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Contents

Experimental and Numerical Investigations on formability of AA1200

Manoj Kumar[1], Suresh kumar[2], Vijay Gautam[3] and Prahlad Tewari[4]
[1,2] Assistant professor, Department of Mechanical and Automation Engineering,
HMR Institute of Technology and Management, Delhi, India
[3,4]Department of Mechanical Engineering, DTU, Delhi-110042.
[1]manozme@gmail.com, [3]Vijay.dce@gmail.com, [4] prahlad.tewari@gmail.com

A B S T R A C T

The ability of a sheet metal to be formed in a given forming process without failure or necking is known as its form ability. Form ability is a measure of the amount of deformation a material can withstand prior to fracture or excessive thinning. Forming Limit Diagram is a graphical representation of limit strains at which necking/fracture occurs in a sheet metal under all possible modes of deformation. In the present paper, tensile properties of AA1200 sheet are determined as per ASTM-E8M standard. Anisotropy of the sheet is also determined by giving 20% elongation to the tensile specimens in a UTM. The values of yield strength, tensile strength and ductility show a huge variation because of the differences in as rolled specimens, annealed specimens, and different thickness of the Al sheets. The standard limiting dome height test is conducted on the specimens of different thicknesses and it is found that form ability of the sheet metal increases with increase in sheet thickness.

Keywords— AA1200 Aluminum Alloy, Sheet Metal Forming, Forming Limit Diagram, Stretch forming, and Anisotropy.

1. INTRODUCTION

Sheet metal forming is a process in which flat thin blanks are deformed permanently to produce a wide range of products. These operations are widely used in the industries and hence the knowledge of various sheet metal forming processes and deformation criteria are essential to manufacture good quality products. Common parts made by sheet metal forming processes include automobile body panels, fuel tanks, aircraft parts, various parts for building industries and also for making domestic home appliances, food and drink cans. Aluminium alloys are now-a-days replacing the steel in automobile industry since they have higher strength to weight ratio, comparable strength and high corrosion resistance. With advent of manufacturing technology, many researchers have been attracted to determine the forming limit curves of various aluminium alloys which may reduce the vehicle weight to achieve better fuel efficiency[1-3].

Aluminium alloy selection depending on the above mentioned properties may look better, but the manufacturing aspect also needs to be considered.. Hence the formability of aluminium alloys needs to be studied thoroughly. Because of their inferior forming properties, advanced methods are being used to exploit their full potential. The experimental determination of forming behavior of these modern materials is time consuming which necessitates some easier methods of determining formability. Finite element simulation or theoretical methods are finding wider importance now-a-days. This can lead to the optimization of process and design variables to achieve better quality stampings.

Some lab tests used to determine formability of sheet metals are quite common. The Swift-cup test[4] is a drawing test. A series of blanks with steadily increasing diameters are deep drawn, and at one point a diameter is reached, where the punch penetrates but not yet completely drawn cup. The Swift cup test is the determination of the limiting drawing ratio (LDR) for flat-bottom cups. A simulative test in which circular blanks of various diameters are clamped in a die ring and deep drawn into a cup by a flat-bottomed cylindrical punch.

The Erichsen & Olsen tests [5] are used to estimate sheet metal formability under pure stretching conditions. The sheet is clamped between two flat plates and is stretched by a ball. Cups are formed by stretching over a hemispherical tool. The height of the cup represents the formability index. Cups with larger height represent good resistance to necking. The results depend on stretchability rather than drawability. The Erichsen and Olsen test produce bending strains in the test and hence no longer used in the industry.

The cupping tests discussed above are losing favour because of irreproducibility. Hecker[6] attributed this to “insufficient size of the penetrator, inability to prevent inadvertent drawing in of the flange, and inconsistent lubrication.” He proposed the limiting dome height test (LDH)[7]. The specimen width is adjusted to achieve plane strain and the flange is clamped to prevent draw-in. The limiting dome height (LDH) is the greatest depth of cup formed with the flanges clamped. The LDH test results correlate better with the total elongation than with the uniform elongation. This test is widely used in the industries.

2. METHODOLOGY

2.1 Selection of materials.

Sheet metal for present work is Aluminium Alloy 1200 grade in as rolled and annealed state of thickness 1mm and 1.6mm.As rolled metal sheets are those sheets which are come directly from the roll mill. The properties of as rolled sheets are unfavorable for forming due to accumulated strains.

Moreover, it depicts an isotropic behaviour which changes to anisotropic soon after the annealing of the sheet metal. The sheet metal received was in as-rolled condition which has high strength and low ductility and strain hardening exponent. To bring the material in formable state needed heat treatment in vacuum. The distorted, dislocated structure resulting from cold working of aluminium is less stable than the strain free, annealed state, to which it tends to revert. The chemical compositions of the selected material is given in Table 1.

Table.1: Chemical composition of the as rolled AA1200 (by weight %).

Si	Fe	Cu	Mn	Al
0.0929	0.451	0.0026	0.0022	Remainder
Mg	Cr	Ni	Zn	
0.0017	<0.0005	0.0022	0.0073	
Ti	Pb	Sn	V	
0.0271	0.0148	0.0067	0.0013	

2.2 Preparation of Tensile Specimens

The Laser cutter works by directing a high powered laser beam very precisely at the chosen material to cut right through. The cutting beam is very fine focus (typically around 0.1mm) and precise resulting in incredibly detailed and accurate cuts. By reducing the beam power we can mark the surface of the material, this is known as etching or engraving and can give some stunning effects on materials. The specification of the machine used is given in Table 2.

The sub-sized specimens of AA1200 as per ASTM standard E8M were used for tensile testing. The rolling direction of the sheet was determined with help of stretcher roll marks. The specimens were prepare d by laser cutting of annealed and as rolled aluminium alloy sheets in different directions relative to rolling direction (RD), i.e., 0° in RD, 45° w. r. t RD and 90 ° w. r. t RD as shown in Fig. 1.

Table.2: Specification of laser cutting machine

Match type	CNC Laser cutting
Elect/voltage	440V,60Cy, 3Phase
Maximum cutting dimension	80"x148"
Maximum cutting thickness	0.375 mild steel
Laser power	2600 watt
Laser gas	CO_2
X travel	1524mm
Y travel	3048mm
Z direction	101mm

Fig. 1 Laser cutting of tensile specimens

The specimens were tested in uniaxial tension on Instron machine. Load elongation data was obtained for all the tests which were converted into engineering stress strain curves. The standard tensile properties such as yield stress, ultimate tensile stress, uniform elongation and total elongation were determined from the stress- strain data.

2.3 Determination of anisotropy

The plastic strain ratio, which is a measure of anisotropy, was determined using specimens prepared according to ASTME517 specification. The specimens were elongated to predetermined longitudinal strain (15%depending on the % elongation up to UTS) and the testing was stopped before the onset of necking. Final width and gauge length were measured and the plastic strain ratio (R) is calculated as below [George E Dieter, Mechanical metallurgy]. The R value was determined in three directions as mentioned in the tensile tests by repeating the above procedure. The normal anisotropy or average plastic strain ratio and planar anisotropy were calculated using the formula:

$$R_{avg} = (R_0 + 2R_{45} + R_{90})/4$$
$$\Delta R = (R_0 - 2R_{45} + R_{90})/2$$

R_0, R_{45} and R_{90} represent the R value in three directions.

