Web-based toxic gas dispersion model for Shuttle launch operations

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ABSTRACT

During the launch of the Space Shuttle vehicle, the burning of liquid hydrogen fuel with liquid oxygen at extreme high temperatures inside the three space shuttle main engines, and the burning of the solid propellant mixture of ammonium perchlorate oxidizer, aluminum fuel, iron oxide catalyst, polymer binder, and epoxy curing agent in the two solid rocket boosters result in the formation of a large cloud of hot, buoyant toxic exhaust gases near the ground level which subsequently rises and entrains into ambient air until the temperature and density of the cloud reaches an approximate equilibrium with ambient conditions. In this paper, toxic gas dispersion for various gases are simulated over the web for varying environmental conditions which is provided by rawinsonde data. The model simulates chemical concentration at ground level up to 10 miles (1 KM grids) in downrange up to an hour after launch. The ambient concentration of the gas dispersion and the deposition of toxic particles are used as inputs for a human health risk assessment model. The advantage of the present model is the accessibility and dissemination of model results to other NASA centers over the web. The model can be remotely operated and various scenarios can be analyzed.

Keywords: Toxic gas dispersion, Shuttle Launch, Virtual test bed, Modeling and Simulation

1. INTRODUCTION

NASA, particularly Marshall Space Flight Center (MSFC), has pursued the development of computerized atmospheric dispersion models for predicting the behavior of rocket exhaust clouds in the troposphere since the mid 1960's.\textsuperscript{1} These models are used to assess the environmental impact of exhaust products from rocket engines with respect to air quality standards, toxicity thresholds and potential bio-ecological effects and to evaluate requirements, if any, for launch constraints. In 1973, a joint program for rocket exhaust prediction and launch monitoring was initiated by NASA for all Titan launches from Kennedy Space Center (KSC). Now for all launches, the gas dispersion model provides a ground concentration prediction which will be validated against a database for Go/No-go decision.

Meteorological conditions at the time of launch are a critical factor in the behavior of rocket exhaust buoyant cloud rise and subsequent downwind transport and diffusion. The rocket engines also leave an exhaust trail from normal launches, which extends throughout the depth of the troposphere and beyond. The most important factor is the vertical temperature profile of the lower atmosphere, followed in importance by the wind speed and direction vertical profiles. As with the classical air pollution meteorology, the presence of stable air layers determines whether or not emissions will get trapped near the ground surface or will mix through a deeper, well-ventilated air volume. The presence of temperature inversion and its proximity to the thermally stabilized rocket exhaust cloud are significant parameters affecting ground level concentrations of rocket exhaust gases. The model uses a generalized concept of multilayer Gaussian dispersion approach which is outlined in the next section.

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2. GAUSSIAN DISPERSION MODEL

The generalized gaussian dispersion equation for a continuous point source plume,

\[ C = \frac{Q}{2u\sigma_x \sigma_y} e^{-y^2/(2\sigma_y^2)} \left[ e^{-(x-H)^2/(2\sigma_x^2)} + e^{-(x+H)^2/(2\sigma_x^2)} \right] \]

where \( C \) = concentration of emission \( g/m^3 \) at any receptor located at \( x \) meters downwind; \( y \) meters crosswind from the centerline and \( z \) meters above ground. \( Q \) is the source emission rate \( g/sec \), and \( u \) is the horizontal velocity expressed in \( m/sec \). \( H \) is the plume centerline height above ground in meters. \( \sigma_x \) and \( \sigma_y \) are vertical and horizontal standard deviations of the emission distribution. Equation (1) represents the constant emissions of gases from a fixed stack. In this model, a single average wind speed and wind direction is used, where as in our model, the exhaust cloud column is partitioned into disks of cloud material that correspond to layers of the atmosphere defined from rawinsonde sounding measurements. In our model, the exhaust material is assumed to be uniformly distributed in the vertical and to have a bivariate Gaussian distribution in the plane of the horizon at the point of cloud stabilization. The dosage and concentration formulas are written in a rectangular coordinate system with the origin at the ground beneath the cloud stabilization point in the \( K^{th} \) layer. The \( x \)-axis is directed along the axis of the mean wind direction in the \( L^{th} \) layer and the \( y \)-axis is directed crosswind or perpendicular to the mean wind direction. The origin of the coordinate system is at the launch pad.

![Diagram](image)

**Figure 1.** Schematic diagram of algorithms involved in the Toxic Gas Dispersion Model.

Figure (1) shows a schematic flow chart of the major components of toxic gas dispersion computation. Rawinsonde data provides vertical profiles of wind direction, wind speed, air temperature, atmospheric pressure and dew point or relative humidity between the earth's surface and 3000 m. Rawinsonde measurements are performed routinely at scheduled times throughout the pre-launch countdown and after the launch has taken place. The rawinsonde data can be manually edited to reflect any projected weather forecasting. The Wind System is a series of 30-m towers located throughout Kennedy Space Center and one 152-m tower instrumented to measure wind direction, wind speed, turbulence and air temperature. Depending upon the type of rocket, fuel, and type of launch, the rising cloud will be defined.

