On numerical modelling of atmospheric gas dispersion

Using computational fluid dynamics approach

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Mostly all human activities are affected by Atmospheric boundary layer (ABL). This is also where most air pollution phenomena are occurred. Understanding of the processes taking place in the ABL has attracted various research study.

Computational Fluid Dynamics (CFD) is increasingly being used in simulation of ABL flows. Ensuring accurate description of the ABL is an important task in any ABL flow study. This can be done by simulating the horizontally homogeneous ABL flow prior of dispersion study. Either the Reynolds Averaged Navier–Stokes (RANS) equations or Large Eddy Simulations (LES) are used for atmospheric turbulence modelling. The RANS turbulence models are still widely used in practical approach to overcome boundary conditions sensitivity and computational intensive of the LES. Two equation turbulence models: standard $k-\varepsilon$ and SST $k-\omega$ turbulence models are modified substantially using open source CFD tool OpenFOAM to validate its usage in simulating ABL flow.

Monin-Obukhov similarity theory, well validated for flow in ABL surface layer over homogeneous surface, is used to model the profiles of velocity, turbulent kinetic energy and turbulence dissipation rate at inlet of computational domain. Consistency of these profiles across the domain are ensured by deriving the relation between turbulence model constants for horizontally homogeneous constant shear stress flow. This verified turbulence model is then validated using simulated atmospheric dispersion flow of dense gas and field experiments of Liquefied Natural Gas (LNG) vapour dispersion. For simulation of LNG vapour dispersion, the proposed model also takes into accounts the heat transfer from the ground to the vapour cloud, the effect of variable temperature on gas properties. Statistical Performance Measures (SPM) are compared with LES code FDS (Fire Dynamics Simulator) and specified dispersion code FLACS (FLame

ACceleration Simulator) under Model Evaluation Protocol (MEP) proposed for LNG vapour dispersion.

Nomenclature

Acronyms

Symbol	Description
ABL	Atmospheric Boundary Layer
FAC2	Factor of 2
FDS	Fire Dynamics Simulator
FLACS	FLame ACceleration Simulator
LES	Large Eddy Simulations
LFL	Lower Flammability Limit
LLNL	Lawrence Livermore National Laboratory
LNG	Liquefied Natural Gas
MBSE	Mean Relative Square Error
MEP	Model Evaluation Protocol
MG	Geometric Mean Bias
MRB	Mean Relative Bias
NFPA	National Fire Protection Agency

RANS	Reynolds-Averaged Navier-Stokes
SPM	Statistical Performance Measures
SST $k-\omega$	Menter's Shear Stress Transport $k-\omega$
VG	Geometric Variance

Dimensionless Numbers/Quantities

Symbol	**Description**	**Definition**
Pr	Prandlt number	ν/α
Sc	Schmidt number	ν/D

Greek Symbols

Symbol	**Description**	**Units**
α	Thermal diffusivity	m^2/s
α_P	Numerical under-relaxation factor	
ε	Turbulence dissipation rate	$\mathrm{m}^2/\mathrm{s}^3$
ε^+	Near wall scale of turbulence dissipation rate	
κ	von Karman constant	
μ	Dynamic viscosity	kg/ms
ν	Kinematic viscosity	m^2/s
ν^+	Near wall scale of kinematic viscosity	
ω	Turbulence specific dissipation rate	$1/\mathrm{s}$
ω^+	Near wall scale of turbulence specific dissipation rate	

ϕ_h	Monin-Obukhov universal temperature similarity function	
ϕ_m	Monin-Obukhov universal momentum similarity function	
ρ	Fluid density	$\mathrm{kg/m^3}$
τ, τ_{ij}	Viscous stress tensor	$\mathrm{N/m^2}$
τ_s	Surface shear stress	$\mathrm{N/m^2}$
θ	Potential temperature	K
θ_*	Friction temperature	K
$\boldsymbol{\delta}$	Kronecker symbol	

Roman Symbols

Symbol	Description	Units
$\boldsymbol{g}$	Gravitational acceleration vector	$\mathrm{m/s}$
$\boldsymbol{u}$	Velocity vector	$\mathrm{m/s}$
A	matrix of coefficients	
C_m	Experimental measured concentration	
C_p	Predicted concentration from simulation	
c_p	Specific heat	$\mathrm{J/kgK}$
D	Mass diffusivity	$\mathrm{m^2/s}$
E	Smooth wall constant	
h	Enthalpy per unit mass	$\mathrm{J/kg}$
h_{ABL}	Height of ABL	m

k	Turbulence kinetic energy	$\mathrm{m^2/s^2}$
k^+	Near wall scale of turbulence kinetic energy	
L_{MO}	Monin-Obukhov length	m
M	Specie molecular weight	kmol/kg
p	Fluid pressure	$\mathrm{N/m^2}$
p'	Numerical pressure correction	$\mathrm{N/m^2}$
p_{rgh}	Pressure defined without hydrostatic pressure	$\mathrm{N/m^2}$
q_s	Surface heat flux	$\mathrm{W/m^2}$
S_ε	Source term in turbulent dissipation rate equation	
S_k	Source term in turbulent kinetic energy equation	
T_s	Surface temperature	K
u'	Numerical velocity correction	m/s
u^+	Near wall region velocity scale	
u_*	Friction velocity	m/s
w_*	Convective velocity	m/s
Y	Specie mass fraction	
y^+	Near wall region length scale	
z_0	ABL roughness length	m

Subscripts

Symbol **Description**

α	Species index
eff	Sum of turbulence and laminar part of properties
t	Turbulence part of properties
P	Properties at cell point adjacent to wall
w, s	Properties value at wall/surface

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