	$\varepsilon_{R.F}$
8	γ	V
9		t_g
10		



$$\overline{c} = \frac{\gamma G(1-\varepsilon_L \varepsilon_{L.F})}{(Q+\varepsilon_{R.F} Q_R) + \varepsilon_{L.F} Q_L}$$

2Box Models

Standard



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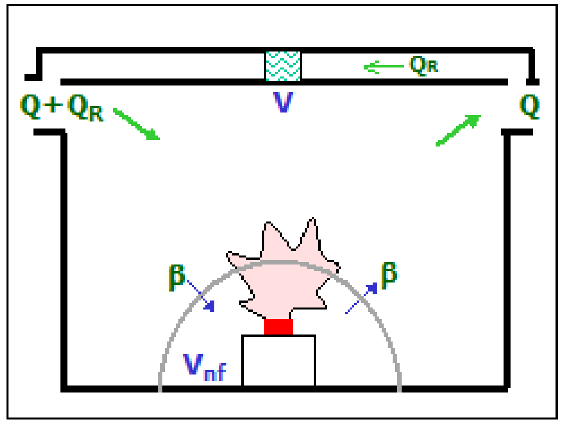

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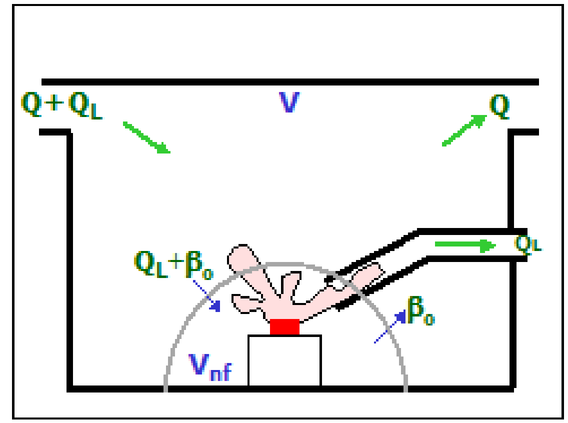

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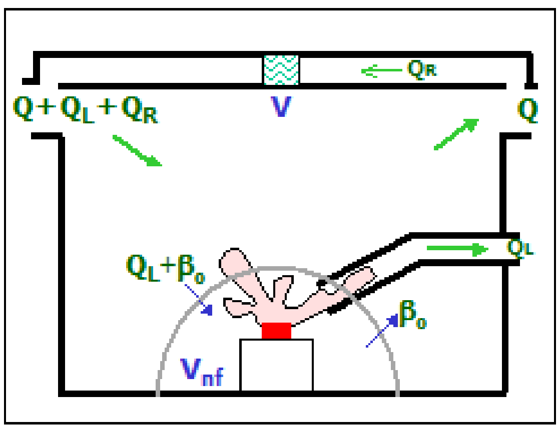

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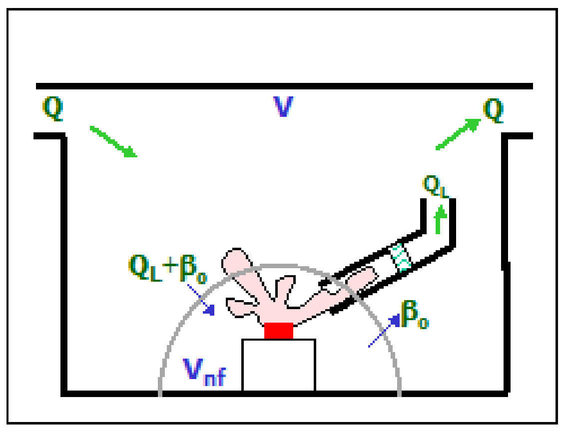

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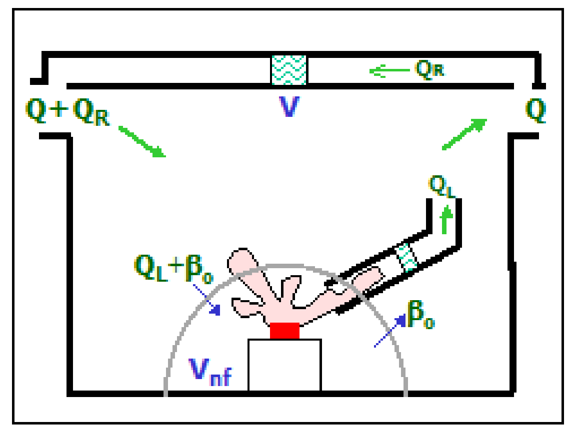

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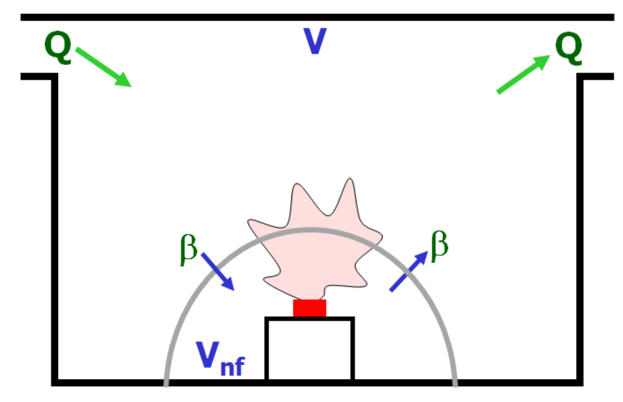
2Box.CE.GvR (standard) (2Box.CE.GvR)

