# After a Year of Comparing Two Vapor Intrusion Models: What We Learned

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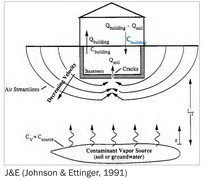
## 1. Introduction

Recently, the Johnson and Ettinger (J&E) model has been compared to a second vapor intrusion (VI) model (ViM) at sites across the United States where soil or groundwater was contaminated with VOCs. The J&E model is the standard VI model that has been used by regulatory agencies in the United States for the past two decades to evaluate the risks associated with vapor intrusion from groundwater and soil sources. More recently, an alternative, but somewhat more complex, vapor intrusion model named ViM has been developed that is also intended to be applied at the regulatory level.

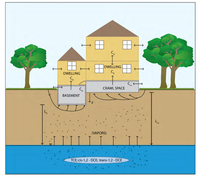
Conceptual models for J&E and ViM are shown in Figure 1. The J&E model (JEM) is a one compartment model and can simulate buildings with basements or slab-on-grade foundations. ViM can simulate up to three compartments in a building. A comparison of the capabilities of the two models is shown in Table 1.

**Table 1**
**ViM and J&E Comparison**

| Capability | ViM | J&E/ EPA |
|---|---|---|
| Basements, slab-on-grade | ✓ | ✓ |
| Crawl space | ✓ | |
| Multiple compartments | ✓ | |
| Outdoor air intrusion | ✓ | |
| Non-steady conditions | ✓ | |
| Lifetime exposure | ✓ | ✓ |
| Monte Carlo: Uncertainty analysis | ✓ | |
| Chemical Processes: biodecay, adsorption | ✓ | |
| Sensitivity analysis | ✓ | ✓ |




J&E (Johnson & Ettinger, 1991)




ViM (Mills et al., 2007)

Figure 1. Conceptual models.

## 2. How We Know ViM Works Correctly, and Several of Its Unique Features

While the J&E model has been tested and used many times over the past 20 years, ViM (developed much more recently) has not been as well tested. During the course of its development, however, the model has undergone both verification testing (successfully model-to-model comparison) and validation (successful comparison with field data at specific sites).

| | |
|---|---|
| **Initial Testing:** ViM's numerical Laplace Inverse routines | Feb - Aug 2005 |
| **Verification:** ViM vs. T&R | Sept - Oct 2005 |
| **Verification:** ViM vs. Jury Model | Jan - Feb 2006 |
| **Validation:** Building 20 Moffett Field | Feb - July 2006 |
| **Documentation:** Research paper to ES&T | July 2007 |

### Verifcation Tests

#### *Comparison with Turcynowicz and Robinson (T&R, 2001)*

Turcynowicz and Robinson developed a model that is in some ways is similar to ViM. The model they developed focused on calculating the time varying cumulative indoor air dose of benzene, defined as:

$$\mathrm{Dose}(t) = \int_0^t I \cdot C_{in}(\tau)\,d\tau$$

where $C_{in}(t)$ is the indoor vapor concentration at time $\tau$ [M/L$^3$], and I is the inhalation rate (L$^3$T$^{-1}$)

The residence simulated by T&R consists of a crawl space beneath a dwelling space. T&R did not report the predicted concentrations in the dwelling or crawl space, so the comparison with their results was to dose. Figure 2 compares the dose curve predictions over a 1,600 day (i.e., 4.4 year) exposure period, and indicates that the results are essentially identical.

#### *Comparison with Sanders and Talimcioglu (S&T, 1997)*

Sanders and Talimcioglu used the Jury Model to estimate indoor air concentrations for a variety of conditions. The scenario assumed a zone of benzene-contaminated soil at a concentration of 1 µg/g.

Sanders and Talimcioglu performed 30 tests, where soil moisture content, soil moisture advection, and decay were varied. Table 2 shows the comparison between the Sanders and Talimcioglu's results and ViM. Both time-to-peak concentration and peak concentration comparisons are shown. In all cases, the predictions were in good agreement.

