

THE PASQUILL-PROFILES FACILITY IN PHOENICS

1. INTRODUCTION

Both PHOENICS and PHOENICS-FLAIR are used extensively for modelling the atmospheric boundary layer (ABL) in wind-engineering applications, such as, for example, pollutant dispersion, urban and wind-comfort studies, and optimization of wind-farm placement. For such studies, the wind inlet profiles and associated boundary conditions can be specified automatically through use of the WIND object of the VR Menu, but only for neutral ambient conditions with a uniform temperature.

In this release of PHOENICS 2023, the WIND object has been extended to allow for stable and unstable atmospheric conditions. For this purpose, the widely-used Pasquill-profile classes [1,2] have been coded into Subroutine GXBLIN of the PHOENICS code. These classes define six atmospheric-stability classes labelled from A to F and based on wind speed, sun insolation and cloud cover, as shown in Table 1.1.

Wind speed (m/s)	Daytime Insolation			Night time conditions	
	Strong	Moderate	Slight	Thin overcast >= 4/8 low cloud	<=3/8 cloud
< 2	A	A-B	B	-	F
2-3	A-B	B	C	E	E
3-5	B	B-C	C	D	D
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

Table 1.1 Pasquill Stability Classes: A (very unstable), B (moderately unstable), C (slightly unstable) , D (neutral), E (slightly stable), F (moderately stable)

For unstable classes, increased vertical mixing occurs because solar heating of the ground increases the near-surface air temperature, which decreases its density. Neutral class D occurs in the early morning or evening when this solar heating is negligible and wind speed dominates vertical mixing. For stable classes, solar heating is less than ground cooling, which usually occurs at night, and the near-surface air density is increased, and so vertical mixing is suppressed. In modelling the dispersion of hazardous gases, stable conditions are used to represent worst-case scenarios due to the reduced mixing and dilution of hazardous gases into the atmosphere.

The implementation in PHOENICS is generic in terms of the gravitational and wind directions, and it covers Pasquill stability classes A through to F by use of the Monin-Obukhov Similarity Theory (MOST) [3, 4] for specification of boundary conditions. However, in this first release, no account is taken of MOST in the turbulence transport equations and wall functions. Also, no provision is made to solve for the energy equation in terms of the potential temperature. These extensions will be subject of future releases.

The purpose of this report is to document the Pasquill-Profiles facility in terms of listing the model equations, the model input data, and the test cases used to check the basic functionality. The remainder of this document comprises four sections, of which the first is Section 2 which presents

the model equations. Section 3 deals with the model input data, and Section 4 lists the test cases created for validation of the implementation. Section 5 provides some concluding remarks together with suggestions for further developments and testing.

2. MODEL EQUATIONS

2.1 Potential Temperature

In the literature, Pasquill temperature profiles are expressed in terms of the potential temperature θ , which is defined by:

$$\theta = T \left(\frac{p_d}{p} \right)^{R/C_p} \quad (2.1.1)$$

where p_d is the datum pressure, which is taken as 1 bar in the literature. PHOENICS solves for the actual thermodynamic temperature T , and so the following approximation is used to relate the two temperatures

$$\Delta\theta = \Delta T \Gamma \Delta z \quad (2.1.2)$$

where Γ is the dry adiabatic lapse rate in K/m, which is given by

$$\Gamma = \frac{g}{C_p} = 0.00977 \quad (2.1.3)$$

where g is the gravitational acceleration and C_p is the specific heat of air at constant pressure.

2.2 Profile Equations

Velocity

$$u = \frac{u_*}{\kappa} \left[\ln \left(\frac{z}{z_0} \right) - \psi_m \right] \quad (2.2.1)$$

Potential Temperature

$$\theta = \theta_0 + \frac{T_*}{\kappa} \left[\ln \left(\frac{z}{z_0} \right) - \psi_h \right] \quad (2.2.2)$$

Temperature

$$T = T_0 - \Gamma(z - z_{T0}) + \frac{T_*}{\kappa} \left[\ln \left(\frac{z}{z_0} \right) - \psi_h \right] \quad (2.2.3)$$

Turbulent kinetic energy

$$k = \frac{u_*^2}{\sqrt{c_\mu}} \left(\frac{\varphi_\varepsilon}{\varphi_m} \right)^{1/2} \quad (2.2.4)$$