2.1. Launch Types

There are two types of launches viz., normal and abnormal (launch failures). For a normal launch, the assumption is made that all engines operate normally. In the case of a launch failure (single engine burn on pad), one solid
engine of the Space Shuttle, Titan III and Delta vehicles is assumed to fail to ignite, causing the vehicle to remain on hold-down configuration while the other solid engine is assumed to ignite and burn with the pad deluge system operating normally. In the other failure mode (slow burn on pad), an on-pad explosion is assumed to rupture the casings of the solid engines, scattering solid propellant over the area in the vicinity of the launch pad.

2.2. Fuel Expenditure

The fuel expenditure rates for normal launches are obtained by averaging the fuel expenditure rates for the engines over the approximate period from lift-off until the vehicle is about 3000m above the surface. The fuel expenditure rates for the single engine burn are an average of the normal firing period of the engine. For the slow burn, the rates are an average over the estimated total burn time of the scattered propellants. Table (1) provides the effective fuel heat contents, which are used in calculating buoyant cloud rise for normal launches and plume rise for launch failures, including the effects of heat produced by after burning as well as heat losses due to radiation.¹

Table 1. Fuel Expenditure and Heat Content.

<table>
<thead>
<tr>
<th>Property</th>
<th>Space Shuttle</th>
<th>Titan III</th>
<th>Delta 2914</th>
<th>Delta 3914</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal Launch</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fuel Expenditure Rates W (gs⁻¹)</td>
<td>1.5219 × 10⁷</td>
<td>5.4375 × 10⁶</td>
<td>8.3607 × 10⁵</td>
<td>1.0576 × 10⁶</td>
</tr>
<tr>
<td>Effective Fuel Heat Content H (calg⁻¹)</td>
<td>1479.1</td>
<td>2021.1</td>
<td>1766.0</td>
<td>1449.9</td>
</tr>
<tr>
<td>Single Engine Burn</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fuel Expenditure Rates W (gs⁻¹)</td>
<td>3.8451 × 10⁶</td>
<td>2.1788 × 10⁶</td>
<td>Not Available</td>
<td>Not Available</td>
</tr>
<tr>
<td>Effective Fuel Heat Content H (calg⁻¹)</td>
<td>1062.4</td>
<td>1010.6</td>
<td>Not Available</td>
<td>Not Available</td>
</tr>
<tr>
<td>Burn Time t_B (s)</td>
<td>132.0</td>
<td>60.0</td>
<td>Not Available</td>
<td>Not Available</td>
</tr>
<tr>
<td>Slow Burn</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fuel Expenditure Rates W (gs⁻¹)</td>
<td>9.8873 × 10⁵</td>
<td>1.3594 × 10⁶</td>
<td>2.729 × 10⁵</td>
<td>3.7073 × 10⁵</td>
</tr>
<tr>
<td>Effective Fuel Heat Content H (calg⁻¹)</td>
<td>1000.0</td>
<td>1000.0</td>
<td>690.0</td>
<td>411.2</td>
</tr>
<tr>
<td>Burn Time t_B (s)</td>
<td>1027</td>
<td>240.0</td>
<td>69.0</td>
<td>126.0</td>
</tr>
</tbody>
</table>

2.3. Cloud Constituents

Table (2) shows exhaust cloud constituents, expressed as a fraction of the total weight of the exhaust products. These fractions have been adjusted to yield the weight of HCl, Al₂O₃, CO₂ and CO in the exhaust cloud multiplied by the appropriate fuel expenditure rates in table (1).

Table 2. Exhaust Cloud Constituents (Fraction by Weight).

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Space Shuttle</th>
<th>Titan III</th>
<th>Delta 2914</th>
<th>Delta 3914</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCl</td>
<td>0.1146</td>
<td>0.1932</td>
<td>0.1218</td>
<td>0.1589</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>0.1826</td>
<td>0.2819</td>
<td>0.2214</td>
<td>0.1936</td>
</tr>
<tr>
<td>CO₂</td>
<td>0.2503</td>
<td>0.2655</td>
<td>0.2055</td>
<td>0.2783</td>
</tr>
<tr>
<td>CO</td>
<td>0.00042</td>
<td>0.0222</td>
<td>0.0156</td>
<td>0.0331</td>
</tr>
</tbody>
</table>

The cloud rise and dispersion calculations for normal launches require specification of the time height profile of the launch vehicle. The vehicle flight profile data for the first 3000m above the surface are used to obtain a
least-squares fit to the expression

\[ T_k = az^b + c \]  (2)

where \( T_k \) time for the vehicle to reach the altitude \( z \). The values of the coefficients are tabulated in table (3).