	SS	Transient
1	G	G
2	Q	Q
3	β	V
4	γ	V_{NF}
5		β
6		t_g
7		
8		
9		
10		



$$\bar{c}_F = \frac{\gamma G}{Q}$$

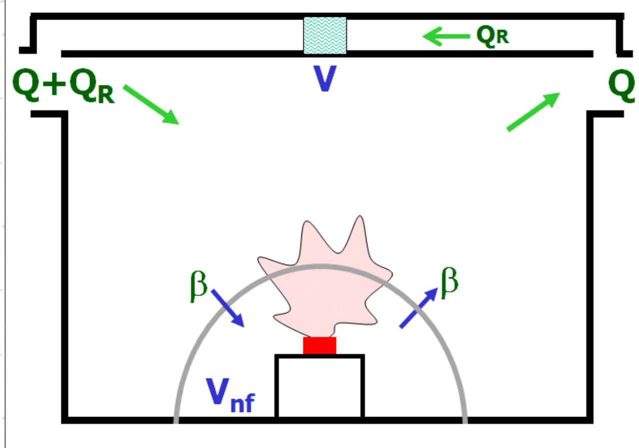
$$\bar{c}_N = \bar{c}_F + \frac{\gamma G}{\beta}$$

- β = near field flowrate

New !!

2Box.CE.GvR

	SS	Transient
1	G	G
2	Q	Q
3	Q_R	Q_R
4	$\varepsilon_{R.F}$	$\varepsilon_{R.F}$
5	β	V
6	γ	V_{NF}
7		β
8		t_g
9		
10		



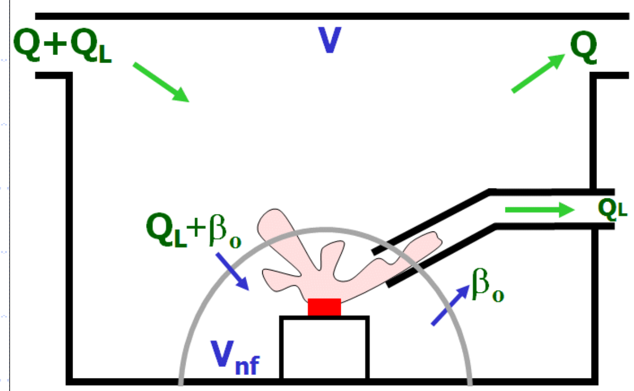
$$\bar{c}_F = \frac{\gamma G}{Q + Q_R \varepsilon_{RFilter}}$$

$$\bar{c}_N = \bar{c}_F + \frac{\gamma G}{\beta}$$

New !!

2Box.CE.Lev.Gv

	SS	Transient
1	G	G
2	Q	Q
3	Q_L	Q_L
4	ε_L	ε_L
5	β	V
6	γ	V_{NF}
7		β
8		t_g
9		
10		



$$\bar{c}_F = \frac{\gamma G(1-\varepsilon_L)(1-\varepsilon_{NF})}{Q+Q_L}$$

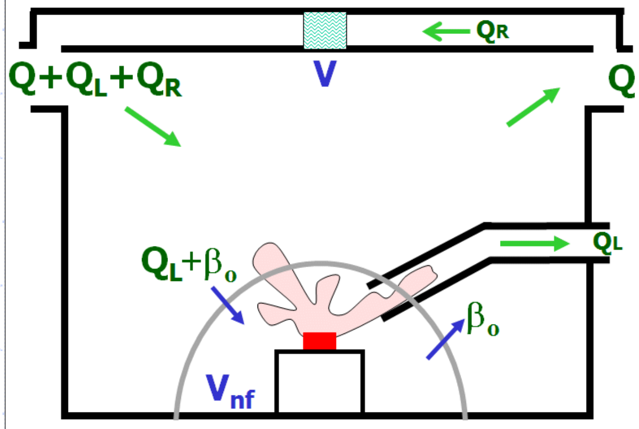
$$\bar{c}_N = \bar{c}_F + \frac{\gamma G(1-\varepsilon_L)\varepsilon_{NF}}{Q_L}$$

$$\text{where } \varepsilon_{NF} = \frac{Q_L}{Q_L+\beta_o}$$

New !!

