

Air Emissions Modeling Advances for Oil and Gas Production Facilities

Barry L. Burr and Adam M. Georgeson
Bryan Research & Engineering, Inc.
Bryan, TX, USA

Kha Mach
Chesapeake Energy
Oklahoma City, OK, USA

ABSTRACT

Hydrocarbon processing systems and storage tanks are a significant source of volatile organic compound (VOC) emissions in the United States. Emissions rates from process units and tanks have historically been calculated individually for permit applications and at a single operating point once design engineering is complete. Now with EPA's new NSPS OOOO rule, operating companies must perform far more VOC emissions calculations than ever before to comply with increased reporting requirements. With more focus on the quantities emitted and possible control alternatives, there is more interest in using the emission calculation methods during the oil and gas production site design stage.

More sophisticated modeling systems using chemical process simulators permit more accurate emissions estimation over a wider range of conditions and configurations. Recent advances in simulation interface technology permit automation of these modeling tasks for more efficient enterprise-wide reporting.

INTRODUCTION

Oil, gas and process industries affect the atmosphere due to the quantity of emissions and types of chemicals emitted. Their environmental performance is becoming increasingly regulated by government agencies. Air emissions in the United States are regulated by the Environmental Protection Agency (EPA), often in conjunction with state or local agencies.

Coinciding with the rise in regulation and scrutiny of air emissions, there has been a rise in computer and simulation software performance. Such technology allows producers to create detailed emissions predictions using the best available scientific methods. It also allows permitting and reporting tasks to be executed with minimal economic burden and provides a framework for further engineering and optimization tasks.

This paper will describe recent advances toward automated methods for calculating both tank flash emissions and working, breathing, and loading loss emissions from oil and gas site storage tanks.

Types of Air Emissions

Due to the wide variety of industrial activities in the United States, there are many different classifications of air emissions. Let's take a look at the most common classifications affecting the upstream oil and gas sector:

- A hazardous air pollutant (HAP) is a chemical specifically designated by the EPA as having adverse human health or ecological impacts. At the time of the 1990 Clean Air Act, 187 chemicals were designated as hazardous, although additions and removals have been made.¹
- Volatile organic compounds (VOC) are defined as any carbon compound which participates in atmospheric photochemical reactions, unless the compound is excluded or specifically exempted. Excluded are carbon monoxide, carbon dioxide, carbonic acid, metallic carbides and ammonium carbonate. Methane and ethane are exempted along with a list of compounds in 40 CFR 51.100(s).²
- Benzene, toluene, ethyl-benzene and xylene (BTEX) are aromatic hydrocarbons classified both as VOCs and HAPs. These compounds make up a considerable fraction of the hydrocarbon produced from oil & gas wells, and thus are of concern to operating companies and environmental regulators alike.
- Greenhouse gases (GHG) are believed to contribute to climate change. Carbon dioxide is the most prevalent greenhouse gas, released from both process and combustion sources. Other common greenhouse gases include methane and nitrous oxide, which are

reported to have 21 and 310 times the global warming potential of carbon dioxide, respectively.³

- Nitrous oxides (NO_x) refer to a group of highly reactive gases including NO, NO₂ and N₂O, which are formed in high temperature combustion. Of this group, NO₂ is considered of the highest interest and tracked as an indicator for the larger group of nitrous oxides.⁴
- Sulfur dioxide (SO₂) is a toxic gas which also contributes to acid rain through a reaction with atmospheric water. Sulfur dioxide is a product when sulfur-rich fuels or process streams are burned.⁵ Particulate matter (PM) is a measure of the tiny solids suspended in the atmosphere with a size between 0.1 and 10 μm. The majority of particulates are naturally occurring, including mineral dust and sea salt. Industrial activity such as fuel combustion can contribute to particulate pollution.⁶
- Criteria pollutants are ozone, lead, carbon monoxide, nitrogen oxides, sulfur dioxide and particulate matter. They may be directly emitted or the product of atmospheric reactions. Criteria pollutants are the subject of national ambient air quality standards.⁷

Air emissions from a facility are categorized as point source or fugitive. Point source emissions come from a single, identifiable location such as a tank vent or exhaust stack. Point sources may be equipped with continuous emissions monitoring systems to measure pollutant type and rate at regular intervals. For the vast majority of point sources, pollutant type and rate are estimated with engineering calculations or process simulation. Fugitive emissions escape through valve packing, pump seals, flanges and the like; they are usually estimated on a plant-wide basis using emissions factors. For most of oil and gas production sites, continuous emissions monitoring is excessive. Operating companies typically develop their own mechanisms for meeting emission tracking requirements by EPA and state agencies. The development of such tracking mechanisms is discussed in this paper.

Oil and Condensate Tanks

Oil and condensate tanks at production sites are point sources and several types of emissions are estimated from this type of source. The primary emissions are atmospheric tank flash emissions which result when production liquids originally at their bubble point in a high pressure separator are transferred to a storage tank held at near atmospheric pressure. The change to new equilibrium conditions at a lower pressure usually vaporizes hydrocarbons which vent to the atmosphere or some emissions control system. Secondary types of VOC emissions which must be estimated are Working, Breathing, and Loading Losses produced from unsteady state operation of the atmospheric storage tank. The standard method for calculating these is defined in the EPA AP-42 specification⁸.

Usually these emissions are predicted for the purpose of obtaining construction and/or operating permits for a well-site from a state environmental regulatory agency. During this task, the

operating company through their own employees or environmental consultants prepare permit documents containing estimates of well-site emission. Storage tank VOC emissions are also predicted annually at each well-site for the purpose of compiling operating emissions inventories for all sites and segregated by geographical regions. For permitting, compliance demonstration, and inventory purposes, the short term emissions (lb/hr or lb/day of VOC), and the long term emissions (12 month rolling total of VOC emissions) are usually required by EPA, states and local agencies.

Also in recent years, the emission thresholds differentiating permit requirement levels have been dropping. This motivates operators to reduce emissions and also estimates of those emissions. Operators are using more accurate emissions calculation methods and tools which let them design well-site facilities with emissions reduction in mind.

Emissions may also be predicted for the purpose of implementing control methods such as vapor recovery compressors or flares. For this prediction, maximum instantaneous rates are used, rather than monthly or annual averages.

Finally, any hydrocarbon lost to the atmosphere is a hydrocarbon not available as a saleable product. Through adjustment of the well site equipment and pressure profile, the possibility exists to increase product rates.

All of these emissions calculating and reporting efforts incur considerable costs. Companies are always looking for better ways to streamline the work process while also providing high-quality and accurate estimates.

Technology Solutions

Several tools have been used for estimating VOC and other types of emissions. Nearly all jurisdictions allow use of process simulators that are based on Peng-Robinson or SRK equations of state when performing physical property and equilibrium flash calculations. Some less rigorous methods such as Vasques-Beggs Equation (VBE)⁹ or E&P Tank^{®10} are allowed and used in many cases.