### Validation Tests

Model validation was performed at a former naval BOQ (Bachelor Office Quarter) at Moffett Field, CA. The chemicals of concern there were TCE, cis-1, 2-DCE, and trans-1, 2-DCE. Predictions of TCE concentrations were made in the building's basement (green lines), crawl space (blue lines), and dwelling space (red lines) (see Figure 3). The multiple traces of each line color denote Monte Carlo simulations. The few observed data were collected in the dwelling space and crawl space, as show by the red and blue symbols, and compare well against ViM predictions for the few years of data availability. Two further validation tests were performed at Moffett Field for cis-1,2-DCE and trans-1,2-DCE. Once again a good agreement resulted. (The solid lines in the figures represent results from the steady-state J&E model, and illustrate that steady state cannot represent the time variable predictions, except for a limited time frame.)

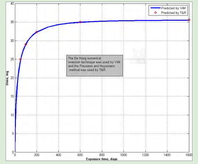
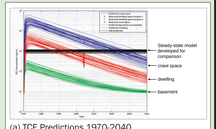
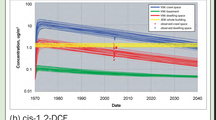


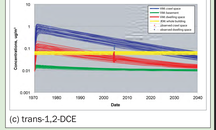

Figure 2. Comparisons of predicted benzene dose to a young child.




(a) TCE Predictions 1970-2040




(b) cis-1,2-DCE




(c) trans-1,2-DCE

Figure 3. ViM Validation Simulations, Bld 20 Moffett Field: These validation results show ViM's ability to predict indoor air concentrations that range over many orders of magnitude.

**Table 2**
**Comparison of Predicted Indoor Air Concentrations Using Jury Model and ViM Using Conditions Presented in Sanders and Talimcioglu**

| Description of Test | | | | A: No degradation | | B: Half life=180 d | | C: Half life = 16 d | |
|---|---|---|---|---|---|---|---|---|---|
| Scenario Number | Soil Moisture (% v/v) | Soil Moisture Advection (cm/d) | Model | Time to Peak (days) | Peak Concentration (ug/m³) | Time to Peak (days) | Peak Concentration (ug/m³) | Time to Peak (days) | Peak Concentration (ug/m³) |
| 1 | 10 | 0 | Jury | 25 | 450 | 22 | 409 | 16 | 198 |
| | | | ViM | 25 | 446 | 25 | 406 | 15 | 193 |
| 2 | 20 | 0 | Jury | 110 | 97 | 87 | 66 | 42 | 7 |
| | | | ViM | 110 | 96 | 90 | 66 | 40 | 7 |
| 3 | 30 | 0 | Jury | 1100 | 9 | 445 | 0.8 | 150 | 0.0001 |
| | | | ViM | 1200 | 9 | 400 | 0.7 | 155 | 0.00013 |
| 4 | 19 | 0 | Jury | 100 | 116 | 75 | 84 | 38 | 12 |
| | | | ViM | 100 | 115 | 80 | 83 | 40 | 11 |
| 5 | 19 | 0.016 | Jury | 100 | 110 | 75 | 80 | 38 | 11 |
| | | | ViM | 100 | 109 | 80 | 79 | 40 | 10 |

## 3. Solution of ViM Equations: Numerical Inversion of Laplace Transforms

The equations that form the mathematical basis for ViM are coupled linear partial differential equations. An exact analytical solution to the equations was not found. While a numerical finite-difference scheme could have been used to solve the equation, such a solution would have required large amounts of computational time to simulate the typical 70 year period of exposure. The problem of excessive computational time was addressed by taking Laplace Transforms of the equations, and numerically inverting the equations to find the required indoor air concentrations over the 70 year period of simulation. However, numerical inversion from Laplace space back into the time domain can introduce enough round-off error that the actual solution is overwhelmed. Figure 4 illustrates that inverse Laplace solutions are expressed as series, where (without round-off error) the numerically inverted solutions approach the exact solution. Experience with this solution technique has shown that 16 to 20 terms are sufficient for convergence. However, if round-off error creeps in before convergence is attained then the calculated solution will diverge (see Figure 4).

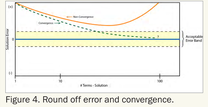



Figure 4. Round off error and convergence.