2Box.CE.Lev.GvR

	SS	Transient
1	G	G
2	Q	Q
3	Q_L	Q_L
4	ε_L	ε_L
5	Q_R	Q_R
6	$\varepsilon_{R.F}$	$\varepsilon_{R.F}$
7	β	V
8	γ	V_{NF}
9		β
10		t_g



$$\bar{c}_F = \frac{\gamma G(1-\varepsilon_L)(1-\varepsilon_{NF})}{(Q+\varepsilon_{R.F}Q_R)+Q_L}$$

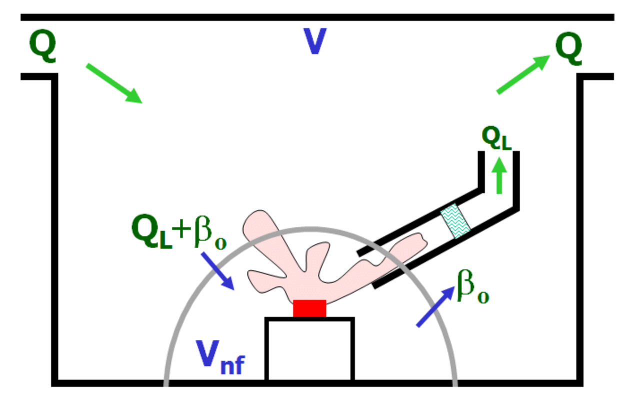
$$\bar{c}_N = \bar{c}_F + \frac{\gamma G(1-\varepsilon_L)\varepsilon_{NF}}{Q_L}$$

where $\varepsilon_{NF} = \dfrac{Q_L}{Q_L+\beta_o}$

New !!

2Box.CE.LevR.Gv

	SS	Transient
1	G	G
2	Q	Q
3	Q_L	Q_L
4	ε_L	ε_L
5	$\varepsilon_{L.F}$	$\varepsilon_{L.F}$
6	β	V
7	γ	V_{NF}
8		β
9		t_g
10		

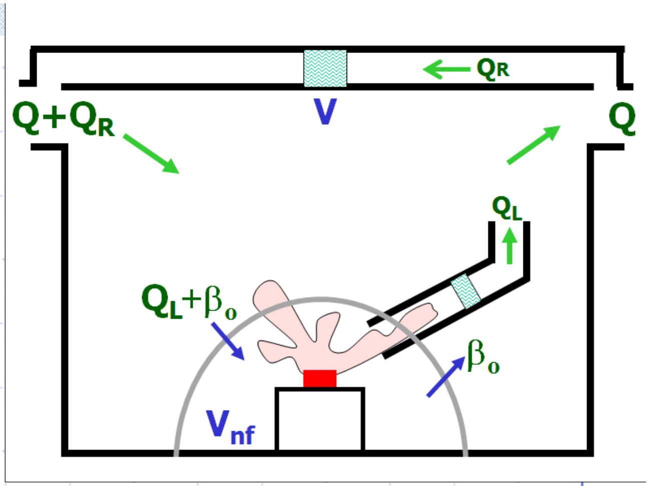


[under construction]

New !!

2Box.CE.LevR.GvR

	SS	Transient
1	G	G
2	Q	Q
3	Q_L	Q_L
4	ε_L	ε_L
5	$\varepsilon_{L.F}$	$\varepsilon_{L.F}$
6	Q_R	Q_R
7	$\varepsilon_{R.F}$	$\varepsilon_{R.F}$
8	β	V
9	γ	V_{NF}
10		β
11		t_g



[under construction]

Model Number	1Box Models	Model Number	2Box Models
100	1Box.CE.Gv.SS	200	2Box.CE.Gv.SS
101	1Box.CE.Gv	201	2Box.CE.Gv
102	1Box.CE.GvR.SS	202	2Box.CE.GvR.SS
103	1Box.CE.GvR	203	2Box.CE.GvR
104	1Box.CE.Lev.Gv.SS	204	2Box.CE.Lev.Gv.SS
105	1Box.CE.Lev.Gv	205	2Box.CE.Lev.Gv
106	1Box.CE.Lev.GvR.SS	206	2Box.CE.Lev.GvR.SS
107	1Box.CE.Lev.GvR	207	2Box.CE.Lev.GvR
108	1Box.CE.LevR.Gv.SS	208	2Box.CE.LevR.Gv.SS
109	1Box.CE.LevR.Gv	209	2Box.CE.LevR.Gv
110	1Box.CE.LevR.GvR.SS	210	2Box.CE.LevR.GvR.SS
111	1Box.CE.LevR.GvR	211	2Box.CE.LevR.GvR
112	1Box.DE.Gv	212	2Box.DE.Gv
113	1Box.DE.GvR	213	2Box.DE.GvR
114	1Box.DE.Lev.Gv	214	2Box.DE.Lev.Gv
115	1Box.DE.Lev.GvR	215	2Box.DE.Lev.GvR
116	1Box.DE.LevR.Gv	216	2Box.DE.LevR.Gv
117	1Box.DE.LevR.GvR	217	2Box.DE.LevR.GvR

