COMPLEX/PFM Air Quality Model, User's Guide

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Environmental Research and Technology, Inc. Concord, MA

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COMPLEX/PFM AIR QUALITY MODEL

User's Guide

by D.G. Strimaitis J.S. Scire A. Bass

Environmental Research & Technology, Inc. Concord, Massachusetts 01742

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Project Officer

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A user's guide has been assembled to des of the COMPLEX/PFM air quality modeling syste the Potential Flow Model (PFM) with those of to produce a potential flow complex terrain m flow dispersion calculations may be selected this option is selected, the model requires h profiles in order to calculate hourly mixing layered plume rise equation), and hourly valu height. A preprocessor is provided to interp and evening radiosonde data. Potential flow the plume lies above the dividing streamline stability class is D, E, or F. COMPLEX I (22 performed whenever plume lies below the divid calculations are performed whenever the surfa	Cribe the purpose, des m. The system combine the EPA COMPLEX I and odel for routine appli as an option within CO ourly wind speed and t heights, hourly plume es of the critical div olate hourly profile d calculations are perfo height, providing that .5° sector averaging) ing streamline height, ce stability class is MENT ANALYSIS DENTIFIENS/OPEN ENDED TERMS MENT ANALYSIS DENTIFIENS/OPEN ENDED TERMS SECURITY CLASS (This Report) UNCLASSIFIED SECURITY CLASS (This page) UNCLASSIFIED	ign, and operations the features of Complex II modelss cation. Potentia MPLEX/PFM. When emperature rise (using a iding streamline ata from morning rmed whenever the surface calculations are and COMPLEX II A, B, or C.

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NOTICE

This document has been reviewed in accordance with U.S. Environmental Protection Agency policy and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

PREFACE

This publication contains a user's guide for the COMPLEX/PFM dispersion model which applies potential flow theory for calculating the impact of non-reactive pollutants on the windward side of the first significant terrain feature downwind of a point source. The potential flow model offers a realistic physical description of the interaction of plumes with terrain features; plume path and dispersion coefficients are modified based on the height of the plume relative to the height and shape of the terrain feature.

The PFM option within COMPLEX/PFM requires twice-daily representative radiosonde data as input and incorporates an algorithm to interpolate a temperature sounding for each hour of the day. The interpolated sounding is used to calculate the mixing height, plume rise, and critical dividing streamline for that hour. Plumes above the critical streamline are assumed to pass over the terrain feature and, for neutral and stable stratification, potential flow theory is the basis for specifying the interaction of the plume with the terrain feature. Plumes below the critical streamline are assumed to impact on the terrain. Since potential flow theory does not apply for plume impaction, concentrations are calculated as in the COMPLEX I dispersion model.

Potential flow theory has not been extensively applied to dispersion problems. The COMPLEX/PFM model is being made available through this document and the UNAMAP system to encourage its application for the purpose of accruing evaluation statistics for diversified complex terrain applications. No regulatory standing should be ascribed to COMPLEX/PFM. Its use for any regulatory application should be considered in light of EPA's Guideline on Air Quality Models.

The model represents a first step towards a refined complex terrain model and may be modified in the future based on feedback from users and on the results of the EPA multi-year complex terrain model development project. Corrections and modifications of this model may be obtained as they are issued by completing and sending the form on the last page of this guide. In addition, the mailing form may also be used to obtain a sensitivity analysis comparing concentration, mixing height, and plume rise calculations by COMPLEX/PFM with those for COMPLEX I and COMPLEX II. The report should be available by October 1983.

The computer code for COMPLEX/PFM will be available on version 5 of the User's Network for Applied Modeling of Air Pollution (UNAMAP) system by spring 1983. The UNAMAP system may be purchased on magnetic tape from NTIS for use on the user's computer system. For information on UNAMAP contact: Chief, Environmental Operations Branch, MD-80, U.S. Environmental Frotection Agency, Research Triangle Park, NC 27711.

ABSTRACT

A user's guide has been assembled to describe the purpose, design, and operation of the COMPLEX/PFM air quality modeling system. The system combines the features of the Potential Flow Model (PFM) with those of the EPA COMPLEX I and COMPLEX II models to produce a potential flow complex terrain model for routine application.

Potential flow dispersion calculations using the theory of Hunt and Mulhearn (1973) and Hunt and Snyder (1978) may be selected as an option within COMPLEX/2FM. When this option is selected, the model requires hourly wind speed and temperature profiles in order to calculate hourly mixing heights, hourly plume rise (using a layered plume rise equation), and hourly values of the critical dividing streamline height. A preprocessor is provided to interpolate hourly profile data from twice daily (morning and evening) radiosonde data. Potential flow calculations are performed whenever the plume lies above the dividing streamline height, providing that the surface stability class is D, E, or F. COMPLEX I (22.5° sector averaging) calculations are performed whenever the plume lies below the dividing streamline height, and COMPLEX II calculations are performed whenever the surface stability class is A, B, or C.

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Preface	CONTENTS
Abatasat	•••••••••••••••••••••••••••••••••••••••
Abstract.	
rigures.	
Abbreviet	· · · · · · · · · · · · · · · · · · ·
Abbreviat	
Acknowled	gement
1 2	
1.2	COMPLEX/DEM Modeling Package
1.4	Summary of Date Required for PEN Options
2	1.4.1 Meteorological Data.
	1.4.7 Source Data
	1.4.3 Receptor Data
	1.4.4 Program Control Parameters
2. Tech	
2.1	Introduction
2.2	The Potential Flow Model
	2.2.1 Diffusion Theory
	2.2.2 PFM Factors
	2.2.3 Plume Trajectory Analysis - Neutral Flow
	2.2.4 Plume Trajectory Analysis - Stratified Flow
2.3	The COMPLEX/PFM Option
	2.3.1 PFM Option: Long and Short
	2.3.2 Plume Rise
	2.3.3 Froude Number and HC Analysis
2.4	Temperature and Velocity Profile Interpolation
	2.4.1 Required Data and Defaults
	2.4.2 Mixing Heights and Profile Interpolation • • • •

			, set
	2.5	Terrain Description Guidance	· • •
		2.5.1 PMF-Short Obstacle Selection	
		2.5.2 PMF-Long Obstacle Selection	
3.	User	's Instructions	
$\frac{\partial f}{\partial t} = \frac{1}{2} \frac{\partial f}{\partial t} = \frac{1}{2$	3.1	SETUP Instructions	
	3.2	READ56 Instructions	
	3.3	PROFIL Instructions	
	3.4	COMPLEX/PFM Instructions 61	
		3.4.1 COMPLEX/PFM Options 61	
		3.4.2 Input Format Specifications 63	
Ref	erence	8	
Арре	endice	S	
	A.	PFM Bluff Cross-Sections	
1. 1.16	В.	Program Description - PROFIL	
	C.	Program Description - COMPLEX/PFM	
	D.	Subroutine Description - SPFM	
	Е.	Test Case	

FIGURES

Number		Page
1	The COMPLEX/PFM modeling system	5
2	Horizontal dispersion coefficients for neutral flow over a circular ridge	16
3	Vertical dispersion coefficients for neutral flow over a circular ridge	17
4	Horizontal dispersion coefficients for neutral flow over a hemispherical hill	18
5	Vertical dispersion coefficients for neutral flow over a hemispherical hill	19
ба	Velocity speed up factors for neutral flow over a circular ridge	20
6b	Velocity speed up factors for neutral flow over a hemispherical hill.	20
7	Plume path and surface streamlines derived from flow over a step	25
8	Height of the source streamline above the hill crest for various stack heights and Froude Numbers.	29
9	Relationship between PFM and actual sources and receptors in PFM-Long	35
10	Relationship between PFM receptors and COMPLEX receptor in PFM-Short	37
11	Calculation of neutral plume rise	40
12	Relationship between PFM geometry and plume height when HC, the dividing streamline height, is not zero	43
13	Sample construction of temperature profile for fourth hour after A.M. sounding	46

51. V-

FIGURES

Number		Page.
14	Relationship between north and the orientation of the bluff coordinate system	49
15	Definition sketch for selecting cross-wind and along-wind aspect ratios	51
16	Relationship between XO, YO, and OBSANG	52
17	The COMPLEX/PFM modeling system	56
18	Input data deck setup for COMPLEX/PFM	64

TABLES

Number		Page
1	Obstacle shapes available for applications of PFM-Long	53
2	PARAMS namelist - READ56	57
3	Data identification record - READ56	58
4	PROFIL program control card variables	60
5	Options available in COMPLEX/PFM	62
6	COMPLEX/PFM card type 1, 2, and 3 - title	65
7	COMPLEX/PFM card 4 - control and constants	66
8	COMPLEX/PFM card 5 - options	67
9	COMPLEX/PFM card 6 - wind and terrain	68
10	COMPLEX/PFM card type 7 - point source	69
11	COMPLEX/PFM card type 8 - specified significant sources	70
12	COMPLEX/FFM card type 9 - met. data identifiers	71
13	COMPLEX/PFM card type 10 - polar coordinate receptors	72
14	COMPLEX/PFM card type l1 - polar coordinate receptor elevations	73
15	COMPLEX/PFM card type 12 - receptors	74
16	COMPLEX/PFM card type 13 - obstacle information	75
17	COMPLEX/PFM card type 14 - grid center	76
18	COMPLEX/PFM card type 15 - receptors	77

', ix

No 14

TABLES

,	<u>Number</u>		Page
	19	COMPLEX/PFM card type 16 - segmented run	78
dje de	20	COMPLEX/PFM card type 17 - meteorology	79
	21	COMPLEX/PFM optional input file - meteorological data	81
	22	COMPLEX/PFM optional input file - emission data	82
	23	COMPLEX/PFM optional input file - hourly sounding data	83

, sh

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LIST OF SYMBOLS AND ABBREVIATIONS

SYMBOL

 a height of obstacle a,b,c half the length of the primary axes of an ellipsoid c concentration C' dimensionless concentration D depression of a neutral streamline to approximate stratified flow D1,2 normal and crosswind dimensionless diffusivities D1,2 normal and crosswind "effective" diffusivities p1,2 trial solution functions F buoyancy flux FR Froude number g(s) trial solution function h step height (bluff problem) H plume height above flat terrain HC critical dividing streamline of the flow HE effective source height (above H_c) HH net plume height above the surface K1(s) normal dimensional diffusivity k2(s) crosswind dimensional diffusivity k2(s) crosswind dimensional diffusivity k2(s) crosswind dimensional from plume centerline to surface N brunt-Vaisala frequency Q emission rate of pollutant R(s) distance from axis of symmetry to plume centerline for axisymmetric obstacle s path length along plume centerline s,n,Y curvilinear coordinates for system that follows the plume centerline s stability parameter S speed-up factor t advection time along plume centerline t parametric complex variable in bluff streamline equations T(s) line integral for crosswind flow deformation un local velocity along the plume in neutral flow 		_	
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us local velocity along the plume in stratified flow		un	local velocity along the plume in neutral flow
		us	local velocity along the plume in stratified flow

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~	and also attached and and the
	along-streamline velocity
Um line	uniform velocity upwind of source (u-component)
Vm	uniform velocity upwind of source (v-component)
v(s)	scaled velocity normal to streamline
_V(s)	velocity normal to streamline
x	distance along X axis from source
Xs	downwind distance from source to obstacle center
zC	height of streamline above crest for neutral flow
zCF	height of streamline above crest for stratified flow
ß "	entrainment parameter
n	plume height perturbation factor
λ	ellipsoidal coordinate
ρ	density
σ _{y,z}	crosswind and vertical dispersion coefficients
^o yf,zf	crosswind and vertical dispersion coefficients in flat
	terrain
φ(s)	dafermetion
м.) М	velocity potential
	stream function along surface
* *O	stream function through source
. ⊬ຣ ີ ຟ_	streamline equation of plume centerline
, ™P	errantine adaptation of brand samarerus

ABBREVIATIONS

Cm	centimeter
EPA	U.S. Environmental Protection Agency
ERT	Environmental Reasearch & Technology, Inc.
FMF	Fluid Modeling facility
К	Kelvin
km	kilometer
'n	meter
NCC	National Climate Center
NWS	National Weather Service
PGT	Pasquill-Gifford-Turner
s	seconds

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SECTION 1

INTRODUCTION

1.1 Objective

The focus of the development work that produced the modeling system described in this manual has been the application of potential flow theory to the problem of predicting pollutant concentrations on significant terrain features. Two classes of meteorological conditions are often associated with the likelihood of large ground-level concentrations: (1) low wind speed and stable cases and (2) moderate or high wind speed and neutral or slightly stable cases. The first class of conditions generally leads to high concentrations through direct plume impingement or terrain blocking. The second class of situations promotes high concentrations because, as the plume is transported over terrain features, it is forced to pass close to the terrain surface. Physical mechanisms relevant to this class of conditions include terrain-induced alteration of the plume centerline trajectory and kinematic constraints on horizontal and vertical dispersion. Potential flow theory is particularly useful in modeling concentrations produced by the second class of conditions.

Other methods have been used to account for plume trajectory deformations over terrain features. For example, those EPA models suggested for use in complex terrain on a site-specific basis (COMPLEX I, COMPLEX II, and MPTER, all available on UNAMAP-Version 4) modify the height of the plume centerline over the terrain. This is done by using plume path coefficients that vary according to the dispersion stability class of the surface layer. These coefficients do not vary with obstacle shape or position along the plume path and are only weakly responsive to the magnitude of the speed of the flow relative to the density stratification. Consequently, a better representation of plume dynamics near terrain is sought through the application of potential flow theory.

The first phase in the study of the potential flow theory approach culminated in the construction and testing of what has become known as the Potential Flow Model, PFM (Bass et al. 1981). That version of PFM contained potential flow streamline solutions for flows over the center of an isolated hemisphere and an isolated circular cylinder. Flow over obstacles of intermediate shape between these two was approximated by a streamline weighting scheme. The model was designed to estimate pollutant concentrations from a single plume over a single terrain feature only when the atmosphere's density stratification is neutral to slightly stable (that is, no blocking or impingement). A more general model is needed, however, to apply potential flow theory calculations in regulatory permitting situations. Concentration estimates are needed when the flow is either very stable or well-mixed (unstable) as well as when it is neutral to slightly stable. In addition, several sources often need to be modeled simultaneously for sequential hourly periods totaling as much as one year so that three hour, 24- hour, and annual pollutant concentration averages at many receptors can be estimated.

Potential flow calculations themselves must also be generalized. Hill shapes other than the sphere-cylinder variants are needed to better approximate single terrain features. Moreover, plume trajectories that do not pass over the center of a terrain feature are necessary, as the proper simulation of wind direction variability is an essential feature of a successful sequential model.

The objective of the second phase of this study was the generalization of the PFM code, and the design of a complete modeling system that would satisfy each of these requirements. That modeling system is COMPLEX/PFM. The FFM calculations performed by this model are applicable to more general terrain shapes and wind flow angle. And the host model (EPA COMPLEX) contains the structure for handling many point sources, many hourly simulation periods, and any averaging time for reporting air pollutent concentration statistics. The host model also provides pollutant concentration algorithms for impingement situations and strongly convective situations.

1.2 Major Features

COMPLEX/PFM is a modified version of COMPLEX I/COMPLEX II which contains the PFM algorithm as an option. If the PFM option is not invoked, the model performs COMPLEX I (22.5° crosswind sector averaging and Gaussian vertical spread based on σ_z) computations for stability classes five and six (E, F), and COMPLEX II (bivariate Gaussian spread based on σ_y and σ_z) computations for stability classes one through four (A through D). Both COMPLEX versions are based on the MPTER model (Pierce et al. 1980) with an expanded list of terrain algorithms. Major features of COMPLEX include:

- o Averaging periods of longer than one hour, if selected by user.
- Hourly meteorological data that may be read off punched cards for each hour, or from a tape (or disk) containing a year's data (same data as used for RAM or CRSTER).
- o Optional terrain adjustments as a function of stability class.
- c Inclusion or omission of stack downwash.
- o Inclusion of gradual plume rise, or final rise only.
- o Inclusion or omission of buoyancy-induced dispersion of pollutant during plume rise using the Pasquill method.
- o Input of anemometer height.
- Input of wind profile power law exponents as functions of stability.

