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## ANALYSIS OF SURFACE WATER QUALITY IN KALINGARAYAN CANAL BY NUMERICAL MODELING USING COMPUTATIONAL FLUID DYNAMICS (CFD)

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### Abstract

Kalingarayan canal is the oldest canal constructed in 1271 AD – 1283 AD located in Erode district and it is useful for irrigation purposes. This canal receives polluted water from various industries located nearby and also polluted by domestic activities and now is subjected especially to heavy metal pollution. This paper examines the pollutant status in the surface water of the Kalingarayan canal. The objective of the study is to find the dispersion of the pollutant concentrations, particularly heavy metals in surface water of canal. It is important to predict the environmental impact of new emissions in rivers, especially during periods of drought. Computational fluid dynamics (CFD) has proved to be an invaluable tool to develop models which identifies the dilution distance of pollutants along and across the Kalingarayan canal. The problem of heavy metal is addressed because water in the canal is polluted by anthropogenic activities, industrial and other uses. The study relies on experimental data gathered during monitoring campaigns conducted for a period of three years from 2014 to 2016. Every month surface water samples were collected from 8 stations along the canal. Heavy metal concentration was analyzed in the water samples for three seasons namely summer, pre-monsoon and post-monsoon periods. From CFD, it is observed that the distance at which the concentration of pollutant species becomes very much low and constant, reached i.e., across the canal is about 13 meters from the source point. The concentration of pollutant species along the canal is comparatively higher to that of the previous case (across the canal) till the distance of about 450 m. The results are in agreement with the experimental data obtained from the Kalingarayan canal. The geometrical model of the canal is developed in ANSYS - ICEM CFD. The domain is discretized using "MULTI BLOCKING TECHNIQUE" through which one can achieve a good quality structural mesh. It is highly recommended in computing for a better result.

*Keywords:* ANSYS, CFD, heavy metals, pollutant, surface water

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### 1. Introduction

Water polluted by anthropogenic activities is harmful to humans and animals. Unbalanced river and lake ecosystems cannot support full biological diversity (Kumar et al., 2017a). Deforestation, acid rain and many other sources are causes for water pollution. Surface water are important sources for drinking, irrigation, washing, and industrial uses.

Among the surface water sources of irrigation, canal irrigation is the most important form of irrigation in India (Owa, 2013). There is a necessity to analyse the aquatic system to see the status of surface water for irrigation purposes (Bhateria and Jain, 2016).

Heavy metals have a particular significance in ecotoxicology due to their long persistence, bioaccumulation and biomagnification in the food chain (Yin et al., 2018). Kumar et al. (2019)

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determined the presence of maximum toxicity in As, Co, Cr and Ni in the surface water bodies through the median lethal toxicity index database collected throughout the world from 1994 to 2019. In addition to that, to avoid the human risk, aquatic phytoremediation plant species and adsorbents introductions in the land management plans are recommended (Kumar et al., 2016, 2017b, 2018a; Setia et al., 2020).

The pollutant dispersion can be studied by CFD and also the dispersion trend with time (Marusic et al., 2016a). The spatial and temporal evolution of the transportation process and pollution dispersion is found and proven to be most appropriate in the mathematical and numerical modeling by using Navier-Stokes equations (Marusic et al., 2016b). Some author's tried Hydrological Engineering Centers River Analysis System (HECRAS) with Modified Streeter Phelps equations to study the water quality (Fan et al., 2012). The combined equations are used to simulate the water quality of rivers. Pollutants like conductivity, COD, Mn and BOD<sub>5</sub> are also useful in analyzing the upstream and downstream of the critical points of water bodies (Petrescu and Sumbasacu, 2010). Application of 2D mathematical model is useful to assess the variation of velocity, sediment transport and bed level changes (Sarfaraz and Matin, 2013).

CFD model is helpful in suggesting possible future development in the river to estuary. The draft scarcity, silt variation, hydrological and change in morphology in the river can be studied by using a mathematical modeling like HEC-RAS 4.1.0 (Chowdhury and Navera, 2015). With modifications of CFD, the 2.5D non-hydrostatic model in the Boussinesq approximation (Tsydenov and Starchenko, 2013; Tsydenov et al., 2015, 2016), takes heat fluxes into effects of wind and other forces and shows the variation of impurities entering in the water bodies along the variation of thermal bar movement.

Pollution discharges are expected more nowadays from industrial and urban areas. In different monitoring stations, field data can be compared with two computational models during evaluation. Parameter estimation can be developed from models in the form of non-linear equation with flow rate. Derived coefficient of the equation which is known for a particular stream, can be used for calculating parameters for other streams (Ani et al., 2009; Ani, 2010). This study is useful, by developing a pollutant transport model for assessing pollution and to take correct management decision. Modelling was framed for the surface water to find the diffusion patterns along and across the canal and finally validated with field data (El-Alfy et al., 2017; Kachiashvili et al., 2007; Petrescu and Sumbasacu, 2010; Prem et al., 2017; Vasarevicius et al., 2010).

A stretch of 140-kilometers along the Kalingarayan canal is fed by the Bhavanisagar dam and the canal serves as a main source of water to the Erode district, being further taken for conducting the water pollution study.

Kalingarayan canal which gives life to hundreds of farmers in Erode district, now faces pollution problems (Divahar et al., 2019; Kulandaivel et al., 2009). Untreated effluents from the tannery units and textile processing plants are dumped into Kalingarayan canal which is affecting the water quality (Divahar et al., 2020; Mohanakavitha et al., 2019a, 2019b). As a consequence of this, deterioration of the soil and the productivity of crops has dropped dramatically. Thus, due to the destroyed quality of the canal which is meant for irrigation purpose, undesirable results is met by the people who consume the canal water for drinking and agricultural purposes (Palanisamy et al., 2007; Sivakumar et al., 2010). The study basically concentrates on the pollution by industrial disposal of effluents rather than the solid waste dumping (Cheema et al., 2018).

Any type of physical conditions can be simulated theoretically in CFD, which have the best control over the processes and support to simulate any specific theoretical environment need for the study. An analyst can examine any numbers of specific locations in a region of interest and extract a comprehensive set of flow parameters for examination through CFD. The CFD model uses the technique of approximate numerical computation (Dunn et al., 2015). Thus, the model CFD can be applied to present field data of the Kalingarayan canal to know the diffusion patterns along and across the canal by the surrounding environmental activities.