Calibrating a Model

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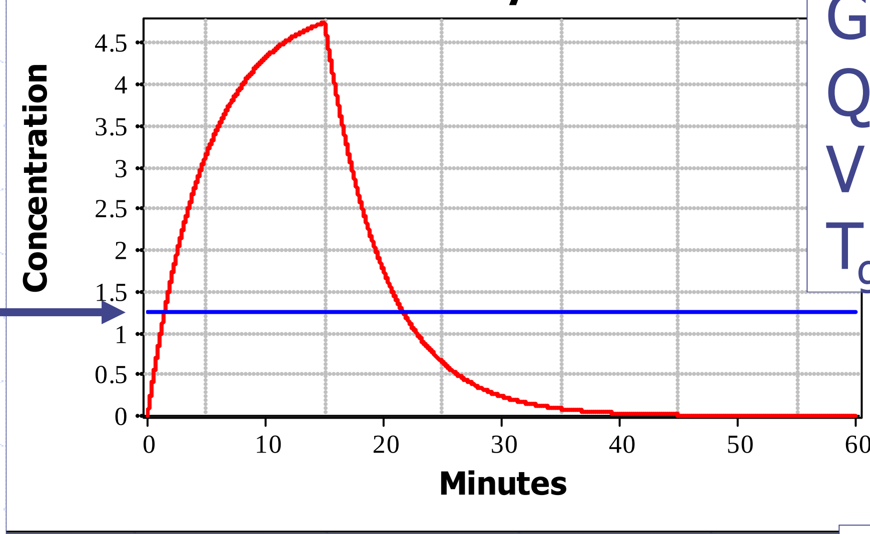
Proposition:

- The Steady State (SS) equations can be used to calibrate *any* to a task with a few TWA measurements, provided …
  - (a) the task starting and ending concentrations are zero (or near zero), or
  - (b) the sample time is long.
- Under either of these conditions this procedure can be applied to both *continuous* and *cyclic (or irregular)* processes.

(a)