- Concentration contributions that are available per hour and/or for the selected averaging period at each receptor from up to 25 sources.
- Concentrations available hourly and/or for the selected averaging period at each receptor.
- Optional output of the following information: average concentration over length of record, plus highest five concentrations for each receptor for four end-to-end averaging times (1-, 3-, 8-, and 24 hour), and an additional averaging time selected by the user.
- o Optional output files for further processing of concentrations that are available per hour and for each averaging period.
- o Up to 50 spatially separated point sources.

o Up to 180 receptors with no restrictions on location.

Several new features are introduced when the PFM option is invoked. These include the following:

- o Refined hourly mixing height calculation based upon twice daily radiosonde profiles of wind and temperature.
- Layered plume rise calculations that use hourly wind and temperature profiles interpolated from twice-daily radiosonde observations.
- o Assessment of wind flow characteristics by means of a critical dividing streamline (HC) and Froude number (FR) analysis based on the hourly wind and temperature profiles.
- o Selection of the COMPLEX I, COMPLEX II, or PFM algorithm based on the surface stability class, FR, HC, and initial plume height instead of on the stability class alone.
- o Inclusion of explicit plume size and trajectory deformations computed from potential flow theory when PFM is applicable.
- o An economical long-term version (PFM-Long) for computing annual average concentrations, for assessing regions of frequent high concentration and for identifying critical periods of meteorology that produce the highest expected pollutant concentrations.
- A short-term, worst-case or critical period version (PFM-Short) for a refined analysis of maximum pollutant concentrations expected.

Along with these new features come several added restrictions to the original COMPLEX features:

- o all sources (maximum = 50) are at the same point,
- o the receptor pattern is radial; and
- o there is no gradual plume rise option.

These restrictions arise from the necessity of maintaining a simple, fixed source-terrain relationship.

The new features should be viewed as a natural extension of the COMPLEX modeling system when representative profiles of wind and temperature are used. Characterization of the relationship between HC, FR, plume height, and terrain height is essential to assessing plume behavior and to choosing the most appropriate algorithm to simulate it. When plume impingement is likely, based upon these quantities and not simply upon the dispersion stability class of the surface layer, a VALLEY-like (Burt 1977) (COMPLEX I with the recommended parameter choices) computation is performed. When potential flow theory applies, a PFM computaton is performed. If the boundary layer is convectively unstable, a COMPLEX II computation is performed with a suitable plume path coefficient.

1.3 COMPLEX/PFM Modeling Package

The COMPLEX/PFM modeling package is schematically illustrated in Figure 1. The meteorological preprocessing steps on the left side of the figure are required by most sequential air quality dispersion models in use today, especially those available through UNAMAP. This preprocessor requires hourly surface data and twice-daily mixing height data. For further information about the preprocessor program, consult the User's Guide for the Single Source (CRSTER) Model (EPA 1977).

The preprocessing steps on the right side of the figure pertain only to the use of the PFM option within COMPLEX/PFM. For short-term runs, user-specified meteorological data may be input on cards. Hourly temperature and wind profiles are required when the PFM option is invoked. These can be constructed by the PROFIL preprocessor from twice-daily profile data and hourly surface data. When on-site tower data are available, tower wind and temperature data should also be included by the user although the code for doing this is not yet included in the preprocessor.

Two sources of twice-daily profile data may be available: representative profiles obtained at a National Weather Service (NWS) Upper-Air Network Station, or on-site profiles obtained for site-specific model application. The NWS data are obtained from the National Climate Center (NCC) on their TDF5600 series data tapes. When the NWS data are used, program READ56 reads the TDF5600 tape, checks for missing data, and reformats the wind, temperature, and pressure data. At this point, the user must ensure that missing data is properly flagged. When on-site data are used, the user is responsible for formatting the data and flagging missing or bad data.

All source, receptor, and program control data are entered by card deck. The control information determines which algorithms are to be used in the computations and what sort of program output is desired.

Prior to execution, an unformatted look-up table of intermediate PFM computations must be prepared for use with the PFM-Long option. A formatted file of this table accompanies the COMPLEX/PFM source code. Program SETUP (lower right on Figure 1) converts this file to the form needed at execution time. SETUP must be run only once, when the model is first compiled on a new system.



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Figure 1. The COMPLEX/PFM modeling system.

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1.4 Summary of Data Required for PFM Options

Four types of input data are required for the COMPLEX/PFM dispersion model:

o meteorological data,

o source data,

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- o receptor data, and
- o program control parameters.

Most of this data is needed by the host model and therefore has been described at length in the MPTER user's guide (Pierce et al. 1980). Only those data required to operate the PFM option will be discussed here.

1.4.1 Meteorological Data

The PFM option requires hourly temperature and wind profiles. These are interpolated from twice daily observations in program PROFIL. When short periods of time are simulated, the user should analyze these profiles by hand and create the hourly sequence file directly. The hourly data should include:

the number of data levels,
the mixing height (m),
the height of each data level (m),
the wind speed (m/s) and wind direction from which the wind blows (degrees from North) at each data level, and
the temperature at each data level (°K).

1.4.2 Source Data

The PFM option requires the same source data as COMPLEX I and II, but two restrictions are imposed:

- o no more than 50 point sources are allowed and
- o all sources must be placed at the same location (as in CRSTER).

1.4.3 Receptor Data

A total of 180 receptors may be used with the PFM option. These must be aligned along rays from the source. The position and number of receptors along any ray is independent of the position and spacing of receptors on other rays. Also, the angular spacing between rays need not be regular.

The receptor information required for PFM-Long includes:

- o coordinates of the origin (source location)(user units),
- o receptor name,
- o receptor bearing and distance (user units),
- o receptor height above terrain (user units),
- o the height of terrain above sea level at receptor position (user units),
- o relief height of controlling terrain feature (user units),

- the distance between the source and the controlling terrain feature (user units), and
- o the obstacle shape code that best describes the controlling terrain shape.

When PFM-Short is invoked, additional obstacle information is needed:

- source coordinates relative to the obstacle coordinate system (user units),
- o the relief height of the terrain feature (user units),
- the angle of rotation from North of the obstacle coordinate system (degrees clockwise),
- cross-wind and along-wind obstacle aspect ratios, if the obstacle is a hill, and
- o the bluff shape code, if the obstacle is a bluff.

1.4.4 Program Control Parameters

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COMPLEX/PFM requires one more program control parameter than needed to run COMPLEX I or COMPLEX II. The PFM option is set by option number 26. A value of one (1) will invoke the PFM-Long algorithm, whereas a value of two (2) will invoke the PFM-Short option. If zero is specified, no PFM computations will be done.

SECTION 2

TECHNICAL DESCRIPTION

2.1 Introduction

COMPLEX/PFM is a modified version of COMPLEX (I and II) which contains an option for potential flow computations. The potential flow computations are derived from PFM. Section 2 presents the theoretical background of PFM and the method of implementing the theory within the framework of the COMPLEX model system.

Section 2.2 contains a description of the diffusion theory appropriate for deforming potential flow streamlines and the methods of solution for potential flows over isolated simple bluffs and hills. It also describes how computations based on the theory are used to modify the flat terrain Gaussian diffusion equation. Section 2.3 presents a description of the PFM option within COMPLEX. Both the long-term and short-term versions are discussed.

Sections 2.4 and 2.5 deal with data requirements for COMPLEX/PFM. The need for hourly temperature and velocity profiles requires a new meteorological preprocessor to interpolate twice-daily profile observations when more frequent soundings are unavailable. Section 2.4 describes how the preprocessor interpolates between soundings to produce hourly soundirg information. Section 2.5 provides guidance in specifying bluff shapes and ellipsoid aspect ratios to represent real terrain features.

2.2 The Potential Flow Model

2.2.1 Diffusion Theory

The potential flow complex terrain model incorporates the theory developed by Hunt and Mulhearn (1973) and Hunt and Snyder (1978) for turbulent plumes embedded within potential flow fields. They developed solutions to the diffusion equations describing flow fields over two-dimensional and three-dimensional axisymmetric terrain obstacles. Qualitatively, these solutions are of Gaussian form, with crosswind and vertical dispersion coefficients evaluated as line integrals of the velocity field along the plume centerline trajectory. Because the mathematics used are not immediately familiar, some details of the derivation are presented; the reader is urged to consult the original references. The modeling technique applies potential flow theory to a Gaussian point source model. It permits explicit evaluation of the terrain-induced kinematic constraints and trajectory variations. In adopting the present technique, an attempt has been made to broaden its applicability. Approximations have been developed to extend the neutral formulation to slightly stable cases and to allow for three-dimensional terrain obstacles that are not axisymmetric. This approach is suggested for the following topographic and meteorological situations:

- o isolated, simple bluffs of arbitrary height and slope and simple hills of arbitrary height and arbitrary aspect ratio in the crosswind and downwind directions, and
- o neutral to slightly stable density stratifications.

At the outset, the limitations of the potential flow model should be stressed. These limitations arise mainly from physical effects that are not described by the model:

- o The presence of a realistic surface boundary layer is ignored.
- Relevant physical phenomena such as velocity shear, radiative heating, and flow separation are omitted.
- o The theoretical model requires that the plume remain "thin" compared to its height above the terrain. This criterion is often violated near the hill crest.

[Strictly speaking, the first two of these limitations also restrict the theoretical validity of a conventional Gaussian solution in <u>flat terrain</u> <u>situations</u> (Pasquill 1978), unless the set of dispersion coefficients specifically accounts for these effects.] It is prudent to apply the potential flow theory approach only to the windward side of obstacles and not to situations dominated by lee wake or separation effects not treated by potential flow theory. In many cases, the computed plume dimension will violate the restriction to "thin plumes", but it is not unreasonable to "stretch" the theoretical formulation in these cases (Hunt, Puttock, and Snyder 1979, Bass et al. 1981).

Two-Dimensional Obstacles

The starting point for the calculation is the two-dimensional advection diffusion equation in the streamline coordinate system (s,n,y):

$$u(s) \quad \frac{\partial C'}{\partial s} + n \frac{\partial v}{\partial n} \frac{\partial C'}{\partial n} = D_1(s) \frac{\partial^2 C'}{\partial n^2} + D_2(s) \frac{\partial^2 C'}{\partial v^2}$$
(2-1)

Here s, n, and y are dimensionless directional coordinates in the along plume, normal (nearly vertical), and crosswind directions relative to the plume trajectory. When the terrain is flat and the trajectory is level, the s and n directions correspond to the downwind distance, x, and the vertical distance from plume centerline, z. In Equation 2-1, u and v are velocities along and normal to the trajectory, and $D_1(s)$ and $D_2(s)$ are diffusivities in the n and y directions that vary along the trajectory. C' is the dimensionless concentration. The variables in Equation 2-1 are nondimensionalized by the height of the obstacle, a, and the uniform velocity upwind of the source, U_∞, so that:

$$C' = C U_{\infty} a^2/Q \qquad (2-2a)$$

$$u(s) = U(s)/U_{\infty} \qquad (2-2b)$$

$$v_{\rm V}(s) = V(s)/U_{\rm co} \qquad (2-2c)$$

$$D_1(s) = K_1(s)/[aU_{\infty}]$$
 (2-2d)

$$D_2(s) = K_2(s)/[aU_{\infty}]$$
 (2-2e)

where Q is the source strength (mass/unit time), U(s) and V(s) are the dimensional velocities (length/unit time), and $K_1(s)$ and $K_2(s)$ are the dimensional diffusivities (length squared/unit time). The relationship between these diffusivities and the PGT dispersion cc fficients (Turner 1970) will be discussed later.

Substituting the continuity equation:

$$\frac{\partial v}{\partial n} + \frac{\partial u}{\partial s} = 0 \qquad (2-3)$$

into Equation 2-1 yields:

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$$u(s) \quad \frac{\partial C'}{\partial s} - n \frac{\partial u}{\partial s} \frac{\partial C'}{\partial n} = D_1(s) \frac{\partial^2 C'}{\partial n^2} + D_2(s) \frac{\partial^2 C'}{\partial v^2}$$
(2-4)

Solutions to Equation 2-4 are sought that are Gaussian in form:

$$C'(s,n,y) = \frac{1}{g(s)} \exp \left[-f_1(s) n^2 - f_2(s) y^2\right]$$
 (2-5)

and also satisfy the additional constraint that the mass flux across the plume is constant, i.e.:

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} u(s) C' dn dy = 1.0 \qquad (2-6)$$

This constraint requires that:

$$g(s) = \pi u(s) / [f_1(s) f_2(s)]$$
(2-7)

Substituting Equation 2-5 into 2-4 yields:

$$f_1(s) = [u(s)]^2 / [4\phi(s)]$$
 (2-8a)

$$f_2(s) = 1/[4T(s)]$$
 (2-8b)

where:

$$\phi(s) = \int_{0}^{s} D_{1}(s') u(s') ds' \qquad (2-3)$$

and

$$T(s) = \int_{0}^{s} [D_2(s')/u(s')]ds'$$
 (2-10)

By Equation 2-7:

$$g(s) = 4\pi [\phi(s) T(s)]^{1/2}$$
 (2-11)

In more familiar terms, the dispersion coefficients in the Gaussian form of the diffusion equation solution, σ_n and σ_y , are given by:

$$f_1(s) = 1/[2\sigma_n^2]$$
 (2-12a)

$$f_2(s) = 1/[2\sigma_y^2]$$
 (2-12b)

$$\sigma_n^2 = 1/[2 f_1(s)] = 2\phi (s)/[u(s)]^2$$
 (2-13)

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$$\sigma_y^2 = 1/[2 f_2(s)] = 2T(s)$$
 (2-14)

Three-Dimensional Axisymmetric Obstacles

or or

The arguments for three dimensions proceed much the same as in the previous section. The appropriate non-dimensional diffusion equation is:

$$u(s) \frac{\partial C'}{\partial s} + n \frac{\partial v}{\partial n} \frac{\partial C'}{\partial n} = D_1(s) \frac{\partial^2 C'}{\partial n^2} + D_2(s) \frac{\partial^2 C'}{\gamma^2} \quad (2-15)$$

where the coordinate system is now with respect to (s,n,γ) . Here, γ is the angular, azimuthal coordinate from the axis of symmetry along the flow with:

$$y \simeq \gamma R(s)$$
 (2-16)

where R(s) is the distance from the axis of symmetry of the obstacle to the plume centerline, and y is the crosswind distance from the plume centerline. The continuity equation in this coordinate system becomes:

$$\frac{\partial \mathbf{v}}{\partial \mathbf{n}} + \frac{1}{\mathbf{R}(s)} \frac{\mathrm{d}}{\mathrm{d}s} \left[\mathbf{u}(s) \mathbf{R}(s) \right] = 0 \qquad (2-17)$$

The trial solution sought is of the form:

$$C'(s,n,\gamma) = \frac{1}{g(s)} \exp[-f_1(s) n^2 - f_2(s)\gamma^2]$$
 (2-18)

subject to the constraint:

.

$$\int_{0}^{2\pi} \int_{-\infty}^{+\infty} u(s)C'(s,n,\gamma)R(s) dnd\gamma = 1.0$$
(2-19)

Substitution of Equation 2-18 into 2-15 yields:

$$f_1(s) = [u(s)R(s)]^2 / [4\phi(s)]$$
 (2-20a)

$$f_2(s) = 1/[4T(s)]$$
 (2-20b)

where

$$\phi(s) = \int_{0}^{s} D_{1}(s') [R(s')]^{2} u(s') ds' \qquad (2-21)$$

$$T(s) = \int_{0}^{s} [D_{2}(s')/[u(s') R^{2}(s')]]ds' \qquad (2-22)$$

and substitution of Equations 2-18 and 2-20 into 2-19 gives:

$$g(s) = 4\pi [\phi(s) T(s)]^{1/2}$$
 (2-23)

The forms of the familiar Gaussian dispersion coefficients are obtained by substituting Equation 2-20 into Equation 2-12a and b:

$$\sigma_{n}^{2} = 2 \phi(s) / [u(s) R(s)]^{2} \qquad (2-24)$$

$$\sigma_y^2 = 2 [R(s)]^2 T(s)$$
 (2-25)

PGT Scaling of Dispersion Coefficients

Evaluating the terrain-influenced dispersion coefficients (Equations 2-13, 2-14 and 2-24, 2-25) with this formulation requires specifying the crosswind and the normal diffusivities, D_2 and D_1 . To compare model calculations with analogous flat terrain situations, an approximation scheme was implemented, using the PGT dispersion coefficients (Turner 1970) as a calibrating scale. Other dispersion coefficient systems can be easily incorporated within the basic methodology used here.

