# ALOFT-PC A SMOKE PLUME TRAJECTORY MODEL FOR PERSONAL COMPUTERS

by

William D. Walton, Kevin B. McGrattan
Building and Fire Research Laboratory
National Institute of Standards and Technology
Gaithersburg, MD 20899
and
Joseph V. Mullin
Technology Assessment and Research Branch
Minerals Management Service
U.S. Department of Interior
Herndon, VA 22070

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William D. Walton
Kevin B. McGrattan
National Institute of Standards and Technology
U.S. Department of Commerce
Gaithersburg, MD 20899

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Joseph V. Mullin
Technology Assessment and Research Branch
Minerals Management Service
U.S. Department of Interior
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### **ABSTRACT**

As the understanding of the capabilities and limitations of in situ burning of oil spills increases, in situ burning continues to gain acceptance as an oil spill mitigation tool. One widely imposed criteria for the use of in situ burning is limiting the exposure of downwind populations to smoke particulate. Since the downwind distribution of smoke particulate is a complex function of the fire parameters, meteorological conditions, and topographic features, a computer based model is required to predict the smoke plume trajectory. Measurements and observations at experimental burns have shown that the downwind distribution of smoke is not Gaussian and simple smoke plume models do not capture the observed plume features. To resolve these problems, NIST has developed a smoke plume trajectory model that solves the fundamental Navier-Stokes equations using an eddy viscosity over a uniform grid which spans the smoke plume and its surroundings. This large eddy simulation smoke plume model has been refined over a period of years using a computer workstation and the results have compared favorably with the limited data available from experimental burns. ALOFT-PC (A Large Open Fire plume Trajectory model) is the public domain version of the model for windows based personal computers. The model inputs include wind speed and variability. atmospheric temperature profile, and fire parameters and the output is the average concentration of smoke in each of the computational cells from ground level to the top of the plume. ALOFT-PC is designed to aid in the in situ burn planning process. For this purpose a "foot print" of the ground level smoke concentration is the most commonly used model output.

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### INTRODUCTION

In situ burning has grown in acceptance as an oil spill mitigation tool as the capabilities and limitations are better understood (Buist et al., 1994). Although in situ burning has been included in a number of regional response plans, limiting the exposure of downwind populations to smoke particulate remains a concern. The downwind distribution of smoke particulate is a complex function of the fire parameters, meteorological conditions, and topographic features. Simple smoke plume models designed for smoke stack emissions do not adequately capture the observed features of plumes from large in situ oil spill burns. Under the sponsorship of the Minerals Management Service, U.S. Department of Interior, the National Institute of Standards and Technology has developed a computer based model, ALOFT, to prediction the smoke plume trajectory from in situ oil spill burns.

ALOFT (A Large Open Fire plume Trajectory model) is a model to prediction the downwind concentration of smoke particulate from a large outdoor fire. The model was previously known as the NIST LES model based on the large eddy simulation technique used (Walton, et al., 1993). ALOFT-PC<sup>2</sup> is a public domain, personal computer implementation of version 2 of the ALOFT model for level terrain. The development of the ALOFT-PC program is a continuing process and the future addition of new features will change the model inputs and outputs. Detailed instructions for using the model are included with the program.

ALOFT-PC is envisioned as a prototype tool for developing in situ burn plans. It also has the potential for use as a training tool and perhaps an operational tool. At the present time the model has not been officially certified. ALOFT has, however, been used to examine the expected downwind particulate deposition under meteorological conditions common to Alaska (McGrattan, et al., 1994).

It is difficult to verify models such as ALOFT. The model has the ability to predict the downwind concentration of smoke particulate from a fire over a large area. Large oil spill fire experiments occur infrequently and it is difficult to accurately measure smoke concentrations as well as the input parameters required for the model. To date there has only been limited verification testing of model although the comparisons of the model predictions with measurements from large experiments have been favorable (McGrattan, et al., 1994).

# PLUME TRAJECTORY MODEL

The mathematical model consists of the Navier-Stokes equations simplified for the problem at hand. This is accomplished in part by assuming the component of the plume

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velocity in the direction of the ambient wind is literally the wind speed. Once this approximation is made, the plume can be viewed as two-dimensional in the crosswind direction with the downwind direction represented by time. The large scale structure of the plume can then be computed in detail and the small scale "sub-grid" mixing and dissipation is represented with a constant eddy viscosity. This permits the mathematical structure of the Navier-Stokes equations to be retained. The effective Reynolds number, defined by the buoyancy induced velocity, plume height and eddy viscosity, is chosen to be above 104. It is in this sense that ALOFT is a large eddy simulation.