Used in this study is ProMax^{®11}, the process simulator developed by Bryan Research and Engineering, which is one of the commercially available design-quality simulators employing both Peng-Robinson and SRK equation of state options.

CONVENTIONAL CALCULATION OF OIL AND GAS WELL SITE

Traditional Forward Calculation

The traditional method for calculating VOC emissions from oil or condensate tanks starts with sampling the liquid from the separator upstream of the atmospheric tank while it is still at separator pressure. The sample is sent to a laboratory for analysis by gas chromatograph while separator pressure and temperature are recorded along with storage tank temperature.

Process information is entered into a process simulation which then calculates the amount and composition of vapors generated upon equilibrium flash to atmospheric pressure at the measured tank temperature. From those vapors, the propane and heavier hydrocarbons are summed to yield the tank flash VOC emissions which are typically reported in tons per year.

From there, the residual atmospheric tank liquid product is used along with information about tank dimensions, paint color and quality, roof type, and location to calculate working and breathing losses using EPA's AP-42 methodology (and very similar to EPA Tanks 4.09d software). Working losses result from vapors being forced out of tank as the liquid level rises. When the level falls, unsaturated vapors enter which have new capacity for bringing VOC's out of the stored liquid. Breathing losses are similar except that they are the result of thermal expansion and contraction of the vapor space caused by diurnal temperature cycles. Loading losses are calculated based on the type of liquid unloading system and the efficiency of any emissions control system also according to AP-42's methodology¹²

A very typical example (Exercise 3 in the ProMax: Air Emissions Training Manual¹³, Marathon-Peacock Study¹⁴) for calculating a single storage tank is specified here along with the results from a ProMax simulation.

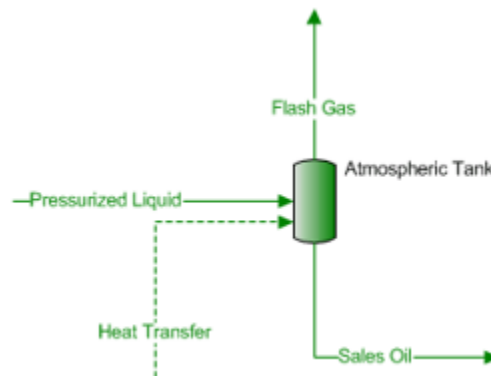


Figure 1. Simulation of atmospheric tank in ProMax

The Sales Oil flows at 188 bpd from a storage tank near Sioux Falls, SD where the atmospheric pressure is 13.98 psia and ambient temperature is 64.2°F. The Pressurized Liquid comes from a separator operating at 42 psig and 66 F. The tank data and dimensions are:

- Five tanks
- Diameter of 12 ft., height of 25 ft.
- Conical roof with a slope of 0.05
- Filled 50% on average, 90% on maximum
- Medium gray paint, good condition
- The vacuum breaker opens at -0.03 psig
- The breather opens at 0.03 psig

The following screenshot is the Working and Breathing Loss utility dialog window for this case.

The screenshot shows the 'Tank Losses.50' dialog window with the following parameters:

Property	Value	Units
Process Stream	Sales Oil	
Tank Geometry	Vertical Cylinder	
Shell Length	25	ft
Shell Diameter	12	ft
Number of Storage Tanks Employed	5	
Location	Sioux Falls, SD	
Annual Net Throughput	185.5	bbl/day
Include Non-VOC components in calculations?	<input type="checkbox"/>	
Maximum fraction fill of tank	90	%
Average fraction fill of tank	50	%
Material category	Heavy Crude	
Tank Color	Medium Grey	
Shell Paint Condition	Good	
Operating Pressure	0	psig
Breather Vent Pressure	0.03	psig
Breather Vacuum Pressure	-0.03	psig
Roof Type	Cone	
Radius of domed roof		ft
Slope of coned roof	0.05	
Roof Color	Medium Grey	
Roof Paint Condition	Good	

At the bottom left of the dialog, there is an 'Edit Source ...' button.

Figure 2. Tank Loss interface in ProMax

The pressurized liquid sample has the following composition where the C10+ material has a molecular weight of 262.7 lb/lb-mol and specific gravity of 0.87872.

Table 1. Pressurized Liquid Composition

Composition	Mol%
Methane	0.93
Ethane	2.59
Propane	5.46
i-Butane	1.33
n-Butane	6.22
i-Pentane	2.30
n-Pentane	4.15
2-Methylpentane	2.17
n-Hexane	2.26
2,2,4-Trimethylpentane	0.12
n-Heptane	10.04
n-Octane	8.92
n-Nonane	3.71
Benzene	0.28
Toluene	0.92
Ethylbenzene	0.33
p-Xylene	1.41
C ₁₀₊	46.86

The Peng-Robinson equation of state is used for this case. The C10+ component is configured as a Single Oil in the ProMax Oil Characterization utility which takes the molecular weight and specific gravity as input to create a pseudo-component representing the entire C10+ material.

An equilibrium flash of the above composition to 13.98 psia and 64.2 F produces 110.8 ton/yr of tank flash VOC emissions. ProMax has a Working and Breathing Losses utility provided in the ProMax Property Stencil. This utility incorporates the EPA AP-42 methodology in a very easy to use format that relieves the user from having to export intermediate results and running them in another program. The total working and breathing losses for this case are 12.65 ton/yr.

The pressurized liquid pressure and temperature are not necessary for computing the flash emissions but are useful for validating the results. A good check on the quality of the sampling and laboratory analysis is to compute the bubble point of the above composition at separator pressure and compare to the measured separator temperature. The two values should correspond well with one another. In this case, the pressurized liquid has a predicted bubble point of 67.4°F which compares very well to the measurement of 66°F.

This case is from the Marathon-Peacock Study¹⁴ which reports direct measurements of emissions from an oil or condensate storage tank. The table below shows ProMax results for tank flash emissions compared to direct measurements and several other emissions calculation methods. These results are from that study's case having 188 BPD of tank oil production.

Table 2. Flash Emissions from Several Calculation Methods

Flashing Losses Method	VOC (ton/yr)
V-B Flash	19
GOR Flash	23
Generic E&P Tank	34
Direct Measurement	94
ProMax Flash Only	111
E&P Tank Flash	236

ProMax' predicted VOC emissions are 18% higher than and considerably closer to direct measurements than any other method. A method that over-predicts emissions by too much (like E&P Tank) will place a significant portion of well sites into a more complex permitting category. Methods which typically under-predict emissions, if accepted by state agencies, will place more wells into the simpler permitting category. However, well sites are subject to operating inspection tests and compliance reporting. Permits based on gross under-predictions of VOC emissions may present considerable challenges to operators during compliance testing and reporting.