Qualitatively, the diffusivity at a given distance from the source along the plume centerline streamline is taken as that for the same transit time in flat terrain. The consequence of this assumption is that model calculations of dispersion coefficients reduce to flat terrain values in the limits of large downwind distances or small obstacles. Substituting Equations 2-21 and 2-22 into Equations 2-24 and 2-25 gives explicit expressions for σ_z and σ_y . (From here on, the dispersion coefficient in the normal direction is denoted as σ_z .) At a distance, s, from the source along the streamline, the dispersion coefficients are given by:

$$\sigma_{z}^{2}(s) \simeq \frac{2 \overline{D}_{1}(s)}{u^{2}(s) R^{2}(s)} \int_{0}^{s} R(s') u(s') ds' \qquad (2-26)$$

$$\sigma_{y}^{2}(s) \simeq 2R^{2}(s) \overline{D}_{2}(s) \int_{0}^{s} ds' / [R^{2}(s') u(s')]$$
 (2-27)

where $\overline{D_1}$, $\overline{D_2}$ are typical mean diffusivity values at distance s.

These values are assumed to be given by the PGT values ($\sigma_{zf},$ $\sigma_{yf}):$

$$\overline{D}_{1}(s) \simeq \sigma_{zf}^{2}(s)/2t \qquad (2-28)$$

$$\overline{D}_{2}(s) \simeq \sigma_{yf}^{2}(s)/2t \qquad (2-29)$$

where s is the integrated path length along the plume trajectory and t is the advection time:

$$s \approx \int_{0}^{s} ds' \qquad (2-30)$$

$$t = \int_{0}^{s} \frac{ds'}{u(s')}$$
 (2-31)

Substituting Equations 2-28 through 2-31 into Equations 2-26 and 2-27 yields the final form of the dispersion coefficients:

$$\sigma_z^2 \simeq \sigma_{zf}^2 \begin{bmatrix} \int_{0}^{s} R^2(s') u(s') ds' \\ 0 \\ t u^2(s) R^2(s) \end{bmatrix}$$
(2-32)

$$\sigma_{y}^{2} \simeq \sigma_{yf}^{2} \left[\frac{R^{2}(s)}{t} \int_{0}^{s} \frac{ds'}{R^{2}(s') u(s')} \right]$$
(2-33)

The bracketed quantities approach 1 as streamline deformation becomes negligible, and σ_z , σ_v reduce to their flat terrain values.

Figures 2 and 3 illustrate the plume spread statistics σ_y and σ_z , respectively, for neutral flow over a circular ridge. The ridge is 1.0 km high; the point source, 200 m high, is 4.5 km from the ridge center. Calculations are shown for diffusivities scaled to reproduce the PGT neutral stability class values for σ_y , and σ_z in the flat terrain case. This illustrates that only the vertical dimensions of the plume (as characterized by σ_z) differ from flat terrain values in flow over two-dimensional obstacles. (In each of Figures 2 through 5, the center of the ridge is indicated by a short vertical bar at the downwind distance 4.5 km; the horizontal bar extending from 3.5 km to 5.5 km denotes the windward-leeward extent of the ridge.)

As streamlines diverge to the leeward and windward side of the hill, σ_z increases. Over the ridge, vertical compression of the streamlines leads to a drastic decrease in σ_z . Over the ridge crest the vertical plume thickness is about equal to the height of the plume centerline above the surface, n_s . This marginally obeys the thin plume approximation.

With the same source-obstacle geometry retained, but the terrain obstacle type changed from a circular ridge to a hemispherical hill, Figures 4 and 5 display the three-dimensional neutral flow results developed from Equations 2-24 and 2-25. In this case, both σ_y and σ_z are affected by the potential flow field, as evidenced by a marked increase in σ_y over the hill top. Comparing σ_z values in Figures 2 and 4 at x = 4.5 km reveals that the vertical thickness of the plume is more severely restricted in three-dimensional flow than two-dimensional flow. In fact, as indicated ia Figure 5, downwind of the hill σ_z never recovers from the deformation over the hill top.

Figure 6 shows the evolution of the velocity speed-up factor (the ratio of the source streamline velocity in the presence of the hill to that in the absence of the hill) for potential flows over the circular ridge and over



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Figure 3. Vertical dispersion coefficients for neutral flow over a circular ridge.



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Figure 5. Vertical dispersion coefficients for neutral flow over a hemispherical hill.

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Figure 6a. Velocity speed up factors for neutral flow over a circular ridge.



Figure 6b. Velocity speed up factors for neutral flow over a hemispherical hill.

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the hemispherical hill. Both streamline patterns upwind and downwind of the obstacle crests are symmetric; therefore, the speed-up factor has been plotted only from source to crest. The theoretical speed-up value at the surface of each of the crests is 2.0 for the cylindrical ridge, and 1.5 for the hemispherical hill. Because the source streamline does not touch the surface at the crest, the surface speed-up values are approached, but not attained, in Figure 6. Note that the influence of the cylindrical ridge extends farther upstream (and downstream) than does the influence of the hemispherical hill.

2.2.2 PFM Factors

The discussion of the previous section presented the theory used in PFM for calculating concentrations on the surface of a simple obstacle, when a potential flow streamline trajectory had been computed. The method for scaling diffusivities using sigma-curves (e.g. PGT) was also presented. This scaling approach provides a simple way of quantifying the plume deformations predicted by PFM so that "PFM-like" computations can be simulated within other Gaussian plume models.

The Gaussian plume equation for surface concentrations under unlimited mixing conditions for level terrain is:

$$C = 2 C_0 \exp(-0.5(H/\sigma_z f)^2) \exp(-0.5(y/\sigma_y f)^2)$$
(2-34)

where

$$C_{0} = Q/(2\pi \sigma_{vf} \sigma_{zf} u_{\infty})$$
(2-35)

and

Q	**	pollutant emission rate
uco	=	wind speed
H	=	plume height above the surface
у	=	lateral distance to plume centerline
σzf	2	standard deviation of concentration in the vertical (flat terrain)
σyf	=	standard deviation of concentration in the horizontal (flat terrain)

The corresponding equation in the PFM for a plume near an obstacle is Equation 2-5 (or 2-18). However, when the functions g(s), $f_1(s)$, and $f_2(s)$ are rewritten in terms of u(s), $\sigma_z(s)$, and $\sigma_y(s)$ the form of Equation 2-5 (or 2-18) is the same as Equation 2-34:

$$C_h = 2 C_{oh} \exp(-0.5(n/\sigma_z(s))^2) \exp(-0.5(y/\sigma_y(s))^2)$$
 (2-36)
where

$$C_{oh} = Q/(2\pi\sigma_{y}(s) \sigma_{z}(s) u(s))$$
(2-37)

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The subscript h is introduced to denote a "hill" value.

This equation can be rewritten further in terms of the flat terrain equation and ratios of sigmas, velocity, and plume height when Equations 2-34 and 2-35 are combined with Equations 2-36 and 2-37:

$$C_{h} = 2C_{oh} \exp(-0.5(\frac{H}{\sigma_{zf}})^{2} (\frac{n(s)\sigma_{zf}}{H\sigma_{z}(s)})^{2}) \exp(-0.5(\frac{y}{\sigma_{yf}})^{2} (\frac{\sigma_{yf}}{\sigma_{y}(s)})^{2}) (2-38)$$

$$C_{oh} = Q/(2\pi \sigma_{yf} \sigma_{zf} u_{\infty} - \frac{\sigma_{y(s)} \sigma_{z(s)} u_{(s)}}{\sigma_{yf} \sigma_{zf} u_{\infty}})$$
(2-39)

Now the utility of the sigma scaling is apparent. Ratios n(s)/H and $u(s)/u_{\infty}$ are computed from potential flow theory within PFM. Ratios of the sigmas are readily found according to Equations 2-32 and 2-33 and their properties have already been discussed. For convenience, four PFM "factors" are defined in terms of these quotients:

$$CFAC(s) = \frac{\sigma_y(s) \sigma_z(s) u(s)}{\sigma_{vf} \sigma_{zf} u_{\infty}}$$
(2-40a)

$$S2FAC(s) = \sigma_z(s)/\sigma_{zf}$$
(2-40b)

$$SYFAC(s) = \sigma_{y}(s)/\sigma_{yf} \qquad (2-40c)$$

$$HFAC(s) = n(s)/H$$
 (2-40d)

These factors are independent of wind speed and dispersion parameters. They depend only on the source-terrain geometry, receptor distance, and the density stratification of the atmosphere. Hence, more complicated computations such as plume trapping and buoyant plume enhancement may readily extend the usefulness of PFM computations. In particular, these PFM factors are central to the PFM option within COMPLEX, as discussed in Section 2.3.2.

2.2.3 Plume Trajectory Analysis - Neutral Flow

Streamlines are computed for two basic obstacle shapes in PFM – a two-dimensional bluff and a three-dimensional ellipsoid. In each case, the shape is kept simple to minimize computer costs. Although few real terrain features resemble pure ellipsoids or simple bluffs, it should be remembered An that potential flow itself is an approximation to the wind field over the earth's surface. The intent of the model is to compute first-order changes in the plume trajectory and shape as it passes over major terrain obstacles.

Flow Over a Bluff

Potential flow is non-divergent flow of a constant density fluid without vorticity. The only condition placed on the velocity field of such a flow near a solid surface is that there should be no velocity component into the surface. This means that the velocity component normal to the surface must be zero. The component parallel to the surface may take on any value. Therefore, the surface must represent a streamline of the flow and conversely, any streamline of the flow may be considered a solid surface.

This property of potential flow is used to generate streamlines for flow over a family of bluff shapes. The basic solution contained in PFM is for flow over a step (Milne-Thomson, 1960). However, by considering any streamline of this solution as a possible solid surface, the PFM actually contains an infinite nuber of bluff shapes. Of the twenty shapes explicitly incorporated, each streamline has its own characteristic slope (they range from 0.15 to 3.2). A user only has to select the shape most like the terrain feature to be modeled. Section 2.5 contains instructions for selecting the most appropriate bluff shape.

Caution must be used in applying potential flow theory to very steep bluffs. As the bluff face becomes steeper, the probability of streamline separation and secondary circulation increases. The potential flow solution completely neglects these effects and therefore becomes inappropriate. In fact, the theoretical velocity field close to the crest of the step feature tends to infinity. Consequently, the maximum bluff slope represented in PFM is about 3:1.

The solution to the step problem requires complex variables and the final equations are transcendental functions of a complex parametric variable, t. Let RT be the real part of t, and MT be the imaginary part of t; then:

π Ψ/(U∞h) =	(sinh RT)(sin MT)	(2-41a)
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 $\pi x/h = RT + (\sinh RT)(\cos MT)$ (2-41b)

 $\pi y/h = MT + (\sin MT)(\cosh RT) \qquad (2-41c)$

$$u = Real (SP)$$
(2-41d)

$$v = -Imag (SP)$$
(2-41e)

$$SP = \left[-U_{\infty} \frac{\cosh t - 1}{\cosh t + 1} \right]^{1/2}$$
(2-41f)

$$\cosh t = (\cos MT)(\cosh RT) + i (\sin MT)(\sinh RT)$$
 (2-41g)

In these equations, x and y are the space variables in the horizontal and vertical directions, respectively; ψ is the streamfunction, a constant along a particular streamline; u and v are the velocity components along the streamline. Their values depend upon the height of the step (h), and the upstream velocity (U_m) (see Figure 7).

An iterative technique (Newton-Raphson) is used to evaluate a streamline trajectory and the along-streamline velocity. A value for the streamfunction (Ψ) is defined when a bluff shape is specified, and numerous points along the x-axis are specified between the source position and the position of the last downwind receptor. For each x, RT and MT are evaluated through iteration using Equations 2-41a and b. Then the streamline height (y) and the velocity (u,v) are computed.

This process works only when U_{∞} and h are properly specified, because the streamfunctions used in PFM correspond to the particular choices $U_{\infty} = 2$ and h = 100. Therefore, user's dimensions are rescaled into "step space" for computation of the streamline coordinates and velocities and then scaled back again before the PFM line integrations are performed.

As shown in Figure 7, the scaling process depends on which bluff shape is chosen. Equations 2-41a through 2-41g are based on a coordinate system with its origin at the base of the step. The heights of all streamlines are measured from this reference point. The operational bluff height in any application, however, is measured from the upwind height of what is labeled the surface streamline. The net height change (DH) of this streamline between a position 100 step heights upwind of the step and a position 2 step heights downwind of the step is defined as the scaling measure for the bluff height and plume height in the real setting. This model bluff height (DH) decreases as surface streamlines farther from the origin are chosen (smaller slopes).

In practice, PFM scales all space dimensions by the hill (bluff) heights, and it scales all velocities by the mean flow speed. This is done at the start of the program. When the plume path over a particular bluff is later computed, all length scales are multiplied by DH, and the new velocity is multiplied by U_{∞} (=2). This transforms the flow speed, source location, plume height, and bluff height into the dimensional units of "step space." The scaled plume height at the source is then added to the height of the surface streamline at the source position, and the streamline through this point (the plume streamline) is obtained. Once the series of points along this streamline and the corresponding velocity components are calculated, the height of the bluff base (indicated by the dashed line in Figure 7) is subtracted from the streamline height, and old lengths and velocities are made nondimensional once again by dividing by DH and U_{∞} .

This analysis has been based on the two-dimensional problem of flow normal to an infinitely wide terrain obstacle. Because flows of oblique incidence are just as likely to occur, a simple geometric approximation has been incorporated in PFM.



Figure 7. Plume path and surface streamlines derived from flow over a step.

As the angle between the wind direction and the direction normal to the crest line becomes nonzero, trajectory distances to the crest increase. The trajectory no doubt tends to curve along the face of the bluff somewhat before sweeping back over the crest. Also, the effective slope of the bluff face along the trajectory changes. If the streamline curvature is neglected, then the problem remains two-dimensional and can be handled in the model by changing the source to obstacle distance and by changing the effective bluff shape. Each of these changes depends on the cosine of the wind angle. When the geometry is altered and a new bluff shape is computed, the plume trajectory analysis along the wind direction proceeds as before.

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Flow Over an Ellipsoid

The general case of flow over an ellipsoid of arbitrary shape is neither two-dimensional nor axisymmetric. Consequently, a unique streamfunction cannot be defined for each streamline as it was in the bluff analysis. This means that streamline trajectories must be generated by selecting a point in space, solving for the velocity at that point and moving a short distance along the indicated trajectory to select another point, and start the process over again.

Outside an ellipsoid moving along its positive x-axis at a speed U_{∞} in a fluid at rest, the velocity at any point is derived from the velocity potential Φ (Lamb, 1945).

$$\Phi = K \times \int_{\lambda}^{\infty} \frac{d\lambda'}{(a^2 + \lambda')\Delta}$$
(2-42a)

$$\Delta = ((a^2 + \lambda')(b^2 + \lambda')(c^2 + \lambda))^{1/2}$$
 (2-42b)

when the equation of the ellipsoid surface is:

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$$
 (2-43)

The integral is a function of the elliptic coordinate λ , defined in terms of x, y, z, a, b, and c by :

$$\frac{x^2}{a^2+\lambda} + \frac{y^2}{b^2+\lambda} + \frac{z^2}{c^2+\lambda} = 1$$
 (2-44)

26

Hence, λ = constant corresponds to one of a family of confocal ellipsoids, with λ = 0 being the surface of the obstacle. The constant K also involves an integral over λ :

$$K = a b c U_{\infty}/(2 - A_0)$$
 (2-45a)

$$A_{o} = abc \int_{0}^{\infty} \frac{d\lambda'}{(a^{2} + \lambda')\Delta}$$
(2-45b)

Having obtained the velocity potential, the velocity of the fluid surrounding this translating ellipsoid is:

$$(\mathbf{u}, \mathbf{v}, \mathbf{w}) = (\partial \Phi / \partial \mathbf{x}, \partial \Phi / \partial \mathbf{v}, \partial \Phi / \partial \mathbf{z})$$
(2-46)

This relationship changes when the ellipsoid is stationary and when the fluid is moving along the positive x-axis at a speed U_{∞} :

$$(u, v, w) = (\partial \Phi / \partial_X + U_{\infty}, \partial \Phi / \partial_Y, \partial \Phi / \partial_Z)$$
(2-47)

This is the form used in PFM to address air flow over ellipsoidal obstacles.