2.4 LDH test of Al alloy sheets.

As suggested by Hecker [6], samples were deformed using a hemispherical punch. The All the LDH specimens were etched with the circles of 2.5mm diameter. The width was varied to obtain all possible deformation modes i.e. biaxial tension, plane strain tension and tension-compression. The width of the samples varied from 20mm to 100mm. The experimental setup is shown in Fig. 2. The plane strain deformation width was found to be approx 50mm. The specimens tested for the LDH are shown in Fig. 3. The necking strains are clearly seen in both the specimens. The necking strains were measured using a trinocular microscope.

Fig. 2 Experimental setup on 100 tonne double action hydraulic press

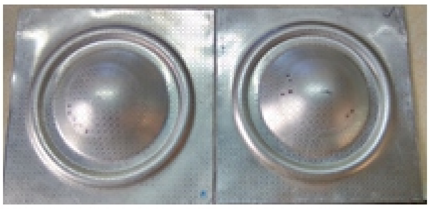

Fig. 3 LDH tested specimens showing biaxial stretch

2.5 Finite Element Analysis

Computer based simulations are widely used by sheet metal engineers to meet the demand for better quality products. These simulations using finite element are used for predicting the failures, assessing a proposed forming process, designing tools and also in troubleshooting the manufacturing problems.

In the this work, the finite element simulation was carried out for the prediction of failure in stretch forming of aluminium alloys. The FE simulation was carried out in Abaqus 6.11, commercially available dedicated software for sheet metal forming applications. This system provides preprocessing (auto meshing, tool positioning, draw bead representation) and post processing (animation, formability plot, forming limit diagram). Default input parameters are generally chosen to give efficient, accurate simulation results. The FE simulations as shown in Fig. 4 were done to check the accuracy of failure prediction in stretch forming of aluminium alloys. The failure predictions based on the developed as well as existing correlations were compared with the experimental results. The forming limiting diagram developed from the software is shown in Fig. 5.

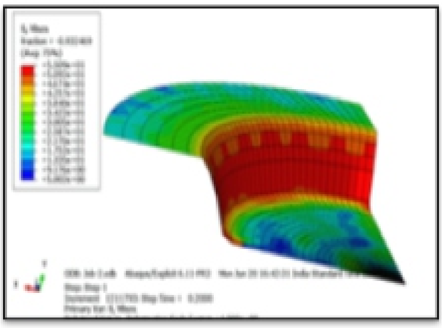

Fig. 4 Simulation of deep drawn specimen with flat punch

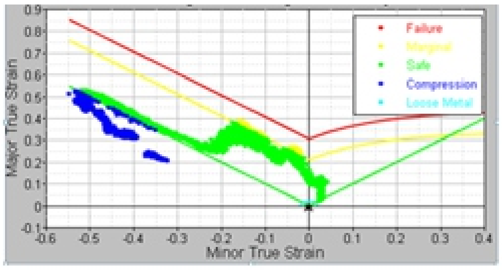

Fig. 5 Forming limit diagram developed from the simulations

3. RESULTS AND NDISCUSSION

The tensile properties of the tested specimens of both the thicknesses and as rolled sheets are given in Table 3 and 4. It is observed that 1mm thick sheet is stronger than the 1.6mm thick sheet. This could be attributed to the higher reduction in the thinner sheet and higher dislocation density. The tensile results of 1mm thick sheet depicts higher strength in the specimens oriented transverse to the rolling direction and minimum strength in the direction inclined w.r.t. the rolling direction. The values of strain hardening exponent are very low, which indicates that the sheet is almost unworkable at room temperature. Similar results are seen with the sheets of 1.6mm thickness, although in this case the percentage elongation is higher than the 1mm thick sheet. Experiment shows that these sheets are completely isotropic.

Table 3 Tensile properties of as Rolled AA1200 (Thickness: 1mm)

Orientation wrt RD	YS (Mpa)	UTS (Mpa)	n	k	% elongation
0^0-1	77.6	97.6	0.029	312.9	9.94
0^0-2	67.4	75.5	0.098	117.6	7.13
0^0-3	68	72.2	0.072	103.7	7.27
45^0-1	47.2	52.7	0.072	71.8	6.85
45^0-2	62	69.5	0.09	103.2	6.09
45^0-3	93.2	104	0.042	596.4	7.84
90^0-1	91.4	104	0.043	684.7	5.99
90^0-2	90.4	103	0.035	487.8	6.08
90^0-3	91.4	107	0.051	882.7	7.03

Table 4 Tensile properties of as Rolled AA1200 (Thickness: 1.6mm)

Orientation wrt RD	YS (MPa)	UTS (Mpa)	n	k	% elongation
0^0-1	56.9	64.9	0.092	91.6	9.74
0^0-2	51.8	60.2	0.089	87.26	9.12
0^0-3	43.8	50.8	0.077	68.4	11.6
45^0-1	57.2	64.1	0.088	97	7.66
45^0-2	51.9	59.4	0.078	85.6	9.09
45^0-3	47.8	54.6	0.07	74.8	8
90^0-1	48	52.6	0.082	76.6	6.68
90^0-2	51.8	57.7	0.094	88.2	7
90^0-3	56.7	62.4	0.192	142.4	6.89

The sheets of both the thicknesses are annealed at 220°C in an inert atmosphere to prevent oxidation. The tensile properties of the tested specimens of both the thicknesses and as annealed sheets are given in Table 5 and 6. It is observed that the strength of the sheets have reduced but ductility has improved significantly which can be attributed to the formation of new strain free grains after annealing. The percentage elongation of the specimens oriented at 45° to the rolling direction is the highest followed by the specimens along and transverse to the rolling direction. In the annealed sheets also, the strength of the thinner sheet is higher than the thicker sheet. The results of the normal and planar anisotropy for the annealed sheets are given in Table 7. The average normal anisotropy of the sheets are 0.45 (approx.) which indicates that these sheets are poor in deep drawability. The drawability of these sheets may be improved by warm working.