$\bar{C}$=1.249

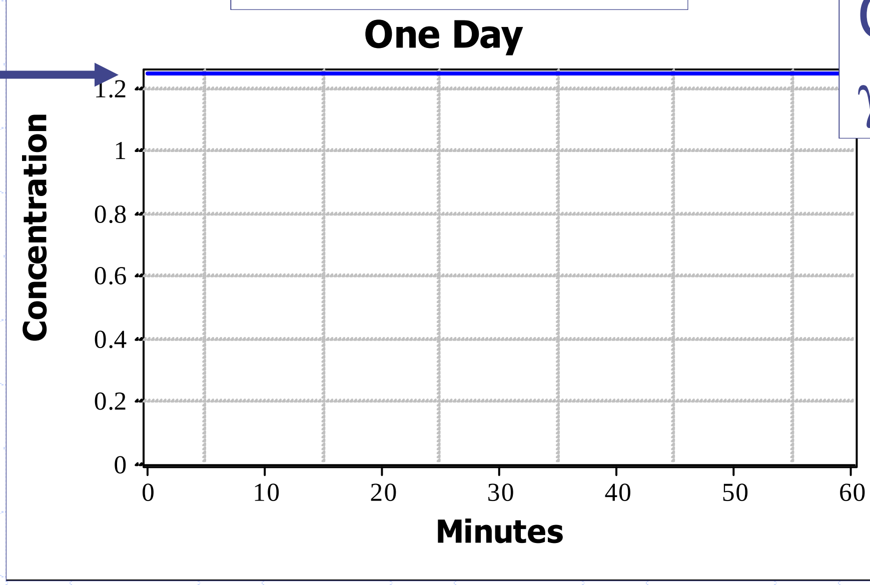
1Box.CE.Gv



G = 100 mg/min
Q = 20 m^3/min
V = 100 m^3
T_g = 15 min

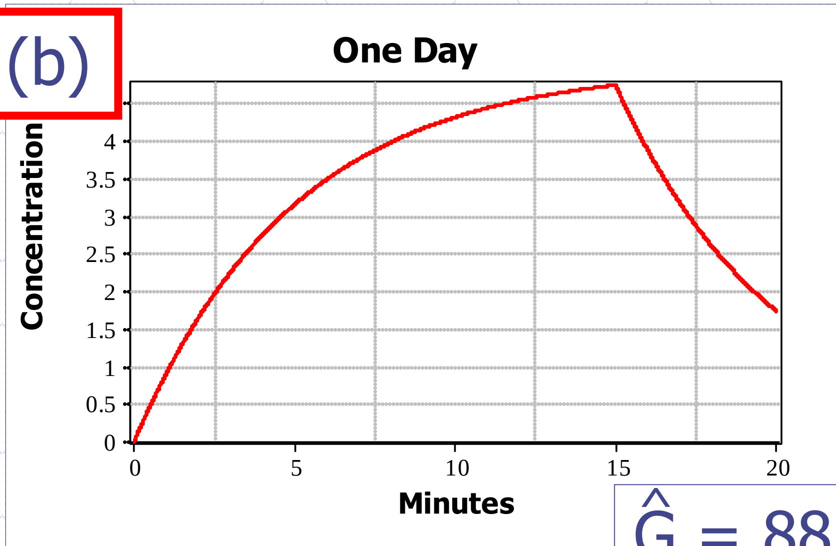
$\bar{C}$=1.25

1Box.CE.Gv.SS

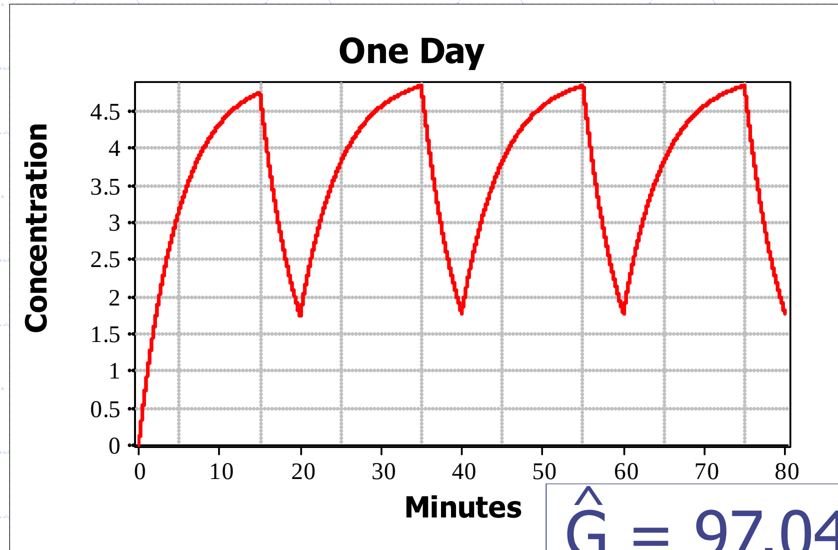


G = 100 mg/min
Q = 20 m^3/min
γ = 0.25

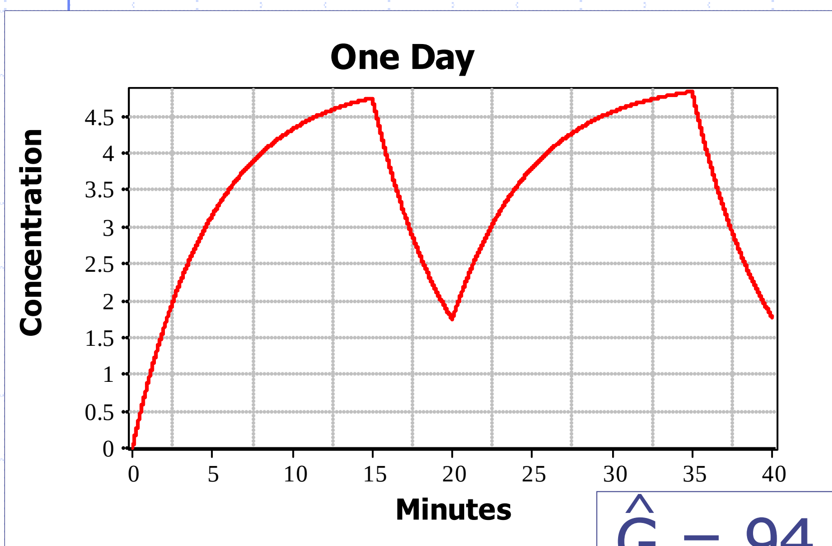
(b)



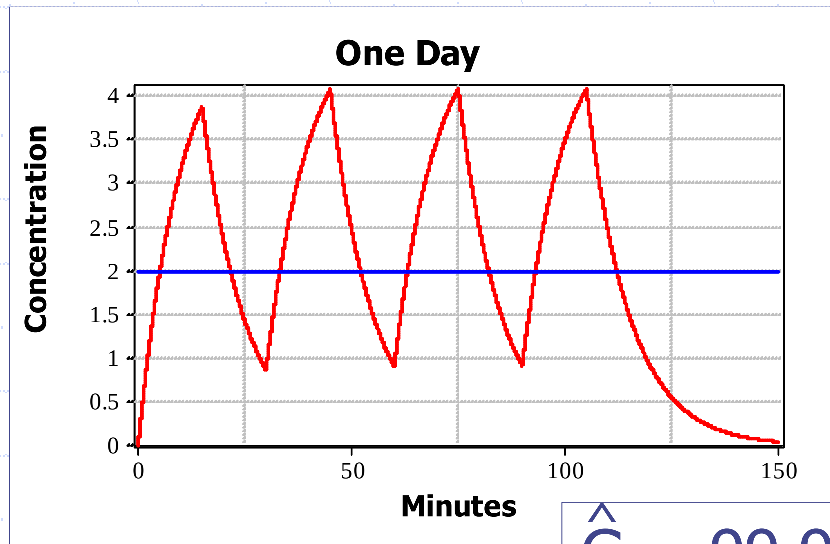
$\hat{G} = 88.38$



$\hat{G} = 97.04$

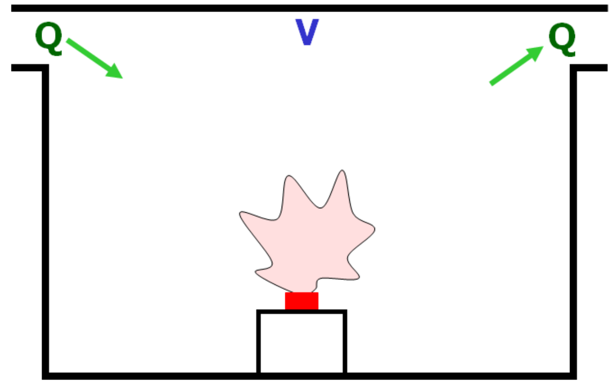


$\hat{G} = 94.08$



$\hat{G} = 99.93$

Example 1



- Assume a 1Box scenario:
  - G = ?   (unknown)