After the emissions results are obtained, they are manually compiled into a report. The steps must be repeated if the well conditions change, if the separator conditions change, or on an annual basis as required by law. The same steps must then be completed for each well site in the field.

RECENT DEVELOPMENTS IN EMISSIONS CALCULATIONS

The traditional method for calculating VOC emissions from a well site oil and condensate storage tanks requires permitting and compliance personnel to manually transfer data from databases or spreadsheets into calculation software such as E&P Tank and EPA Tanks 4.09 and then the results back to permit or compliance reports. This effort was tolerable so long as:

1. the number of wells to permit and pass compliance were manageable

2. there was little concern for optimizing the well-site design for VOC emissions minimization
3. measurements existed for pressurized liquid at current operating pressure.

With shale oil and gas booms, production companies now must contend with far more wells than in years past. Furthermore, these wells often run at production rates and separator pressures considerably different than when original measurements were taken.

Emissions thresholds for initiating more intensive permitting regimes have fallen in recent years. Operators have responded by designing additional equipment into well-sites which can substantially reduce tank flash VOC's. Some examples are heater-treaters, secondary low pressure separators, vapor recovery compressors, and flares. These intermediate separators work by driving off most of the traditional tank flash emissions at slightly above atmospheric pressure into a vapor recovery compressor and back to sales gas pipeline. The liquids leaving these intermediate separators have very low levels of VOCs that will flash at atmospheric tank conditions. These VOC-reducing additions to the well-site design not only put the well into a simpler permitting category, they recover valuable material into the sales gas which would have otherwise been lost to the atmosphere. They also have the benefit of not allowing air (containing oxygen) into the recovered vapors which would happen if the Vapor Recovery Unit (VRU) were applied directly to the atmospheric tank vent.

Case Study #1

Some major challenges for operating companies when entering a new production play are the lack of infrastructure and unstable oil and gas production forecast. To improve production forecast, reservoir engineers typically collect a few pressurized oil and gas samples at the inlet separator and request laboratories to perform a recombination of the oil and gas samples to obtain a full wellstream of a representative site in a new play (new formation). These recombination studies are also known as Pressure-Volume-Temperature (PVT) studies. Operating companies that do not want to spend effort and resources for PVT studies could take the same pressurized oil and gas samples and recombine using process simulation. Utilizing process simulation with oil and gas pressurized samples collected at the most upstream point and top-side point of the process can help operating companies solve different emission scenarios with minimal sampling effort and cost.

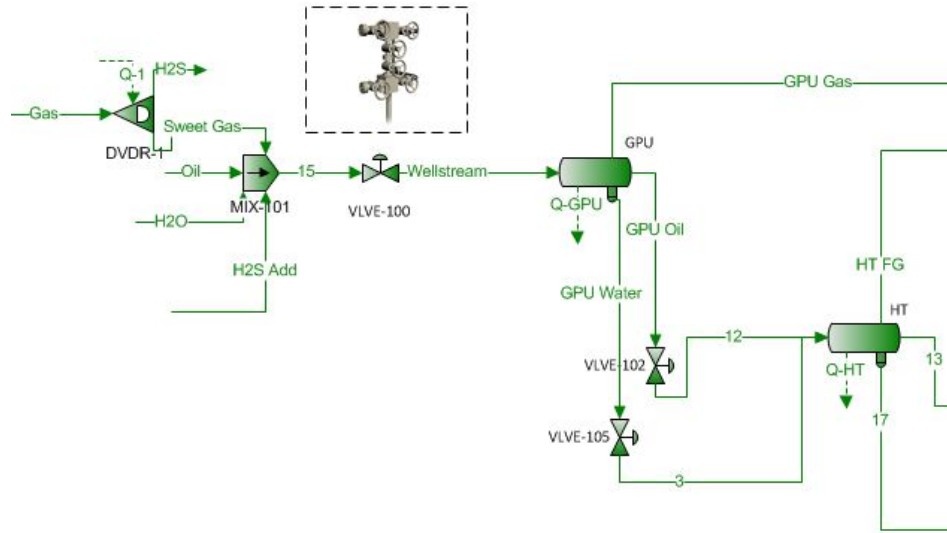


Figure 3. Partial Well Site Model

Recreate Wellstream Fluid by Mass Balance

Recombination of inlet stream compositions to match measured product rates for oil, gas, and water provides a wellstream inlet flow and composition suitable for evaluating cases at any operating condition or configuration for that well site. Creating this wellstream requires the sales gas composition and flow rate to be measured simultaneously with the pressurized liquid sample. However, knowledge of this wellstream can be applied to this well over many alternative or future operating conditions. The wellstream may also be applied to differently-operated well sites within the same formation or Play which greatly reduces sampling and analytical requirements.

To perform inlet stream recombination to create a wellstream, ProMax Simple Solvers are employed. These are calculators in the simulation which iteratively adjust one specification (such as an inlet stream flow rate) until another simulation property (such as one of the product stream flow rates) matches a target (such as that product stream's measured flow rate).

In order to recombine the gas and oil samples, temperature and pressure as well as gas/oil ratio at the inlet separator need to be recorded. After entering temperature, pressure, oil and gas composites in the inlet stream of the inlet separator, ProMax solvers for inlet gas, oil and water streams should be activated to simulate the 3 phase inlet separator. The rest of the surface facility should be set up as operated during the time the samples were collected. To run ProMax to simulate the wellstream fluid, tune the solvers in the inlet streams to drive oil/gas/water product streams of the process to match the recorded oil/gas and water production flows obtained during the sampling. The oil stream solver is presented below to tune the inlet oil stream flow rate to match the product measured flow rate of 1,000 bbl/d in the Oil_Loading stream (see the next two figures below).