### Mathematical Model

The mathematical model assumes that the plume is described in terms of steady-state convective transport by a uniform ambient wind of heated gases and particulate matter introduced into the atmosphere by a continuously burning fire. A detailed description of the equations used in the ALOFT model have been presented previously (Walton, et al., 1993). The model does not predict features of the fire itself, but rather the plume of smoke which emanates from it. Only the convective heat release rate and smoke particulate release rate of the fire need be specified. The simulation begins several fire diameters downwind of the fire, where the flow field is characterized by relatively small temperature changes, minimal radiation effects, and a velocity field dominated by the prevailing wind. The plume gases ascend to a point in the atmosphere of neutral buoyancy, and then gradually disperse. The trajectory of the plume is governed by the ambient wind, the atmospheric stratification and the level of turbulent motion. The wind is taken as uniform, but the temperature may vary with height according to a prescribed profile.

Given these assumptions, the mathematical model of a smoke plume consists of the conservation equations of mass, momentum and energy which govern the absolute temperature, pressure, density, and crosswind velocity components in a plane normal to the direction of the uniform ambient wind. It is convenient to divide the temperature and pressure fields into mean background values plus perturbations induced by the fire. Similarly, the density is decomposed into an ambient density and a small thermally induced perturbation, which is related to the temperature perturbation through the equation of state taken in the small disturbance, low Mach number form appropriate to this problem. The ambient density is related to the background pressure through the hydrostatic balance.

The uniform ambient wind speed is assumed to be constant and larger than the crosswind velocity components. This assumption is quite realistic several flame lengths downwind of the fire. Since the wind speed does not change, there is no need for a windward component of the momentum equations. Since the details of the fire are not being simulated, the only information about the fire required is the overall convective heat release rate and the particulate mass release rate. The model does not take into account the heat loss due to thermal radiation. The initial temperature distribution in the plume cross section is assumed to be Gaussian, but the temperature downwind is not assumed to be Gaussian and is computed from the conservation equations.

The equations of motion are made non-dimensional with the windward spatial coordinate replaced by a temporal coordinate where the plume height is given in terms of the potential temperature of the undisturbed atmosphere. Following this scaling, the three-dimensional, steady state system of equations can be considered as a two-dimensional, time-dependent system. This is an initial value problem in which the initial conditions are prescribed in a plane perpendicular to the direction of the prevailing wind a few fire diameters downwind of the fire.

Initially, the crosswind velocity components are assumed to be zero. No-flux, free-slip boundary conditions are prescribed at the ground, consistent with the assumed uniformity of the prevailing wind and the resolution limits of the calculation. At the outer and upper edges of the computational domain, the perturbation temperature, perturbation pressure, and windward component of vorticity are set to zero.

Atmospheric turbulence effects mixing on a wide range of scales, extending to scales which are smaller than the resolution of the calculations performed here. There are two mechanisms by which turbulent atmospheric motions are introduced into the simulation. First, the small scale mixing is represented by a constant eddy viscosity, which is taken to be three orders of magnitude greater than the viscosity of air. The choice is governed by the desire for resolution limits in the five to fifteen meter range which are needed to capture the large scale fire induced eddy motions.

#### Numerical Method

The uniform wind assumption and the subsequent scaling of the equations transforms the three dimensional, steady state problem into a two dimensional, time dependent problem. sometimes referred to as an initial value problem. The equations constitute a mixed system of partial differential equations; i.e., the equations for the temperature and velocity components are parabolic and the equation for the pressure (which is derived from the incompressibility condition) is elliptic. The equations and the associated boundary conditions are solved using a relatively simple finite difference technique. The computational domain spanning the crosswind plane is one unit in the vertical direction and four units in the horizontal direction and is divided into uniformly sized rectangular cells. The size of the cells is computed by the model so that the plume will fit within the computational space. The horizontal velocity is assigned on the left and right boundaries of each cell, the vertical velocity is assigned at the top and bottom, and the perturbation temperature and pressure are taken at cell centers. This placement of the flow variables leads to a natural and efficient differencing scheme for the equations. Central differences are used for all spatial derivatives, and the solution is advanced in time (i.e. follow the evolution of the plume downwind) with a second order Runge-Kutta scheme. The model automatically adjusts the time steps to assure stability.

## Particle Tracking

A fixed number of particles are used to represent the particulate matter carried aloft and downwind by the plume. The particles are introduced into the flow at the start of the calculation and convected with the induced flow. The initial distribution of particles,

like the temperature distribution is uniform within an elliptical area in the crosswind plane. All particles move at the same downwind speed equal to that of the wind. The average of the velocity at the start and at the end of a time step is used to update the particle position. Particles that reach the ground level cells are considered to have been deposited on the ground and are not carried forward in the calculation.