The problem of round off error was overcome by using Symbol Mathematics (Matlab, 2009) and variable precision arithmetic to emulate higher precision processors. In Figure 5a the predictions of TCE concentrations clearly shows signs of round off error affecting the solutions. Figure 5b shows the corrected solution, where 64 significant digits were emulated to remove the round off error.

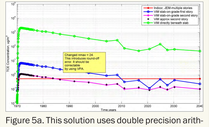



Figure 5a. This solution uses double precision arithmetic, and round off error corrupts the solution.

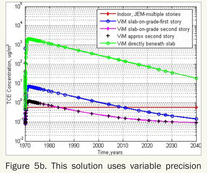



Figure 5b. This solution uses variable precision arithmetic (VPA). Note that round-off error has disappeared.

## 4. Comparison of ViM and J&E Predictions at U.S. Air Force Bases in the United States

Since ViM can simulate the effects of a time-variable groundwater plume, Figure 6 was developed to provide estimates of groundwater concentrations not only in 2009 (when the site investigation at Travis AFB was done), but also in 2006-2007 when groundwater concentrations in the vicinity of Building 828 may have been higher.

Using these data, indoor air and sub-slab concentration were predicted by both ViM and JEM. See Figure 7. It is noticed that ViM predicted concentrations while initially very low, eventually exceeded JEM predictions beginning in 2008 and continuing until 2014. The groundwater concentration used in the JEM predictions correspond to the upper end of the observed groundwater data collected in 2009, which was 27,400 µg/m³. While the ViM model used the same groundwater concentrations for 2009, earlier concentrations in 2006-2007 may have been higher as shown previously in Figure 6. During that time vadose zone vapors were predicted to have been migrating through the unsaturated zone, and it was these vapors that caused the predicted indoor air concentrations to be higher than the JEM predictions.

At Kelly AFB a Monte Carlo analysis was performed using observed data, as available, or otherwise using a realistic range about the mean value. The predicted indoor air concentrations and sub-slab concentrations are shown in Figure 8. Predictions are shown for median concentrations (solid lines) and 5% and 95% confidence limits (dashed lines). It is noteworthy that the confidence limits of the predicted results, for the most part, encompass the observed data(the blue patches). This indicates that the predicted variability associated with the Monte Carlo analyses may be close to the actual system variability. Predictions using a modified version of the J&E model are included, where a Monte Carlo framework was added.

For Cape Canaveral AFS, Table 3 shows specific comparisons of alternative predictions using J&E, ViM, and EPA's 95% attenuation factor approach for different source concentrations as specified by different metrics (such as the arithmetic means of source data). Based on the different metrics used to develop the source concentration, the source strength varied by a factor of 3. When ViM is used in a Monte Carlo mode, ViM's 50% predictions are similar to the observed data when sub-slab or near-slab data are used as source terms.

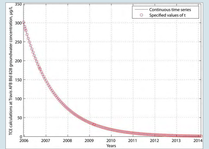



Figure 6. Time series of groundwater TCE concentrations at Travis AFB, in the vicinity of Building 828.

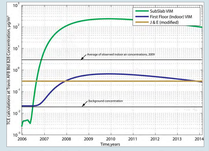



Figure 7. TCE Concentrations at Travis AFB Building 828

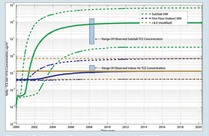



Figure 8. Monte Carlo predictions of TCE concentrations of sub-slab and indoor vapor concentrations at Building 1416 on Kelly AFB. (Note: The range of observed concentrations is shown by the blue patches.)

**Table 3**
**Summary of All Model Predictions:**
**Comparison of J&E[1] and ViM Indoor Air Predictions at CCAFS Deterministic Predictions of Indoor Air Concentrations, µg/m³**

| Source Generation Metric | Source | | | | | | 95 % Attenuation factor[3] | Average Indoor air concentration |
|---|---|---|---|---|---|---|---|---|
| | Sub-slab[2] | | Near-slab | | Groundwater | | | |
| | J&E | ViM | J&E | ViM | J&E | ViM | | |
| Arithmetic mean | 28 | 35 | 20.6 | 29 | 3 | 4.2 | 71 | 28 |
| Spatially averaged mean | 32 | 40 | 22.5 | 32 | 2.8 | 3.9 | 77 | 28 |
| Maximum value | 77 | 95 | 71.3 | 100 | 13.5 | 18.7 | 193 | 28 |
| UCL95 | 42 | 53 | 76 | 107 | 12.4 | 17.4 | 102 | 28 |