Turbulence dissipation rate

$$\varepsilon = \frac{u_*^3}{\kappa z} \varphi_\varepsilon \quad (2.2.5)$$

Turbulent frequency

$$\omega = \frac{u_*^3}{\kappa Z} (\varphi_\varepsilon \varphi_m)^{1/2} \quad (2.2.6)$$

Eddy Viscosity

$$\nu_t = \frac{\kappa u_* z}{\varphi_m} \quad (2.2.7)$$

2.3 Stability Parameters

$$\varphi_m = 1 - \psi_m \quad (2.3.1)$$

For stable weather conditions ($L > 0$)

$$\psi_m = \psi_h = -\beta \zeta \quad (2.3.2)$$

$$\varphi_\varepsilon = \varphi_m - \zeta \quad (2.3.3)$$

For unstable weather conditions ($L < 0$)

$$\psi_m = 2 \ln \left(\frac{1+x}{2} \right) + \ln \left(\frac{1+x^2}{2} \right) - 2 \tan^{-1} x + \frac{\pi}{2} \quad (2.3.4)$$

$$\psi_h = 2 \ln \left(\frac{1+x^2}{2} \right) \quad (2.3.5)$$

where

$$x = (1 - b\zeta)^{1/4} \quad (2.3.6)$$

$$\varphi_\varepsilon = 1 - \zeta \quad (2.3.7)$$

For neutral weather conditions :

$$\psi_m = \psi_h = 0 \quad (2.3.8)$$

In the foregoing, $\beta=5$, $b=16$, and

$$\zeta = \frac{z}{L} \quad (2.3.9)$$

where L is the Monin-Obukhov length, defined by:

$$L \equiv - \frac{u_*^3 T_o \rho C_p}{\kappa g Q_w} \quad (2.3.10)$$

Here, u_* is the friction velocity, T_o is the surface temperature, Q_w is the surface heat flux, ρ_a is the atmospheric density, and κ is von Karman's constant.

2.4 Pasquill Classes and the Monin-Obukhov Length

The Monin-Obukhov (MO) length L is an estimation of the height where the turbulent buoyancy production is comparable with the shear-stress production of turbulence. It can be estimated from measurements, and it is positive for stable ABLs, negative for unstable BLs, and infinity for neutral BLs. In practice, the value of L is generally not known, and so it must be estimated, for instance by using the most hazardous or dominant Pasquill stability class.

In PHOENICS, the MO length may be specified directly if the value is known, but otherwise it is estimated automatically by using the Pasquill stability classes. This is done by means of one of two alternative equations. The first uses the TNO formula given by Bosch [5]:

$$L = \frac{L_s}{\log_{10} \left(\frac{z_o}{Z_s} \right)} \quad (2.4.1)$$

where z_o is the surface roughness length. For $0.001 \leq z_o \leq 0.5$ m, the constants L_s and Z_s differ for each stability class according to the values given in Table 2.4.1. For $z_o > 0.5$ m, the MO length calculated for $z_o = 0.5$ m should be used. For Pasquill stability class D, equation (2.4.1) leads to $1/L = 0$.

As an alternative to equation (2.4.1), the MO length can be estimated from the following power-law formula [6] which can be derived from Golder's nomogram [7]:

$$L = a_m \cdot z_o^{b_m} \quad (2.4.2)$$

where z_o is the roughness height, and the constants a_m and b_m are defined in Table 2.4.1 below.

Pasquill Stability Class	Weather condition	TNO eqn(2.4.1)		Golder eqn(2.4.2)	
		L_s	Z_s	a_m	b_m
A	Very unstable ($L < 0$)	33.162	1117.0	-11.4	0.1
B	Moderately unstable ($L < 0$)	32.258	11.46	-26.0	0.17
C	Slightly unstable ($L < 0$)	51.787	1.324	-123.0	0.3
D	Neutral ($L = 0$)	∞	-	-	-
E	Slightly stable ($L > 0$)	-48.33	1.262	123.0	0.3
F	Moderately stable ($L > 0$)	-31.325	19.36	26.0	0.17

Table 2.4.1 Pasquill Stability Classes and the Monin-Obukhov Length

2.5 The Friction Velocity and Friction Temperature

The friction velocity is computed from

$$u_* = \frac{\kappa u_r}{\left(\ln \left(\frac{z_r}{z_0} \right) - \psi_{m,zr} \right)} \quad (2.5.1)$$

where u_r is the reference wind velocity at the reference height z_r .