Therefore, in this research, in the evaluation of the surface water quality status of Kalingarayan canal, we have applied a combination of numerical modelling using CFD with a computation of heavy-metal contamination indexes, which was different from the usual and found to be unparalleled compared with any other previous studies made. To achieve this goal we have conducted: (i) a compilation of heavy-metal concentration in the Kalingarayan canal surface water for the period of three years from 2014 - 2016; (ii) a water quality comparison among the guidelines of Bureau of Indian Standards (BIS) and World Health Organization (WHO), to study the suitability of water for irrigation (IS 2296: 1982) and drinking water purpose (IS 10500: 1991 & WHO); (iii) numerical modelling using CFD to identify the dilution distance of pollutants along and across the Kalingarayan canal.

## 2. Experimental

### 2.1. Description of the study area

Kalingarayan canal was constructed in the period 1271AD - 1283AD. The canal starts from Kalingarayan dam located on River Bhavani. The canal starts and flow through the district Erode and ends in Kodumudi. This canal is having more irrigation area as its path on its way. It covers a length of 92 km. It is covering the entire Erode district. This canal is having its mean sea level starting from 125.75 m to 162.80 m. In River Cauvery banks the Kalingarayan canal is on the west side with an extent of 7621 Sq. kms (Fig. 1).

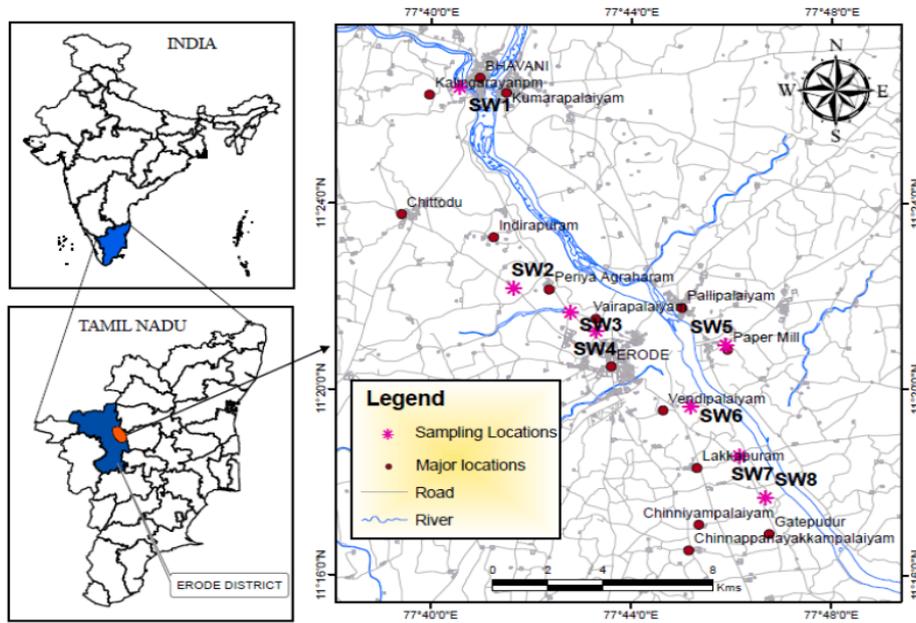


Fig. 1. Locations of the monitoring stations on Kalingarayan canal in Erode

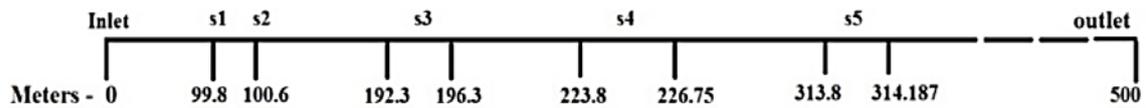


Fig. 2. Effluent discharge port distances (S1- first source point, S2- second source point, S3- third source point, S4- fourth source point, S5- the fifth source point)

Tropical climate is prevailing in the area and which makes the canal enriched with dense population and industries. A length of 500 m along the canal with different effluent openings are studied (Fig. 2). Openings are the inlet of the source point (point of entry of pollutants into the canal). In the model, the openings (inlets) S1 and S2 are placed at 99.8 m and 100.6 m, respectively away from the inlets. The openings S3, S4, S5 is placed in the distance of 192.3 m - 196.3 m, 223.8 m - 226.75 m, 313.8 m - 314.87 m, respectively.

## 2.2. Sample collection and analysis

The basic data pertaining to the canal by the impact of domestic, industrial, agricultural and other activities are presented in this section. Since, the canal water is degraded, monitoring of the canal water for heavy metals is necessary to make this water useful for domestic, agricultural and industrial purposes in the future.

This study is based on spatial and temporal variation of E in heavy metal in eight surface water stations along the canal where water quality is suspected to be affected by the heavy metals/Pollutants (Table 1). The water quality is tested during three seasons namely summer, pre-monsoon and post-monsoon for the heavy metals content

(Ismail and Robescu, 2018). Parametric analysis of surface water was done once in a month for three years (January 2014 to December 2016) for 8 months. A total of 24 samples were collected from 8 different sampling locations. The average values for every season has been determined and projected in Table 2. A five liters polyethylene cans are used to collect water for the study and stored in 4°C in cool condition after measuring pH at the site itself. Atomic absorption spectrophotometer has been used in measuring heavy metals.

The amount of heavy metals present in the water is negligible during the monsoon season. While comparing with these three seasons in post monsoon season the heavy metal concentration is low. This is due to the dilution of canal water in that season. According to BIS (1991), the parameters analyzed are tested for the concentrations. The average concentration of heavy metals in the surface water range from 0.045-8.530, 0.040-0.710, 0.023-0.723, 0.002-1.557, 0.001-0.009, 0.002-0.053, 0.009-0.097 and 0.140-2.698 mg/L for the metals Fe, Mn, Zn, Cu, Cd, Ni, Pb and Cr, respectively. The dominance of various heavy metals in the surface water follows the sequence: Fe > Cr > Cu > Zn > Mn > Pb > Ni > Cd. The concentrations of Zn, Cd, Ni and Pb are within the limits prescribed for drinking and agricultural purposes.