When the wind is not directed along the x-axis, the incident flow has a v-component as well as a u-component. In that case, velocities due to each component are calculated separately, then added together. The solution for flow along the y-axis may be written from symmetry with Equations 2-42 and 2-45:

$$\Phi = K y \int_{\lambda}^{\infty} \frac{d\lambda^{4}}{(b^{2} \cdot \lambda^{4})\Delta}$$
(2-48a)

$$K = a b c V_{\infty} / (2 - B_0)$$
 (2-48b)

$$B_{0} = a b c \int_{0}^{\infty} \frac{d\lambda'}{(b^{2} + \lambda')\Delta}$$
(2-48c)

The velocity is obtained again from derivatives of the velocity potential Φ :

$$(u, v, w) = (\partial \Phi / \partial x, \partial \Phi / \partial y + V_{\infty}, \partial \Phi / \partial Z)$$
(2-49)

It is important to emphasize that computed plume trajectories over these arbitrary ellipsoids are approximate because a streamfunction cannot be specified. The local velocity-increment scheme will either undershoot or overshoot the actual trajectory each time the tangential velocity is used to advance to the next point. The accuracy attained is directly related to the density of sampling points and the curvature of the flow.

2.2.4 Plume Trajectory Analysis - Stratified Flow

Potential flow trajectory solutions presented in Section 2.2.3 are appropriate for neutral density stratification only. Ambient stratification can significantly affect plume behavior and resultant atmospheric pollutant concentrations. For moderate plume heights relative to hill size and for moderately stable stratification, laboratory experiments suggest that the plume will go over the top of the hill, but the path of the plume will be closer to the surface and the flow over the crest will be faster than in neutral flow. For small plume heights under strong stratification, the plume will tend to go around the hill rather than over it. If the hill is a long ridge, the flow may be "blocked" and stagnate upwind. To approximate first-order effects of moderate stratification, results of EPA Fluid Modeling Facility (FMF) experiments on plume behavior in a stratified water channel flow over a polynomial hill (Hunt et al. 1978) have guided the development of a streamline modification algorithm.

Stratification is assessed in terms of the Froude number (FR) based upon the hill height (H):

$$FR = \frac{U_{\infty}}{NH}$$
(2-50a)
N = [(g/ θ)($\partial \theta$ / ∂z)]^{1/2} (2-50b)

When FR is small, the density layering is strongly stable compared to the kinetic energy of the flow and vertical motion on the scale of the hill height is suppressed. This is the case of strong stratification. If FR is very large, density stratification has little effect on vertical motion over the hill and the flow is said to be neutral.

Experimental results of the FMF tow-tank experiments on plume behavior in stratified flow over a polynomial hill are reproduced in Figure 8 (Hunt et al. 1978). The height of a streamline at the hill crest (n_s) is shown as a function of stack height (H_s) for various stratifications denoted by Froude number, FR, including the neutral flow case, FR = ∞ . For any given stack height and Froude number, the height of the streamline at the hill crest can be compared with the neutral flow case. To calculate the streamline displacement at positions upwind of and over the hill crest in the model, an aproximation is made.



Source: Hunt et al. 1978

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Figure 8. Height of the source streamline (n_S) above the hill crest (height = a) for various stack heights (H_S) and Froude numbers (F_r).

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Call the streamline lift at the crest in neutral flow L_n . Then an approximate form with the right asymptotic limits (L_n and U_{∞}/N) for the streamline lift in stratified flow (L) is:

$$L = FR H/(1 + FR H/L_n)$$
 (2-51)

Because the neutral lift is also known away from the hill crest from the potential flow solutions, Equation 2-51 is assumed to hold everywhere. Note that as L_n becomes vanishingly small far from the hill, L goes to zero as well.

PFM keeps track of the actual streamline trajectory, not the streamline lift near the hill. Therefore, Equation 2-51 is transformed from a lift expression to a depression expression:

$$D_0 = L_n - L = L_n / (1 + FR_L)$$
 (2-52a)

 $FR_{L} = FR (H/L_{n}) = U_{\infty}/(NL_{n}) \qquad (2-52b)$

In the neutral limit where $U_{\infty}/N >> L_n^2$, D_o approaches zero, and no stratification effects are simulated. In the strongly stratified limit where $U_{\infty}/N << L_n$, D_o approaches $L_n - U_{\infty}/N$, the difference between the neutral streamline deflection, and the length scale for vertical deflections in stratified flow. When L_n is zero, so is D_o .

Application of D_0 to potential flow streamlines tends to "relax" vertical streamline deflections around a hill with increasing stratification, without regard for the consequences of allowing streamlines to pass through the hill. Although some of the flow should not pass over the crest for Froude numbers less the one, comparison of Equation 2-52 with Figure 8 shows that the computed relaxation is much too severe. Streamlines are straightened out too rapidly with increasing stratificaton. The expression for D_0 must include some adjustment for the presence of the hill.

An adjustment region of order U_{∞}/N close to the hill surface is missing in Equation 2-52. This is the length scale in which significant vertical motion is allowed. All streamlines that rise over the hill must be compressed into this region. This adjustment region is incorporated in the depression equation (2-52a) by adding an exponential adjustment factor. The factor is ad hoc and merely requires the computed depression to tend toward zero when the neutral streamline passes very close to the obstacle (compared to the length scale U_{∞}/N). If the neutral streamline is several scale heights above the local surface, the correction factor tends to 1 and the depression is equal to D_0 . The corrected streamline depression is called D:

$$D = D_0 (1 - \exp(-\ell/FR H))$$
 (2-53)

where L is the local neutral streamline height above the obstacle.

When the streamline height is adjusted using Equation (2-53), the along streamline velocity must be recomputed. Conservation of mass indicates that the ratio of the stratified flow velocity (u_8) to that in neutral flow (u_n) depends upon the vertical rate of change of the streamline depression:

$$\frac{u_s}{u_n} = 1/(1 - \frac{dD}{dz})$$
(2-54)

Furthermore, a change in the trajectory requires a redistribution of the along-streamline wind speed among the u, v, w, components so that the velocity still points along the streamline. PFM adjusts the streamline wind speed according to Equation 2-54 and then computes the individual components based upon the slopes of the depressed streamline trajectory.

2.3 The COMPLEX/PFM Option

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The COMPLEX models (COMPLEX I and COMPLEX II) are multiple point source sequential terrain models formulated by the Complex Terrain Team at the EPA Workshop on Air Quality Models held in Chicago in February, 1980. COMPLEX I is a univariate Gaussian horizontal sector-averaging model (sector width = 22.5°), while COMPLEX II computes off-plume-centerline concentrations according to a bivariate Gaussian distribution function. Both models are very closely related to the MPTER model in both structure and operation. Anyone who is not familiar with either COMPLEX or MPTER should consult the MPTER user's manual (Pierce, et al. 1980).

Terrain treatment in COMPLEX varies with stability class. Neutral and unstable classes use a 0.5 terrain adjustment, while stable classes use no terrain adjustment when the recommended options are selected. With 22.5° sector averaging, COMPLEX I performs sequential VALLEY plume impingement calculations for stable cases. COMPLEX II plume impingement calculations are similar, with the exception that sector averaging is not used.

COMPLEX/PFM has the ability to utilize PFM calculations for neutral to moderately stable flows. The PFM option invokes either COMPLEX I, COMPLEX II, or PFM computations depending upon the stability class and the Froude number. Unlike previous versions, however, all sources must be located at the same point (as in CRSTER).

COMPLEX II is invoked whenever the stability class is either 1, 2, or 3 (A, B, or C), regardless of the Froude number. In these cases plume growth is rapid and the details of terrain adjustment are not so important. A 0.5 terrain adjustment is an adequate representation of average plume behavior. PFM is invoked for stability classes 4, 5, and 6 (D, E, and F) whenever the flow along the plume streamline has enough kinetic energy to rise against the stable density gradient and surmount the highest terrain elevation along the wind direction. Such a plume is said to be above the critical dividing streamline of the flow (Section 2.3.3).

COMPLEX I is invoked whenever the plume is found to be beneath the critical dividing streamline of the flow. Plumes beneath the dividing streamline no longer pass over the terrain peak and therefore may impinge on the face of the the hill somewhere. Thus, the PFM option defaults to VALLEY-like computations for impingement cases. This can potentially occur in conjunction with stability classes 4, 5, and 6; but, class 4 occurrences may be rare.

The PFM option enhances the ability of COMPLEX to perform complex terrain Gaussian plume dispersion computations in two important areas. Firstly, it incorporates plume deflections and distortions derived from potential flow theory. This enhancement approximates at least first-order terrain effects on plume geometry. And, because the streamline computations vary with obstacle shape, plume height and Froude number, plume distortions are coupled directly to meteorological variations and the approximate terrain geometry in a way that no single terrain adjustment could be. Secondly, the use of the PFM option requires vertical temperature and velocity information to characterize the Froude number, the critical dividing streamline, and stable plume rise. Availability of the Froude number and the dividing streamline removes the assumption of coupling between the surface dispersion stability class and the dynamics of the flow aloft at plume elevation under stable conditions. It is not necessary to identify plume impingement with class E or F dispersion conditions.

Elements of the PFM option are presented in the following sections. Section 2.3.1 explains how PFM computations are made in both a long- and short-term version of COMPLEX/PFM; Section 2.3.2 summarizes the plume rise computations; Section 2.3.3 addresses the computation of dividing streamlines and Froude numbers and their use in the model; Section 2.3.4 describes incidental changes to COMPLEX required for the PFM option.

2.3.1 PFM Option: Long and Short

Two PFM option choices are provided in COMPLEX/PFM. The short-term option calls PFM as a subroutine and is designed for critical period analyses in which 3-hour or 24-hour concentrations near one particular terrain feature are to be evaluated. The long-term option searches a look-up table of intermediate PFM results and is designed to be run for a full year of sequential hourly meteorological data, producing concentrations and concentration statistics for up to 180 receptors. It may have as many terrain features as there are receptors. The long-term version of the PFM option should be used as a sequential analysis model for calculating annual average concentrations, for siting air quality monitors, and for identifying those periods within the meteorological data which produce the highest predicted concentrations.

PFM-Long

PFM-Long is constructed around a series of PFM calculations for 5 plume heights, 6 Froude numbers, and 20 discrete obstacles shapes. It is not designed to reproduce actual PFM results for the specific plume heights, meteorological conditions, and obstacle shapes of a particular application. Instead, it is designed to provide credible, conservative approximations.

All of the PFM computations in the look-up table assume that the plume travels directly over the crest of the obstacle, perpendicular to the crest line. The user must supply the model with those obstacle shapes that best represent each of the terrain features. The user is given 4 bluff choices and 16 ellipsoid choices. These are summarized in Section 2.5.

One controlling obstacle must be identified for each receptor. Usually, there will be one obstacle specified along each receptor ray and all receptors along that radial will have the same controlling obstacle. However, if it is not clear which of a series of terrain features along a radial is most important, several obstacles may be specified. In this case, receptors more than one hill height downwind of the nearest obstacle should be identified with the next closest obstacle downwind of the receptor.

Note that PFM (or COMPLEX) does not include wake physics. If a plume is strongly deformed by the leading obstacle along a receptor ray, then model predictions downwind of this obstacle are invalid. Predicted concentrations downwind of the first terrain feature should be considered adequate only if upwind terrain features are no larger than one half of the expected plume heights.

The look-up table of PFM calculations contains 8 variables at 49 non-dimensional downwind distances for each possible plume height, Froude number, and obstacle shape combination (440 in all). Of these eight variables, six are presently used to calculate PFM factors. These six are: PTA, the elapsed time from the source along the plume trajectory; ANS, the distance from the plume centerline to the surface; US, the wind speed along the plume centerline; R2S, the square of the local effective radius of curvature of the obstacle; PHI, the line integral of UR² along the plume trajectory; and TEE, the line integral of 1/(UR²) along the plume trajectory.

The source position and the position of the last PFM receptor in the tabulated computations are selected so that the source is located upwind of the region of substantial influence around the obstacle and the final receptor is about one obstacle length downwind of the obstacle. This allows PFM factors (Equation 2-40) to be calculated for arbitrary source positions. If the source is located closer to the obstacle than the source in the PFM computations, the Case 1 version of Equation 2-40 is used. If the source is located farther from the obstacle, the Case 2 version is used (see Figure 9).

Case 1 assumes that the source is located at the one downwind PFM receptor point (S) c^{*} sest to the actual source position and all actual receptors are located at the nearest PFM receptor point downwind of the source. Then, approximate PFM factors for each of these receptors (R) are computed using the following equations:

$$CFAC(R) = \sqrt{\frac{(PHI(R) - PHI(S))(TEE(R) - TEE(S))}{(US(S)(PTA(R) - PTA(S)))^2}}$$
(2-55a)

$$SZFAC(R) = \sqrt{\frac{PHI(R) - PHI(S)}{R2S(R)(PTA(R) - PTA(S))}} \quad (\frac{1}{US(R)}) \quad (2-55b)$$

$$SYFAC(h) = \sqrt{\frac{R2S(R)(TEE(R) - TEE(S))}{PTA(R) - PTA(S)}}$$
(2-55c)

$$HFAC(R) = ANS(R) / ANS(S)$$
 (2-55d)

Here PHI, TEE, and PTA are the line integrals $\phi(s)$, T(s), and t(s); therefore, only the change in these values from S to R are needed. All other quantities are evaluated at the receptor point R. US(s) is u (s), R2S(s) is R²(S), and ANS(s) is the distance from the plume centerline to the surface (see Equations 2-32, 2-33, and 2-40).

Case 2 assumes the nondimensional distance from the actual source to the PFM source is d. Because plume deformation is negligible over this distance, the line integrals along the plume streamline are constant and all PFM factors are unity. Consequently, PFM factors only need to be calculated for receptors that fall within the 49 array entries. Again, the PFM receptor points closest to actual receptors are selected, and PFM factors are calculated with the following equations:

$$CFAC(R) = \sqrt{\frac{(R2S(1)US(1)d + PHI(R))(d/(R2S(1)US(1)) + TEE(R))}{(US(1)(d/US(1) + PTA(R)))^2}} (2-56a)$$

$$SZFAC(R) = \sqrt{\frac{R2S(1)US(1)d + PHI(R)}{R2S(R)(d/US(1) + PTA(R))}} (\frac{1}{US(R)}) (2-56b)$$

$$= \sqrt{\frac{R2S(R)(d/US(1) + PTA(R))}{R2S(R)(d/US(1) + PTA(R))}} (\frac{1}{US(R)}) (2-56b)$$

$$SYFAC(R) = \sqrt{\frac{R2S(R)(d/(R2S(1)US(1)) + TEE(R))}{d/US(1) + PTA(R)}}$$
(2-56c)

$$HFAC(R) = ANS(R) / ANS(1)$$
(2-56d)



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Case I: Actual source is located downwind of the PFM source

Case II: Actual source is located upwind of the PFM source



Figure 9. Relationship between PFM and actual sources and receptors in PFM-Long.

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Note: PFM receptors labeled R,S, or 1 are used in Equation 2-55 and Equation 2-56.

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Again, the line integrals PHI, TEE, and PTA are adjusted so that they encompass the entire interval between the source and the receptor. For $e \ge ample$, R2S(1)US(1)d is the "PHI" integral from the actual source to the PFM source and PHI (R) is its value from the PFM source to the receptor evaluation point (R).

PFM-Long starts out by setting up factor arrays for each receptor. Because each receptor has a fixed relationship to its own controlling obstacle and the location of the sources, factors are calculated for all plume height-Froude number combinations (22). This is done once at the start of the program.

Receptor-specific PFM factors modify the COMPLEX model's concentration equations in much the same way as they modified Equations 2-34 and 2-35. Within a particular hour loop, one of the six Froude number classes is selected on the basis of the hourly Froude number, and the PFM factors at each receptor are interpolated for each source. Each source can have a different plume height, so the PFM factors are interpolated in height only. These factors do not affect computed downwind and off-axis distances within the host model.