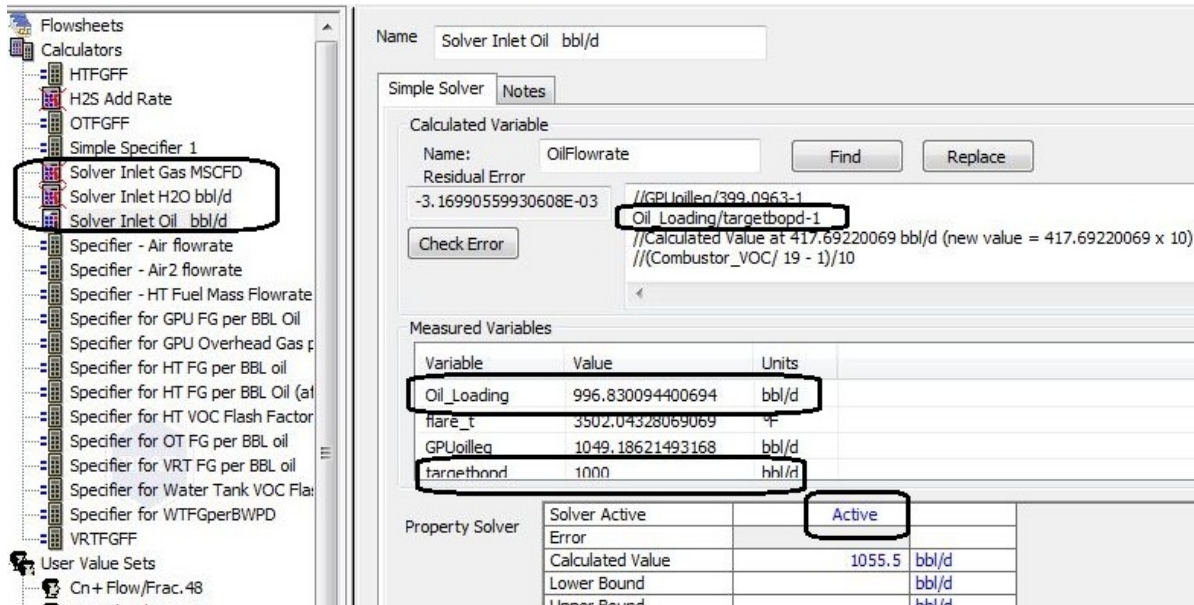


Figure 4. Solver Configuration for Wellstream Recombination

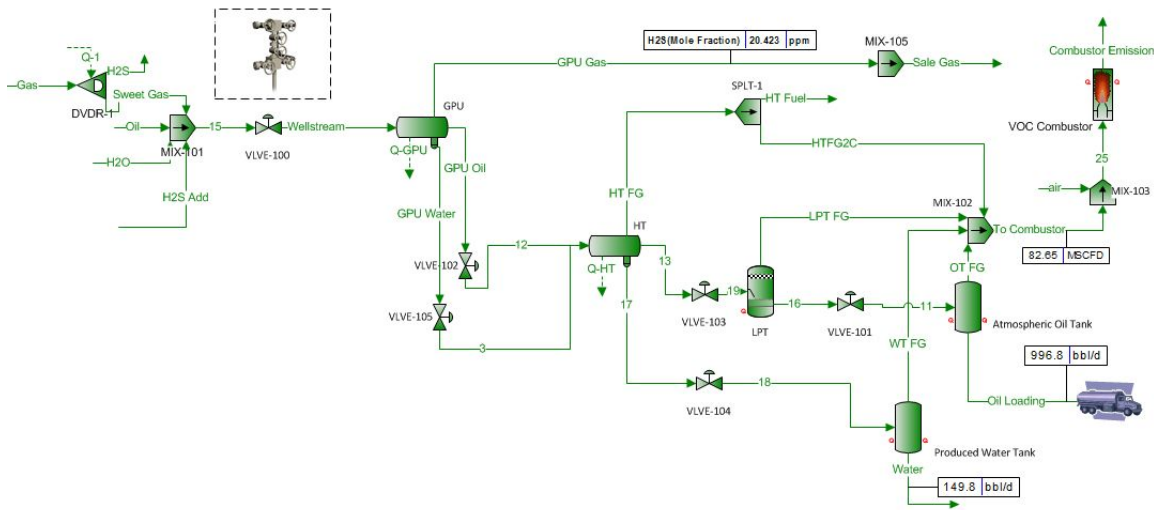


Figure 5. Full Well Site Model for Recreating Wellstream

The results of the simulated wellstream composition are comparable to the PVT wellstream provided by the laboratory. The maximum difference on a component-by-component basis between the laboratory results and the simulation is 2.7% as shown in Table 3. The simulation model can now be used to recreate or simulate wellhead streams to obtain appropriate wellhead compositions and GORs for different wells in the same formation. The model now provides more flexibility and prompt results.

Table 3. Accuracy of Wellstream Composition by Recombination

Composition (mol fraction)	PVT Wellstream	Simulated Wellstream	% Difference
Oxygen	0.0000	0.0000	--
Water	0.0000	0.0000	--
H2S	0.0330	0.0322	2.63
Nitrogen	0.1260	0.1249	0.89
Carbon Dioxide	0.4500	0.4454	1.03
Methane	34.1203	33.6889	1.28
Ethane	9.0621	8.9936	0.76
Propane	6.1961	6.1872	0.14
i-Butane	1.0330	1.0356	0.25
n-Butane	3.1970	3.2114	0.45
2,2-Dimethylpropane	0.0060	0.0061	2.30
i-Pentane	1.3390	1.3490	0.74
n-Pentane	1.9400	1.9555	0.79
2,2-Dimethylbutane	0.0140	0.0139	1.05
Cyclopentane	0.0110	0.0107	2.63
2,3-Dimethylbutane	0.1790	0.1811	1.16
2-Methylpentane	0.7210	0.7271	0.84
3-Methylpentane	0.4180	0.4226	1.09
n-Hexane	1.2010	1.2127	0.97
Methylcyclopentane	0.4350	0.4399	1.11
Benzene	0.1870	0.1887	0.88
Cyclohexane	0.4330	0.4370	0.92
2-Methylhexane	0.3140	0.3169	0.92
3-Methylhexane	0.3990	0.4032	1.04
2,2,4-Trimethylpentane	0.0010	0.0000	--
n-Heptane	1.6540	1.6711	1.03
Methylcyclohexane	0.7560	0.7645	1.11
Toluene	0.4550	0.4597	1.03
n-Octane	2.7250	2.7556	1.11
Ethylbenzene	0.2480	0.2505	1.00
m-Xylene	0.2970	0.3001	1.02
o-Xylene	0.1890	0.1917	1.39
n-Nonane	2.7780	2.8088	1.10
n-Decane	3.1720	3.2076	1.11
pseudoC11	2.6660	2.6964	1.13
pseudoC12	2.2600	2.2862	1.15
pseudoC13	2.2250	2.2508	1.15
pseudoC14	1.9070	1.9286	1.12
pseudoC15	1.8070	1.8275	1.12
pseudoC16	1.4220	1.4379	1.10
pseudoC17	1.2760	1.2905	1.12
pseudoC18	1.1990	1.2122	1.09
pseudoC19	1.1780	1.1917	1.15
pseudoC20	0.9350	0.9455	1.11
pseudoC21	0.8360	0.8455	1.12
pseudoC22	0.7700	0.7792	1.18
pseudoC23	0.6700	0.6781	1.19
pseudoC24	0.6130	0.6193	1.01
pseudoC25	0.5620	0.5684	1.13
pseudoC26	0.5470	0.5536	1.19
pseudoC27	0.5190	0.5250	1.14
pseudoC28	0.5070	0.5124	1.06
pseudoC29	0.4270	0.4313	1.00
pseudoC30	0.4370	0.4422	1.17
pseudoC31+	3.1470	3.1831	1.13

Re-evaluate the system at different separator pressures:

With the full wellstream simulated, the operating company has a good estimate of the expected oil and gas production for a similar well in the same formation. A major challenge for a developing area are the frequent changes in sales gas pipeline pressure available due to the midstream company implementing various compressor stations to meet the gas gathering demand. A fluctuating sales line pressure causes differences in inlet separator pressures at the production sites. Demonstrating air emission compliance in the face of such operational swings is the main reason to re-evaluate the surface facility by simulating at different separator pressures.