**Table 1.** Location of surface water samples in Kalingarayan canal

S. No	Latitude	Longitude	Sample code	Sampling locations (Polluting factors)
1	11°26'26.69"N	77°40'36.27"E	SW1	KalingarayanAnicut (Agricultural Activities)
2	11°23'13.92"N	77°41'43.78"E	SW2	Chunnambuoodai (Tanneries)
3	11°21'49.29"N	77°42'43.45"E	SW3	Convent School (Domestic area)
4	11°21'44.96"N	77°43'16.18"E	SW4	Vairapalayam (Dyeing units)
5	11°21'27.98"N	77°44'12.87"E	SW5	Pallipalayam (Paper mills)
6	11°19'37.77"N	77°45'9.56"E	SW6	Vendipalayam (Domestic area)
7	11°18'39.08"N	77°46'13.97"E	SW7	Lakkapuram (Domestic area)
8	11°17'37.41"N	77°46'39.02"E	SW8	Colony Pudur (Domestic area)

**Table 2.** Average concentrations of pollutant parameters in surface water of the Kalingarayan canal in Tamilnadu

Metal	Season	Average concentration of metal (mg/L)								Statistical data			
		SW <sub>1</sub>	SW <sub>2</sub>	SW <sub>3</sub>	SW <sub>4</sub>	SW <sub>5</sub>	SW <sub>6</sub>	SW <sub>7</sub>	SW <sub>8</sub>	Min	Max	Mean	SD
Fe	Summer	1.58	8.53	4.19	3.25	5.27	1.23	1.15	1.15	1.15	8.53	3.29	2.63
	Pre monsoon	1.25	2.34	1.74	1.3	0.65	1.00	0.79	0.79	0.65	2.34	1.23	0.57
	Post monsoon	0.091	1.421	0.121	0.11	0.32	0.091	0.045	0.045	0.05	1.42	0.28	0.47
Mn	Summer	0.41	0.43	0.4	0.26	0.28	0.36	0.25	0.24	0.24	0.43	0.33	0.08
	Pre monsoon	0.71	0.64	0.42	0.13	0.18	0.24	0.18	0.18	0.13	0.71	0.34	0.23
	Post monsoon	0.08	0.06	0.07	0.08	0.05	0.06	0.04	0.04	0.04	0.08	0.06	0.02
Zn	Summer	0.065	0.084	0.053	0.082	0.071	0.064	0.023	0.023	0.02	0.08	0.06	0.02
	Pre monsoon	0.35	0.66	0.512	0.723	0.642	0.524	0.326	0.326	0.33	0.72	0.51	0.16
	Post monsoon	0.024	0.095	0.111	0.083	0.058	0.084	0.062	0.062	0.02	0.11	0.07	0.03
Cu	Summer	0.017	0.283	0.347	0.426	0.585	0.427	0.302	0.302	0.02	0.59	0.34	0.16
	Pre monsoon	0.804	0.885	0.748	0.645	0.682	1.557	1.424	1.424	0.65	1.56	1.02	0.38
	Post monsoon	0.003	0.007	0.095	0.012	0.086	0.004	0.002	0.002	0.00	0.10	0.03	0.04
Cd	Summer	0.008	0.006	0.006	0.007	0.005	0.004	0.003	0.003	0.00	0.01	0.01	0.00
	Pre monsoon	0.001	0.008	0.008	0.009	0.004	0.003	0.003	0.003	0.00	0.01	0.00	0.00
	Post monsoon	0.003	0.002	0.001	0.001	0.001	0.001	0.001	0.001	0.00	0.00	0.00	0.00
Ni	Summer	0.045	0.053	0.044	0.052	0.052	0.031	0.025	0.025	0.03	0.05	0.04	0.01
	Pre monsoon	0.035	0.041	0.038	0.035	0.032	0.026	0.02	0.02	0.02	0.04	0.03	0.01
	Post monsoon	0.021	0.005	0.005	0.006	0.005	0.002	0.002	0.002	0.00	0.02	0.01	0.01
Pb	Summer	0.015	0.015	0.091	0.097	0.092	0.09	0.09	0.09	0.02	0.10	0.07	0.04
	Pre monsoon	0.015	0.015	0.012	0.012	0.009	0.009	0.009	0.009	0.01	0.02	0.01	0.00
	Post monsoon	0.006	0.008	0.01	0.01	0.009	0.009	0.009	0.009	0.01	0.01	0.01	0.00
Cr	Summer	0.804	2.698	2.28	2.424	1.56	1.424	0.84	0.84	0.80	2.70	1.61	0.77
	Pre monsoon	0.283	1.56	1.54	1.14	1.17	0.302	0.302	0.302	0.28	1.56	0.82	0.58
	Post monsoon	0.14	0.94	0.14	0.685	0.585	0.28	0.28	0.28	0.14	0.94	0.42	0.29

Note: Max: Maximum; Min: Minimum; SD: Standard deviation; SW: Surface water.

But other parameters like Fe, Mn, Cu and Cr exceed the limitation during all the seasons. These parameters Fe, Mn and Cu are also within available limits during rainy seasons, whereas Cr is not in the acceptable limit in all the seasons.

More than 500 tanneries are established along the canal and discharging the effluents into the canal (Rao et al., 2020; Yuce and Altundag, 2020). This is the reason for the appearance of Cr in surface water of the canal. The water used for drinking purpose should be free from organic pollution and heavy metals. Therefore, the canal water cannot be used for drinking purpose before further treatment. The long-term usage of canal for irrigation also causes adverse effects in the soil as well as in the yield of crops (APHA, 1995; Jindal and Sharma, 2011; Kumar et al., 2018b; Nivetha et al., 2019).

### 3. Numerical simulations using CFD

#### 3.1. Introduction to CFD

Computational fluid Dynamics is a useful tool to study the dynamics of the flow, to analyze and solve the problems related to fluid flow. The CFD interprets the process of fluid flow, including turbulent flow and also the characteristics of the flow at any distance and time. The result obtained from this model is widely used because of its precision. It is advantageous that the simulations of physical conditions can be executed in short period of time in CFD. In this study, CFD is used to understand the diffusion pattern of different pollutants and also to determine the diffusion distance of the pollutants along and across the canal (Bosneagu et al., 2019).

