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SPECIFICATIONS OF CFD MODELLING TO ESTIMATE THE EFFECTIVENESS OF LARGE-SCALE AIR CLEANING SYSTEMS IN URBAN ENVIRONMENT

Installation, testing, and validation (using measured data) of CFD model to calculate the concentration distribution of pollutants in various locations in Urban areas under background situation and when a large-scale outdoor air cleaner is in operation. The detailed specifications are given below.

I	General Features	Compliance “Yes” or “No” (or remarks, if required)
1	Atmospheric Boundary Layer generation using 3D CFD with sufficient validation for turbulent mixing due to complex hilly, vegetated, urban and industrial topography	
2	User friendly graphical interface for environmental and risk analysis engineers with no/little numerical knowledge	
3	Multiple sources: point/ line, stacks, surface sources and volume sources	
4	Simulation of clean air and pollutants dispersion for long term impacts using wind data	
5	Domain area of 5 km*5 km*1 km (height depends on the stability)	
6	Clean/polluted air plume interaction with structures (buildings, reservoir, tanks)	
7	Spatial resolution of 50 m and 10 m horizontal and vertical respectively with provision for variable grid spacing	
8	Provision to export results in terms of tables and generic formats such as Tecplotetc.	
9	Facility to read solution from mesoscale models like WRF and MM5 to generate initial and boundary conditions for CFD simulation	
II	Air cleaner system and performance evaluation	
1	Profiling pollutant at the tower inlet and outlet	
2	Modelling the tower system and the perturbation induced in the atmospheric flows	
3	Modelling the air flow velocity distribution, temperature and RH profile at the tower inlet and outlet	
4	Height and width of clean air zone in all the directions w.r.t wind direction	
III	Topographical Set-up	
1	Integrated CAD-GIS for terrain modeling with: a) Site data: location, major land use pattern b) Altitude curves that define the terrain undulations	

	c) Buildings and obstacles: cubical, cylindrical, arbitrary shaped, porous/packed	
2	Facility in the pre-processor to read topography data in standard formats including: a)GTOPO	
	b) ETOPO	
	c) Surfer Grid	
	d) ASCII XYZ	
3	Map projection including Transverse Mercator (TM), Universal Transverse Mercator (UTM) and Lambert Conformal Conic to convert topography data in geographic coordinates to plane coordinates	
IV	Pollutant Database	
1	Thermodynamic properties e.g. molecular weight and Cp used for air and its mixture with pollutant species.	
2	Transport properties such as viscosity and diffusion coefficient of the pollutants	
3	Built-in chemical database from which the properties of species can be read. The database can be edited by the user to modify/add/delete species.	
4	Considers PM across a broad spectrum of sizes ranging from 1 nm to 20 micrometres and chemical composition including hygroscopicity along with trace gases	
5	Capable to incorporate available PM concentration data on a continuous basis	
V	Emission Sources and Sinks	
1	Multiple types of sources and sinks: Handling of multiple sources and sinks <ul style="list-style-type: none"> • Point: Emissions directed vertically, horizontally, or other direction • Line: Emissions from road traffic • Area: Emissions from a surface patch on the ground or obstacle • Volume: Emissions from a volumetric region 	
2	Pollutant release– continuous or over a specific duration with changing emission rate	
3	Incorporation of size dependent, dry and wet deposition velocities to estimate PM removal	
VI	Meteorological Data	
1	Incorporation of constant or time varying weather conditions	
2	Dedicated fast CFD solvers for the generation of wind field taking in to account measured values	
3	Ability to incorporate meteorological data such as wind data, solar insolation, etc.into CFD simulation at discrete locations	
4	Interpolate meteorological data from other global software if "measured data" not available	
5	Predict seasonal and diurnal effects on air pollutants	
VII	Numerical Modelling Features	
1	Higher order CFD schemes for solving non-linear partial differential equations of conservation of mass, momentum, energy, and species concentrations	
2	Automatic optimal discretization – meshing and time stepping – for stable and optimal mesh independent solution	
3	Meshing capability to generate terrain fitting hexahedral grid for Atmospheric Dispersion applications	
4	Built-in adaptive mesh refinement capabilities based on function of any primitive and/or derived variable	