Prior to adjusting the inlet separator pressures, the three original inlet flow solvers in the ProMax model should be deactivated to preserve the wellstream compositions as the down-hole fluid composition presumably stays while operators physically adjust the wellhead choke valve only for pressure variation. At an oil and gas production pad, the sale of oil and gas is documented using gas meter and an oil run ticket. The emission calculation concept presented here is to develop the flash factors tied to the available production data that all operating companies would record and maintain. Flash factors at each unit operation are defined in term of pounds of VOC emission from the overhead stream per barrel of oil produced at the stock tank. These flash factors hold to a tight range as long as operating conditions downstream of the inlet separator are unchanged. However, changes in separator conditions or settings will change the flash factors and these changes can be captured by the ProMax model. The Scenario Tool within ProMax helps automate the runs as the inlet separator pressures are varied. More details about the Scenario Tool are contained in Case Study #2. The result of several flash factors at each unit operation versus the inlet separator pressures are tabulated below.

Table 4. Flash Factors of Different Unit Operations at a Well Site as Varying Inlet Separator Pressures

Separator Pressure (psig)	GPU Flash (lb/bbl)	HT Flash(lb/bbl)	LPT Flash (lb/bbl)	OT Flash (lb/bbl)	WT Flash (lb/bbl)
1000	8.729	33.497	1.534	0.776	0.010
950	9.056	32.578	1.608	0.814	0.011
900	9.411	31.617	1.687	0.854	0.011
850	9.800	30.610	1.772	0.897	0.011
800	10.227	29.549	1.864	0.942	0.011
750	10.699	28.429	1.962	0.990	0.011
700	11.227	27.239	2.068	1.040	0.012
650	11.820	25.971	2.182	1.092	0.012
600	12.492	24.611	2.303	1.147	0.012
550	13.261	23.146	2.433	1.203	0.012
500	14.149	21.558	2.569	1.261	0.013
450	15.187	19.827	2.710	1.320	0.013
400	16.415	17.931	2.853	1.377	0.013
350	17.892	15.843	2.991	1.431	0.013
300	19.702	13.536	3.110	1.476	0.013
250	21.973	10.991	3.185	1.502	0.014
200	24.922	8.212	3.167	1.493	0.014
150	28.943	5.279	2.956	1.408	0.013
100	34.917	2.465	2.363	1.159	0.012
50	45.607	0.447	1.195	0.588	0.009

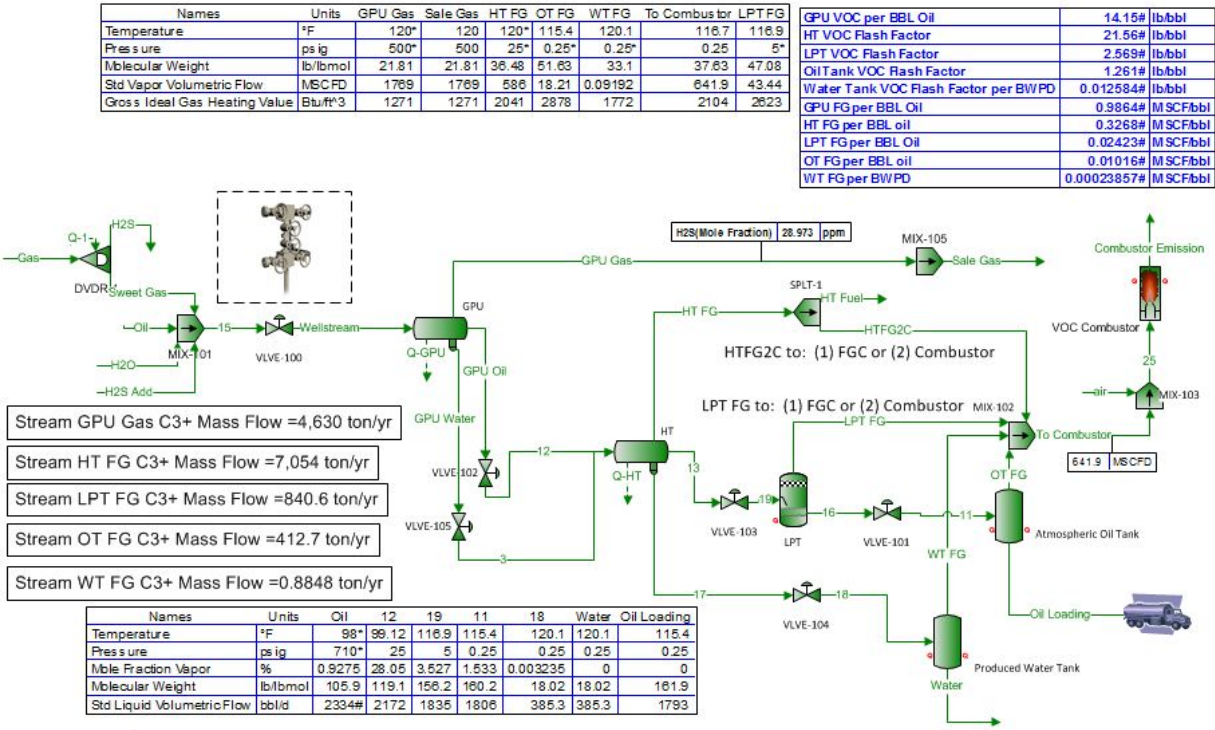


Figure 6. Wellsite Model with Flash Factors at 500 psig Gas Production Unit (GPU)

Multiple samples in an area or a shale formation can be run using this same ProMax model so long as the wells are drawn from the same reservoir to produce similar wellstream composition. A library of flash factors can be loaded into a company-built data base or environmental management system (EMS) for emission tracking or permitting purposes. As inlet pressures change from time to time, an appropriate set of flash factors can be selected. The selection of flash factors can be automated with the automatic oil and gas production reading such that as soon as the SCADA system picks up a new pressure reading at a remote production site, the compliance officer can immediately update the 12-month rolling total emissions or can quantify the emissions from an event. The collection of flash factors will also speed up the permitting process as well as other periodic reporting requirements.