The surface heat flux Q_w is computed from

$$Q_w = -\frac{u_*^3 T_0 \rho C_p}{\kappa g L} \quad (2.5.2)$$

This heat has to be applied at the ground in the CFD simulations, which leads to requirement for a compensating heat flux at the top (sky) boundary. The former has been implemented in this first release, but not the latter.

The friction temperature, which is needed for the inlet temperature profiles, is computed from:

$$T_* = -\frac{Q_w}{u_* \rho_a C_p} \quad (2.5.3)$$

where ρ_a is the atmospheric density at the reference height and C_p is the atmospheric specific heat capacity, and κ is von Karman's constant.

2.6 Buoyancy

There are two options for representing buoyancy forces in the momentum equations, as follows:

Boussinesq

The source of momentum due to buoyancy is given by:

$$S_m = -\nabla p' + \rho \beta \mathbf{g} (T_r - T) \quad (2.6.1)$$

where T_r is the reference temperature, which varies with height according to equation (2.2.3).

Density difference

$$S_m = -\nabla p' + \mathbf{g} (\rho - \rho_r) \quad (2.6.2)$$

where ρ_r is the reference pressure, which varies with height.

2.7 Turbulence Model Equations

The standard k - ϵ and k - ω model equations are not consistent with the Monin-Obukhov profiles, and so, strictly, modifications are needed to these equations in order for the inlet profiles to be preserved from inlet to outlet in open-field simulations. Similarly, the standard wall functions need to be modified for consistency with Monin-Obukhov similarity theory. Both of these modifications have not been implemented in time for this first release of the Pasquill-Profiles facility.

3. MODEL INPUT

The model inputs can be set automatically by the [WIND](#) object. To do this manually, the PHOENICS User needs to specify the following input parameters in the Q1 input file:

- 1) Retrieve the following log-law parameters from the WIND object:

```
ZO=0.1 ! roughness height ; QREF=2.0 ! wind speed at reference height
ZREF=10.0 ! reference height
```

These will be needed to compute the ground heat flux for use in the TEM1 COVAL statement, as discussed in 8) below.

- 2) In the VR Menu, under "Menu">"Sources"> activate "Gravitational Forces", set the gravitational vector, and then select either "Density Difference" or "Boussinesq" for the buoyancy model.
- 3) Deactivate the buoyancy forces in the non-gravitational grid directions by using:

```
COVAL(BUOYANCY,U1,ZERO,ZERO ) ; COVAL(BUOYANCY,W1,ZERO,ZERO )
```

- 4) Create 3d whole-field storage using STORE for the variables listed in Table 3.1.
- 5) Set the integer-control variables ITPRO and MONIN, as follows:

```
ITPRO = 0 uniform temperature (default)
      MOLEN = 0 user-specified value of the MO length
      = 1 TNO equation (2.4.1) (default)
      = 2 Golder equation (2.4.2)
```

```
SPEDAT(SET,BLIN,MOLEN,I,MOLEN)
```

- 6) Set Surface Temperature : GT0=10.0 , SPEDAT(SET,BLIN,GT0,R,GT0).
- 7) Select Pasquill Stability Class by setting the INTEGER variable ITPRO to 1, 2, 3, 4, 5 or 6 (see tables 2.4.1 above and Table 3.2 below):

```
SPEDAT(SET,BLIN,ITPRO,I,ITPRO);
```

The variable ITPRO will be set automatically for each class, according to Table 3.2 below.