Table 5 Tensile properties of annealed AA1200 (Thickness: 1mm)

Orientation wrt RD	YS (Mpa)	UTS (Mpa)	n	k	% elongation
0^0-1	33.8	54.5	0.349	122.3	42
0^0-2	29.1	47.2	0.349	122.3	38.4
0^0-3	26.5	42.8	0.364	97.4	42.3
45^0-1	32.7	54.3	0.394	117.5	59.1
45^0-2	40.2	64.8	0.358	130.3	61.7
45^0-3	39	64.7	0.363	132.1	49.7
90^0-1	25.2	41.4	0.405	108.7	32
90^0-2	26.3	43.2	0.375	102.1	41.7
90^0-3	24.3	40.6	0.405	99.2	42.1

Table 6 Tensile properties of annealed AA1200 (Thickness: 1.6mm)

Orientation wrt RD	YS (Mpa)	UTS (Mpa)	n	k	% elongation
0^0-1	26.2	43.2	0.405	109	39.7
0^0-2	26.7	44.4	0.389	103.5	48.9
0^0-3	28.3	45.9	0.393	109.9	46.1
45^0-1	31.3	52	0.418	115.8	63
45^0-2	31.3	51.9	0.426	118	57.4
45^0-3	31.9	52.6	0.434	122.3	54.2
90^0-1	30.6	50.6	0.381	116.1	44.9
90^0-2	28.8	47.5	0.375	107.7	45.9
90^0-3	16.8	27	0.392	65	39.4

Table 7 Values of anisotropy of the sheets

Thickness	R_0	R_{45}	R_{90}	R_{avg}	(ΔR)
1mm	0.64	0.22	0.73	0.45	0.46
1.6mm	0.54	0.27	0.71	0.45	0.34

The results for the LDH tests of as annealed specimens of AA1200 of both the thicknesses are given in Table 8. The limiting strain values and the formability of sheet metal were found to increase with increase in the sheet thickness. The plane strain condition is observed to occur with a width sample of 50mm in both the thicknesses. The maximum dome height of the specimen measured is 22.26mm, whereas the dome height is 24.14mm with the thicker sheet. This can be attributed to the higher thinning resistance of the thicker sheet.

As discussed, stretch forming with a flat punch of different sheet thicknesses was simulated using ABAQUS 6.11 to predict failure and LDH for the cases of biaxial stretching, plane strain condition and tension-compression. The simulation results agree closely with the experimental results. The LDH has been found to be 24.14 mm which is significantly higher LDH which means formability increases with the increases of thickness. There has been a significant improvement in accuracy of prediction of limiting dome height and limit strains in FE simulations. The blow figure explains the finite element analysis.

Table 8 LDH test values of annealed AA1200 for different thickness

Failure points 1mm thick sheet	Minor strain	Major strain
1	0.073342	0.661675
2	0.092124	0.744198
3	0.09039	0.634173
Failure points 1.6mm sheet	Minor strain	Major strain
1	0.079043	0.635564
2	0.100723	0.819158
3	0.114481	0.661271
Safe points 1mm sheet	Minor strain	Major strain
1	0.086052	0.512572
2	0.093698	0.564837
3	0.084842	0.498685
Safe points 1.6 mm sheet	Minor strain	Major strain
1	0.102691	0.498895
2	0.092319	0.534202
3	0.100613	0.554041
Specimens	LDH(mm) thickness 1mm	LDH (mm) thickness 1.6mm
1	21.9	23.74
2	22.1	23.8
3	22.26	24.14

4. CONCLUSIONS

Based on the results and discussion presented in the previous chapter the following conclusions are drawn:

1. The tensile tests showed a large variation in mechanical properties of the aluminium alloys.
2. The annealed specimens have high strain hardening exponent indicating good stretchability.
3. Anisotropy influences both mechanical and physical properties of metals. The value of the average plastic strain ratio in annealed specimens is less than 0.5 which indicates poor drawability of the sheets. The value of planar anisotropy is almost found to be equal to the average plastic strain ratio indicating the earing tendency of the sheets.
4. From the LDH test the limiting strain values and the formability of sheet metal were found to increase with increase in the sheet thickness.
5. There has been a significant improvement in accuracy of prediction of limiting dome height and limit strains in FE simulations.

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For a fixed set X, IFS of A is defined as:

$A = \{< x, \mu_A(x), \nu_A(x) > | x \in X\}$

Where

$\mu_A(x): X \rightarrow [0,1]$ *and* $\nu_A(x): X \rightarrow [0,1]$

define the degree of membership and degree of non-membership of the element $x \in X$ to the set A.

For every $x \in X$, $0 \le \mu_A(x) + \nu_A(x) \le 1$ and the amount $\pi_A(x) = 1 - \mu_A(x) - \nu_A(x)$ is called the intuitionistic index or hesitation index, which may require to membership value, non-membership value or both. Let A be an IFS of the set X and let R be an IF relation from $X \to Y$, then Max-min-max composition B of IFS X with the IF relation R($X \to Y$) is defined as $B=RoA$ with membership and non-membership function.

Let $F = \{ f_1, f_2, \ldots, f_m \}$; $P = \{ p_1, p_2, \ldots, p_n \}$; $C = \{ c_1, c_2, \ldots, c_q \}$; be the finite set of feed stock, parameters and constraints respectively. According to Kumar [4, 5], two fuzzy relations (FR), Q and R are defined as:

$$Q = \{ < (f, p), \mu_Q(f, p), \nu_Q(f, p) > | (f, p) \in F \times P \} \}$$

$$R = \{ < (p, c), \mu_R(p, c), \nu_R(p, c) > | (p, c) \in P \times C \}$$

Where $\mu_Q(f, p)$ indicate the degree to which the parameter p appear in feedstock f and $\nu_Q(f, p)$ indicate the degree to which the parameter p does not appears in feedstock f. Similarly $\mu_R(p, c)$ indicate the degree to which parameter p confirm the constraints c and $\nu_R(p, c)$ indicate the degree to which the parameters p does not confirms the constaints c.

The composition T of IFRs R and $Q(T = R \circ Q)$ describe the state of feedstock f_i in terms of the undertaken for the process from $StoC$ given by membership and non-membership as:

$$\mu_T(f_i, c) = \max_{i \in I} \{\min [\mu_Q(f_i, p), \mu_R(p, c)]\} \quad and$$

$$\nu_T(p_i, c) = \min_{i \in I} \{\max [\nu_Q(f_i, p), \nu_R(p, c)]\}; \quad \forall \ f_i \in F \ and \ c \in C$$

We can estimate the labels of parameters of different feed- --stocks using the information obtained from the chart of given case study. From Q and R, one may compute new measure of IFR T for which, in general, the parameteteric labels of feedstock f for any constraint c such that the following is to be satisfied:

(i) $F_T = \mu_T - \nu_T \cdot \pi_T$ is greatest and (ii) The equality $T = R \circ Q$ is retained.

This new measure of T will translate the higher degrees of association and lower degree of non-association of property as well as lower degrees of intuitionistic index to the processing.
If there is almost equal values for different processing in T is obtained, we consider the case for which intuitionistic index is least.

2. CASE STUDY

To see the application of the method, let us frame a hypothetical case study:

Let $F = \{ f_1, f_2, f_3, f_4, f_5, f_6 \}$ be the set of feed stocks and $P = \{ P_1, P_2, P_3, P_4, P_5 \}$ be the set of available parameters of different feedstocks .