PFM-Short

PFM-Short contains the PFM code as a subroutine. Instead of approximating the source-terrain geometry, plume height, and meteorology as in PFM-Long, PFM-Short performs the appropriate PFM calculation. This means that more obstacle shapes are at the user's command, the obstacle orientation to the wind trajectory is preserved, and actual plume heights and Froude numbers are incorporated in the computation.

The user may specify only one terrain obstacle. This is consistent with the refined purpose of the short-term model. Additional obstacle descriptors required for PFM-Short are described in Section 2.5.

PFM factors are computed at 49 points along the wind trajectory for each source. COMPLEX determines the downwind distance and crosswind distance to each model receptor and selects the PFM factors from the PFM receptor point closest to the downwind distance. The geometry is summarized in Figure 10. When the particular factors are selected, concentrations are computed as in PFM-Long.

2.3.2 Plume Rise

Wind and temperature information available from upper dir soundings is used in the plume rise calculation when the PFM option is selected. A stepwise integration is performed through each vertical layer, allowing different vertical potential temperature gradients and wind speeds in each layer. Thus, the effects of elevated inversion and vertical wind shear can be accounted for in the plume rise calculations.



The technique described by Briggs (1975) is used to integrate the stable plume rise equation. The reduction of buoyancy flux is calculated layer-by-layer, until all of the plume's buoyancy is consumed. The height at which the buoyancy flux goes to zero is the equilibrium or final plume rise height.

For a vertical plume,

$$\mathbf{F}_{z} = \mathbf{F}_{1} - 0.027 \, \mathbf{S}_{1} \, \mathbf{F}_{z}^{1/3} \, (\mathbf{z}^{8/3} - \mathbf{z}_{1}^{1/3})$$
 (2-57)

where F_z is the buoyancy flux at height Z (height above stack height);

F; is the buoyancy flux at the bottom of the jth layer;

 F_0 is the initial buoyancy flux of the plume;

S; is a stability parameter $[(g/T_a)\partial \Theta/\partial Z]$ in the jth layer.

For a bent-over plume,

$$F_{z} = F_{j} - (1/3)g^{\prime 2} S_{j} u_{j} (z^{3} - z_{j}^{3})$$
(2-58)

where B' is an entrainment parameter, and

uj is the average wind speed in layer j.

The formulation (either bent-over or vertical plume) that gives the largest decrease in buoyancy flux in a given layer is used in that layer.

The entrainment parameter, β' , is assumed equal to 0.41314. Thus, with a single layer of constant potential temperature gradient and wind speed, Equation 2-58 reduces to standard Briggs final stable plume rise equation.

 $Z = 2.6 (F_{0/u_1}S_1)^{1/3}$ (2-59)

To calculate neutral plume rise, the Briggs (1969) neutral plume rise equation is applied in a stepwise fashion with a constant wind speed assumed in each layer. Plume rise is calculated in each layer by means of the average wind speed in that layer. A virtual source technique is used to match the plume rise at the interface of layers. Figure 11 illustrates the procedure for calculating neutral plume rise. The virtual distance (X_v) ; at which the plume enters layer j is:

$$(X_v)_j = (\frac{H_j u_j}{1.6 F_0^{1/3}})^{3/2}$$
 (2-60)

The actual downwind distance, X_a , at which the plume enters layer j is:

$$\mathbf{x}_{\mathbf{a}} = \begin{cases} x_{1} & j = 2 \\ j & (2-61) \\ x_{1} + \sum_{i=3}^{j} [(x_{v})_{i} - (x_{v})_{i-1}] & j \ge 3 \end{cases}$$

The layer, J, in which final plume height is reached is determined when $X_a \ \geq \ X_f,$ where

$$X_{f} = 3.5 X^{*}$$
 (2-62)

$$X^* = \begin{cases} 14F^{5/8} & F \leq 55 \text{ m}^{4}/\text{s}^{3} \\ & & & & & (2-63) \\ 34F^{2/5} & F > 55 \text{ m}^{4}/\text{s}^{3} \end{cases}$$

Thus, the virtual final rise distance, $(X_v)_f$, is:

$$(x_v)_f = (x_v)_J + (x_f - x_{J-1})$$
 (2-64)

The final neutral plume rise, Z_f, is:

$$z_{f} = \frac{1.6 F_{0}^{1/3} (x_{v})_{f}^{2/3}}{u_{J}}$$
(2-65)

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If the wind speed does not vary with height, $(X_v)_f$ equals X_f and Equation (2-65) reduces to single layer Briggs final plume rise equation.

The stable plume rise equation allows unrealistically large plume rise when the vertical potential temperature gradient obtained from the sounding data is negative or near zero. Likewise, the layered neutral plume rise equations may overpredict plume rise under conditions when an elevated inversion exists above a neutral layer. For these reasons, the plume rise used by the model when the PFM option is requested is always the minimum of the layered stable and neutral plume rise equations, regardless of stability classification at the surface.

If sounding data are missing for a particular hour (or if the PFM option is not requested), the single layer Briggs stable and neutral plume rise equations are used to determine plume height.

2.3.3 Froude Number and HC Analysis

The Froude number characterizes the balance of inertial and buoyancy forces over the scale of the obstacle height. If it is less than one, streamlines close to the surface upwind of the hill are more likely to go around the obstacle than over it. PFM computations do not address these streamlines, so it is important to define the height of the critical dividing streamline (HC), and apply PFM calculations only to the flow above this level.

The height HC is found from a simple energy argument suggested by Snyder, et al. (1981). The kinetic energy of the dividing streamline upwind of the obstacle must just balance the energy required to lift the streamline from its initial height (HC), to the top of the obstacle (H) through the density gradient:

$$0.5 \rho u^{2} = g \int_{HC}^{H} (H-Z)(-d\rho/dz)dz$$
 (2-66)

If the potential energy gained in lifting a streamline exceeds the initial kinetic energy, then that streamline must lie below HC. Conversely, if the potential energy is less then the initial kinetic energy, the streamline must lie above HC. When the kinetic energy of the surface streamline exceeds the accrued potential energy, there is no critical dividing streamline (HC=0).

COMPLEX/PFM evaluates HC through Equation 2-66 by integrating over the temperature soundings. The temperature gradient is constant between observation levels, and the wind speed is obtained by linear interpolation between observation levels.

A bulk Froude number for the layer above HC is calculated from:

$$FR = \frac{\overline{U}_{\infty}}{N(H-HC)} | HC$$
 (2-67)

where NT is a height above the obstacle equal to the maximum of either 1.5 the obstacle height, or the sum of plume height and obstacle height. The wind speed is the mean for the layer between HC and HT, and N is based upon the temperature difference across the layer.

Both the HC and FR computations are treated as local analyses for the plume streamline. Each must be based upon terrain heights along the plume trajectory. In PFM-long, each receptor radial is assumed to pass over the crest of the controlling obstacles. PFM-short incorporates details of the plume trajectory over a single three-dimensional obstacle; the maximum terrain height along the wind direction in this case is computed from the equation of the ellipsoidal hill surface.

After the dividing streamline height and Froude number are computed, effective plume and obstacle heights are defined. The layer beneath HC has been assumed to either stagnate, or flow around rather than over the obstacle. Plumes in this layer are treated in the COMPLEX I branch of the model. Plumes above HC still pass over the obstacle, but now they pass closer to the surface since the lower layer no longer competes for space above the obstacle. Consequently, the depth of the lower layer is subtracted from both the plume height and the obstacle height before PFM factors are calculated.

The resulting factors for plume deformation and centerline concentration can be used directly as before, but a correction must be made for the plume centerline height (Figure 12). The net plume height above the surface is not solely determined by the effective plume height times HFAC. Away from the obstacle, the net height should be equal to the full plume height before the HC correction. Closer to the obstacle, the surface of the terrain rises toward HC, and the net height decreases.

This process is accounted for by setting the net plume height (HH) equal to the sum of the effective plume height (HE) times HFAC and the difference between HC and the local terrain height (ZH, less than or equal to HC):

HH = (HE)(HFAC) + (HC - ZH) (2-68)



HH(A)=HE*HFAC+HC-ZH

. . .



Figure '2. Relationship between PFM geometry and plume height (HH) when HC, the dividing streamline height, is not zero.

This is done only when ZH is less than HC. When ZH exceeds HC, the second term in Equation 2-68 is set equal to zero.

2.4 Temperature and Velocity Profile Interpolation

Adequate meteorological profile information is essential to modeling elevated plumes in complex terrain. The behavior of streamlines at plume height depends on wind speeds and temperature gradients from the surface to the top of the important terrain features and beyond. If such profiles of temperature and wind speed are not available, then the utility of fabricating Froude numbers and dividing streamline heights from standard surface observations alone is questionable. COMPLEX/PFM predictions using such Froude numbers offer no advantage over predictions of either COMPLEX I or COMPLEX II.

2.4.1 Required Data and Defaults

The most desirable meteorological data include hourly wind velocity and temperature soundings from the modeling site. The next most desirable on-site data include at least twice-daily temperature and velocity soundings (early morning and evening) and an on-site instrumented tower at least as tall as the source stack. The least desirable (but still modelable) data set includes representative off-site upper-air data and surface data. This last choice is essentially equivalent to using standard available airport data.

Only the first of the above possible data sets contains hourly profiles for calculating hourly values of plume rise, FR, and HC. Consequently, a profile preprocessor has been constructed to interpolate between twice-daily soundings and thereby create an hourly data set. It is described in the next section.

A full year of hourly modeling data requires a complete set of twice-daily profiles, including an evening sounding from the last day of the preceeding year and a morning sounding from the first day of the following year. If the complete set is not available, then gaps will exist in the interpolation set. These gaps will be flagged in the program, and default calculations will be performed in COMPLEX/PFM using the host COMPLEX I or COMPLEX II algorithms, depending on the surface stability class.

2.4.2 Mixing Heights and Profile Interpolation

The sounding preprocessor is designed to be used with the data obtained from the National Climate Center (NCC). Sounding data from the national network of upper-air stations are contained on "TDF 5600" tapes.

The first part of the preprocessor, READ56, reads pressure, temperature, wind speed, and wind direction data from the sounding tape. These are formatted for further analysis and written to a file for editing. Only pressure levels with good temperatures are placed into the file, and missing winds are flagged. The user must elect to either remove pressure levels with bad winds, or replace the missing data with "reasonable values". The user must also specify the uppermost standard pressure level needed for profile interpolations. The default is the 700 mb level. Temperature data must be available at this level on all soundings. Any missing entries are flagged by the preprocessor. When data other than an NCC TDF 5600 tape is used, the user must prepare and format the data to look like the output from READ56.

The second part of the preprocessor, PROFIL, computes hourly mixing heights and interpolates the temperature and wind data to construct hourly sounding profiles between the actual sounding times. Mixing height computations are based in part upon the Benkley-Schulman scheme (1979). Temperature and wind velocity interpolation methods are consistent with the hourly mixing height determinations.

Temperature Interpolation - Morning to Evening

Interpolated soundings between the early morning (1200 GMT) and the evening (0000 GMT) observations must account for the growth and partial decay of the daytime convective layer when this layer depth exceeds the mechanically mixed layer. The interpolation begins with a calculation of the maximum height of the convectively mixed layer (HLMAX) for the day. First, a temperature profile for the time of the maximum relative surface temperature is constructed by interpolating all vertical profile levels in time. Then a dry adiabat is drawn from the maximum surface temperature to the constructed temperature profile. The point of intersection defines HLMAX. This method differs from the Benkley-Schulman method in that each data point in the profiles determines the local temperature shift in time due to advection, rather than just the 700 mb level.

Once HLMAX is determined, the profile interpolation above and below HLMAX is handled differently. All profile points above HLMAX are unaffected by surface heating; therefore, hourly temperatures are found by simple linear interpolation in time at all levels greater than or equal to HLMAX (Figure 13). Below HLMAX, the surface temperature progression must be incorporated. The hourly adjustment is as follows:

- adjust profile below HLMAX by shifting temperature an amount equal to the shift at HLMAX;
- o follow the adiabat from the surface temperature to the point of intersection with the shifted profile;
- compare the height of the intersection with the mechanical mixed layer height (see Benkley et al. 1979);
- create a new profile point at the maximum of these two heights and neglect all profile points below it; and
- o call this height the mixing height for this hour (HL).



Figure 13. Sample construction of temperature profile for fourth hour after A.M. sounding.

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If HL is less than the previous value of the mixing height, and if the surface temperature has not reached its maximum value for the day, HL is set to its preceeding value, and the temperature at HL is incremented an amount equal to the change at HLMAX.

Once the maximum surface temperature has been reached, the profile below HLMAX will slowly relax, approaching the shape of the evening sounding. The mixing height persists at HLMAX until the night-time mechanical shear layer becomes dominant, and this transition is determined as in the Benkley-Schulman method. Consequently, temperatures below HLMAX are linearly interpolated from the dry adiabat to the actual evening sounding.

Throughout this discussion, reference has been made to a "surface" temperature. If on-site meteorological tower data are available, the "surface" temperatures referred to above should actually be the uppermost measurement height. In this way, site-specific surface layer changes can be included directly. The user may then merge the lower tower measurements into the profile data set with a suitable data manipulation routine.

Temperature Interpolation - Evening to Morning

The remnants of the daytime mixed layer continue to decay in the evening. Cooling proceeds more rapidly at the surface than at the middle levels of the profile. Therefore, linear interpolation of temperatures at all sounding levels is appropriate. Regions of greatest temperature change will have the greatest hourly rate of change, so the lower profile will stabilize most rapidly.

Velocity Interpolation

Wind velocity interpolation is likely to be far less accurate than temperature interpolation. For this reason, the results of the wind speed interpolation are used for FR-HC analysis and plume rise calculations only, and the wind directions are not used at all. Linear interpolation is used throughout after profile height levels are computed for the temperatures.

The interpolation proceeds as follows:

- interpolate all speeds and directions between soundings;
- interpolate in height to compute winds at new pressure levels
 created in the temperature profile interpolation (i.e., HLMAX); and
- compute wind speed and direction at the hourly HL heights using the surface stability class, the recommended power law exponents, and the "surface" wind speed and direction from the surface meteorology data file.

This interpolation method separates the surface layer flow from the upper level flow. Winds measured on-site or at the nearest NWS station control the wind speed and direction throughout the mixed layer. Radiosonde winds observed only twice a day are not allowed to influence low-level winds at all.

2.5 Terrain Description Guidance

Two classes of obstacle shapes are incorporated in PFM: bluffs and ellipsoids. Bluffs are strictly two-dimensional features with one ascending face, but no descending face. Ellipsoids are truly isolated hills, and may be either two- or three-dimensional. The two-dimensional ellipsoid is applicable to long ridges, while the three-dimensional ellipsoid is applicable to mounds, peaks, or short ridge elements.

Twenty bluff profiles and an infinite number of ellipsoid shapes are available within PFM-Short. A subset of four bluff profiles and sixteen ellipsoid shapes is contained in PFM-Long.

2.5.1 PMF-Short Obstacle Selection

Profiles of twenty bluff sections are presented in Appendix A. Each section has a characteristic mean slope, and a characteristic crest location.

To pick the bluff shape most like an actual terrain feature, construct a terrain section through a representative part of the feature. Make sure that the section is along a cut perpendicular to the crest line. Scale the length units by the crest height in such a way that the profiles are the same size as the bluff profiles contained in Appendix A.

Now match the general shape of the terrain profile to one of the twenty bluff shapes. The most important features to match are terrain slopes near the top, and the overall scale of the terrain shape. The number of the bluff shape most like the terrain section should be specified as parameter "BLFSH." The actual bluff height should be entered as "HAO."

The source location (XO, YO) relative to the center of the obstacle, and the orientation (OBSANG) of the obstacle must also be specified. Each bluff shape has a zero point identified on the horizontal axis. The actual perpendicular distance of your source from the corresponding point on your terrain section is XO. YO is zero. Note that the value entered for XO must be negative, since the positive X-direction points from the source to the obstacle, and the source is positioned on the negative side of the origin (unless your source lies between the zero point and the crest).

The direction of the positive X-axis also defines the bluff orientation. OBSANG is the angle between North and the vector direction X. This angle is measured in a clockwise direction (Figure 14).