The viscosity and thermal conductivity terms included do not account for larger scale atmospheric motions, which may be thought of as variations of the prevailing wind over a time scale of minutes to hours. These deviations can be measured, and are introduced into the model through random perturbations to the trajectories of the particles. In a smoke plume the path of particles originating from a given area on the fuel surface changes over time with fluctuations in the wind. Thus, the motion of each particle is governed by the fire-induced velocity field, found by solving the conservation equations, plus a perturbation velocity field which represents the random temporal and spatial variations of the ambient wind. The perturbation velocities are determined from the input standard deviations of the prevailing wind direction in the horizontal and vertical directions.

The present version of the model decouples the random spatial and temporal motion of the advected particles and the governing hydrodynamic equations. The reason for this is that the hydrodynamic equations describe the steady-state plume structure and cannot readily accommodate temporal fluctuations. As a result use of this model for high wind fluctuation values (>25°) is not recommended.

### ALOFT-PC

ALOFT-PC includes an interactive input/output routine which 1) allows the user to select the input units. 2) performs error and range checks on the data, 3) provides methods to estimate input values based on observed conditions, 4) allows convenient input and output file selection, 5) provides explanations for inputs, and 6) provides a simple graphical display of the results.

In addition to the outputs displayed by the program, ALOFT generates a number of output files. These files provide the particulate concentration profiles and information on the computational grid. These files allow the user to display the output in other formats or use the output as input to another program. A complete description of the output files is included with the program.

The ALOFT-PC is written for the Windows953 environment and is presently undergoing testing and refinement. Typical run times are on the order of 10 minutes with a Pentium

<sup>&</sup>lt;sup>3</sup> Certain trade names and company products are mentioned in the text in order to adequately specify the procedure used. In not case does such identification imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the products are necessarily the best available for the purpose.

based computer. The user should refer to material provided with the program for the latest information.

### ALOFT-PC INPUTS

The input parameters for ALOFT-PC are the same as those for the ALOFT version 2 workstation program however the parameters related to grid size are fixed by the input routine at optimum values and the user is not given the opportunity to change them. Many of the required inputs are values that would difficult to obtainable by the user. ALOFT-PC offers the user the choice of either directly entering the parameters used by the model or utilizing estimates based on more readily available observations and measurements.

Many of the inputs have units associated with them. ALOFT-PC provides the user with the choice of a number of common units for the input parameters. The input file and output files generated are all in SI units regardless of the input units selected by the user.

The following is a description of the inputs required for the model, methods used by ALOFT-PC to obtain estimates if selected by the user, and the range of acceptable values. The units associated with the values in the input file are also given.

Title: This is a title to identify the data set to the user. The maximum length is 80 characters.

Wind Speed: The model assumes the wind speed to be constant with height and downwind distance. The user should estimate the average speed of the wind at the height to which the plume will eventually rise over the distance to be calculated. The units for wind speed are m/s. The model predictions should not be used for wind speeds below 2 m/s or above 15 m/s. Usually wind speeds are measured near ground level and the corresponding wind speed at the height to which the plume will rise is generally greater. Correlations can be found in the literature which relate the wind speed near the surface with the wind speed at elevations up to a few hundred meters (Brode, 1988). These correlations are usually of the form:

$$u = u_i \left(\frac{h}{h_i}\right)^p$$

where:

u = the wind speed at elevation h

u, = the measured wind speed at elevation h,

p = function of the stability and terrain

Based on this correlation using a typical value of p. the wind speed 200 meters above the ground would equal approximately twice the wind speed measured 2 meters above the ground. Since the wind speed can be a function of many factors, this information is

provided as guidance for the user has not been incorporated into the input routine. It is recommended that the user obtain specific information for the location of interest.

Wind direction is not an input since the wind direction is assumed to be constant with altitude and the plume always travels in the direction of the wind. It is not uncommon, particularly in the marine environment, for the wind direction to change with altitude. The model cannot at this time accommodate changes in wind direction with altitude and user should be aware that the predictions can be misleading when that condition exists.

Standard Deviation of lateral and vertical wind speed: These represent time-averaged deviations of the wind from the prevailing direction in degrees. These are normally obtained with special anemometers with readings taken over time periods of the order of the burn time. Typically these values cannot be obtained directly and are obtained from correlations. Table 1 gives relationships between Pasquill-Gifford stability category and the standard deviation of the wind direction (Randerson, 1984). Table 2 provides the relationship between observed weather conditions and Pasquill-Gifford stability category (Randerson, 1984, Slade, 1968).

Table 1. Pasquill-Gifford stability category for observed weather conditions

				Nighttime conditions		
Surface	Daytime insolation			Thin overcast	≤ <sup>3</sup> /8	
wind speed - (m/s)	Strong	Moderate	Slight	or ≥ 1/8 cloudiness	cloudiness	
2	A-B	В	С	Е	F	
4	В	B-C	С	D	Ē	
6	С	C-D	D	D	D	
>6	С	D	D	D	D	

Use D for heavy overcast day or night

The degree of cloudiness is defined as that fraction of the sky above the horizon which is covered by clouds.