Suppose the IFR $Q(S \to I)$ is given by (hypothetically):

Q	P_1		P_2		P_3		P_4		P_5	
Feedstock	μ_Q	ν_Q	μ_Q	ν_Q	μ_Q	ν_Q	μ_Q	ν_Q	μ_Q	ν_Q
F_1	0.8	0.1	0.6	0.1	0.2	0.8	0.6	0.1	0.1	0.6
F_2	0.0	0.8	0.4	0.4	0.6	0.1	0.1	0.7	0.1	0.8
F_3	0.8	0.1	0.8	0.1	0.0	0.6	0.2	0.7	0.0	0.5
F_4	0.6	0.1	0.5	0.4	0.3	0.4	0.7	0.2	0.3	0.4
F_5	0.6	0.1	0.2	0.8	0.6	0.1	0.1	0.6	0.8	0.1
F_6	0.2	0.8	0.6	0.1	0.1	0.6	0.8	0.1	0.6	0.1

Let the Constraints $C = \left\{ \begin{matrix} EasternIndia, Western, NorthernIndia, \\ SouthernIndia, CentralIndia \end{matrix} \right\}$

be the set of options available for their availability.
Suppose the IFR $R(P \to C)$ is given by (hypothetically):

Table 1:

R	EI		WI		NI		SI		CI	
Parameter	μ_R	ν_R	μ_R	ν_R	μ_R	ν_R	μ_R	ν_R	μ_R	ν_R
P_1	0.4	0.0	0.7	0.0	0.3	0.3	0.1	0.7	0.1	0.8
P_2	0.3	0.5	0.2	0.6	0.6	0.1	0.2	0.4	0.0	0.8
P_3	0.1	0.7	0.0	0.9	0.2	0.7	0.8	0.0	0.2	0.8
P_4	0.4	0.3	0.7	0.0	0.2	0.6	0.2	0.7	0.2	0.8
P_5	0.1	0.7	0.1	0.8	0.1	0.9	0.2	0.7	0.8	0.1

The Composition $T = R \circ Q$ is follows as:

Table 2:

T	EI		WI		NI		SI		CI	
Feedstock	μ_T	ν_T	μ_T	ν_T	μ_T	ν_T	μ_T	ν_T	μ_T	ν_T
F_1	0.4	0.1	0.7	0.1	0.6	0.1	0.2	0.4	0.2	0.6
F_2	0.3	0.3	0.2	0.6	0.4	0.4	0.6	0.4	0.2	0.8
F_3	0.4	0.1	0.7	0.1	0.6	0.1	0.2	0.4	0.2	0.5
F_4	0.4	0.1	0.7	0.1	0.5	0.3	0.3	0.4	0.3	0.4
F_5	0.4	0.1	0.6	0.1	0.3	0.3	0.2	0.1	0.2	0.1
F_6	0.4	0.3	0.7	0.1	0.6	0.1	0.2	0.4	0.6	0.1

Now, we calculate S_T :

Table 3:

F_T	EI	WI	NI	SI	CI
F_1	0.35	0.68	0.57	0.04	0.08
F_2	0.18	0.08	0.32	0.6	0.2
F_3	0.35	0.68	0.57	0.04	0.05
F_4	0.35	0.68	0.44	0.18	0.18
F_5	0.35	0.57	0.18	0.13	0.13
F_6	0.31	0.68	0.57	0.04	0.57

From the table, we conclude that feedstock $f_1, f_3, f_4, f_5 and\ f_6$ are suitable for Western India [7-9] and feedstock f_2 [6] is suitable for Southern India for production of biodiesel.

3. CONCLUSION.

In this paper, we use generalized concept of fuzzy set theory. A study for selecting and promoting the feedstock selection in different zones of India has been made with IFS theory. IFS method is an efficient tool for decision making problem. A fuzzy base feedstock selection for biodiesel production is being made which may prove to be an optimized selection.

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Job Shop Scheduling Optimization Using Genetic Algorithm

Rohitash Singh[1‡], Ajai Jain[2]
[1]Department of Mechanical Engineering, Delhi Technological University, Delhi, Ph.D. Scholar
rohitashsingh2703@gmail.com,
[2]Department of Mechanical Engineering, Professor, N.I.T, Kurukshetra (Haryana),
ajayjainfme@nitkkr.ac.in
[‡] Corresponding Author; Tel: +91 9412557868

A B S T R A C T

Production scheduling is generally considered to be one of the most significant issue in the planning and operation of a manufacturing system. Better scheduling system has significant impact on cost reduction, increased productivity, customer satisfaction and overall competitive advantage. Job Shop Scheduling problem is one of the challenging combinatorial optimization problems that has drawn the attention of researchers. In job shop scheduling, there are 'n' jobs to be processed at 'm' machines with the objective of minimizing the makespan, total tardiness or any other objective.

In the present work an attempt is made to optimize the job shop scheduling problem using simulation based Genetic Algorithm Approach in the presence of multiple process plans with the objective of minimizing the makespan. Four case studies are considered to optimize the JSS problem. Sequence Oriented representation is used to encode the chromosome for Genetic Algorithm. GA operators such as Two-Point Crossover, Linear rank Selection with Stochastic Universal Sampling Method, Exchange Mutation and Elitism are applied on the chromosome and new offsprings are created. Evaluation of fitness value is done through simulation as it yields better performance than mathematical functions. A restart scheme, as suggested in literature, is also taken into consideration to avoid premature convergence. These four case studies reveal that there are more than one process plan combinations that yield the same optimized makespan.

Keywords- Job Shop Scheduling; Genetic Algorithm; Simulation; Optimization; Multiple Process Plans.

1. INTRODUCTION

Scheduling is broadly defined as the process of assigning a set of tasks to resources over a period of time [1]. Scheduling has considerable significance in manufacturing domain. The environment of scheduling problem is called the job shop. Several types of manufacturing shop configurations exist in real world such as single machine, job shops, flow shops, etc. In industries job shop problems arises because of the diverse characters of the jobs and order sizes are relatively small. Job shop problems have a set of '*n*' jobs to be processed on a set of '*m*' machines. Each job has a set of operations to be performed on set of machines in a particular order and each machine can process at most one operation at a time.

Job shop scheduling (JSS) deals with the allocation of jobs to various machines with the objective of minimizing the makespan, the time to complete all jobs, or minimizing the tardiness (not meeting the due date) in jobs or any other required objectives. Job shop scheduling problems are one of the most challenging Non Polynomial hard problems [2]. Thus it has drawn the attention of researchers because of its theoretical, computational and empirical significance since it was introduced. Optimization is the act of obtaining the best result under given circumstances. There are various optimization algorithms that have been developed to implement the various optimization techniques. An optimization algorithm is a procedure, which is executed iteratively by comparing various solutions till the optimum or a satisfactory solution, is found. There are two categories of optimization algorithms. One category includes those algorithms that are deterministic with specific rules for moving from one solution to another (for example Lagrangian, Branch and Bound, etc.). Another category includes those algorithms that are stochastic in nature and with probabilistic transition rules (for example, Genetic Algorithm, Simulation Annealing, Tabu Search, etc.). These algorithms are called "Metaheuristics".

In this work, a simulation based GA is used for optimization of makespan performance measure as GA is well suited for hard combinatorial problems. Genetic Algorithm uses basic Darwinian mechanism of "survival of the fittest" and repeatedly utilizes the information contained in the solution to generate new solutions with better performance. Simulation is used in this work as it yields better results than mathematical calculations [3].