Case Study #2

In this case study, we discuss a technique for automatically calculating emissions for numerous well sites using a single model linked to an Excel spreadsheet filled with well-site data. Installed with ProMax is an Excel Add-in called the Scenario Tool which manages the transfer of input and output data between ProMax and Excel along with executing the ProMax simulation for each case. Due in no small part to requests from ProMax users involved in calculating VOC emissions, the Scenario Tool has been enhanced with some unique capabilities such as:

- Importing properties like specific gravity and molecular weight (often used to characterize C10+ component in oil and gas analyses) from Excel into ProMax to define ProMax Single Oils
- Transferring Working, Breathing, and Loading tool properties even including text selections like Geographic Location or Tank Type
- Producing custom Excel Report files separate from the Excel workbook containing the data
- Producing ProMax project files for each case within a Scenario

There are two objectives for this study. First, all of the well-sites are to have their emissions calculated and stored in Excel. The well-site emissions will be summed to generate a total area inventory for VOC emissions. The second objective is to generate a distinct emissions report for each well-site during the course of automatically running the simulations.

These calculations must be performed each year. Well conditions vary from year to year bringing the need to calculate emissions for all wells each year. Usually, the reservoir composition is assumed to remain constant, so well test data can be used as the basis for calculation subsequent year emissions rates. Sales gas and oil production rates vary from year to year and are inputs. Just as in Case Study #1, the ProMax model shown below contains calculators (Simple Solvers) which adjust the inlet oil, gas, and water stream flow rates so that the simulated sales gas, produced oil, and produced oil rates match the observed values for a given year.

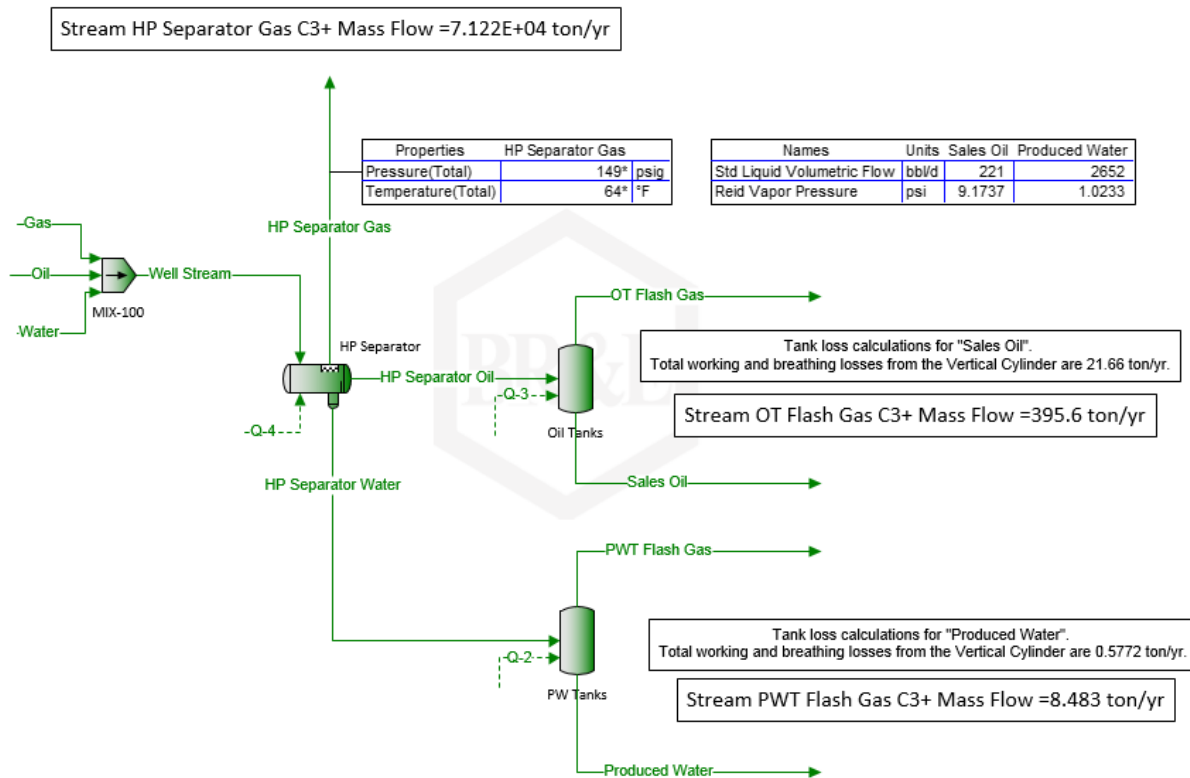


Figure 7. Complete Well Site Model in ProMax

We start with an Excel workbook containing all data required to calculate emissions for each well site. In this case, an Excel column will contain all data for a single well. The first segment shown in Table 5 is the composition of oil sampled from the high pressure separator during a well test for four different wells. Tables 6-9 also have four data columns each which refer to these same four wells respectively.

Note the C10+ component at the bottom of the component list which was created from the ProMax Oil characterization utility as a Single Oil and added to the component list. This C10+ component generally comprises a large amount of oil compositions but the properties of this C10+ fraction vary significantly from well to well. A Single Oil can be defined by supplying a Specific Gravity and Molecular Weight and these properties are usually available in oil analyses. It is an important, and perhaps unique, capability of ProMax' Scenario Tool that it can change a Single Oil's Specific Gravity and Molecular Weight for each case in the Scenario.

Table 5. Process Data Input Spreadsheet

INPUT VALUES	1	2	3	4
Facility ID	Zachry	Polo Field	Bizzell	Duncan Field
Representative Station Name	Coryatt 2H	Teichelman 2H	Corrington 2H	Wallace 2H
Oil Sample Information				
C10+ Molecular Weight	174.28	174.28	174.28	174.28
C10+ Specific Gravity	0.791	0.791	0.791	0.791
Oil to Separator - Component (mol%)				
Water	0	0	0	0
H2S	0	0	0	0
Nitrogen	0.17	0.17	0.17	0.17
Carbon Dioxide	0.03	0.03	0.03	0.03
Methane	7.44	7.44	7.44	7.44
Ethane	4.37	4.37	4.37	4.37
Propane	3.32	3.32	3.32	3.32
Isobutane	1.01	1.01	1.01	1.01
n-Butane	3.18	3.18	3.18	3.18
Isopentane	2.1	2.1	2.1	2.1
n-Pentane	3.03	3.03	3.03	3.03
2-Methylpentane	1.83	1.83	1.83	1.83
3-Methylpentane	1.23	1.23	1.23	1.23
n-Hexane	4.01	4.01	4.01	4.01
Methylcyclopentane	0.59	0.59	0.59	0.59
Benzene	2.23	2.23	2.23	2.23
2-Methylhexane	0.48	0.48	0.48	0.48
3-Methylhexane	1.97	1.97	1.97	1.97
Heptane	5.59	5.59	5.59	5.59
Methylcyclohexane	2.84	2.84	2.84	2.84
Toluene	0.62	0.62	0.62	0.62
Octane	11.57	11.57	11.57	11.57
Ethylbenzene	2.19	2.19	2.19	2.19
m-Xylene	2.35	2.35	2.35	2.35
o-Xylene	0.04	0.04	0.04	0.04
Nonane	7.3	7.3	7.3	7.3
C10+	30.52	30.52	30.52	30.52

Appearing next is the composition of the gas from the same test. Note that even though some components are not present in the gas composition, there are storage locations for all of the same components that are present in the oil. It is important to maintain consistent component lists when employing simulation. The simulation streams all use the same composition set defined in the flowsheet environment. It is important to match the Excel-side compositions to the same component list and order as exists within the simulation.