- 8) Compute Ground heat flux from equation (2.5.2), and then set TEM1 boundary condition:

```
AKA=0.41;ZRDZO=ZREF/ZO ; ZETAR=ZREF/GLMO
PSIUR=-5.*ZETAR ; LOGZDZ=LOG(ZRDZO) ; QTAU= AKA*QREF/(LOG(ZRDZO)-PSIUR);
USDK=QTAU/AKA ; RHOAMB=PRESS0/(286.7*(GT0+TEMP0))
GQWALL=-(QTAU**3)*(GT0+TEMP0)*RHOAMB*CP1/(AKA*9.81*GLMO)

COVAL(BLIN6,TEM1,FIXFLU,GQWALL) ; SPEDAT(SET,BLIN,GQWALL,R,GQWALL)
```

Name	Inlet variable	
TIN	Temperature	Optional
RHIN	Density	Optional
PIN	Pressure	Optional
TREF	Temperature	Optional
UIN	Inlet velocity component in the x direction	Optional
VIN	Inlet velocity component in the y direction	Optional
WIN	Inlet velocity component in the z direction	Optional
KEIN	Turbulence kinetic energy	Optional
EPIN	Turbulence dissipation rate	Optional
OMIN	Turbulence frequency	Optional
TPOT	Potential temperature	Optional

Table 3.1 Whole-field variables

Class	A	B	C	D	E	F
	Very unstable	Moderately unstable	Slightly unstable	Neutral	Slightly stable	Moderately stable
ITPRO	1	2	3	4 or 0	5	6

Table 3.2 Pasquill Class input variables

** temperature profile
 SPEDAT(SET,BLIN,ITPRO,I,ITPRO)
 GZT0=0.0 ; SPEDAT(SET,BLIN,GZT0,R,0.)
 GALR=-9.81/CP1 ! adiabatic lapse rate
 TSTAR=-GQWALL/(RHOAMB*CP1*QTAU) ; TSDK=TSTAR/AKA
 TKCON=QTAU*QTAU;EPCON=QTAU**3/AKA

4. SOURCE FILES

The following source files have been modified to implement the Pasquill-Profiles facility:

/phoenics/d_earth/d_core/gxblin.for
 /phoenics/d_earth/d_core/grex3.for
 /phoenics/d_earth/d_core/gxbuoyso.for

5. BASIC TEST CASES

Table 4.1 below provides a list of the Q1 files produced to test basic functionality:

Core Library Case No	Test case	Remarks
676	Case1a-3d-Zup-Xflo-PasqF3_DensD	Gravity in Z Flow in X
677	Case1b-3d-Zup-Xflo-PasqF3_Buoss	Gravity in Z Flow in X
678	Case2a-3d-Yup-Xflo-PasqF3_DensD	Gravity in Y Flow in X
679	Case2b-3d-Yup-Xflo-PasqF3_Buoss	Gravity in Y Flow in X
680	Case3a-3d-Xup-Yflo-PasqF3_DensD	Gravity in X Flow in Y
681	Case3b-3d-Xup-Yflo-PasqF3_Buoss	Gravity in X Flow in Y
682	Case4a-3d-Xup-Zflo-PasqF3_DensD	Gravity in X Flow in Z
683	Case4b-3d-Xup-Zflo-PasqF3_Buoss	Gravity in X Flow in Z
684	Case5a-3d-Yup-Zflo-PasqF3_DensD	Gravity in Y Flow in Z
685	Case5b-3d-Yup-Zflo-PasqF3_Buoss	Gravity in Y Flow in Z
686	Case6a-3d-Zup-Yflo-PasqF3_DensD	Gravity in Z Flow in Y
687	Case6b-3d-Zup-Yflo-PasqF3_Buoss	Gravity in Z Flow in Y

Table 5.1 Flat-terrain Pasquill-F Test Cases: - Wind speed 3 m/s unless stated otherwise; DensD denotes density-difference buoyancy, whereas Buoss denotes Boussinesq buoyancy.

6. CONCLUDING REMARKS

PHOENICS 2022 has been equipped with the facility to use Pasquill profiles facility for use in simulations of the ABL with conditions of both stable and unstable stratification. This first release of the facility will be subject to further upgrades because further work is needed as follows:

- For density-difference cases, allow the inlet density to vary with height.
- Sky heat-flux boundary condition to compensate for ground heat flux
- Modify the turbulence transport equations and wall functions to account for MO theory.
- Option to solve for the energy equation in terms of the potential temperature.
- Validate the implementation against measurements and other CFD simulations.
- Logarithmic temperature profile for neutral conditions (ITPRO=4).

7. REFERENCES

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