2. LITRATURE REVIEW

GA has been applied to scheduling problem since Davis (1985) [4] first suggested and demonstrated the feasibility by using a GA on a simple JSS Problem [5]. Kumar and Srinivasan (1996) [6] solved the JSS problems faced by an organization using GA and a combination of dispatching rules. The proposed algorithm showed an improvement of about 30% in makespan over the present system. Bierwirth and Mattfeld (1998) [7] proposed a general model for JSS which can be applied to static, dynamic and nondeterministic production environment. The algorithm was tested in a dynamic environment under different workload condition. Werner *et al.* (2000) [8] solved JSS problem using genetic programming. Results for a set of benchmark problems with both conventional and evolved GA were obtained. Gupta (2002) [9] discussed an excursion into various scheduling problems arising in the manufacturing environment and possible approaches that could be taken to solve them. Ombuki and Ventresca (2004) [10] proposed a hybrid GA for JSS on local search strategy. This proposed algorithm is based on scheduling scheme that is deadlock free. Omar *et al.* (2006) [11] used GA to solve JSS, the initial populations were randomly including the results obtained from some well known priority rules such as the Shortest Processing Time (SPT) and the Longest Processing Time (LPT). From there the population would go through the process of reproduction, crossover and mutation to create a new population for new generation. A 5 job 5 machine problem was solved. The number of generation which in this case was 200 generations was used as stopping criteria.

Mendes (2010) [12] presented an optimization approach for the JSS problem based on GA. The algorithm produced good results in comparison to other approaches. Bagheri A. and Zandieh M. (2011) [13] consider Flexible Job Shop Scheduling Problem (FJSP) with sequence-dependent setup times to minimize makespan and mean tardiness.

Phanden *et al.* (2012) [14] used GA for Flexible Job Shop Scheduling. The authers introduced a simulation-based GA approach to solve flexible job shop scheduling problem. Tsung-Che Chiang et al. (2013) [15] proposed A Simple and Effective Evolutionary Algorithm for Multi-Objective Flexible Job Shop Scheduling (MOFJSP) regarding minimizing the makespan, total workload, and minimum workload.

2.1 Research Gaps & Problem Formulation

Literature review reveals that few researchers focused on JSS optimization problem with the consideration of flexible process plan. Therefore, there is a need to carry out further study in this area using GA and simulation. Thus, in the present work, an attempt will be made to optimize JSS with the consideration of flexible process plans. A Genetic algorithm based approach is planned to be utilized where simulation will be used to evaluate the fitness function as simulation yields better results than mathematical functions. Thus, the problem statement is described below:

"There is a job shop consisting of 15 machines. It can process a production order consisting of '*n*' part types. Each part type can be processed with several multiple process plans. The objective is to select the process plan of each part type in order to minimize makespan using simulation based Genetic Algorithm approach". The various assumptions that will be taken into consideration are given below:

- Production quantity of each part type is unity
- Infinite buffer capacities are assumed in front of individual machine and each part enters buffer location before the processing at machine.
- All parts are available at the start of processing.
- A part may return to an earlier visited machine. However, two consecutive operations are not allowed in the same machine.

- Shortest Processing Time (SPT) is used as dispatching rule with First Come First Serve rule as tie breaker to process the part.
- All machines are available at zero time.

3. METHODOLOGY

Following are the parameters and their values taken for our case studies:

- Number of Machines (m) = 15
- Number of Parts (n) = 12
- Crossover Probability (p_c) = 0.8
- Mutation Probability (p_m) = 0.2
- Elitism Rate (e_rate) = 0.9
- Population Size (pop_size) = 10

3.1 Representation/ Encoding

In this work, sequence oriented encoding is used for representation of chromosome. Here, a bit (gene) of chromosome is formed by a process plan number (i.e. alphabets) of a job type. Each bit of the chromosome is in fixed order to represent associate process plan of a job type. For example, there are twelve job types 1, 2, 4, 6, 7, 8, 10, 12, 14, 15, 17 and 18 having one, two, four, three, nine, ten, two, two, four, four, sixteen and eight process plans respectively and each job type can be processed through any of its given Multiple Process Plan (MPP). A chromosome following sequence oriented encoding for the above parts can be coded as [11 11 13 11 16 15 11 12 11 14 112 18]. Here the first gene i.e. 11 represents processing of job type 1 by following its 1st Process Plan of sequence 1st and the second gene i.e. 11 represents processing of job type 2 by following its 1st Process Plan of sequence 1$^{st.}$ Similarly third gene i.e. 13 represents processing of job type 4 using its 3rd Process Plan of sequence 1st and so on. These numbering of process plans for the particular job type as well as the job sequence are already known. In a chromosome the number in the ith position represents the selected process plan of the job type j.

3.2 Initialization

For the initialization, population is generated randomly as performance of Genetic Algorithm is found better with a random start than from a reselected starting population [16]. The population is generated randomly, covering the entire range of possible solutions.

3.3 Evaluation Of Fitness Function

After the generation of new population, fitness value of each chromosome is calculated. Fitness is the performance evaluation of chromosomes [17]. Higher the fitness value, better the performance of the chromosome. Hence, parents with higher fitness values have more chances to survive. Genetic Algorithm is naturally suitable for solving maximization problems [18]. The objective function in this research work is the minimization of makespan *f(x)*. This minimization problem is transformed into maximization problem by using the following relation:

$F(x) = 1/(1+f(x))$

Where $f(x)$ = makespan of a chromosome

$F(x)$ = fitness function of GA

For finding out the makespan of each chromosome i.e. job mix f(x) simulation is used. Simulation is preferred to mathematical functions as it results in good performance close to actual system performance. Mathematical calculations are time consuming and sometimes tedious to solve. Moreover, the results obtained from mathematical functions may not reflect the performance of actual system. ProModel® software is used for simulation and to calculate the makespan for the part mix due to its adaptability and easy to use functions. Modelling of job shop for each chromosome is carried out using ProModel® and makespan is provided by software after simulation. Further, this value of the makespan is converted into the fitness value as discussed above.

3.4 Selection

Linear Ranking Selection is used for selection in the present study. In this method, individuals are sorted first according to their fitness value and the rank *N* is assigned to the best individual and the rank 1 to the worst individual. The individuals in the population are ranked according to their fitness and the expected value of each individual depends on its rank rather than on its absolute fitness. Once the expected value has been assigned, Stochastic Universal Sampling (SUS) method is applied to sample the population (i.e. choose parents). In this manner, a mating pool consisting of selected individuals is created.

3.5 Crossover

A two point crossover is used and applied on the individuals of mating pool. In order to carry out crossover two strings are selected randomly from the mating pool to make a pair. Each pair is then assessed for the desirability of crossover operation with the crossover probability of 0.8. During crossover, the crossover sites are selected randomly from first to last position. Due to above crossover methodology, some illegal offspring may generate. Then repairing is done to resolve the illegitimacy of the offspring.

3.6 Mutation

In the present study, exchange mutation is utilized. In this method, two genes of a chromosome are randomly selected and their positions are swapped. The mutation probability (p_m=0.2) is used and is applied on offspring produced after crossover operation. Then process plans at randomly selected sites get interchanged due to this process.

As discussed above during mutation, some illegal offsprings may generate. These illegal offsprings are generated due to limited number of multiple process plans of each part type and it may happen that during mutation one job type exceeds the limit of available multiple process plans. Thus, a repairing strategy is necessary to sort out this illegitimacy. Initially, a check is performed to find out the job types that are exceeding the limit of available multiple process plans. If there is no job type that exceeds the limit, the offspring is not illegal and does not require repairing process. However, if there is/are job type(s) that exceed the limit of available multiple process plans, then repairing process is activated. It repairs the genes of the illegal offspring by replacing it with randomly selected multiple process plans of the part type.