Table 2. Relationships between Pasquill-Gifford stability category and the standard deviation of the wind direction

Pasquill-Gifford stability category	Standard deviation of the horizontal wind direction (°)	Standard deviation of the vertical wind direction (°)
A: Extremely unstable	25	16
B: Moderately unstable	20	12
C: Slightly unstable	15	10
D: Neutral	10	6
E: Slightly stable	5	3
F: Moderately stable	2.5	2

Tables 1 and 2 have been combined and included in the input routine so the user can select standard deviations of the wind based on observed conditions if measurements are not available. The range for standard deviation of lateral wind speed is 2.5 to 25° and for the vertical wind speed is 2 to 17°.

**Downwind Distance:** This is the distance downwind of the fire that the plume is tracked, in kilometers. Distances should me in the range from 0.5 to 20 km. Although results are for distances less then 1 km the predictions may not be valid for areas close to the fire since the details of the fire are not modeled. Beyond 20 km the assumption that the wind and temperature conditions do not vary with downwind distance are less likely to be valid.

Fire Heat Release Rate: This is the convective heat release rate of the fire in MW. Radiative heat is not considered by the model. For very sooty fires, it is often assumed that about 10% of the total heat release rate is lost to radiation so the convective heat release rate is 90% of the total heat release. The heat release rate per unit burning area is a function of the fire size since the rate of fuel vaporization is a function of the thermal radiation from the flames to the fuel. It is also a function of the type of fuel being burned. For fires of the size normally considered for *in situ* burning, that is larger than 10 m in diameter, the rate of heat release per unit area is nearly constant. The heat release rate per unit area for a particular fuel can be determined in the laboratory by enhancing the thermal radiation to the fuel surface with an external source. The heat release rate should be in the range of 50 MW to 2000 MW.

Since convective heat release rates per unit burning area are not normally available for crude oils a typical value for crude oil has been provided in the input routine. The user has the option of entering either the convective heat release rate of having the input

routine determine it from the rate of heat release per unit area and a specified burning area

Fire Smoke Particulate Mass Release Rate: This is the mass rate of particulate being generated by the fire in units of kg/s. The smoke particulate mass release rate is normally calculated from measurements of the surface regression rate, smoke yield, and fuel properties in a large scale fire experiment. The user may select a typical smoke particulate mass release rate per unit area in the input routine which is multiplied by the burning area to provide an estimate of the mass release rate. If the downwind concentration of particles in a particular size range is desired then in input release rate should be the fraction of the total mass in the desired size range. Although the input is identified as smoke particulate, the model can calculate the downwind concentration of any non-reacting product of combustion.

Fire Area: This is the area of burning fuel in m<sup>2</sup>. The fire area is not directly used in model however it may be used in several places by the input routine in conjunction with user specified alternative input methods. In order to avoid conflicts between parts of the input routine a fire area is required. The fire area should be in the range of 25 m<sup>2</sup> to 1000 m<sup>2</sup>.

Initial Plume Height, Width, and Centerline Elevation: The model prediction begins with the source of heat and smoke distributed over an ellipse shaped area in a vertical orientation, located at a specified elevation above ground level. Normally the starting size and elevation would correspond to the plume conditions several fire diameters downwind of the fire. Downwind concentrations however, are not sensitive to small changes in these inputs. Since the actual shape of the fire area is often unknown, the normally the user selects the option for a circle with an area equal to the specified fire area and a centerline elevation equal to the diameter of the circle. The units for the initial plume height, width, and centerline elevation are meters.

Temperature Profile: Starting at ground level, the elevation and temperature of the atmosphere. The units for the elevation are meters and the temperature degrees C. and the maximum number of points is 200. The user may either enter specific points defining a temperature profile or a lapse rate for a linear profile. The limitation for a user specified profile is the slope using any two of the points must be greater than -9 °C km. The profile should be specified to the elevation to which the plume is expected to rises which is typically 1 km. If the plume rises to an elevation greater than the highest point in the specified profile, the profile will be linearly extrapolated using the highest two specified points. If a lapse rate is used the rate must be greater than -9 °C/km. Since a temperature profile is often difficult to obtain, the input routine contains the estimates made by the authors shown in table 3 based on the Pasquill-Gifford stability category determined from table 1.

Table 3. Relationships between Pasquill-Gifford stability category and the temperature lapse rate

Pasquill-Gifford stability category	Temperature lapse rate (°C/km)
A: Extremely unstable	-9
B: Moderately unstable	-6
C: Slightly unstable	-3
D: Neutral	0
E: Slightly stable	0
F: Moderately stable	0

#### ALOFT-PC STATUS

The Beta test version of ALOFT-PC with draft user guide is presently available for evaluation and comment. The authors anticipate that the program and user guide will be published in the fall of 1996.

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