The main contribution of the present work is that it proposes a three-dimensional model capable of predicting the dispersion of effluents in open channels using a very fast in-house code, an unusual feature for CFD models. Due to this, it is possible to predict the diffusion of different pollutants and also to determine the diffusion distance of the pollutants along and across the canal kilometers long. The end product of

this research has applications as a predictive tool to support and guide management decisions of an industrial nature.

Using CFD, it would be possible to calculate all the parameters in each point of the current, compared to experimental method, where only few points can be obtained. To explain it more clearly, by using the CFD technique, complete information and very precise details can be obtained for solving the problem. On the other hand, the CFD method has been used by many researchers in recent years and has been mentioned as a powerful method to study different issue in the water quality. This method has many advantages in comparison with traditional methods.

### 3.2. Preprocessing

In preprocessing, grid generation and fluid domain extraction play an important role with a good quality mesh. Here, the CAD model is imported into the CFD model tool. By removing the extra parts from the base model, geometry is simplified.

### 3.3. Problem formulation

#### 3.3.1. Governing equation

There are two components necessary to study quality of water. One is a mathematical equation for that particular sector of the river. Second part is the evaluation of the model by the numerical equations (Gagescu et al., 2011; Kachiashvili et al., 2007; Marusic et al., 2012, 2015; Marusic, 2013). The Navier-Stokes equation is followed and also continuity equation.

The governing equation is a non-homogeneous flow and it follows the second order partial differential equations. The governing equations should describe the flow and dispersion because the pollutant dispersion is heterogeneous in space. The assumptions to be observed are: (1) flow is turbulent, (2) no chemical reaction occurs and (3) physical properties are constant. The following equations are useful in solving the flow behavior. The conservation of mass equation is distributed over the cross section of the canal giving subject to a first order decay process.

Conservation of mass is shown in Eq. (1):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m \quad (1)$$

where: the first part represents unsteady term, the second represents convective and  $S_m$  is the mass source term.

The momentum equation (for  $i = 1, 2, 3$ ) is shown in Eq. (2):

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \cdot \vec{v}) = -\nabla p + \nabla \cdot (\bar{\tau}) + \rho \vec{g} + \vec{F} \quad (2)$$

where:  $i$  is the invariant mass;  $v = (U_i, U_j, U_k)$  is the mean velocity. The first term in the right represents pressure gradient, second term represents shear and other body forces are represented by third and fourth

term. The flow is assumed to be turbulent and turbulence is modelled by using the K-epsilon model. K-epsilon model includes two extra transport equation in order to represent the turbulent properties of the flow, thus it identified as a ‘two-equation’ model. This extra equations accounts the convection and diffusion effects of turbulent energy. The first transported variable ‘ $k$ ’ represents the turbulent kinetic energy and the second transported variable ‘ $\epsilon$ ’ represents turbulent kinetic energy dissipation rate. The variable  $k$  determines the energy of the turbulence instead of its scale (Chung, 2019; Chau and Jiang, 2002; Mohammad et al., 2019; Nakkina et al., 2016). The turbulent kinetic energy  $k$ , and its rate of dissipation  $\epsilon$ , for this model are obtained by Eqs. (3- 4).

The conservation of turbulence kinetic energy ( $k$ ) (Eq. 3):

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \epsilon - Y_M + S_k \quad (3)$$

The conservation of turbulence kinetic energy dissipation rate ( $\epsilon$ ) (Eq. 4):

$$\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial x_i}(\rho \epsilon u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + C_{1\epsilon} \frac{\epsilon}{k} (G_k + C_{3\epsilon} G_b) - C_{2\epsilon} \rho \frac{\epsilon^2}{k} + S_\epsilon \quad (4)$$

In Eqs. (3- 4),  $G_k$  represents the generation of turbulence kinetic energy due to the mean velocity gradients;  $G_b$  is the generation of turbulence kinetic energy due to buoyancy;  $Y_M$  represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate;  $C_{1\epsilon}$ ,  $C_{2\epsilon}$ , and  $C_{3\epsilon}$  are adjustable constants;  $S_k$  and  $S_\epsilon$  are user-defined source terms;  $Y_i$  is the local species mass fraction;  $\sigma_k$  and  $\sigma_\epsilon$  are the turbulent Prandtl numbers for  $k$  and  $\epsilon$ , respectively.

#### 3.3.2. Modelling of mass diffusion in turbulence flow

Fluent software predicts the local mass fraction of each species from the  $i^{\text{th}}$  specie’s convection – diffusion equation while solving the conservation equations chemical species. As the flow is assumed to be turbulent, mass diffusion is computed by Eq. (5):

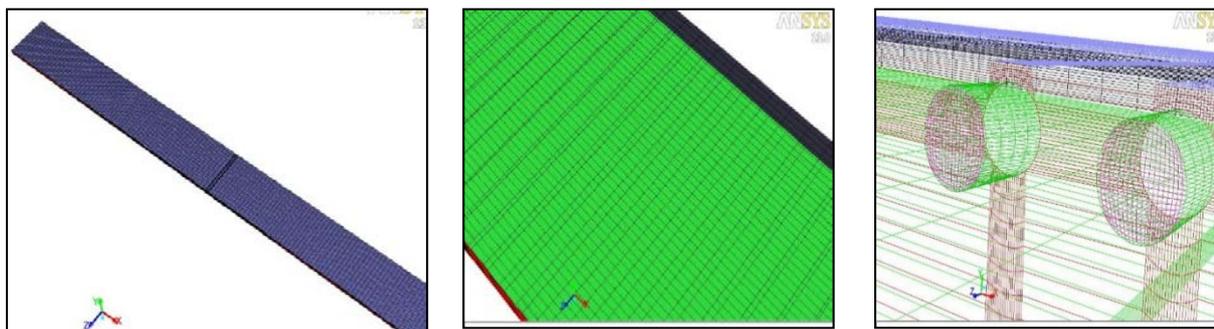
$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \quad (5)$$

where:  $R_i$  - the net rate of production of species  $i$  by chemical reaction;  $S_i$  - the rate of creation by addition from the dispersed phase;  $J_i$  - the mass diffusion of the species.