Figure 14. Relationship between north and the orientation of the bluff coordinate system.

C ¥ Ellipsoid shapes are based on along-wind (AWARO) and cross-wind (CWARO) aspect ratios (Figure 15). An aspect ratio is defined as one-half the obstacle length (or breadth) divided by the obstacle height. The along-wind aspect ratio is calculated using the major ellipse axis that penetrates the windward face. The cross-wind aspect ratio is calculated using the major ellipse axis perpendicular to this axis. The "windward" face assumes that a wind is blowing from the source toward the center of the obstacle. When the windward face is correctly chosen, the source should lie within a 45° cone about the -x axis.

As with the bluff, the user should try to pick aspect ratios that produce an ellipsoid most like the shape of the actual terrain feature. A good starting point is to calculate aspect ratios based on the shape of the terrain feature along its one-half-height contour. Sketches of the resulting ellipsoids should then be compared to terrain cross-sections.

After selecting the ellipse axes, the obstacle origin is defined (center of ellipse), and the source position (XO, YO) and obstacle orientation can be determined. The positive X-axis points away from the source along the "along-wind" ellipsoid axis. Therefore, XO and YO are readily obtained and OBSANG is once again the angle measured clockwise from North to the vector pointing along the positive X-axis (Figure 16). The terrain height (HAO) is the maximum height of the terrain feature that is consistent with the specification of the ellipsoid.

2.5.2 PFM-Long Obstacle Selection

Specification of obstacle shapes and position parameters for PFM-Long is a simplified version of the PFM-Short process. The user may select a bluff shape from four possible profiles, or an ellipse shape from sixteen possible combinations of along-wind and cross-wind aspect ratios. Once this is done, only the source-to-obstacle distance and the maximum obstacle height need be obtained since obstacle orientation to the wind is neglected.

All available obstacle shapes are numbered one through twenty. The first four are bluff shapes, the rest are ellipsoids. Table 1 summarizes which bluff shapes and ellipsoids are included. The obstacle shape is specified as parameter IOBSH. The distance between the source and the obstacle center is specified as parameter ODIST. This quantity should not be negative. It is a true distance and not a source coordinate relative to the obstacle center.

Selection of a controlling obstacle for each receptor depends on the complexity of the terrain. FFM computations are only valid for plumes upwind of and over obstacles. No wake effects in the lee of obstacles are included. Therefore, only the dominant terrain features surrounding the source should be considered.



• Source

Wind -



Cross-wind aspect ratio CWARO = B/C

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IOBSH	BLFSH	CWARO	AWARO	
			, , <u>, , , , , , , , , , , , , , , , , </u>	
1	1	0	0	
2	8	0	0	
3	12	0	0	
4	16	0	0	
5	0	1	1	
6	0	2	1	
7	0	5	1	
8	0	10	1	
9	0	1	2	
10	0	2	2	
11	0	5	2	
12	0	10	2	
13	0	1	5	
14	0	2	5	
15	0	5	5	
16	0	10	5	
17	0	1	10	
18	0	2	10	
19	0	5	10	
20	0	10	10	

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TABLE 1. OBSTACLE SHAPES AVAILABLE FOR APPLICATIONS OF PFM-LONG

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However, when major plumes rise above nearby obstacles, the most important terrain features may lie farther away. In cases where the dominant features are not readily apparent, more than one obstacle may be specified along a single receptor radial. In this case, receptors more than one obstacle length downwind of one obstacle should be associated with the next obstacle along the radial. This method effectively treats succeeding features in isolation from one another.

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SECTION 3

USER'S INSTRUCTIONS

The COMPLEX/PFM modeling package is schematically illustrated in Figure 17. User's instructions for the SETUP file restructuring program, the READ56 and PROFIL preprocessing programs, and the COMPLEX/PFM model program are presented below.

3.1 SETUP Instructions

The SETUP program rearranges the data contained in the formatted PFM look-up table supplied with COMPLEX/PFM. No program control variables are required to run SETUP because the structure of both the input and the output file is predetermined. System channel unit 8 is assigned to the formatted input file, and unit 20 is assigned to the random access output file. This program should be run only when the COMPLEX/PFM modeling system is first installed on the user's system.

3.2 READ56 Instructions

The READ56 program reads an NCC TDF 5600 data tape of upper air data, selects those sounding levels within a pressure window specified by the user, checks each sounding time for missing or multiple entries, and flags entries that contain missing data. Pressures, temperatures, calculated heights, and wind velocities are written to a formatted file for editing, and for later use in the program PROFIL (see Section 3.3).

One program control card is needed to reset namelist variables when other than default values are desired. The namelist variables are described in Table 2.

Two system channel units are needed for data file input and output. The file containing TDF 5600 data is assigned unit 10, and the output file is assigned unit 7.

The first record in the output file created by READ56 repeats the namelist variables in PARAMS. This record is followed by one data identification record and several data records for each sounding. Table 3 describes the contents of the data identification record. Data from each sounding level follows, with four strings of pressure (mb), height (m), temperature (°K), wind direction (degrees), and wind speed (m/s) per record. If missing data were found in the sounding, or if a sounding is



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TABLE 2. PARAMS NAMELIST - READ 56

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Variable	Туре	Description	Default
START	Integer	Year and Julian day number	-
		of the first complete day of	
		profiles (e.g., 81001)	
STOP	Integer	Year and Julian day number of	-
		the last complete day of	
		profiles (e.g., 81365)	
SPT00Z	Real	Starting pressure level for	2000.
		data to be extracted from the	
		00Z sounding (mb)	
EPT00Z	Real	Ending pressure level for data	700.
		to be extracted from the 00Z	
		sounding (mb)	
SPT12	Real	Starting pressure level for data	2000.
		to be extracted from the 12Z	
		sounding (mb)	
EPT12	Real	Ending pressure level for data	700.
		to be extracted from the 12Z	
		sounding (mb)	

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TABLE 3. DATA IDENTIFICATION RECORD - READ 56

	Variable	Туре	Description	Default
`				
	ITPDK	3X, 14	Label identifying the tape	-
			as series "5600"	
	NOSTA	5X, 15	Identification number for the	-
			upper air station	
	IOBTM(4)	5X,4I2	Year, month, day, and hour	-
			of the sounding (GMT)	
	LVL	5X,I2	Total number of sounding	-
			levels in the profile	
	NLVL	80X,I3	Number of sounding levels	-
			extracted from the profile	

missing, or entered more than once, additional records containing warning information are written before the next sounding is obtained.

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3.3 PROFIL Instructions

The PROFIL program requires one input card to specify program control variables, one input disk file containing the processed surface meteorological data, and one input disk file containing edited twice daily temperature and wind velocity soundings. It produces a list file, and a file of hourly wind and temperature profiles. The default system unit number for the sounding file is 7; the default system unit number for the surface data is 2.

Namelist data entry format is used on the program control card. The control variables that make up namelist "INPUT" and their default values are described in Table 4. The user only needs to change variables whose default values are unacceptable.

The surface meteorology file is unformatted and is normally obtained as output from RAMMET or the CRSTER preprocessor. Its content is described in Section 3.4.2 (Table 21).

The file of twice-daily soundings (00Z and 12Z) is a formatted data set. The first record is a namelist statement (PARAMS). Sounding that follows contains one parameter record and several records sounding data. Each record type is described in Section 3.2.

Before the soundings file can be used by PROFIL, the user must add the soundings for the day after the last day to be processed. This is necessary because the 12Z profile on the final day really corresponds to a morning sounding. Both the evening sounding plus the morning sounding of the following day are needed to complete the mixing heights and profile interpolations through hour 23 of the final day.

The user must also edit the soundings file to identify missing data levels or missing soundings. If the wind speed is missing at one level, for example, the user might either interpolate a value based on the values at adjacent levels or remove the sounding level entirely. If the latter action is taken, the number of good levels in the sounding (NLEV) must be reduced accordingly. If an entire sounding is missing, then only the sounding information record should be present, with NLEV set to zero.

PROFILE will interpret this zero as a gap in the sounding data, and no hourly profile data will be calculated. Instead, the output file for this day will contain 24 data entries reporting a mixing height of 9999, and a maximum number of profile points of zero. COMPLEX/PFM will then ignore the sounding data for this day, and perform either COMPLEX I or COMPLEX II computations, depending upon the stability class.

Variable	Туре	Description	Default
NDAYS	Integer	Number of days to be run	-
JTIME	Integer	Local time of the 002	19
		sounding (1900 EST)	
ZMEAS	Real	Anemometer height above the	10.0
		surface (meters)	
20	Real	Roughness length scale	0.05
		representative of the area	
		(meters)	
LMETOT	Logical	Control for writing program	.TRUE.
÷		output to disk	
IMET	Integer	System unit number for the	9
		program output data file	
ISURF	Integer	System unit number for the	2
		surface meteorology file	
IUP	Integer	System unit number for the	7
		upper air meteorology file	
ICARD	Integer	.System unit number for card input	5
ILIST	Integer	System unit number for the program	6
		output list file	
PEXP	Real (7)	Wind profile power law exponents,	0.10
		one for each stability	0.15
		class (1-7)	0.20
			0.25
			0.30
			0.30
			0.30

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TABLE 4. PROFIL PROGRAM CONTROL CARD VARIABLES

3.4 COMPLEX/PFM Instructions

Most program control options available in COMPLEX/PFM are unchanged from MPTER. These will not be restated here to the same depth. The user should read and understand the MPTER user's guide prior to running COMPLEX/PFM.

Portions of the model which are new, or portions which have been changed, are discussed in the following sections. Section 3.4.1 provides a list of all options available in the model, and describes those which are new and those old ones which are not compatible with the PFM options. Section 3.4.2 contains a description of input card and tape format.

3.4.1 COMPLEX/PFM Options

All COMPLEX/PFM options are listed in Table 5. Two of these, options 25 and 26, are not described in the MPTER guide.

Option 25 was added when COMPLEX I and COMPLEX II were designed from the MPTER code. This option controls which of several terrain adjustment algorithms is to be used. In brief, these are:

- OPT 25 = 0 Terrain adjustment follows MPTER.
- OPT 25 = 1 Partial height correction made, but plume may not come closer to the surface than ZMIN (meters).
- OPT 25 = 2 One calculation is made with the receptor at plume height over level terrain. A second calculation is made as in OPT 25 = 1, and the lesser of these two calculations is used.
- OPT 25 = 3 Concentrations are calculated as if there is no terrain, except that the receptor is placed at the actual terrain elevation above sea level.
- OPT 25 = 4 Concentrations are calculated as in OPT 25 = 1 unless the plume path correction is zero and the terrain exceeds the plume height. In that case, the solid ground is placed a distance ZMIN (meters) below the plume, and the receptor is placed at the actual terrain height above the plume.
- OPT 25 = 5 One calculation is made with the receptor at plume height over level terrain. A second calculation is made as in OPT 25 = 4. The lesser of these two calculations is used.

TABLE 5. OPTIONS AVAILABLE IN COMPLEX/PFM

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Option	Description
	Technical Ontions
IOPT(1)	Use Terrain Adjustments
IOPT(2)	No Stack Downwash
IOPT(3)	No Gradual Plume Rise
IOPT(4)	Include Buoyancy Induced Dispersion
	Input Options
IOPT(5)	Met, Data on Cards
IOPT(6)	Read Hourly Emissions
IOPT(7)	Specify Significant Sources
IOPT(8)	Input Radial Distances and Generate Polar
	Coordinate Receptors
	Printed Output Options
IOPT(9)	Delete Emissions With Height Table
10PT(10)	Delete Resultant Met. Date Summary for Averaging Period
IOPT(11)	Delete Hourly Contributions
IOPT(12)	Delete Met. Data on Hourly Contributions
IOPT(13)	Delete Final Plume Height and Distance to Final
	Rise on Hourly Contributions
IOPT(14)	Delete Hourly Summary
IOPT(15)	Delete Met. Data on Hourly Summary
IOPT(16)	Delete Final Plume Height and Distance to Final
	Rise on Hourly Summary
IOPT(17)	Delete Averaging-Period Contributions
IOPT(18)	Delete Averaging-Period Summary
10PT(19)	Delete Average Concentrations and High-Five Tabl
	Other Control and Output Options
10PT(20)	Run is Part of a Segmented Run
IOPT(21)	Write Partial Concentrations to Disk or Tape
IOPT(22)	Write Hourly Concentrations to Disk or Tape
10PT(23)	Write Averaging Period Concentrations to Disk or Tape
10PT(24)	Punch Averaging Period Concentrations on Cards
	Terrain Adjustment Options
IOPT(25)	Complex Terrain Option

Option 26 was added to control the PFM option selection. If zero is specified, standard COMPLEX calculations are made, with the exception that COMPLEX I is called for stability classes 5 and 6 (E and F) and COMPLEX II is called for stability classes 1-4 (A-D). In this sense, the COMPLEX "host" model for PFM computations is a mix of the two previously available COMPLEX models.

When option 26 is set to 1 or 2, PFM calculations are triggered. Selection 1 is the PFM-Long option which is designed to approximate PFM results in a long, sequential calculation mode. Selection 2 is the PFM-Short option which calls PFM as a subroutine. PFM-Short is designed for short runs where refined, critical-period calculations are needed.

Option 26 (non-zero) also triggers the layered plume rise calculations. The user has access to this feature only in combination with the entire PFM option.

A few other options should be specifically set when option 26 equals 1 or 2 to be compatible. Option 3, the gradual plume rise option, should be set for no gradual plume rise because the layered plume rise equations produce only a final rise height. Option 1 should be used because the PFM option requires terrain correction. Option 25 should be set to 1. And option 8, the MPTER polar receptor grid option, should not be used because a more versatile radial receptor package is contained in the PFM option sequence.

3.4.2 Input Format Specifications

Card Input

Tables 6 through 20 list the card input needed to run COMPLEX/PFM. Individual values on a card must be separated by either a comma or a space when the data format is specified as "free."

Table 6 describes card type 1, which applies to the first three cards (see Figure 18). These identify the output run for the user's records. Table 7 describes card type 4, which initializes several program control variables and conversion constants. Table 8 describes card type 5, which controls option branch points within the model. Table 9 describes card type 6, which sets the values for the surface wind measurement height, the wind power law exponents, the terrain adjustment factors, and the minimum plume standoff distance. Table 10 describes card type 7, the source specification cards (up to 50).

Most of the remaining cards depend upon option selections. Table 11 describes card type 8, which is used only when significant source contributions are specified (OPT 7 = 1). Table 12 describes card type 9, which is used when standard meteorological data is read in from a file (OPT 5 = 0). Tables 13 and 14 describe card types 10 and 11, which are used when the CRSTER type of radial receptor pattern is wanted (OPT 8 = 1). Card



Figure 18. Input data deck setup for COMPLEX/PFM.