$$\bar{c} = \frac{\gamma G}{Q}$$

- V and Q are knowable:
  - $V = 100\ m^3$
  - $Q = 20\ m^3/min$
- The process is cyclic:
  - 15 minutes of generation every 60 minutes
- During the generation phase the emissions are continuous.

- Calibration Procedure:
  - Collect a (far field) measurement:
    - $C = 1.249\ mg/m^3$
  - $T = 60$ min and $t_g = 15$ min (time of generation)
    - $\gamma = 15/60 = 0.25$

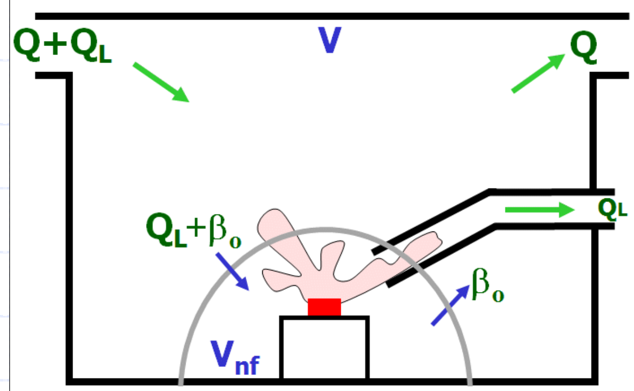
$$\bar{G} = \bar{c}Q = 1.249 \cdot 20 = 24.98\ mg/\min$$

$$\hat{G} = \frac{\bar{c}Q}{\gamma} = \frac{1.249 \cdot 20}{0.25} = 99.92\ mg/\min$$

true G = 100 mg/min

Example 2

- Assume a 2Box w/ LEV scenario:
  - G = ? (unknown)
  - β_o = ?
  - ε_L = ? $\varepsilon_{NF} = f(Q_L, \beta_o)$
- V, V_{NF}, Q, and Q_L are knowable.
  - $V = 100\ m^3$
  - $Q = 20\ m^3/min$ $Q_L = 5\ m^3/min$
- The process is cyclic:
  - 15 minutes of generation every 60 minutes
- During the generation phase the emissions are continuous.



$$\bar{c}_F = \frac{\gamma G(1-\varepsilon_L)(1-\varepsilon_{NF})}{Q+Q_L}$$

$$\bar{c}_N = \bar{c}_F + \frac{\gamma G(1-\varepsilon_L)\varepsilon_{NF}}{Q_L}$$

where $\varepsilon_{NF} = \frac{Q_L}{Q_L+\beta_o}$

- Collect a FF and NF measurement:
  - $C_f = 0.125\ mg/m^3$
  - $C_n = 0.75\ mg/m^3$
- Collect a measurement in the LEV:
  - $C_{Exhaust} = 4.50\ mg/m^3$
  - $T = 60$ min and $t_g = 15$ min (time of generation)
    - $\gamma = 15/60 = 0.25$

- Calculate efficiency of the local exhaust:

$$\hat{\varepsilon}_{Lev} = \frac{(\bar{c}_E - \bar{c}_F)\,Q_{Lev}}{\bar{c}_F Q + \bar{c}_E Q_{Lev}} = \frac{(4.50 - 0.125)\cdot 5}{(0.125\cdot 20) + (4.50\cdot 5)} = 0.75$$

- Calculate the *average* Generation rate:

$$\overline{G} = \overline{c}_F Q + \overline{c}_E Q_{Lev} = 0.125 \cdot 20 + 4.50 \cdot 5 = 25 \ mg/\text{min}$$

- Calculate the actual Generation rate:

$$\hat{G} = \frac{\overline{G}}{\gamma} = \frac{25}{0.25} = 100 \ mg/\text{min}$$

- Calculate the NF "out" flowrate:

$$\hat{\beta}_o = \frac{\gamma \hat{G}(1-\hat{\varepsilon}_L)}{(\bar{c}_N - \bar{c}_F)} - Q_2$$

$$= \frac{0.25 \cdot 100(1-0.75)}{(0.75-0.125)} - 5 = 5\ m^3/\mathrm{min}$$

Checks and Balances

- If G known, compare to the estimated value.
  - Compare the total mass leaving the system with the total mass emitted.
- If β can be measured, compare to the estimated value.
- If the recirculation or return air filtration efficiency is known, compare to the estimated value.