**Monte Carlo Predictions of Indoor air concentrations (5-50-95 percentiles), µg/m³**

| Source Generation Metric | Source | | | | | | 95 % Attenuation factor[3] | Average Indoor air concentration |
|---|---|---|---|---|---|---|---|---|
| | Sub-slab[2] | | Near-slab | | Groundwater | | | |
| | J&E | ViM | J&E | ViM | J&E | ViM | | |
| Arithmetic mean | 10-24-48 | 11-31-56 | 9-19-33 | 10-26-45 | 1.2-2.8-4.9 | 1.3-4.0-7 | 71 | 28 |
| Spatially averaged mean | 12-26-48 | 12-36-60 | 10-21-38 | 11-29-50 | 1.1-2.6-4.7 | 1.5-3.5-6.2 | 77 | 28 |
| Maximum value | 26-64-126 | 33-80-154 | 28-66-113 | 33-92-160 | 6-13-23 | 7-17-31 | 193 | 28 |
| UCL95 | 15-40-73 | 16-51-85 | 33-70-126 | 40-98-180 | 8-18-35 | 6-15-35 | 102 | 28 |

Notes:

1. The version of the J&E model used has been modified to accommodate a Monte Carlo analysis and to execute simultaneously with ViM.
2. Sub-slab simulations assume the soil vapor is directly beneath the slab, and not at depth.
3. The 95 percentile attenuation factor for all simulations is taken as 1.5e-3. These results should only be compared with predictions that use near-slab data as the source terms.

## 5. How ViM can Inform J&E

There are numerous ways ViM can inform J&E (Figure 9):

- Generate additional J&E output/predictions without changing the model
- Expand J&E's capabilities slightly but keep in Excel spreadsheet (don't destroy this convenient feature)
- Add some supplemental external calculations that help to interpret J&E results (but don't modify the model)
- Add a Monte Carlo technique to account for the range of predictions in terms of data uncertainties. While more data are needed to do this, plausible ranges will work (Figure 10)

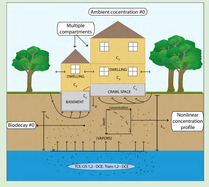



Figure 9. Examples of suggested enhancements to the J&E model.

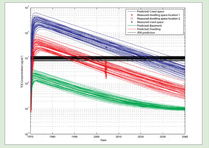



Figure 10. Black lines show how predictions of indoor air concentrations by the J&M model vary in a Monte Carlo framework.

## 6. Exposure Attenuation in Multi-Story Apartment Buildings

Vapor intrusion into multi-story apartment buildings, such as shown below in Figure 11, requires the use of a multi-compartment model to simulate the attenuation between floors. While the J&E model could simulate the entire building as a single-component, such an approach would tend to over estimate indoor vapor concentrations on the upper floors, and under-estimate indoor vapor concentrations on the lower floors.

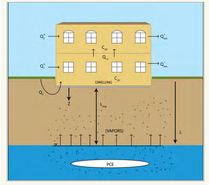



Figure 11. Conceptual model of two-story apartment over hypothetical PCE plume in groundwater.

To accommodate these multi-story apartments, part of the code used by ViM was extracted, simplified, and developed into mathematical formulas to predict attenuation between floors. The analysis focuses on what is happening inside the building.

The ratio of concentrations between the two floors is:

$$\frac{C_{d1}}{C_{d2}} = \frac{X_{d2} \cdot V_{d2}}{Q_{21}} \qquad (1)$$

In the ViM simulation, the following data were used:

$X_{d2}$ = 6/day (EPA's default value)

$V_{d2}$ = (100)(2.44) m3 (EPA's default value)

$Q_{21}$ = 180 m³/day

Therefore,

$$\frac{C_{d1}}{C_{d2}} = \frac{(6)(100)(2.44)}{180} = 8.1$$

, so the attenuation factor is 1/8.1 = 0.12

Where:

$\frac{C_{d1}}{C_{d2}}$ = concentration ratio between the first floor and second floor

Since the ratio is much less than unity, these results show that, in this case, it is not appropriate to treat the two floors as a single compartment.