3.7 Reproduction

Reproduction pertains to the further generating the new generation. Once offsprings are generated after crossover and mutation operations, they along with parent population form the extended population. Elitism method of reproduction is embedded with Linear Rank Selection method. It prevents losing the best found solution. It transfers few good individuals from the previous population to the population of the next generation. In the present study, an elitism rate of 0.9 is considered to transfer the best individual from the previous population to the population of next generation.

3.8 Restart

As GA proceeds, population evolves over time. Sometimes, the population has a low diversity which may cause it to be trapped in a local optimum. In order to avoid premature convergence, a restart scheme is embedded in regular GA. If the best Makespan is not promoted for more than a pre-specified number of generations (i.e. does not change), the restart phase commences to regenerate the population by the following process [19]:

Step 1: Sort the population in ascending order of fitness value
Step 2: Skip the first 10% of the individuals from the sorted list
Step 3: The remaining 90% of the strings in the sorted list are neglected and are reproduced in the following way:

a. From the first 10% best chromosome, first half (50%) of new population is produced by reciprocal exchange mutation
b. Another half (50%) of new population are produced randomly.

All newly generated genetic material will only replace 90% of the worst chromosome of the population if they hold out fitness value better than the worst chromosome of the previous population. Also repetition of the individuals in the newly generated 90% population is not permitted.

In the present work, restart scheme is applied if there is no improvement in the fitness value (makespan) for more than 15 successive generation/iterations.

3.9 Termination Criterion

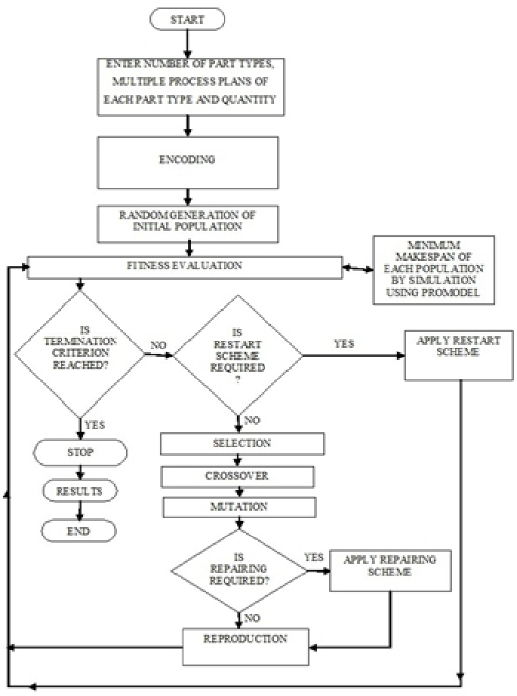

Figure 1: Flow Chart of the Adopted Methodology

Termination criterion refers to the stopping criterion for further exploration in search space. In the present work, maximum number of generation is considered as the termination criteria. The iteration procedure continue until the generation number equals to product of the number of jobs (n) and number of machines (m). For example for a 12 jobs 15 machines problem, the termination criteria is 180 (12 ×15) generations i.e. GA will stop after 180 generations and best fitness value obtained in last iteration is taken as optimal solution. Figure 1 shows the flow chart of the adopted methodology.

4. RESULTS AND DISCUSSION

For Case Study-1, the optimized makespan is 511 Minutes. There are two process plans combinations of part type of the production order that yield same optimized makespan. The convergence curve is shown in Figure 2.

Figure 3 shows the convergence curve for the Case Study-2. The optimized makespan is 506 Minutes and for same optimized makespan, there are twenty one process plans combinations of the part type of the given production order.

Comparison of optimized makespans of case study-I and case study-II reveals that by changing the MPP of part type, optimized makespan is reduced from 511 to 506. For same optimized makespan, there are 21 process plan combinations of part types. It clearly reveals that availability of different MPP of a part type in a production order affects optimized makespan.

Figure 4 shows the convergence curve for Case Study-3. The optimized makespan is 497 Minutes. For same optimized makespan, there are nine process plans combinations of part type of the production order.

Comparison of optimized makespans of case study-II and case study-III reveals that by changing the MPP of part type 2, optimized makespan is further reduced from 506 to 497. For same optimized makespan, there are 9 process plan combinations of part types. It clearly reveals that availability of different MPP of a part type in a production order affects optimized makespan.

For Case Study-4, the optimized makespan is 495 Minutes. Figure 5 shows the convergence curve. It clearly shows that for same optimized makespan, there are nine process plans combinations of part type of the production order.

All the results are tabulated in Table-1. It reveals that if we have a choice of MPP than there are more than one process plan combinations that yield the same optimized makespan.

4.1 Figures And Tables

Table-1

Case Study No.	Process Plan Combinations That Yield The Same Result	Optimized Makespan (in Min.)
1	2	511
2	21	506
3	9	497
4	9	495