<table>
<thead>
<tr>
<th>Vehicle Type</th>
<th>a</th>
<th>b</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Space Shuttle</td>
<td>0.652213</td>
<td>0.468085</td>
<td>0.375</td>
</tr>
<tr>
<td>Titan III</td>
<td>0.42958</td>
<td>0.518422</td>
<td>5.0</td>
</tr>
<tr>
<td>Delta 2914</td>
<td>0.922156</td>
<td>0.432703</td>
<td>0.54</td>
</tr>
<tr>
<td>Delta 3914</td>
<td>1.245756</td>
<td>0.418095</td>
<td>0.0</td>
</tr>
</tbody>
</table>

2.4. Meteorological Layers
The base of the lower layer (L=1) is assumed to be at the earth’s surface and top of the layer is assumed to be given by the base of an elevated inversion (top of mixing layer). The boundaries of the layers must coincide with a height or level reported on the rawinsonde observation. Both gases (vapor) and particulates \((Al_2O_3)\) are assumed to be reflected toward the earth’s surface at the tops of major boundaries. Material is never reflected at the base of the upper layer when gravitational settling or precipitation scavenging calculations are made, but gases are always reflected at the base of the upper layer. The selection of the height of the base and top of the upper layer is made from an interpretation of rawinsonde observations.

2.5. Dosage and Concentration Algorithms
The dosage or time integrated concentration at any point \((x,y,z)\) in the \(L^{th}\) layer due to the source in the \(K^{th}\) layer is given by an equation similar to equation (1).

2.6. Cloud and Plume Rise Model
The determination of the stabilized height of the ground cloud for normal launches and of the plume generated by launch facilities is a vital factor in the dosage/concentration computation, because the maximum dosage/concentration calculated at the earth’s surface is inversely proportional to the cube of the stabilized height. The ground cloud is comprised of buoyant gas emitted over a time period on the order of ten seconds. Hence the buoyant cloud rise is calculated using an instantaneous cloud rise model. The buoyant rise models used are based on Briggs plume rise equations.\(^4\) The time for the ground cloud produced by the normal launch of the Space Shuttle and Titan vehicles to reach a height \(z_k\) in a stable atmosphere is given by equation (3).

\[ t_l = s^{-0.5} \arccos \left[ 1 - \frac{\gamma_x \gamma_y \gamma_z z_k^4}{4 F_I} \right] \]  (3)

where \(s\) stability parameter, and \(\gamma_x, \gamma_y, \gamma_z\) are the alongwind, crosswind and vertical entrainment coefficients respectively. \(F_I\) refers to the initial buoyancy term. The time for a continuous plume to reach the height \(z_R\) in a stable atmosphere is provided by the following equation (4).

\[ t_c = s^{-0.5} \arccos \left[ 1 - \frac{\gamma_x \gamma_y \gamma_z z_R^2}{3 F_c} \right] \]  (4)

where \(F_c\) is buoyancy flux and \(u_c\) height weighted mean wind speed between the surface and the stabilization height \(z_c\).

2.7. Gravitational Deposition Model
The weight of material per unit area deposited on the ground as a result of gravitational settling of particles with velocity \(w_i\) from the source \(i\) in different layers. The wind shear angle is also considered for a particle falling to the earth’s surface.
2.8. Precipitation Scavenging Model

The weight of material from the $K^{th}$ layer deposited on the ground as a result of washout by rain is given by equation (5).

$$W_{K} = \left( \frac{\Lambda P K}{\sqrt{2\pi\sigma_{y}u_{L}}} \exp\left[\frac{1}{2}\left(\frac{y}{\sigma_{y}}\right)^{2}\right]\right) \exp\left[-\Lambda\left(\frac{x}{u_{L}} - t_{i}\right)\right]$$

(5)

where $\Lambda$ is the fraction of material removed per unit time and $t_{i}$ is the time precipitation begins. The basic assumption in equation (5) is that the rate of precipitation is steady over an area that is large compared to the horizontal dimension of the cloud of material. The precipitation originates at a level above the top of the cloud so that hydrometeors pass vertically through the entire cloud. The value of $\Lambda$ for HCl scavenging is $5.2 \times 10^{-4} \times R^{0.567}$ sec$^{-1}$ where $R$ is the rainfall rate in inches/hr.

In the next section, how all these models interact with each other and provide concentration contours for various gases is discussed.