The approach for estimating the attenuation factor between the first floor and second floor, Equation (1), is applicable to more than two stories if using the same assumptions as between the first and second stories. Without showing the steps, the attenuation factor between the first story and Nth floor is:

$$\frac{C_{d1}}{C_{dN}} = \prod_{i=2}^{N} \frac{X_{di} V_{di}}{Q_{i-1,i}} \qquad (2)$$

Where:

$\frac{C_{d1}}{C_{dN}}$ = concentration ratio between first and Nth floors (attenuation factor is inverse of this)

As an example of an application of Equation (2), use the same data as before for a four-story building:

$$\frac{C_{d1}}{C_{d4}} = (8.1)^3 = 530$$

, so the attenuation factor is 1/530

For this example, the first-floor concentration is 530 times greater than the concentration on the fourth floor, assuming all the assumptions made earlier are valid, and shows the need to represent a multi storied building by individual stories.

## 7. Using J&E and ViM Models Jointly to Develop Risk-based Groundwater Goals

Risk-based goals (RBGs) for groundwater were derived to be protective of onsite workers inhaling indoor air. The RBGs were calculated using modeling of vapor intrusion into the buildings using the J&E and ViM modeling approaches.

The Johnson and Ettinger model was first used to calculate preliminary RBGs for four COPCs: trichloroethene (TCE), tetrachloroethene (PCE), vinyl chloride, and benzene. Modeling was conducted using a unitary groundwater source term (i.e., a concentration of 1). Therefore, the following linear relationship was used to calculate RBGs based on the modeling results:

$$\text{Risk - based Goal}_{(gw)} =$$

$$\frac{\text{Risk-Based Concentration}_{(\text{indoor air})}}{\text{Predicted Concentration}_{(\text{indoor air})}}$$

$$\times \text{Unitary Source Term}_{(gw)}$$

ViM was used to refine the RBGs by addressing uncertainties in the input data.

### Johnson and Ettinger Modeling

The Johnson and Ettinger indoor air model calculates the intrusion and subsequent accumulation of contaminant vapors in buildings from subsurface groundwater assuming a steady-state condition. Input data to the Johnson and Ettinger model were primarily obtained from site characterization reports. An indoor air exchange rate of 1 exchange per hour was used instead of the EPA default of 0.25 exchanges per hour. The EPA default of 0.25 is based on residential buildings.

Indoor air RBCs were assumed to be the EPA Region 3 (2009) ambient air regional screening levels (RSLs) for workers. RBCs used in the evaluations were based on both the carcinogenic and non-carcinogenic effects of the four COPCs. The indoor air RBCs are divided by the indoor air concentrations predicted using the Johnson and Ettinger Model with a unitary source term in groundwater to calculate the groundwater RBGs.

### ViM Modeling

The ViM model was used to address uncertainties in the input data used in modeling of this site. For those input data required by both the Johnson and Ettinger model and the ViM model, they were specified to have the same values. ViM has embedded within it a version of the Johnson and Ettinger model (called JEM) that accepts input data from the same file as does ViM. This ensures that both models are using the same data, and that any differences between the two models are not due to data differences.

Figure 12 shows simulated results for both ViM and the JEM model for trichloroethene. The figure shows time-variable results because the ViM model is time-variable; however for this site we did not start with a time-variable source term and are therefore only concerned with the steady-state concentrations, once they are attained. As shown on the plot, the steady-state values of the JEM and ViM model are the same, confirming agreement of the input data between the two models.

ViM was run in Monte Carlo mode with a 10 percent variation in both directions for each input parameter's value. Two hundred Monte Carlo runs were executed to produce the results shown in Figure 13. This figure shows the results of the Monte Carlo analysis that have been processed to show the one percentile, 50 percentile and 95 percentile concentrations. The groundwater source term was set so that the 95 percentile indoor air concentration equaled the RBC. This process was repeated for the 1-50-99 percentiles, and the 0.1-50-99.9 percentiles. The alternative RBGs are shown in Table 3. This process was repeated for PCE, benzene, and vinyl chloride, whose RBGs for those percentiles are also shown in Table 4. As shown in the table, the RBGs calculated using ViM are 50 to 75 percent more restrictive than those predicted using the Johnson and Ettinger model.