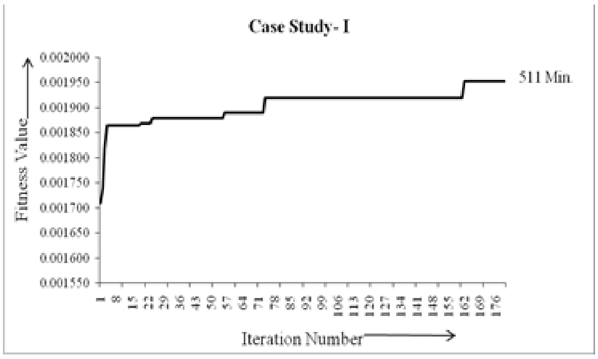

Figure 2: Convergence Curve of case study I

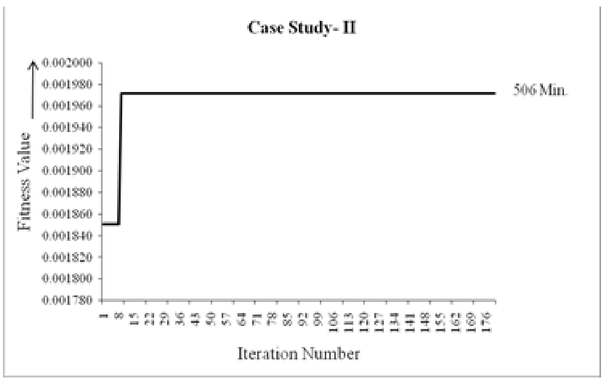

Figure 3: Convergence Curve of case study II

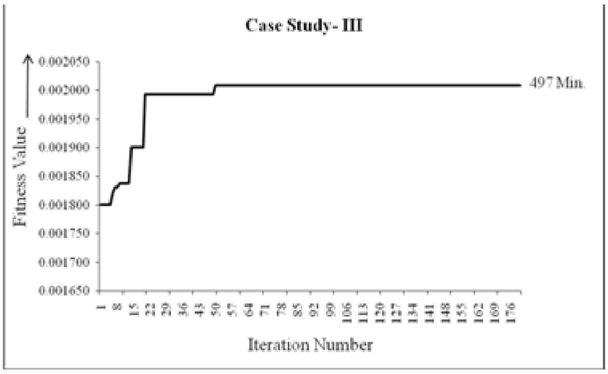

Figure 4: Convergence Curve of case study III

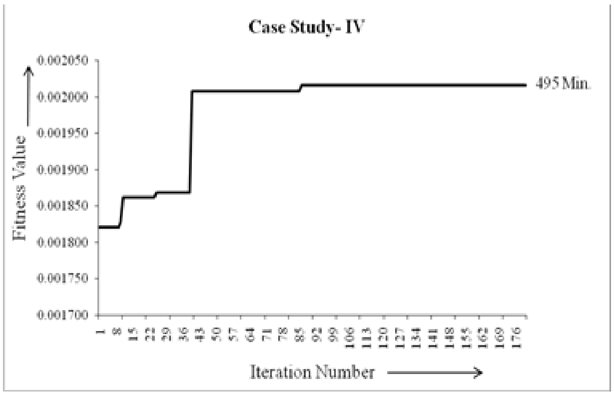

Figure 5: Convergence Curve of case study IV

5. CONCLUSION

In the present work, an attempt is made to optimize job shop scheduling using simulation based Genetic Algorithm approach in the presence of multiple process plans. From the case studies considered, it is concluded that for a given production order in which part type can be processed by multiple process plans, there are more than one process plan combinations of the part types in a production order that yield the same optimized makespan.

6. SCOPE FOR FUTURE WORK

The present work can be extended in several ways. It can be extended by incorporating the aspects of due dates, tardiness, earliness, flow time, throughput, etc. Dispatching rules used in this work is Shortest Processing Time (SPT). The problem can be extended by using other dispatching rules such as Longest Processing Time (LPT), Earliest Due Date (EDD), Most Work Remaining (MWR), etc. and comparative analysis of the results obtained could be done. Different combination of crossover and mutation probabilities can be implemented and results obtained can be compared. The case studies considered in the present work can be solved by other Meta-Heuristics techniques such as Simulated Annealing, Tabu Search, Neural Networks, Fuzzy Logic Techniques, etc. and comparison of the results can be done. Production Quantity used in the case study can be changed.

The jobs and processing time are manually fed to ProModel® software. This is time consuming and likely to cause errors particularly when scheduling larger problems. This can be upgraded by modifying the software by incorporating some external files to capture data from any data files available on the computer. This can considerably reduce the time consumed in entering the job details.

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Mathematical Modelling of Transport of Decaying Contaminants in Groundwater Resulting from Instantaneous Spill

Ashok K. Keshari[1] and Amarsinh B. Landage[2]

[1]Professor, Department of Civil Engineering, IIT Delhi, 110 016, India
[2]Asst. Professor, Govt. Engineering College, Karad, Maharashtra, 415 124, India
Email: akeshari@civil.iitd.ac.in , amarlandage@yahoo.co.in
Telephone/Mobile No.: +91 8860025845, +91 8600430830

ABSTRACT

The growing emergence of groundwater contamination and the increased level of water scarcity problems require appropriate management of groundwater resources in term of both quantity and quality. For better management plans, it is imperative to develop mathematical modelling tools that enable to obtain the response of the considered groundwater system to hydraulic and environmental excitations and to predict resulting changes in groundwater quality in space and time. In this paper, one dimensional finite difference contaminant transport model is presented for an instantaneous spill which incorporates advection, dispersion, diffusion and decay mechanisms of contaminant migration in groundwater system. The developed model is capable of simulating the migration of contaminant species that are characterized by non-linear degradation or decay involving biological or chemical processes. The simulation results were compared with available analytical model, and were found to be in excellent agreement with that obtained from analytical solutions for a wide range of field conditions with regard to dispersion and source definition. The developed numerical model can be used for the forecasting of contaminant dispersion in laboratory and field for the quantitative description of the time-space distribution of the contaminant and to investigate the effect of non-linearity, which will help in addressing a number of real life groundwater quality problems.

Keywords: Groundwater Hydrology, Contaminant Transport, Numerical Modelling, Finite Difference Method, Decay, Biodegradation

1. INTRODUCTION

Water is one of man's basic and precious resources. Contamination of water either on surface or in ground is crucial problem. . In most of groundwater contaminant transport investigations it is not practical to monitor all aspects of the groundwater flow and solute distributions. Information between and beyond monitoring locations and in the future are needed to understand the site and make informed decisions. The role of groundwater models in the study of groundwater flow and transport has long been a topic of interest for water resources people. The growing emergence of groundwater contamination and the increased level of water scarcity problems require appropriate management of groundwater resources in term of both quantity and quality. For better management plans, it is imperative to develop mathematical modelling tools that enable to obtain the response of the considered groundwater system to hydraulic and environmental excitations and to predict resulting changes in groundwater quality in space and time.

The finite difference method is a well known numerical method that has been applied to advection dispersion equation (Akram et al. 1999). The concept of linear "caricature" isotherm and its usefulness in obtaining exact analytical solutions were introduced for concentration profiles under nonequilibrium conditions (Manorajan 1995). An analytical solution for solute diffusion in a semi-infinite two-layer porous medium for arbitrary boundary and initial conditions obtained by Liu and Ball (1998) using the Green's function approach. An improved FDM has been developed by Hossain and Yonge (1999) to provide oscillation free results with the introduction of minimum artificial dispersion. A one-dimensional theory of contaminant migration through a saturated deforming porous media is developed by Smith (2000) based on a small and large strain analysis of a consolidating soil and conservation of contaminant mass. Analytical one-dimensional solutions are obtained by Pang and Hunt (2001) for continuous and pulse contaminant sources in a semi-infinite saturated porous medium when the dispersion coefficient increases linearly with distance downstream. Serrano (2001) used the method of decomposition for obtained series of solutions for the non-linear equation of advection and diffusion. These expressions permit an accurate forecasting of contaminant propagation under non-linearity in laboratory or field investigations at early or prolonged times after the spill. This paper presents the practical scenario of an instantaneous spill, and that of a constant concentration boundary condition for situations of non-linear decay, non-linear Freundlich isotherm, and non-linear Langmuir isotherm. Khebchareon and Saenton (2005) present an initial development of a one-dimensional numerical solution of mass transfer behavior of the entrapped dense non-aqueous phase liquid (DNAPL) in the subsurface environment where the system of equations is solved implicitly. Many analysts worked on the non linearity problem of decay and sorption. But number of analyst considered only one or two parameter of non linearity in there model either in analytical or numerical. In this model proposed combine effect of decay and sorption on account for the solution of governing equation of contaminant transport.