In turbulent flows, Fluent computes the mass diffusion, which is modelled by Eq. (6):

$$\vec{J}_i = - \left( \rho D_{i,m} + \frac{\mu_t}{Sc_t} \right) \nabla Y_i - D_{T,i} \frac{\nabla T}{T} \quad (6)$$

where:  $Sc_t$  is turbulent Schmidt number;  $D_T$  is turbulent diffusivity;  $\mu_t$  is turbulent viscosity.



**Fig. 3.** Structured hexahedron mesh created using multi blocking strategy

### 3.4. CAD model and mesh generation

The geometrical model of the canal is developed in ANSYS - ICEM CFD. An ANSYS - ICEM CFD is suitable for this canal geometry model. ICEM-CFD gives better results which give best structured mesh. The domain is discretized using "MULTI BLOCKING TECHNIQUE" which gives a good quality structured mesh and better results in computation. "MULTI BLOCKING TECHNIQUE" produces the "STRUCTURED HEXA HEDRON", where the cells are parallel to each other and they are exactly perpendicular to the direction of the flow. In this HEXA HEDRON, the cell faces are parallel and the flow is exactly perpendicular to the faces of cells. Grid selection and turbulence selection are important in CFD model. Finally, the mesh is generated being represented in Fig. 3.

### 4. Numerical study

Experimental results are validated or tested by CFD model results. Few assumptions are: (1) Water flow is assumed as 3D flow, (2) Water flow is steady, (3) Flow is turbulent and fully developed. The canal section taken into consideration for the study is a section of 500 m length, 1.595 m depth and 16.76 m breadth. The number of openings and the distance of the openings, quantity of industrial waste water discharged were taken as the boundary.

If we take the full length of the canal for the study, much time is taken for this study. So only 500 m length canal is taken for validation. In between this stretch there are entries of sewage water, dye wastewater entry and inlet of tanneries effluent. They are marked as S1, S2, placed at 99.8 m, 100.6 m, from inlet point (0). The opening like S3, S4, and S5 are as marked in Fig 2. For the numerical modeling the experimental results are tabulated as in Table 3. The mass fraction of various species considered in numerical modelling are within the 500 m length of the canal (Table 3). To perform simulation for the 500m length of the canal, the experimental data and other factors like the number of effluent openings and the amount of industrial waste dumped are taken as boundary conditions.

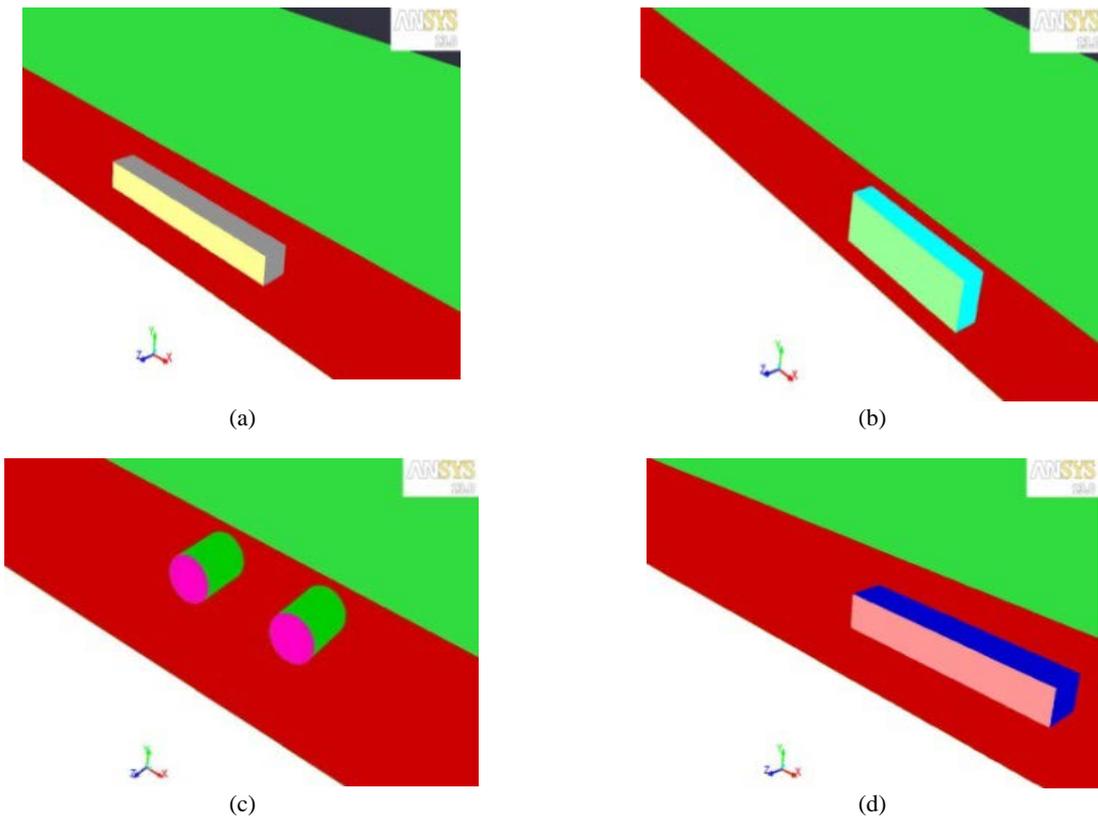
Water flow in the canal is assumed to be 3D, steady, turbulent and fully developed flow. The point sources of pollution through which industry effluent reaches the canal are bare modelled and are shown in Fig. 4. The point source includes sewage inlets, dye inlet and tannery inlets. An incompressible and steady flow is assumed to be flowing inside the canal. The 'no slip' boundary condition is provided for the walls of the canal. In the needle, the inlet and outlet fluid flow condition are given as volumetric flow rate and pressure outlet. For the calculation of numerical equation ANSYS Fluent software is used (Bradbrook et al., 2000; Lin et al., 2002).