Comments

- We view β as an "effective inter-zonal flowrate", a function of …
  - ever changing patterns of local air currents
  - thermal buoyancy effects
  - the position of the worker within the near field.
  - Perhaps best calculated from the calibration measurements.
- Computer simulations show that V_{NF} is usually not a critical factor.
  - Start with a value of 8 or 10 m^3.

- **The revised SS equations can be used to calculate average exposures for cyclic tasks and irregular tasks,**
  - eliminating the need to integrate the transient equations.
- **Note: A “calibrated” model is not yet a “validated” model.**

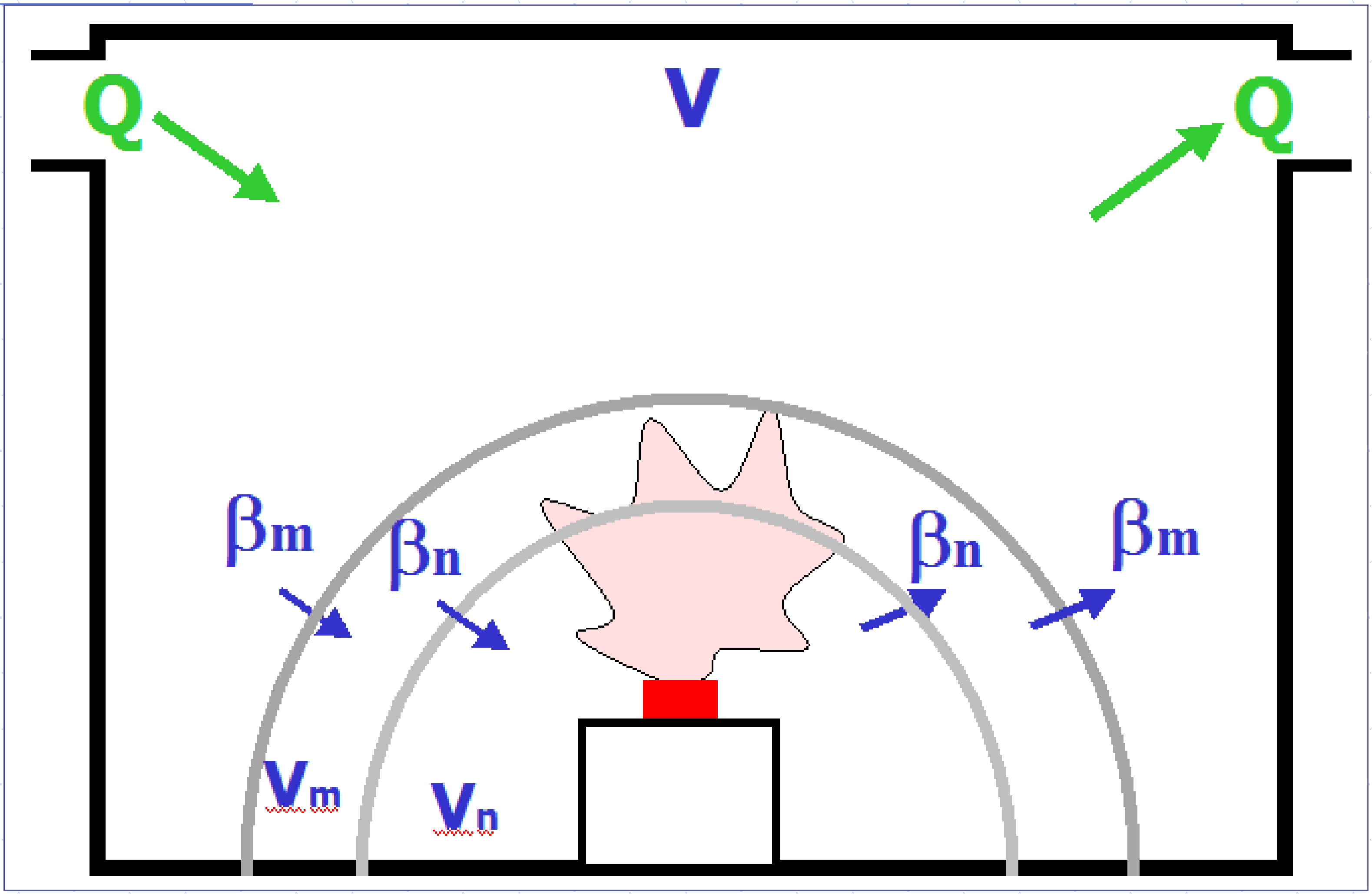
Developing Models

Exposure Assessment Solutions Inc.