3. OPEN MAP ARCHITECTURE AND TOXIC GAS DISPERSION MODEL

The Tomcat web server and openMap GIS software connect the toxic dispersion model to support the model's architecture. OpenMap interacts at the client side and acts as a graphical user interface. The openMap Java toolkit is made up of Java Bean components, of which the MapHandler, MapBean and Layer/PlugIn components play vital roles. OpenMap makes it easy to build components that fit the architecture to present user defined data. The MapHandler can be defined as a conceptual map, which contains MapBean and other components that manage the layers, mouse events and projection controls. The MapHandler is really an extended version of Java's BeanContext. The BeanContext is a mechanism for Java Beans to be used to find other beans which it can interact with. All OpenMap components have been designed to use the MapHandler to locate and connect to other components they need. The MapBean is a drawing Canvas that derives from the Swing JComponent class. Because the MapBean is a Swing component, it can be added to a Java window hierarchy like any other swing windowing component. The MapBean manages a hierarchy of layers, which can paint themselves to the canvas and a projection object to manage the view. Layers are the only component that can be added to a MapBean. When a Layer is added, it becomes a ProjectionListener to the MapBean, and receives a ProjectionEvent whenever the map is panned, zoomed or resized. In figure (2), there are two layers added namely the HRA and TGD layers. The TGD layer invokes the gas dispersion model from the server by sending an http request.

The openMap Applet depends on the viewer application for rendering images on web browsers. The openMap viewer application uses the BufferedMapBean instead of the MapBean precisely because of the increased performance. The BufferedMapBean extends the MapBean by forcing its layers to paint their graphics into a buffer. This drawing buffer is then rendered whenever the AWT causes a redraw. This dramatically increases performance for that particular window since it avoids the layer painting process. Of course if a layer causes a redraw, then regenerate the drawing buffer with the graphics and render the new image. From the web browser, the ToxicRisk applet sends a request to the web server which calls the dispersion models. For dispersion models, rawinsonde data are provided from server2 as inputs. The gas dispersion model performs computations and the output data is provided. This data has been converted to the necessary formats, so that it can be given as an input to openMap for further processing.

3.1. User Inputs

The default launch time and date matches system time and date. The user has an option to edit launch time and date. The user has an option to select type of vehicle among 7 types of vehicles. Once the user has selected a particular vehicle, the type of fuel, the fuel expenditure will be derived from table (1) and (2). The user can select different launch pads available at Cape Canaveral. The user can select chemical species, and their absorption coefficients. The user can use a default rawinsonde or real time data by clicking the appropriate check box. The user can specify cloud characteristics. Once the user has provided all of the information, the client sends data to the server and the toxic gas dispersion model computes the ground level chemical concentration. The user input screen is shown in figure (3).
3.2. Outputs

In figure (4), there are three layers viz., a Florida state map, a local map of Kennedy Space center, and a chemical concentration contour plot. The openMap viewer is an application that can be easily configured to add and remove components, without code modification. The new components can be added by adding a reference to `openmap.properties`. The Florida state GIS information is provided via the properties file. The user can add/remove layers in the application, and turn them on and off. The propertyHandler is a SoloMap component that can search for and parse `openmap.properties` files, directing certain properties to components that need them. At the top level is the MenuBar, which is an extension of the Java JMenuBar. This extension is the implementation of the MapHandlerChild methods that let it use the MapHandler to find MenuBarMenus that will be added to the MenuBar in the order in which they are found. The layerPanel is used to manage the display and order of the layers in the MapBean. Layers are components that get added to the MapBean in a hierarchical stacking order. Painting the graphics of each layer starting with the bottom most one and proceeding up the hierarchy draws the map. Successive layers render their graphics on top of the graphics of lower ones. In figure (5), multiple layers are overlaid. Plugins are components that are used by the PluginLayer to fetch data and prepare graphics for the map. In figure (3), plugins are used to fetch .CSV data formats. Layers and plugins are responsible for acquiring, constructing and rendering their own graphical data. The OMGraphics package provides a simple way to construct vector and raster graphics of geo-spatial and planar data. The Kennedy Space Center location details are used to plot in the map by OMGraphics. The projection interface allows read-only access to the current MapBean projection. The MapBean updates all Layers and other projectionListeners when the view changes. Once the population grid and chemical contour plot are computed, the human health risk
can be estimated. Based on launch commit criteria, a Go/No-go situation can be assessed for a particular toxic chemical concentration at the ground level.

4. CONCLUSION

The toxic gas dispersion model prediction capability coupled with GIS capability over the web and dissemination of information to all centers in real time is the great advantage of this model. Different scenarios for various toxic chemicals can be generated remotely. The model works very well for normal launches but not for any catastrophic launches or failures. The toxic gas model combines gravitational deposition, scavenging and dispersion to compute the maximum available concentration at any given point at ground. Further research is focused on developing a three-dimensional gas dispersion model.

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Figure 4. Contour plot of gas concentration.

Figure 5._layer of population grid over chemical contour.

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