**Table 3.** Mass fraction of various parameters within 500 m

S.No	Particulars	Mass fraction of the wastes within 500 m
1	Lead	1.46E-09
2	Cadmium	2.86E-10
3	Nitrite	8.74996E-10
4	Bicarbonate	4.08E-07
5	Magnesium	4.95698E-07
6	Potassium	1.86991E-07
7	Calcium	1.57379E-06
8	Sodium	4.8103E-06
9	Carbonate	0
10	Chloride	2.91489E-06
11	Sulphate	1.16599E-06
12	Boron	5.24697E-09
13	Manganese	7.3895E-08
14	Iron	4.22494E-08
15	Copper	1.89E-09
16	Zinc	4.07992E-09

### 5. Validation study

CFD procedure has a lot of variables such as Grid count, type, turbulence models, discretization schemes etc. Thus, the end user of CFD has to arrive at an optimal numerical strategy that comprises the optimum mesh count, better turbulence model and the correct numerical methodology/order of discretization. The governing equations have been numerically solved using the CFD solver FLUENT (Soe and Khaing, 2017).



**Fig. 4.** Industry effluent from various sources of pollution: (a) sewage inlet 1, (b) dye inlet, (c) Sewage inlet 2, (d) tannery inlets

### 5.1. Grid generation

One of the most cumbersome and time-consuming parts of the CFD is the grid generation which includes both surface and volume mesh. In this approach the finite volume method is used and the success of CFD procedure implies how best one can convert the flow physics into CFD model initially to start up any optimization using CFD and also validation with experimental results. To find an optimum procedure, a grid independent study is carried out to select a proper grid count where the results are off with a minimal variation with the experimental result and is used for further simulations (Hu et al., 2012).

### 5.2. Grid study

In this study, the different results are obtained by changing the numbers of the mesh count and by keeping the turbulence model constant throughout the grid study. In this case, the turbulence model is a K-epsilon-standard-wall-function. The grid study is conducted for the mesh counts of 0.27 million, 0.4 million, 0.66 million, 0.88 million and 1 million (Table 4). From Table 4, it is clear that the different mesh counts results in the variation of computational results. It was determined that the results obtained using grid count of 0.27 million were close enough to those of grid count of 0.88 million and also required significantly less computational expense than grid count of 0.88 million. Grid counts of 0.4 million and

0.66 million also displayed similar results but the differences between grid counts of 0.27 million, 0.66 million and 1 million suggest the possibility that the mesh needed to be finest to capture accurate results. When comparing with experimental results it is observed that the mesh count of 1 million has shown less variation due to velocity of water increases, than the other mesh counts. The value of concentration is high in other mesh counts of 0.27million, 0.4 million, 0.66 million and 0.88 million, due to decreases in velocity as well as quality of water due to poor diffusion (Fig. 5). It has been concluded that the 1 million mesh count provides an accurate result and will be applied for further analysis (Cable, 2009; Zhang et al., 2014).

### 5.3. Turbulence model study

Turbulence modeling is the computational procedure to solve and analyze the fluid flow introducing some approximations in the governing differential equations so that required solution is obtained approximately consuming feasible computational memory and time. Navier-Stokes equations deal with several turbulence modeling techniques which are in the form of averaging the various ranges of ‘turbulent eddy scales’. The exciting approaches of turbulence modeling using Reynolds Averaged Navier Stokes solution (RANS) were used for the prediction turbulent flow (Rodi, 1997). Five RANS based turbulence model were selected for the numerical simulation of pollutant species prediction in

this research, which are: K-Epsilon- Std, K-Epsilon RNG, K-Epsilon Realizable, K-Omega-Std and K-Omega-SST. The results vary with the change in the selection of turbulent model. In this process, the mesh count is kept constant. The mesh count is 1 million, which is selected from the grid study.

The variation in results of models is compared with the experimental results (Fig. 6). From Table 5, it could be noted that the K-Epsilon-Std turbulent model appear to produce exactly prediction of pollutant species while compared with other RANS based turbulence models. The prediction of pollutant species for those models are very close to the experiments as are the predictions of pollutant species (Wilcox, 2006; Zhang, 2017).

5.4. Results obtained from validation study

It could be noted from Figs. 5- 6, that the peak values are well predicted compared to the pollutant species of K-Epsilon- Std, K-Epsilon RNG, K-Epsilon

Realizable, K-Omega-Std and K-Omega-SST models with experimental results.

Through the Grid and turbulence model study, a steady and validated procedure which is the mesh count of 1 million and K-epsilon realizable turbulence model has been selected as shown in the above graphs with less variation and other RANS based turbulence models shows more variation when compared with the experimental results. The analysis of full length of the canal is applicable by the above specific procedure. As an overview, similar results were obtained from both the k and ε turbulence models used, which were in good agreement with the obtained results (Khalifa et al., 2014; Zhang et al., 2015).

When there were differences between the numerical and the experimental results, it appears that with other RANS based turbulence models, these differences were due more to the assumptions made in defining the physical boundaries rather than with deficiencies in the turbulence models (Mcguirk and Rodi, 1978; Patankar et al., 1977; Rodi, 1980).

Table 4. Mass fraction at 500 m length of canal

S.No	Species	Grid counts (million)				
		0.27	0.4	0.66	0.88	1.0
1	Lead	8e-7	1.5e-9	1.43e-9	7.35e-9	1.26e-9
2	Cadmium	7e-7	3e-10	2.87e-10	3.92e-10	1.87e-10
3	Nitrite	2.2e-7	8.98e-10	8.60e-10	4.29e-10	7.65e-9
4	Bicarbonate	1.25e-4	4.19e-7	4.01e-7	2.45e-10	2.0816e-7
5	Magnesium	2.75e-4	5.09e-7	4.87e-7	2.89e-7	3.96e-7
6	Potassium	7e-4	1.91e-7	1.83e-7	9.38e-7	1.07e-7
7	Calcium	0	1.62e-6	1.55e-6	6.15e-6	1.11e-6
8	Sodium	1.7e-3	4.94e-6	4.73e-6	3.49e-6	3.54e-6
9	Carbonate	8e-5	0	0	0	0
10	Chloride	2.25e-3	3e-6	2.87e-6	2.11e-6	2.45e-6
11	Sulphate	5e-2	1.20e-6	1.15e-6	5.20e-6	1.00e-6
12	Boron	1.25e-3	5.39e-9	5.16e-9	2.83e-9	3.12e-9
13	Manganese	3.2e-6	7.61e-8	7.28e-8	3.59e-8	4.20e-8
14	Iron	1.5e-4	4.34e-8	4.15e-8	1.66e-8	2.21e-8
15	Copper	9e-5	1.9e-9	1.86e-9	9.76e-8	7.21e-9
16	Zinc	5e-6	4.19e-9	4.01e-9	2.13e-9	2.21e-9