5	Built-in functions, without need for writing user defined function code, including logarithmic function, power law function, exponential function, trigonometric function, for specifying velocity and turbulence variable profiles and other higher mathematical functions, if necessary.	
6	Built-in interpolation options, without need to for writing user defined function code, including inverse distance and inverse distance squared interpolations	
7	Various lengths of period for impact simulation	
8	Finite volume based standard dispersion solver	
9	Facility to change turbulence models (within same class of models such different k-epsilon or different k-omega models) on the fly during a simulation.	
10	Different turbulence models for different areas with verified turbulence coefficients	
11	Predict concentration distribution at every 30-minute intervals at various grid points without and with Air Cleaner Operation	
12	Availability of both Eulerian and Lagrangian transport models	
13	Should be able to adopt and recalibrate the model when measured concentration and met data are available	
14	Should take the tower perturbation on wind flow as well as concentration distribution into consideration	
15	Ability to incorporate aerosol dynamics including ground deposition, hygroscopic growth and coagulation	
16	Outlet boundary condition with mass flow correction to allow wind flow to come into the domain at some places and exit the domain at some places	
VIII	User Interface	
1	Pre-Processing: a) Customized interface for the dispersion of air	
	b) Graphical User Interface with prompts for inputs as: <ul style="list-style-type: none"> • Chemical species, pollutants involved in the case and their properties • Study area • Terrain topography • Meteorological data • Source emission data • Sink collection data 	
2	Post-Processing: a) Plots showing the computational mesh in the background for analysis	
	b) Velocity vectors of the wind field	
	c) Contour plots of flow parameters such as temperature, turbulent viscosity, etc. and the selected species concentrations	
	d) Contour plots for the derived properties (user defined property)	
	e) Iso-surface plots of flow parameters and the selected species concentrations.	
	f) Provisions of overlay i.e., super imposing base map and building structures and results there on.	
	g) Ability to save the simulation results data like spatial variation of flow parameters and species concentrations along a line on the ground or in the vertical direction as well as residual and flux balances for all the variables in CSV for further analysis	
3	Predicting the PM concentration w.r.t different sizes, RH, temperature and wind field at every grid point	

IX	Other Important Features	
1	Provision to export results to Grads	
2	Predicting the effective reduction zone (ERZ) of pollutants around their cleaner system including diurnal and seasonal variations	
3	Integrated advanced GIS to generate complex topography interactively or import GIS files and clean them for environmental dispersion applications	
4	PUFF Dispersion solver (for faster simulations)	
5	Meteorological pre-processor generates data based on the user inputs required by the CFD solver	
6	Ability to gather data from real time sensors and predict variations of pollutant concentrations around the air cleaner setup continuously over long periods of time for instance a week	
7	CAD based graphical interface for physical model set up for pre-processing	
8	Access to source code with technical manual for further customization	
X	Installation and Validation	
1	Installation and testing of CFD simulation software at client location by Software Company Officials or Engineers.	
2	Software manual supported by publications; reports should be provided at the time of software delivery.	
3	Documentation i.e. user's manual, developer's manual etc.	
4	Participation in validation and model calibration/modification (depending on the pilot study measurements) during the next 1-year period	
XI	Software Training and Support	
1	Training on CFD simulation software should be conducted at client location or software company premises after installation of software. During the training and for usage thereafter, software company should generate tutorials on cases of specific interest like effect of large-scale air cleaning towers at site.	
2	Technical support throughout the one-year period must be provided (200 working hours)	
XII	Software Maintenance Assistance	
1	Software maintenance assistance should be provided by the company minimum for one-year period after the delivery of software.	
2	Software maintenance assistance should ensure full functioning of the software.	
3	Perpetual software license should be provided while delivery	
XIII	Summary of Deliverables	
1	A CFD based numerical code to predict the PM concentration w.r.t different sizes, RH, temperature and wind field at every grid point	
2	Predicting effective reduction zone (ERZ)	
3	Source code for the calibrated CFD model along with user and developer's manual. Multiple user license and accessibility to modify the code to add new processes if found necessary.	

*The air cleaner basically is a large-scale filtration device which sucks air from a height of 20 m and releases at a height of 5 m at the ground at horizontal flow rates up to 1000 m³/s. For further details, please reach out to Prof. Manoranjan Sahu, ESED, IITB.