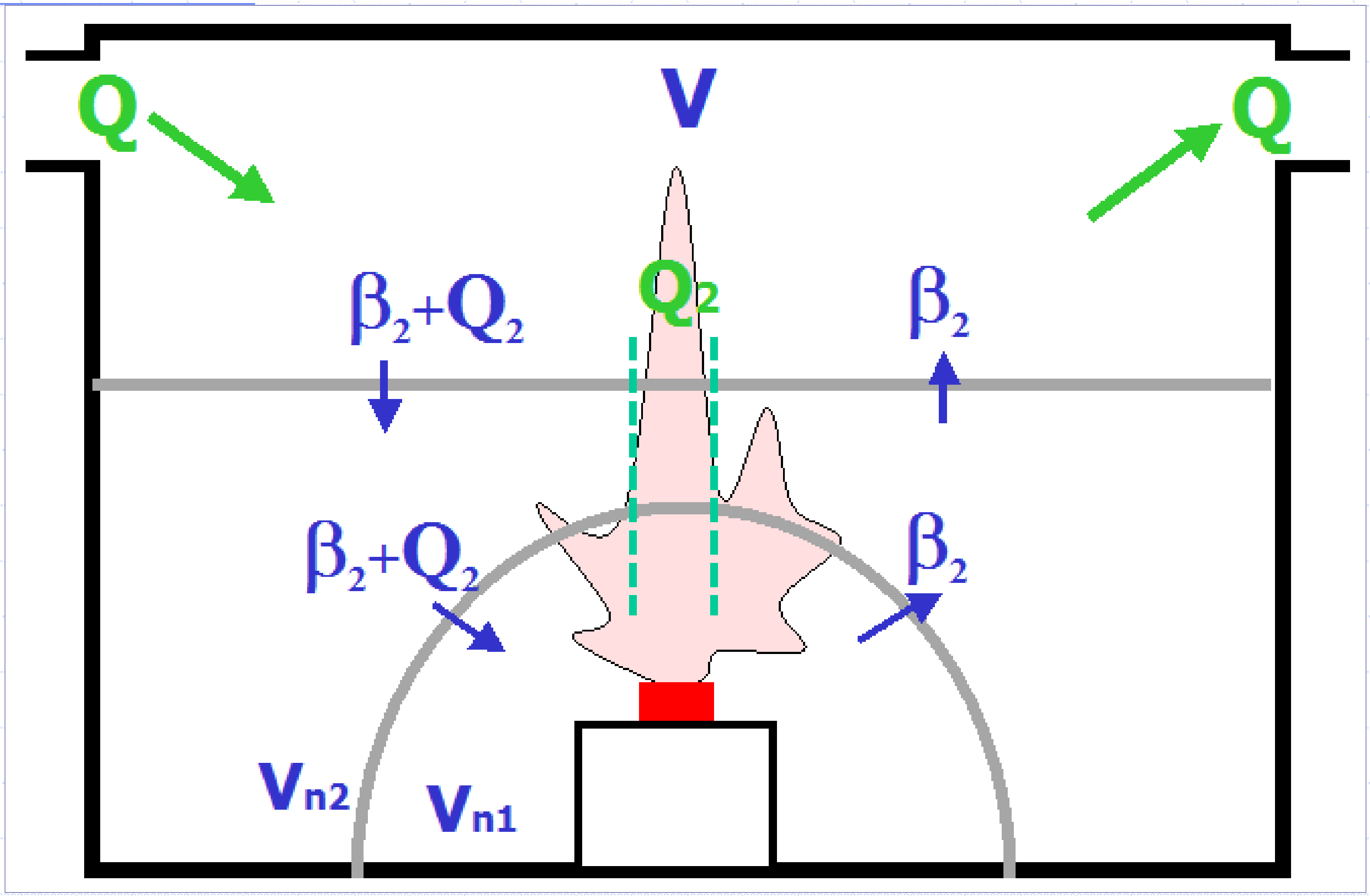
Variations on 1Box and 2Box Models

- Can simple models be devised that account for the effect of … ?
  - room dimensions, floor plan/shape, equipment layout
  - placement and number of intake and exhaust ventilation grills relative to the process
- Special models or guidance on V_{NF} and β when the process is …
  - up against a wall or bluff body
  - in a corner
- Three zone models
- Three zone model + thermally buoyant plumes

Predict exposures in Far, Medium, and Near Fields



The standard "stack effect" equation could be used to estimate the upward flowrate due to thermal buoyancy.



Research Needs

(Dealing with Implementation Issues)

Exposure Assessment Solutions Inc.

Validation of …

- “New” Models
  - Laboratory chamber studies
  - Field validation

Guidance for *Best* Model Calibration Practices

- Our proposed approach to "model calibration"?
- Optimal location of TWA samples and/or DRIs
- Optimal sample sizes
- Statistical analysis of the data:
  - best estimates of the model variables
  - or use to generate inputs into probabilistic modeling
- Characterize the lag times (in the NF and FF) inherent when the agent disperses
- **Walk-through checklist**

Future Research

- Show the value of obtaining *a few extra* measurements.
  - A calibrated and validated model could be very useful in other scenarios.
- Use of direct reading instruments (DRI)
  - Can DRIs be used to *rapidly and cheaply* obtain a useful set of NF and FF exposure measurements, as well as measurements in the LEV and recirculation systems?

Clearing House for “validated” Models

- On-line
- Moderated by an agency or a NIOSH ERC
- Which models work well with combinations of …
  - Substance or class
  - Emission type
  - Unit operation
  - Local controls
  - General ventilation controls
  - Room layout
  - Etc

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