Table 5. Results of turbulence models

S.No	Species	RANS based turbulence models				
		K-Epsilon-Std	K-Epsilon-RNG	K-Epsilon-Realizable	K-Omega-Std	K-Omega-SST
1	Lead	1.46e-9	1.53e-9	1.44e-9	1.38e-9	1.37e-9
2	Cadmium	2.87e-10	3.06e-10	2.88e-10	2.77e-10	2.74e-10
3	Nitrite	8.75e-10	9.16e-10	8.63e-10	8.30e-10	8.21e-10
4	Bicarbonate	4.0816e-7	4.27e-7	4.03e-7	3.87e-7	3.82e-7
5	Magnesium	4.96e-7	5.19e-7	4.89e-7	4.70e-7	4.64e-7
6	Potassium	1.87e-7	1.95e-7	1.87e-7	1.77e-7	1.75e-7
7	Calcium	1.57e-6	1.65e-6	1.55e-6	1.49e-6	1.48e-6
8	Sodium	4.81e-6	5.04e-6	4.74e-6	4.56e-6	4.51e-6
9	Carbonate	0	0	0	0	0
10	Chloride	2.92e-6	3.05e-6	2.88e-6	2.77e-6	2.73e-6
11	Sulphate	1.17e-6	1.22e-6	1.15e-6	1.11e-6	1.09e-6
12	Boron	5.25e-9	5.49e-9	5.17e-9	4.98e-9	4.92e-9
13	Manganese	7.40e-8	7.75e-8	7.3e-8	7.02e-8	6.94e-8
14	Iron	4.23e-8	4.42e-8	4.17e-8	4.01e-8	3.96e-8
15	Copper	1.89e-9	1.98e-9	1.87e-9	1.80e-9	1.78e-9
16	Zinc	4.08e-9	4.27e-9	4.03e-9	3.87e-9	3.83e-9

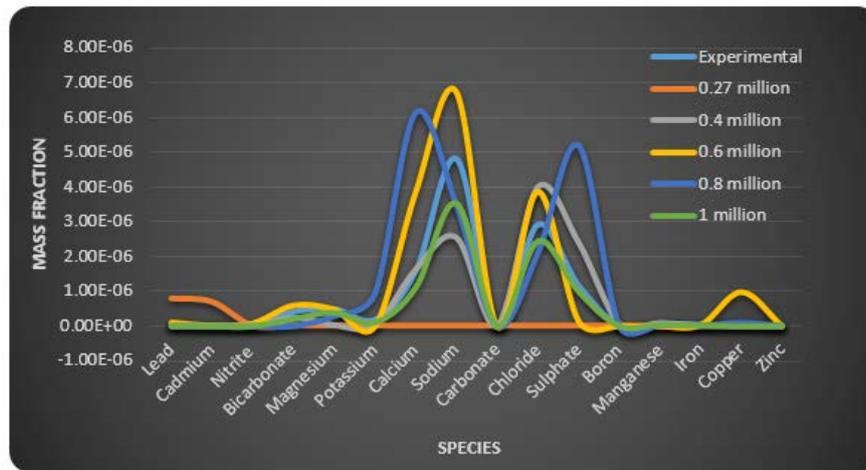


Fig. 5. Comparison of grid study results with experimental results

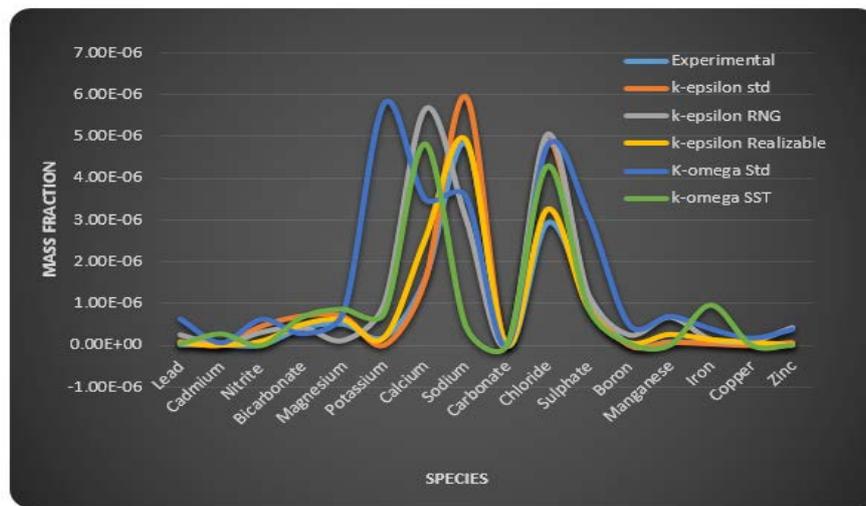


Fig. 6. Comparison of turbulent models with experimental results

## 6. Results of CFD

### 6.1. Dispersion of pollutants across the canal

Across the canal, the dilution distance, i.e. the distance at which the concentration of pollutant species becomes very much low and constant, being reached after a distance of about 13 meters from the source point. Higher water flow rates (e.g. during spring) result in faster transport of the pollutant and lower concentrations due to dilution, while lower flow rates (e.g. during summer) lead to opposite situation (larger residence times and higher concentrations) allowing the pollutant to cause higher environmental damage (Modenesi et al., 2004; Zhang et al., 2016). The concentration predictions are also different in the case of the continuous release, when comparing results obtained with constant vs. variable parameters, in terms of the distance covered by the maximum concentration. The use of constant parameters shows that, after few days from the release start, the entire canal stretch is polluted at maximum concentration, while the use of variable parameters indicates a shorter affected distance. This is because the employment of

constant values of the channel features doesn't allow the model to reflect the real canal behaviour in an accurate manner. The dilution distance and the corresponding concentration of species are shown in Table 6.