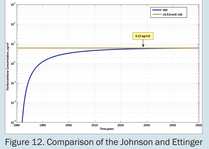



Figure 12. Comparison of the Johnson and Ettinger Model results with the ViM model for indoor air predictions. The models' source terms were chosen to predict the RBC for TCE (6.13 µg/m³)

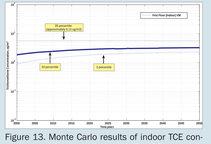



Figure 13. Monte Carlo results of indoor TCE concentrations predicted from ViM. The 95th percentile is set to be the RBC.

**Table 4**

| Percentile | Groundwater RBG (µg/L) | | | |
|---|---|---|---|---|
| | Trichloroethene | Tetrachloroethene | Vinyl chloride | Benzene |
| 95th | 4,800 | 920 | 650 | 3,200 |
| 99th | 4,200 | 800 | 550 | 1,900 |
| 99.9th | 4,000 | 750 | 500 | 1,800 |
| Johnson & Ettinger | 9,505 | 2,342 | 1,558 | 3,639 |

## 8. Air Exchange Rates (AERs): Informing J&E

AERs have an important influence on concentrations of indoor vapor that intrude from subsurface sources. For constant rates of intrusion, indoor air vapor concentrations are approximately inversely proportional to AERs, and exponentially proportional to instantaneous releases of vapor. EPA uses default AERs of 0.25/hr which is between the 10 to 50 percentile values from a study by Hers et al. (2001).

**Table 5**
**Air Exchange Rate at Study Results**

| Description | (per hour) | | |
|---|---|---|---|
| | 10% | 50% | 90% |
| 22 studies | 0.21 | 0.51 | 1.48 |
| Cold climate-winter | 0.11 | 0.27 | 0.71 |
| Warm climate-winter | 0.24 | 0.48 | 1.13 |
| **DoD study (slab-on-grade buildings)** | | | |
| Cape Canaveral AFS, HVAC off | 0.12-0.13 hr$^{-1}$ | | |
| Kelly AFB, vigorous air exchange | 1.1-1.5 hr$^{-1}$ | | |
| Travis AFB | 0.5-0.7/hr$^{-1}$ | | |
| Vandenberg AFB | 0.4-2.4/hr$^{-1}$ | | |

However, results from a recent DoD study indicates that such a default value was not representative of any of the four sites where studies were performed (see Table 5). At three of the four sites AERs were well above the default value (by up to 10 times), and at the remaining site, AERs were found to be lower than the default by a factor of two. Further at sites where wind speed is consistently variable over the course of a day, AERs will be variable as well. Figure 14 illustrates for Vandenberg AFB. Over the two day period AERs ranged from 0.4/hr to 2.4/hr$^{-1}$, a factor of 600%.

The figure shows the results of five methods developed as part of a DoD project. The different methods were developed to determine if cost-effective methods, based on helium releases, would be appropriate. The five methods are:

- Helium is released instantaneously and AER is calculated at multiple times, until detection limits have been reached
- $SF_6$ is released at a steady rate, and an estimate of AER is made once steady-state is attained.
- $SF_6$ is released at a steady-state, but it is not assumed that steady-state concentrations of $SF_6$ are attained.
- A least-squares method that uses the discrete helium concentrations to estimate AER
- A dynamic approach using Helium that does not assume that the AER remains constant.

While all of these methods give generally comparable results and can efficiently be used at different sites, it is important that the dynamic methods (dynamic helium approach, and dynamic $SF_6$ approach) give the best results here.

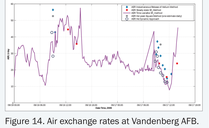



Figure 14. Air exchange rates at Vandenberg AFB.

## 9. Summary

The capabilities and site-specific application of two indoor air models (J&E and ViM) have been compared. Based on these comparisons several suggestions have been developed for the J&E model. Among the suggestions is that more output be generated by the model. Additionally, adding a Monte Carlo capability to J&E would be helpful in understanding variability and levels of confidence of model predictions.

## 10. References

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