Table 6. Process Data Input Spreadsheet (continued)

Gas to Separator - Component (mol%)				
Water	0	0	0	0
H2S	0	0	0	0
Nitrogen	0.67	0.67	0.67	0.67
Carbon Dioxide	0.17	0.17	0.17	0.17
Methane	79.1	79.1	79.1	79.1
Ethane	13.42	13.42	13.42	13.42
Propane	4.43	4.43	4.43	4.43
Isobutane	0.49	0.49	0.49	0.49
n-Butane	0.99	0.99	0.99	0.99
Isopentane	0.26	0.26	0.26	0.26
n-Pentane	0.27	0.27	0.27	0.27
2-Methylpentane	0.06	0.06	0.06	0.06
3-Methylpentane	0.03	0.03	0.03	0.03
n-Hexane	0.07	0.07	0.07	0.07
Methylcyclopentane	0.01	0.01	0.01	0.01
Benzene	0	0	0	0
2-Methylhexane	0	0	0	0
3-Methylhexane	0.01	0.01	0.01	0.01
Heptane	0.01	0.01	0.01	0.01
Methylcyclohexane	0	0	0	0
Toluene	0	0	0	0
Octane	0	0	0	0
Ethylbenzene	0	0	0	0
m-Xylene	0	0	0	0
o-Xylene	0	0	0	0
Nonane	0	0	0	0
C10+	0	0	0	0

The remaining process inputs are the HP Separator pressure and temperature, oil rate, gas rate, water rate, and then tank parameters. There are many more possible tank parameters as displayed in Figure 2 but in this case the only parameters which vary among these wells are the ones shown below. The fixed specifications here are:

- Tank Geometry = Vertical Cylinder
- Location = Charleston, WV
- Material Category = Light Organics
- Tank and Roof Color/Condition = Dark Green/Good
- Roof Type = Cone with 0.0625 slope
- Cargo Carrier = Tank Truck or Rail Tank Car
- Submerged Loading with Dedicated Normal Service
- Overall Reduction Efficiency = 0%

Table 7. Data Input Spreadsheet for Tank Parameters

Tank Parameters				
Oil				
Number of Tanks	8	6	6	6
Shell Height (ft)	20	20	20	20
Shell Diameter (ft)	12	12	12	12
Oil Production Rate (bbl/day)	200	150	75	75
Water				
Number of Tanks	2	2	2	2
Shell Height (ft)	20	20	20	20
Shell Diameter (ft)	12	12	12	12
Produced Water throughput (bbl/day)	660	660	660	660
Operating Parameters				
HP Separator Pressure (psig)	130.74	136.764	127.424	126.834
HP Separator Temperature (F)	72.74	67.3	77.17	69.29
Solver Inputs				
HP Separator H2S Concentration (ppm)	0	0	0	0
Oil Production Rate (bbl/day)	200	150	75	75
Produced Water throughput (bbl/day)	660	660	660	660
Gas throughput (Mscfd)	3977	5510	3860	5657

The flow rate specifications are directed to user values (or custom data storage properties) within ProMax. These become target flow rates in solvers which adjust the flow rates of each feed type (oil, gas, and water) entering the separator. In this way, the measured product flows are achieved and the liquid leaving the separator is at its bubble point.

After supplying input specifications to Excel, this information is tied to respective model properties using the ProMax Scenario Tool. In the Scenario Tool main dialog window, there are selection boxes to select the simulation file to run scenarios against and another for selecting the scenario definition to run. Then follows a section for ProMax Inputs (links for transferring Excel data into the model) and ProMax Outputs (for model to Excel transfer). Each item in these two windows defines a linkage between an Excel range and a ProMax property.

Once the linkages are configured, the Scenario Tool can be run from a starting case to an ending case as set by the user (cases 1 to 95 in the figure below). The Scenario operates by first transferring Excel values into ProMax properties according to the linkages in ProMax Inputs. Next the Scenario Tool executes the ProMax simulation case. After the run completes, values from ProMax stream, block, analyses, system or other properties are transferred into Excel destination cells according to the defined linkages in ProMax Outputs. A very large number of cases can be run at one time with desired results being placed into Excel for later tabulation or graphing.

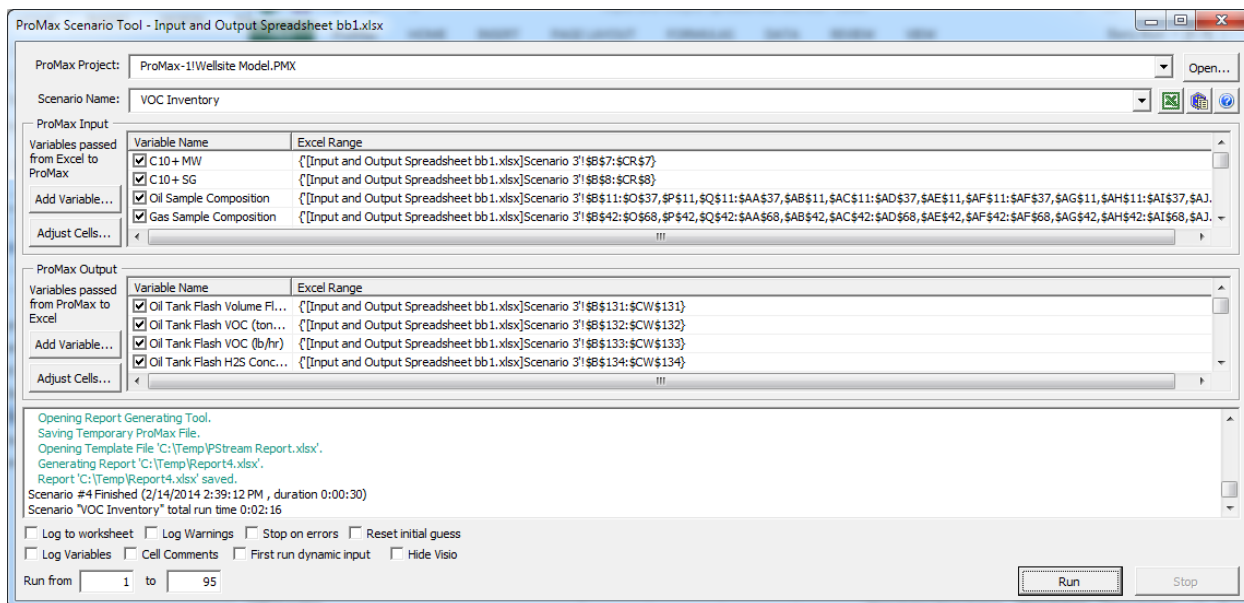


Figure 8. ProMax Scenario Tool – Primary Dialog Window

For the first four well site cases, results in Excel are shown here for flashing, working, breathing, and loading losses from the Oil Tank. Reported, but not shown are speciated compositions of the loss streams and water tank flashing losses,