### 6.2. Dispersion of pollutants along the canal

In this case the dilution starts around 400 m away and still the concentration of pollutant species is comparatively high to that of the previous case (across the canal). The diffusion pattern resembles that of the species having a higher density than that of the water. In such pollution scenarios living organisms and plants along the canal could survive an accident with increased probability than in the case of a continuous release, as for the latter the exposure is longer and at higher concentrations. For continuous events, the pollutant spill has the maximum concentration in the vicinity of the source as long as the pollutant is discharged (Timis et al., 2016). For the species having lower density values due to dilution caused by a large effluent, the diffusion pattern varies with respect to their mass contribution to total mass fraction.

**Table 6.** Species mass fraction

S.No	Species	Mass fraction at dilution distance of 450 m
1	Lead	4.25 e-7
2	Cadmium	5.5 e-7
3	Nitrite nitrogen	2.2 e-7
4	Bicarbonate	1.2 e-4
5	Magnesium	2.7 e-4
6	Potassium	5 e-6
7	Calcium	5.8 e-4
8	Sodium	1.50 e-3
9	Carbonate	5.7e-4
10	Chloride	2 e-3
11	Sulphate	2 e-2
12	Boron	1.25 e-3
13	Manganese	2.6 e-6
14	Iron	1.5e-4
15	Copper	5.75 e-4
16	Zinc	4 e-6

**Table 7.** Species mass fraction at 450 m

S.No	Species	Mass fraction at dilution distance of 450 m
1	Lead	8e-7
2	Cadmium	7e-7
3	Nitrite nitrogen	2.2 e-7
4	Bicarbonate	1.25 e -4
5	Magnesium	2.75 e-4
6	Potassium	1.3 e-5
7	Calcium	7 e-4
8	Sodium	1.7 e-3
9	Carbonate	8 e-5
10	Chloride	2.25 e-3
11	Sulphate	5 e-2
12	Boron	1.25 e-3
13	Manganese	3.2 e-6
14	Iron	1.5 e-4
15	Copper	9 e-5
16	Zinc	5 e-6

The dilution distance and the corresponding concentration of species are shown in Table 7. Compared to the real behaviour the average constant channel features employed for the calculation of the convective and the dispersive transport have larger values at the beginning of the stretch and lower values at the near its tail-end of the canal. It results in faster transport velocity and a larger canal length affected by pollution.

**7. Conclusions**

As a result of the study, it is concluded that computation fluid dynamics model is a good tool for the analysis of the quality of water in the canal. The Grid and turbulence model study, a steady and validated procedure which has the mesh count of 1 million and K-epsilon realizable turbulence model has been selected due to less variation and other RANS based turbulence models shows more variation when compared with the experimental results.

High precision water quality data can be obtained from this model. The diffusion pattern of the pollutants can be obtained along and across the canal. This study is quite useful for the pollution study in a particular sector and in emergency & accidental pollutant study. This serves to be a simple model which helps in deciding for planning urban and farming practices in future. This work presents the numerical modeling of surface water to analyse the diffusion patterns of various pollutants along and across the canal. The results show that the pollutant level gets stabilized at 13 m along the canal and at 450 m across the canal, which can be used for future planning considerations of the water body. Dye effluents should be treated in common effluent treatment plant before it is disposed. Before the disposal of effluents into the canal, the effluents should be checked to find out whether it meets the permissible limit prescribed for its disposal into running water bodies. This CFD provides an alternate way to study the dispersion of pollution in the river without doing heavy experimental work and is handy in analyzing the polluted region. The geometrical model of the canal is developed in ANSYS - ICEM CFD. The domain is discretized using "MULTI BLOCKING TECHNIQUE" through which one can achieve a good quality structural mesh. It is highly recommended in computing for a better result.

Heavy metal analysis can be carried out for soil and groundwater samples. The transportation of pollutants along the aquifers can be studied using CFD.

**Nomenclature**

CFD	Computational Fluid Dynamics	$\epsilon$	Turbulent Kinetic energy dissipation rate ( $m^2/s^2, s^{-1}$ )
HECRAS	Hydrological Engineering Center's River Analysis System	$u_i$	Velocity components in corresponding direction (m/s)
BIS	Bureau of Indian Standards	$\mu$	Viscous diffusion rate (kg/m.s)
SW	Surface Water	$\mu_t$	Turbulent viscosity
CAD	Computer Aided Design	$G_k$	Turbulence kinetic energy due to the mean velocity gradients
RANS	Reynolds-Averaged Navier Stokes	$G_b$	Turbulence kinetic energy due to buoyancy
$\rho$	Water density ( $kg/m^3$ )	$Y_M$	Fluctuating dilatation in compressible turbulence
$t$	Time(s)	$C_{1\epsilon}, C_{2\epsilon}, C_{3\epsilon}$	Adjustable constants in the turbulence model
$\Delta$	Divergence	$\sigma_k, \sigma_\epsilon$	Turbulent Prandtl numbers for k and $\epsilon$ , respectively
$\nu$	Kinematic viscosity( $m^2/s$ )	$S_k, S_\epsilon$	User-defined source terms
$S_m$	Mass source term	$D_{i,m}$	Diffusion coefficient for species $i^{th}$ in the mixture ( $m^2/s$ )
$p$	Pressure of the fluid ( $kg/m s^2$ )	$Y_i$	Local species mass fraction

$\tau$	Turbulent shear stress(kg/m <sup>2</sup> )	$T$	Mean turbulent time
$g$	Acceleration (m s <sup>-2</sup> )	$S_{ct}$	Turbulent Schmidt number
$F$	Body force acting on the fluid	$D_T$	Turbulent diffusivity
$k$	Turbulent Kinetic Energy	$J_i$	Mass diffusion of the species
$v$	Mean velocity (m/s)	$R_i$	Net rate of production of species $i$ by chemical reaction
$U_i, U_j, U_k$	Local velocity for x, y and z direction (m/s)	$S_i$	Rate of creation by addition from the dispersed phase
$i, j, k$	Variables indices for x, y and z direction (subscript)	$S_1, S_2, S_3, S_4, S_5$	Source point

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