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TABLE 6. COMPLEX/PFM CARD TYPE 1, 2, AND 3 - TITLE (3 CARDS)

Variable	Format	Description	Units
	B C L (
LINEL	20A4	80 alphanumeric characters for heading	-
LINE2	20A4	80 alphanumeric characters for heading	-
LINE3	20A4	80 alphanumeric characters for heading	-

والمراجع المراجع والمراجع والمراجع والمراجع والمراجع والمراجع والمراجع والمراجع والمراجع والمراجع والمراجع

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TABLE 7. COMPLEX/PFM CARD 4 - CONTROL AND CONSTANTS (1 CARD)

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Variable	Format	Description	Units
IDATE(1)	Free	Two digit year	-
IDATE(2)	Format	Starting Julian day for this run	-
IHSTRT		Starting hour for this run	-
NPER		Number of averaging periods to be run	-
NAVG		Number of hours in an averaging period	-
IPOL		Pollutant indicator:	-
		$3 = so_{2},$	
		4 = suspended particulates	-
NSIGP		Number of significant point sources,	
		max = 25.	
NAV 5		Number of hours in the user specified	-
		period for which a high-five	
		concentration table is generated,	
		(most likely equal to 2, 4, 6, or 12)	
CONONE		Multiplier constant, user distance units to	-
		km example multipliers:	
		feet to km: 3.048E-04	
		miles to km: 1.609344	
		meters to km: 1.0E-03	
CELM		Multiplier constant, user ht units to m	-
HAFL		Pollutant half-life	second
		(an entry of zero will cause skipping	
		of pollutant loss calculations)	

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TABLE 8. COMPLEX/PFM CARD 5 - OPTIONS (1 card)

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Variable	Format	Description
······································		▝▝▋▙▙▝▆▁▙▖▆▁▙▖▆▁▖▆▁▖▆▁▖▖▆▁▖▖▆▁▖▖▆▁▖▖▆▁▆▖▖▖▆▁▖▖▖▖▆▁▖▖▖▖▆▁▖▖▖▖▆▁▖▖▆▁▖▖▆▁▖▖▆▁▖▖▆▁▖▖▆▁▖▖▆▁▖▖▖▖▖▖
202-(1)	_	Technical Options
10PT(1)	Free	Use Terrain Adjustments
10PT(2)	Format	No Stack Downwash
10PT(3)		No Gradual Plume Rise
10Pr(4)		Include Buoyancy Induced Dispersion
		Input Options
TOPT(5)		Met. Data on Cards
1011(5) 1007(6)		Pagd Howily Emissions
10PT(7)		Specify Significant Sources
TOPT(8)		Input Radial Distances and Constate Polar
1011(0)		Coordinate Receptors
		Printed Output Options
10PT(9)		Delete Emissions With Height Table
IOPT(10)		Delete Resultant Met. Data Summary for Averaging
		Period
IOPT(11)		Delete Hourly Contributions
IOPT(12)		Delete Met. Data on Hourly Contributions
10PT(13)		Delete Final Plume Height and Distance to Final
		Rise on Hourly Contributions
IOPT(14)		Delete Hourly Summary
IOPT(15)		Delete Met. Data on Hourly Summary
IOPT(16)		Delete Final Plume Hieght and Distance to Final
		Rise on Hourly Summary
10PT(17)		Delete Averaging-Period Contributions
10PT(18)		Delete Averaging-Period Summary
10PT(19)		Defere Average Concentrations and High-Five Table
		Other Control and Output Sptions
10PT(20)		Run is Part of a Segmented Run
10PT(21)		Write Partial Concentrations to Disk or Tape
10PT(22)		Write Hourly Concentrations to Disk or Tape
10 PT(23)		Write Averaging Period Concentrations to Disk or
		Tape
IOPT(24)		Punch Averagin_ Period Concentrations on Cards
		Terrain Adjustment Options
<u> </u>		Compley Terrein Option
1011(23) 1097(26)		Potential Flow Option
1011(40)		Inclusion of the observed

Note: Integer values: 0 or 1 (0 means don't use option) on options 1-24.

TABLE 9. COMPLEX/PFM CARD 6 - WIND AND TERRAIN (1 card)

Variable	Format	Decomination	Unite
Variable	roimat	Description	UNILS
HANE	Free	Anemometer height	meters
PL(I), I=1,6	Format	Wind increase with height	-
		exponents for each stability class	
CONTER(1), 1=1,6		Terrain adjustment factors	-
		for each stability class	
		(real numbers from 0 to 1)	
ZMIN		Minimum approach distance of	meters
		plume centerline above the	
		terrain surface	

TABLE 10. COMPLEX/PFM CARD TYPE 7 - POINT SOURCE* (up to 50 cards)

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		Description	Units
RNAME	2A6	12 alphanumeric characters for source identification	-
SOURCE(1,NPT)	F8.2	East coordinate of point source	user units
SOURCE(2,NPT)	F8.2	North coordinate of point source	user units
SOURCE(3,NPT)	F8.2	Sulfur dioxide emission rate	g s ⁻¹
SOURCE(4,NPT)	F8.2	Particulate emission rate	g s ⁻¹
SOURCE(5,NPT)	F8.2	Physical stack height	meters
SOURCE(6,NPT)	F8.2	Stack gas temperature	Kelvin
SOURCE(7,NPT)	F8.2	Stack inside diameter	meters
SOURCE(8,NPT)	F8.2	Stack gas exit velocity	m s ⁻¹
ELP(NPT)	F4.0	Source ground-level elevation	user ht units

*Card with ENDPOINTS in columns 1-9 is read in after the last point source card.

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TABLE 11. COMPLEX/PFM CARD TYPE 8 - SPECIFIED Statisficant SOURCES (1 card)(used with option 7 = 1)

Variable	Format	Description	Unit
NPT	13	Number of user specified significant point sources	-
MPS	2513	Point source numbers user wants to be considered significant	-

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TABLE 12. COMPLEX/PFM CARD TYPE 9 - MET. DATA IDENTIFIERS (used with option 5 = 0)

Variable	Format	Description	Units
ISFCD	Free	Surface met station identifier	5 digit
ISFCYR	Format	Year of surface met data	2 digit
IMXD		Upper-air station identifier	5 digit
IMXYR		Year of mixing-height data	2 digit

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Variable	Format	Description	Units
RADIL(1)	Free	Up to five radial distances at	user units
I=1,5	format	which 36 receptors are generated around points CENTX, CENTY on	
		azimuths 10 to 360 degrees	
CENTX		East coordinate about which radials are centered	user units
CENTY		North coordinate about which	user units

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TABLE 13.COMPLEX/PFM CARD TYPE 10 - POLAR COORDINATE RECEPTORS(1 card) (used with option 8 = 1)

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TABLE 14. COMPLEX/PFM CARD TYPE 11 - POLAR COORDINATE RECEPTOR ELEVATIONS (36 cards) (used if options 1 and 8 are both 1)

Variable	Format	Description	Units
IDUM	12	Azimuth indicator (1 to 36)	-
	8X	(8 blank columns)	
ELRDUM	5F10.0	Receptor ground-level	user ht units
		elevations for this	
		azimuth for up to five	
		distances	

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Variable	Format	Description	Units
RNAME	2A4	8 alphanumeric characters for station identification	-
RREC	F10.3	East coordinate of receptor	user units
SREC	F10.3	North coordinate of receptor	user units
ZR	F10.0	Receptor height above local	
		ground-level	meters
ELR	F10.0	Receptor ground-level elevation	user ht units

TABLE 15. COMPLEX/PFM CARD TYPE 12 - RECEPTORS* (up to 180 cards) (use if option 26 = 0)

*Card with ENDREC incolumns 1-6 should follow the last receptor card (a maximum of 180 receptors are allowed).

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TABLE 16.	COMPLEX/PFM CARD TYPE 13 - OBSTACLE INFORMATION (used if	
(ption 26 = 2)	

Variable	Format	Description	Units
		·	
xo	Free	Source coordinates as represented	user units
YO	format	in hill coordinate system	user units
HAO		Obstacle relief height	user ht units
OBSANG		Angle from North to hill x-axis	degrees
CWARO		Obstacle cross-wind aspect ratio	-
4		(ellipsoid)	
AWARO		Obstacle along-wind aspect ratio	-
		(ellipsoid)	
BLFSH		Obstacle bluff shape number (bluff)	-

ana na kana ana ana ana ana ana ana ana	TABLE 17.	COMPLEX/PFM CARD	TYPE 14 -	GRID CENTER
	é	(Usea if option	20 - 1, 2)	
			÷	

Variable	Format	Description	<u>Units</u>
CENTX	Free	User coordinates for the center	user units
CENTY	Format	of the polar receptor grid (must	user units
		coincide with source position)	

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- TABLE 18. COMPLEX/PFM CARD TYPE 15 - RECEPTORS* (up to 180 cards) (used if option 26 = 1, 2)

Variable	Format	Description	Units
RNAME	2A4	8 alphanumeric characters for	
		station identification	-
-	2X	-	-
RTHETA	F10.0	Angle to receptor (clockwise from	
		north)	degrees
RADIUS	F10.0	Distance to receptor	user units
ZR	F10.0	Receptor height above local	meters
		ground-level	
ELR	F10.0	Receptor ground-level elevation	user ht units
HTERAN	F10.0	Obstacle relief height	user ht units
ODIS	F10.0	Source distance from obstacle	user units
		center	
TOBSH	12	Obstacle shape number (1-20)	-

*Card with ENDREC in columns 1-6 should follow the last receptor card (a maximum of 180 receptors are allowed).

TABLE 19. COMPLEX/PFM CARD TYPE 16 - SEGMENTED RUN (1 card) (used with option 20 = 1)

3 _{1,σ}	<u>.</u>		
Variable	Format.	Description	Units
IDAY	Free	Number of days already processed	-
LDRUN	Format	Last day to be processed in this run	<u> </u>

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Variable	Format	Description	Units
JYR	Free	Year of met data	2 digits
DAY1	Format	Julian day of met data	3 digits
JHR		Hour of met data	2 digits
IKST		Stability class for this hour	-
QU		Wind speed for this hour	m s ⁻¹
QTEMP		Ambient air temperature for	Kelvin
		this hour	
QTHETA		Wind direction for this hour	degrees azimuth
QHL		Mixing height for this hour	meters

TABLE 20. COMPLEX/PFM CARD TYPE 17 - METEOROLOGY(used with option 5 = 1)

type 11 is read only when a terrain correction is also specified (OPT 1 = 1). Table 15 describes card type 12, the free receptor card. It contains the name, coordinates, and heights of receptors placed anywhere in the field. If less than 180 receptors were specified by the radial grid (OPT 8 = 1), additional receptors may be read in here. If the PFM option is used, card type 12 is replaced by card type 14.

Tables 16 through 18 describe the receptor and terrain information cards (types 13, 14, and 15) needed when the PFM option is used (OPT 26 = 1,2). Card type 13 is used only with PFM-Short (OPT 26 = 2). It contains the location, size, shape, and orientation of the single terrain feature under study. Note that the obstacle relief height is the height of the hill above stack base. Card type 14 is used with both PFM options. It contains the user coordinates for the center of the radial receptor grid. These coordinates must be the same as those for each of the sources (card type 7). Card type 15 is also used with both PFM options. It takes the place of the regular receptor card (type 12) and contains receptor coordinates and heights as well as obstacle information for the one terrain feature (if any) closest to the receptor along the receptor radial.

Table 19 describes card type 16, which sets parameters to allow a segmented run to be made (OPT 20 = 1). Table 20 describes card type 17, which contains the surface meteorological data on cards (OPT 5 = 1).

File Input

Table 21 shows the file structure for the meteorological data that are read from unit 11 if option 5 = 0. This file is unformatted and is normally obtained as output from RAMMET or the CRSTER preprocessor.

Table 22 shows the file structure for the emission data that is read from unit 15 if option 6 = 1. This file is unformatted and must be generated by the user.

Table 23 shows the file structure for the hourly profile data that is read from unit 16 if option 26 = 1, or 2. This file is unformatted and is usually generated by the FROFIL preprocessor. If the soundings are prepared and analysed by hand (e.g., in the case of a PFM-Short analysis), the user must generate this file.

TABLE 21. COMPLEX/PFM OPTIONAL INPUT FILS - METECROLOGICAL DATA (unit 11) (input if option 5 = 0)

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varrante	Dimensions	Description	Units
	, 		
Record 1			
ID		Surface station identifier	5 digits
IYEAR		Year of surface data	2 digits
IDM		Mix ht station identifier	5 digits
IYR		Year of mix ht data	2 digits
Record Type	2 (one for eac	ch day of year)	
		Year	
JYR		IÇUI	
JYR IMO		Month	
JYR IMO DAYl		Month Julian day	
JYR IMO DAY1 IKST	24	Month Julian day Stability class	_
JYR IMO DAYI IKST QU	24 24	Month Julian day Stability class Wind speed	m s ⁻¹
JYR IMO DAY1 IKST QU QTEMP	24 24 24	Month Julian day Stability class Wind speed Ambient air temperature	m s ⁻¹ Kelvin
JYR IMO DAY1 IKST QU QTEMP DUMR	24 24 24 24	Month Julian day Stability class Wind speed Ambient air temperature Flow vector to 10°	m s ⁻¹ Kelvin deg-azimuth
JYR IMO DAY1 IKST QU QTEMP DUMR QTHETA	24 24 24 24 24 24	Month Julian day Stability class Wind speed Ambient air temperature Flow vector to 10° Randomized flow vector	m s ⁻¹ Kelvin deg-azimuth deg-azimuth

TABLE 22. COMPLEX/PFM OPTIONAL INPUT FILE - EMISSION DATA (unit 15) (input if option 6 = 1)

		<u></u>	
/ariable	Dimensions	Description	Units
Record Type	1 (one for each	hour of simulation)	
IDATP		Date-time indicator	
		consisting of:	0 11-1-
		lear Tuling land	
		Julian day	J digits
		Hour	2 digits
OURCE			
(IPOL, I), NPT	I = 1,		
		Emission rate for the	
		each source	g s ⁻¹

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Variable	Dimensions	Description	Units
nlevm	-	Number of levels in sounding for this hour	-
HMIX	-	Mixing height for this hour	meters
HT	NLEVM	Height of observation	meters
WSP	NLEVM	Wind speed	n s ⁻¹
WDIR	NLEVM	Wind flow vector	degrees-azimut
TMPURE	NLEVM	Air temperature	Kelvin

TABLE 23.COMPLEX/PFM OPTIONAL INPUT FILE - HOURLY SOUNDING DATA(unit 16) (input if option 26 = 1, or 2)

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APPENDIX A

PFM BLUFF CROSS-SECTIONS

A.1 Preparation of Terrain Profiles

Bluff obstacle shapes should be selected whenever a wide terrain feature has a sharp ascending face and no significant descending face. The condition that the feature be wide helps to differentiate between a two-dimensional bluff-like shape, and a three-dimensional ellipsoid shape which has a large along-wind aspect ratio.

If the feature has a cross-wind aspect ratio greater than ten, then it should be considered two-dimensional (i.e., the feature looks as though it has an infinite extent in the cross-wind direction.) If such a feature then has no apparent descending face, a bluff profile should be chosen for use with the PFM option. Had the feature possessed an apparent descending face, then an ellipsoid with a large along-wind aspect ratio would have been preferable.

Once a decision is made to model with a bluff profile, a representative cross-section of the terrain feature should be prepared. Follow these five steps:

- 1. Select a representative portion of the terrain feature.
- Find the height of the plateau beyond the rising face. Use this hill height as a scaling length for horizontal and vertical measurements.
- 3. Prepare a table of terrain height versus distance starting at least eight hill heights upwind of the crest, and continuing at least two hill heights beyond the crest.
- 4. Divide these measurements by the hill height to form non-dimensional heights and distances.
- 5. Plot the tabulated values. Use a scale of 2 cm equals one length unit for the horizontal distances, and a scale of 10 cm equals one length unit for the heights.

You should now have a cross-section of the terrain feature drawn to the same scale as the model bluff profiles presented in the next section.

A.2 Selection of a Model Bluff

Twenty bluff shapes are contained in the PFM model. The user selects one of these by specifying a bluff shape number (parameter BLFSH) between one and twenty.

Ten of these shapes are presented in Figure A-1. They correspond to bluff shapes 1-19, odd. Each is drawn to the same scale: 10 cm equals one hill height on the vertical axis; 2 cm equals one hill height on the horizontal axis.

To select one of the shapes, place a tracing of the actual terrain shape prepared according to the instructions in Section A.1 over Figure A-1. Slide the tracing back and forth along the horizontal axis to obtain the best general fit to one of the underlying curves. The portion of the bluff above one-half the hill height is most important in the matching process. Now interpolate between the nearest curves to obtain the best bluff shape number.

Once the shape has been chosen, note where the zero line of Figure A-1 cuts across your terrain tracing. This is the "center" or reference point that must be used in specifying distances between your source and the terrain feature. Be sure to convert length units back to your user units before referencing this number.

If PFM-Long is the option being used, then only four of the twenty bluff shapes are available to you. These four are implicity contained in Figure A-1 and must be referenced by parameter "IOBSH". IOBSH 1 is shape 1, IOBSH 2 is shape 8, IOBSH 3 is shape 12, and IOBSH 4 is shape 16.



Figure A-1. Bluff shapes available in PFM-Short (20 in all).

Note: Vertical scale is 5 times the horizontal scale.

APPENDIX B

PROGRAM DESCRIPTION - PROFIL

B.1 Program Structure

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Program PROFIL computes hourly mixing heights and temperature and wind profiles from twice daily temperature and wind velocity soundings. These soundings must either be formatted by READ56 if the data come from NCC 5600 tapes, or they must be formatted by the user if the data comes from some other source.