Table 8. Oil Tank Flash Gas Emissions

Oil Tank Flash Gas				
Std Vapor Volumetric Flow (scf/hr)	792.0429	692.1550	591.9018	491.9295
Flash Loss (ton/yr) (only includes VOC)	230.3656	201.3289	172.1539	143.0326
Flash Loss (lb/hr) (only includes VOC)	52.5949	45.9655	39.3045	32.6558

Table 9. Oil Tank Working, Breathing, and Loading Loss Emissions

Oil Tank Losses					
Oil Tank Working Loss per Tank (ton/yr) (includes non VOC)	1.2412	1.0863	0.9307	0.7756	1.9368
Oil Tank Breathing Loss per Tank (ton/yr)(includes non VOC)	2.2024	2.2035	2.2043	2.2049	2.1964
Oil Tank Total w/B Tank Losses ALL Tanks (ton/yr) (includes non VOC)	27.5493	26.3181	25.0807	23.8436	33.0653
Total Loading Losses (ton/yr) (includes non VOC)	6.2791	5.4953	4.7086	3.9237	9.7969

After all cases are run for each well site (one well per column) the various VOC loss types can be added to produce the inventory.

In addition to the emission totals, there has been interest in user-defined or custom reports for each case or well-site showing input specifications and emissions results. The ProMax Scenario

Tool has a very interesting capability for generating such reports at the end of each case's calculation and then uniquely creating and storing report output files. This report contains the particular results for a case or well site arranged in the format of the User Defined Template. Additional properties help to make the resulting reports more appealing such as the Client Name, Location, and Job properties. The append option can be specified so as to add the report as a flowsheet in the previously-created workbook if desired.

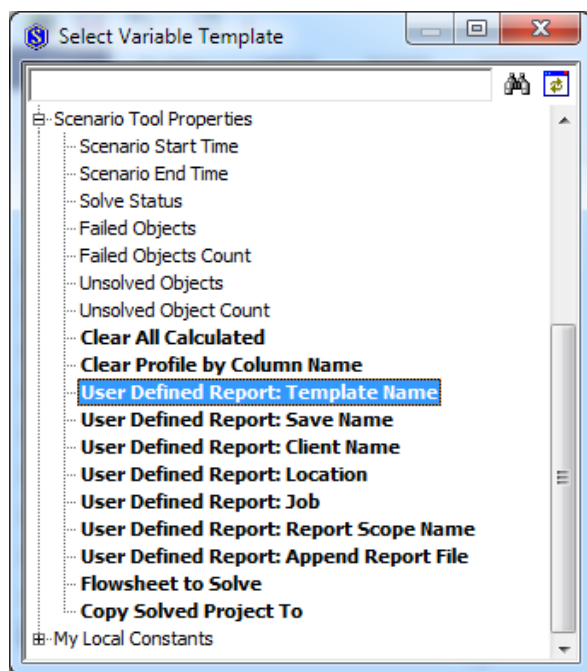


Figure 9. Scenario Tool Properties Available for Transfer Between ProMax and Excel

CONCLUSION

Recent changes in air quality regulations have greatly increased the number of VOC and other emission calculations from oil and gas production sites. Reduction of permitting thresholds has increased operators' incentive to obtain more accurate estimates and to design well sites for minimum emissions. The emissions calculations required for companies can number many thousand per year. The traditional method of manually entering data into simulation tool dialogs and manually entering results into other reports is now too cumbersome. It is now necessary to automate the estimation of large numbers of well-site emissions while simultaneously improving accuracy.

Design-quality process simulators are shown to address these needs with only little customization required by the particular air quality field as applied to oil and gas processing. By adding the EPA AP-42 routines for computing Working, Breathing, and Loading Losses, the

work that was typically handled in two programs collapses to a single one. The Scenario Tool in ProMax is well-suited for processing large numbers of well-site case data stored in Excel and then generating emissions totals and even custom emissions reports. For managing multiple well sites producing the same Play, a simulation design based on a wellstream fluid composition rather yields a simple emission factor model from which environmental group users can easily multiply by individual well site production rates to estimate emissions.

The cases mentioned here are some of the more sophisticated recent developments in this area of providing well site emissions estimates. Much development is in progress at several companies so it is certain that even more effective work processes will be available soon. In any event, design-quality process simulators are likely to be integral to these new developments.

ACKNOWLEDGEMENTS

The authors wish to express their appreciation to Ashley Hull of Bryan Research & Engineering, Inc. for his extremely dedicated work to develop and enhance the Working and Breathing Losses Utility and the Scenario Tool.

REFERENCES CITED

1. US EPA, *Air Toxics Web Site: Rules and Implementation*, April 2011
2. US EPA, *Definition of Volatile Organic Compounds (VOC)*, March 2009
3. US EPA, *Greenhouse Gas Emissions*, April 2011
4. US EPA, *Nitrogen Dioxide*, October 2010
5. US EPA, *Sulfur Dioxide*, March 2011
6. US EPA, *Particulate Matter*, March 2011
7. US EPA, *Six Common Air Pollutants*, July 2010
8. Compilation of Air Pollutant Emission Factors, AP-42, Section 7.1: Organic Liquid Storage Tanks, U.S. Environmental Protection Agency, Research Triangle Park, NC, September 1997
9. Vasquez, M.E. and H.D. Beggs, "Correlations for Fluid Physical Property Prediction", *Journal of Petroleum Technology*, March 1980

10. E&P Tank (Version 2.0), Process Simulation Software, American Petroleum Institute, 1999
11. ProMax 3.2.13330, Process Simulation Software, Bryan Research & Engineering, Inc, Bryan, Texas, November, 2013
12. Michaelson, N.R. and K. Malmquist, "Benefits of Process Modeling Software for Estimating Upstream Oil & Gas Air Emissions", *Proceedings of the 106th Air & Waste Management Association Annual Conference and Exhibition*, Chicago, IL, June, 2013
13. ProMax: Air Emissions, Training Course Manual, Bryan Research & Engineering, Inc., December, 2013
14. Peacock, P., "Bakken Oil Storage Tank Emission Models", *Presented at the Bakken VOC Emission Control Solution Session*, Bismarck, ND, 2010