Major loops and all subroutines are charted in Figure B-1. Within sach day, profiles are interpolated using different methods depending upon the hour (between midnight and the time of the morning sounding, between morning and evening sounding, or between the evening sounding and hour 2300). A brief description of the function of each subroutine follows.

REPLAC	-	This subroutine replaces the surface temperature, wind speed, and wind direction from the sounding with surface data from the surface meteorology file.
INTERP	-	This subroutine interpolates in time between two soundings to create a sounding for an intermediate hour. All variables are interpolated at constant pressure levels.
INSERT	-	This subroutine creates a new measurement level in a sounding to represent the top of the mixing layer.
REMOV	-	This subroutine removes all sounding levels between the surface level and the mixing height to create linear gradients across the mixed layer.
TEXTR	-	This subroutine adjusts surface temperatures during the day according to the temperature shift at the maximum mixing height level. The hour of maximum relative temperature is then computed, as well as the hour of greatest wind speed.
CONV	-	This subroutine follows a dry adiabat from the surface temperature to the temperature profile, and returns the convective mixing depth.
DTINT	-	This subroutine returns the total temperature change at the level of the maximum mixing height.



Figure B-1. Flow chart for program PROFIL.

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APPENDIX C

PROGRAM DESCRIPTION - COMPLEX/PFM

C.1 Program Structure

The COMPLEX/PFM code structure is nearly the same as that for COMPLEX (I, II) and MPTER. Changes required to include the PFM option have been kept to a minimum; most of the new code appears as new subroutines.

Major loops and all subroutines are charted in Figure C-1. When this diagram is compared with the corresponding charts for MPTER or COMPLEX (I, II), the major loops are identical. New branches within these loops are activated when the PFM option is turned on (OPT 26 = 1,2). A brief description of the function of each subroutine follows (*denotes subroutines unique to PFM options).

COMPLEX/PFM -	Main Program: reads and checks input parameters; calls POLAR for PFM receptor information; initializes variables; writes out initial information; determines significant sources; controls loops on days, averaging time, and hours; calls PTR for point source concentrations; reads and writes tapes/discs; calls OUTHR to print concentration contributions and summaries.
	summaries.

POLAR	*-	Subroutine called from Main, POLAR handles receptor and
		terrain input when PFM option is selected. Standard
		terrain information as well as PFM terrain description
		is obtained. If PFM-Long (OPT26=1) is being executed,
		PFMFAC is called to calculate PFM factors.

- PFMFAC *- Subroutine called by POLAR, PFMFAC returns PFM factors for five plume heights and six Froude number classes at each receptor.
- ANGARC Function called from Main, ANGARC calculates the arctan of east resultant wind component over the north resultant wind component and returns the angle between 0° and 360°.
- PTR Subroutine called by Main, PTR calculates the point source contribution at each receptor. It controls the receptor loop and the source loop.



Figure C-1. Flow chart for program COMPLEX/PFM.

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RANK	-	Subroutine called by Main, RANK ordered concentrations for four or five averaging times so that the five highest concentrations are presented for each receptor.
OUTHR	-	Subroutine called by Main, OUTHR arranges and prints tables of pollutant concentration.
HCCALC	*-	Subroutine called by PTR when PFM option is used, HCCALC computes the critical dividing streamline of the flow.
NRISE	*-	Subroutine called by PTR when PFM option is used, NRISE calculates the neutral plume rise in the presence of wind shear.
SRISE	*-	Subroutine called by PTR when the PFn option is used, SRISE calculates the stable plume rise in the presence of wind shear and density stratification.
FRNUM	*-	Subroutine called by PTR when the PFM option is used, FRNUM returns the Froude number controlling the flow above the critical dividing streamline.
CMPLX .	-	Subroutine called by PTR when a PFM calculation is inappropriate, CMPLX adjusts the plume heights according to option 25 and calls either RCP2 or RCP to perform a COMPLEX II or COMPLEX I computation, respectively.
R CP	-	Subroutine called by CMPLX, RCP returns values of σ_z and relative concentrations computed with sector averaging (COMPLEX I) RCP calls PGZ for σ_z .
RCP2	-	Subroutine called by CMPLX or PTR, RCP2 returns values of relative concentrations computed without sector averaging (COMPLEX II) and σ_y and σ_z . When PFM-Long is used, RCP2 calls CSTFAC for PFM factors. When PFM-Short is used, RCP2 calls WCFAC for PFM factors. RCP2 calls PGYZ for σ_y and σ_z .
CSTFAC	*-	Subroutine called by RCP2, CSTFAC obtains approximate PFM factors for each source-receptor combination by interpolating the factors computed by PFMFAC. CSTFAC is used only when the PFM-Long option is selected (OPT 26=1)
WCFAC	-	Subroutine called by RCP2, WCFAC controls the call *o subroutine SPFM and selects PFM factors for each receptor. WCFAC is used only when the PFM-Short (or "worst-case") option is selected (OPT 26-2).
SPFM	*- Subroutine called by WCFAC, SPFM performs the poten flow computations for each specific source-terrain geometry (one obstacle) for this hour. SPFM factor are returned at 49 fixed points along the wind trajectory. (More details are presented in Appendia	tia) ;;; ;; D.)
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PGZ	*- Subroutine called by RCP, PGZ calculates O _Z for a given downwind distance and stability class using Pasquill-Gifford curves.	:he
PGYZ	- Subroutine called by RCP2, PGYZ calculates σ_y and σ_z for a given downwind distance and stability class using the Pasquil offford curves.	

APPENDIX D

SUBROUTINE DESCRIPTION - SPFM

D.1 Program Structure

The SPFM computer code has six primary sections. Section 1 performs data entry and scaling functions; Section 2 performs the appropriate streamline trajectory computations; Section 3 alters the computed streamline if the Froude number is sufficiently small; Section 4 performs the line integrals described in Section 2.2.1; Section 5 computes the distance from the plume centerline to the terrain surface; and Section 6 computes the PFM factors at 49 points along the plume trajectory. Each section is briefly described below.

Data Entry

SPFM version 4.0 is designed to be called as a subroutine within the COMPLEX model described in Section 2.3. Therefore, some of the option switches and variables are set internally and the user no longer has access to them. Their function is still described by means of the comment cards in the listing so readers who are interested should consult the code.

Most source and obstacle information is passed to SPFM through common PFMTER. The source location (XO, YO) is measured from an origin centered on the terrain obstacle of height HAO. The x-axis points along the obstacle axis closest to the wind direction if it is an ellipsoid or if it is perpendicular to the bluff face. The bluff shape is specified through parameter BLFSH, while the ellipse shape is specified by the crosswind and alongwind aspect ratios (CWARO, AWARO). WNDANG is the angle the wind makes with the x-axis.

The remaining source and meteorological information is passed directly through the SPFM subroutine call. NSRCE is the source identification number (no larger than 50), HO is the plume height, and FROUDE is the Froude number.

All length scales are divided by the obstacle height because SPFM computations are nondimensional. Default constant diffusivities are specified, but their actual values are unimportant because the PFM factors are independent of them. And the 49 PFM receptor points are selected along the wind direction. Their dimensional spacing (DELINT) is passed back to the calling program through common PFMTER.

Plume Path and Streamline Velocities

The plume centerline trajectory is defined numerically by placing up to 600 streamline points in an array PATH. Along-streamline velocity components for each of these points is placed in an array VEL. If the bluff shape parameter BLFSH is zero, then subroutine ELLIPS is called and the appropriate streamline path over an ellipsoid characterized by CWARO and AWARO is computed. When BLFSH is non-zero, subroutine BLUFF is called and the appropriate streamline over the specified bluff is computed.

Stratification Adjustment

PATH and VEL array elements are adjusted to approximate first-order effects of stable density stratification when the Froude number is less than or equal to ten. Again, either a bluff subroutine or an ellipse subroutine is called depending on the type of obstacle. Separate routines are needed because the local streamline height required in Equation 2-53 depends on the shape of the ground surface. Subroutine BLFSTR is called for adjustment of bluff streamlines, and ELLSTR is called for the ellipsoid.

Plume Path Line Integrals

Subroutine LININT is called to evaluate the line integrals from the source to each PFM receptor location. These line integrals determine the value of the Φ and T interrals described in Section 2.2.1 and the elapsed time. LININT also obtains the effective radius of curvature of the ellipsoidal obstacles and substitutes this for the distance to the axis of symmetry. (Recall that the theory of Section 2.2.1 was developed for axisymmetric three-dimensional obstacles.) Also, because the PFM receptor points do not coincide with all elements in the PATH and VEL arrays, LIMINT interpolates the y and z coordinate for each receptor point x, and it also interpolates the along-streamline velocity.

Plume Distance From the Surface

The effective plume centerline distance from the surface of the obstacle is not necessarily the vertical coordinate of the plume streamline minus the local terrain elevation. Rather, it must be the distance to the surface along the normal to the streamline because this is the direction in which σ_z is defined.

Two separate subroutines are required for this calculation because the surface is defined differently for the bluff than for the ellipsoid. The value of BLFSH once again determines which is called. The bluff subroutine is BLFDIS and the ellipsoid subroutine is ELLDIS.

PFM Factors

Stored array elements from the line integrations and the centerline displacement above the surface at each PFM receptor are combined to form CFAC, SYFAC, SZFAC, and HFAC arrays (see Section 2.2.2). Each factor array has an element for each receptor point, allowing either exact concentration computations at these points, or interpolated calculations for points in between.

The arrays are also dimensioned for up to 50 individual sources because they are passed back to the calling program through common FACWC. This means that SPFM as a subroutine must be called for each source for each hour that is simulated. The advantage to keeping SPFM a subroutine is that the calling model that has been selected is already established with a well-defined input and output structure (see Section 2.3). Details of averaging times for reporting concentrations and stability class determinations are external to SPFM, so its structure can remain compact and uncluttered. In this form new users may readily become familiar with it.

Figure D-1 also shows the inter-relationship of all subroutines within SPFM. The function of each is summarized below.

- SPFM Subroutine called by WCFAC, SPFM is the main calling program for the PFM branch within COMPLEX/PFM. It controls the transformation and scaling of the input data, provides the structure for the remaining five major sections of the code, and performs the SPFM factor computations.
- BLUFF Subroutine called by SPFM, BLUFF is responsible for computing the plume path and velocities along the path for flow over a two-dimensional bluff. It scales the problem into "step space", computes the plume streamfunction through a combination of calls to BLFHT and GETPSI, and then fills up the "path" and "velocity" arrays through BLFPTH to define the plume trajectory, and the along-streamline velocities.
- BLFHT Subroutine called by BLUFF, BLFDIS and GETPSI, BLFHT returns the height of a streamline over a step given the value of the streamfunction, and the horizontal distance from the step.
- IMRAF Subroutine called by BLFHT, IMRAF uses the Newton-Raphson iterative technique to solve for the real part of the parametric variable "t" (see Section 2.2.3).
- GETPSI Subroutine called by BLUFF, GETPSI returns the value of the streamfunction (psi) that passes through a given point.
- BLFPTH Subroutine called by BLUFF, BLFPTH computes the plume path and the velocities along the plume once the streamfunction for the plume streamline is found. It solves the transcendental equations at up to 600 points along the streamline through repeated calls to IMRAF.



Figure D-1. Flow chart for subroutine SPFM.

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- ELLIPS Subroutine called by SPFM, ELLIPS is responsible for computing the plume path and velocity along the plume path for flow over an arbitrary ellipsoid. It controls the specification of up to 600 points along the streamline, and solves for the net velocity at these points due to mean flow components along each of the two horizontal ellipsoid axes.
 - XRAPH Subroutine called by ELLIPS, XRAPH returns the local velocities at a point along the streamline due to the mean flow component along the "x-axis" of the ellipsoid.
 - YRAPH Subroutine called by ELLIPS, YKAPH returns the local velocities at a point along the streamline due to the mean flow component along the "y-axis" of the ellipsoid.
 - GETLAM Subroutine called by ELLIPS and XRAPH, GETLAM solves a cubic equation for the ellipsoidal coordinate lamda.
 - LAMNEW Subroutine called by XRAPH and YRAPH, LAMNEW returns the ellipsoidal coordinate lamda by using the Newton-Raphson iterative technique, given an initial value for lamda.
 - POTINX Subroutine called by XRAPH, POTINX sets up the integration needed to find the velocity potential due to the mean flow along the "x-axis."
 - POTINY Subroutine called by YRAPH, POTINY sets up the integration needed to find the velocity potential due to the mean flow along the "y-axis".
 - DQATR Subroutine called by POTINX and POTINY, DQATR performs a numerical integration of either the functions F1, F2 (POTINX), or the functions F3, F4 (POTINY).
 - BLFSTR Subroutine called by SPFM, BLFSTR alters the plume path and the along-plume velocities for flow over a bluff to approximate the effect of density stratification.
 - ELLSTR Subroutine called by SPFM, ELLSTR alters the plume path and the along-plume velocities for flow over an ellipsoid to approximate the effect of density stratification.
 - LININT Subroutine called by SPFM, LININT evaluates the "phi" and "tee" line integrals along the plume. These are evaluated at 49 downwind distances.
 - KERNL Subroutine called by LININT, KERNL returns the value of the "phi" and "tee" integral kernels at a point and also computes the advective time and distance along the plume streamline.

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	<u>D</u>	FF	-	Subroutine called by LININT if PGT-scaled diffusivities are requested, DIFF returns dimensionless diffusivities scaled from PGT sigma curves.
	P	GT	~	Subroutine called by DIFF, PGT returns sigma-y and sigma-z given a stability class and a downwind distance.
	BI	LFDIS	-	Subroutine called by SPFM, BLFDIS returns the distance from the plume centerline to the surface along the normal to the streamlines at each of 49 receptor points.
	EI	LDIS	-	Subroutine called by SPFM, ELLDIS returns the distance from the plume centerline to the surface along the normal to the streamline at each of 49 receptor points.
	X	INTER	-	Subroutine called by KERNL, BLFDIS, and ELLDIS, XINTER interpolates between points along a streamline to return the y,z coordinates, and the corresponding velocity components at an arbitrary downwind distance, x.
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APPENDIX E

TEST CASE

The computer code for COMPLEX/PFM is available on version 5 of the User's Network for Applied Modeling of Air Pollution (UNAMAP). It consists of two files. The first file, COMPLEX/PFM file, contains the main program and subroutines, preprocessing programs and test data, and input data streams for test cases. The second file, COMPLEX/PFMFACTORS, contains a formated table of PFM factors. Preprocessor program SETUP converts this formatted file to an unformatted random access file for use with COMPLEX/PFM-Long.

Test cases are provided for the meteorological preprocessors and for both PFM-Long and PFM-Short options of the main program. There are two meteorological preprocessor programs - READ56 and PROFIL. READ56 reads an unformatted TDF 5600 upper air file and produces a formatted file of twice-daily soundings as specified by the program control variables in Table 2. A segment of a formatted TDF 5600 file has been included in COMPLEX/PFM along with program FTOUF-UP which converts these data to an unformatted file for input to READ56. This is the starting point for the test case and the user's output should be compared with the test output of READ56 listed in the test output file of UNAMAP before proceeding.

Program PROFIL requires the formatted output of READ56 and the unformattted surface meteorology output of the preprocessors RAMMET or CRSMET. The surface meteorological preprocessing steps have been omitted here because the code for performing this task (RAMMET or CRSMET) is contained elsewhere in UNAMAP. However, a segment of the processed formatted surface data file for use in the test case has been provided in the COMPLEX/PFM UNAMAP file along with program FTOUF-SFC which converts the data to an unformatted file as required by PROFIL. The output of PROFIL is also unformatted. A formatted version of PROFIL output for the test case is included in the COMPLEX/PFM file along with program SND. The user should format his version of the PROFIL output file using SND to verify that the numbers match.

Four individual test case executions of the main program are included. They represent computations for flow over a bluff and flow over an ellipsoid, using both PFM-Long and PFM-Short options. The cases are needed to verify that the PFM look-up table is constructed correctly (PFM-Long), and to verify that SPFM computations (PFM-Short) for bluffs and ellipsoids are being done correctly. Input data streams are contained in the COMPLEX/ PFM file and output from running the tests are contained in the test output file of UNAMAP. Date ____

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