2. Contaminant Transport Mechanisms

There are three main physical processes effecting contaminant transport namely advection, dispersion and diffusion. In addition, chemical processes that effect transport are decay and sorption. Advection is the mass transport caused by the bulk movement of flowing ground water. The driving force is the hydraulic gradient. In highly permeable materials such as sand and gravel, advection is the most important transport process, and each transport prediction will only be as accurate as the flow description. Advective flow becomes more complex when the density and/or the viscosity of water change with solute concentration. Diffusion is the net flux of the solutes from a zone of higher concentration to a zone of lower concentration. Diffusion is the net flux of the solutes from a zone of higher concentration to a zone

Diffusion over geological time, however, can have a significant impact. The effect of diffusion will normally be masked by the effect of advection in groundwater zones with high flow velocities. Dispersive spreading, within and transverse to, the main flow direction causes a gradual dilution of the contamination plume. Dispersive spreading will lead to increase in plume uniformity with travel distance. The combination of dispersion and diffusion termed as hydrodynamic dispersion. Degradation process also decreases the source of contamination with time. Reactions of the first order are applied to describe radioactive decay or simple degradation processes. Reactions of the first order are a linear and do not change the characteristics of the transport equation. Sorption refers to adsorption and desorption. Adsorption describes the adhesion of molecules or ions to the grain surface in the aquifer. The release from the solid phase is called desorption. Adsorption causes diminution of concentrations in the aqueous phase and a retardation of contaminant transport compared to water movement. The degree of sorption depends on a number of factors, including the concentration and the characteristics of the contaminant, the soil type and its composition, the pH value of water, and the presence of other water solutes. These factors are in time and space, resulting in a variation of retardation in the natural environment. The rate of adsorption onto the solid material as related to the concentration in the groundwater is expressed by adsorption kinetics. The relationship between the concentration of a solute in adsorbed phase and in the adjacent water phase at equilibrium is an adsorption isotherm (C.W. Fetter, 1993 and F.W. Schwartz, 1988).

3. Governing equation for contaminant transport

Assumptions taken in to considerations in model development are that the soil is homogeneous and isotropic, the porosity of soil is constant, saturated hydraulic conductivity is constant, ground water pore velocity is constant, one-dimensional flow is taken, hydrodynamic dispersion coefficient is constant, Freundlich and Langmuir parameters are constant and retardation factor is constant.

The one-dimensional advective-dispersive equations in an infinite aquifer subject an instantaneous point source and linear biological or radioactive decay.

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} + aC = 0 \text{ -------------------------- } -\infty < x < \infty, 0 < t$$

$$C(\pm\infty, 0) =$$

The one-dimensional advective-dispersive equations in an infinite aquifer subject an instantaneous point source and non-linear biological or radioactive decay.

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} + aC^b = 0 \text{ -------------------------- } -\infty < x < \infty, 0 < t$$

$$C(\pm\infty, 0) =$$

4. Analytical solution for decaying contaminant species transport

4.1 Analytical Solution for Linear Decaying Contaminant Species Transport

The one-dimensional advective-dispersive equations in an infinite aquifer subject an instantaneous point source and linear biological or radioactive decay.

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} + aC = 0 \qquad -\infty < x < \infty, C(x,0) = 0$$

$$C(\pm\infty, t) = 0,$$

$$C(x,0) = C_i\delta(x) \tag{1}$$

The solution to equation (1) is

$$C = \sum_{n=0}^{\infty} C_n = \frac{C_i e^{-\left[\left((x-ut)^2/4Dt\right)-\alpha t\right]}}{\sqrt{4\pi Dt}} \tag{2}$$

which is the well-known solution to the advective– dispersive equation with linear decay.

Decomposition series converge to the exact solution to the differential equation. In many instances, however, the closed-form solution may not be identified. This is especially true in many nonlinear equations. While a closed-form solution is mathematically desirable, the series solution constitutes an accurate model of interest to the practicing hydrologist.

4.2 *Analytical Solution for Non Linear Decaying Contaminant Species Transport*

In cases of non-linear biological or radioactive decay, equation (1) becomes

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} + aC^b = 0 \tag{3}$$

solving the equation, we arrive at the closed-form expression

$$C(x,t) \approx C_0(x,t)\, e^{\left[2\alpha C_0(x,t)^{b-1}\right]/(b+1)}, \qquad b>0 \tag{4-22}$$

$C_i > 1$

For the case of linear decay, b=1, and equation (4) is identical to the exact solution of equation (1), that is equation (2).

Thus, equation (4) is a useful, simple, and stable expression for practical applications in the forecasting of contaminant propagation under non-linear decay during early or prolonged-time simulations and a full range of values in the physical parameters.

4.3 Governing equation for contaminant transport

(a) The one-dimensional advective-dispersive equations in an infinite aquifer subject constant point source and linear biological or radioactive decay.

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} + aC = 0 \text{ -------------------------- } -\infty < x < \infty, 0 < t$$

$$C(\pm\infty, 0) =$$

5 Solution of governing equation

Following assumptions are used for developing numerical model of contaminant transport equation:
(1)The porous medium is homogeneous and isotropic.
(2)The solute transport, across any fixed plane, due to microscopic velocity variations in the flow tubes, may be quantitatively expressed as the product of dispersion coefficient and the concentration gradient.
(3)The flow in the medium is unidirectional and the average velocity is taken to be constant throughout the length of the flow field.
(4)The FDM is approximations the higher order terms in Taylor's Series are neglected.
(5)Contaminant is conservative i.e. decay is not considered for sorption cases. Also contaminant is assumed to be non reactive.
(6)Contaminant is non conservative i.e. decay is considered in case of decay and combine effect of decay and sorption. Also contaminant is assumed to be non reactive.
(7)Retardation process is considered in sorption cases.
(8)No other process like pumping, recharge etc. is considered.

5.1 Implicit scheme

The principal models of contaminant transport in groundwater are advection and dispersion. Retardation and degradation can significantly impact the transport. Extensive research has been and is being carried out on the numerical aspect of simulating advective-dispersive transport. A large volume of literature is available on finite difference models (FDMs) and finite element models (FEMs) for simulating advective-dispersive transport, in general and advective-dispersive transport in groundwater, in particular. The FDM for simulating contaminant transport in groundwater is based on either first-order or second-order approximation of the advective term. The first-order approximation of the advective term results in a stable algorithm at the expense of introducing unacceptably large artificial dispersion. The second-order accurate central difference approximation of the advective term,

on the other hand, leads to oscillatory results. Oscillations are usually eliminated by adapting up-winding schemes. Adaptation of upwind FDMs, however, can introduce large artificial dispersion.
The implicit formulation for governing equation is obtained by the replacing the space derivative with its finite difference analog at the (j+1) time level i.e. (t+1). The time derivative is then replaced by a backward difference approximation relative to the j+1 time level i.e. t+1.

To illustrate, let us consider an one dimensional partial differential equation of second order of following type

$$\frac{\partial \Phi}{\partial t} = \frac{\partial^2 \Phi}{\partial x^2}$$

$$\frac{\Phi_i^{j+1} - \Phi_i^j}{\Delta t} = \frac{\Phi_{i+1}^{j+1} - 2\Phi_i^{j+1} + \Phi_{i-1}^{j+1}}{(\Delta x)^2}$$

The truncation error is the approximation is again $O\left((\Delta t) + (\Delta x)^2\right)$ The above equation forms a set of simultaneous linear algebraic equations with the unknowns Φ_i^{j+1}. The unknowns are thus given implicitly. This set of simultaneous equations is solved for the whole aquifer domain at a particular time level. In this passion, the solution is marched forward in time by solving the system of equations at each time level. The beauty of this method is that it is unconditionally stable.

Finite difference by implicit scheme is given by

$$\left[\frac{\partial C}{\partial t}\right] = \left[\frac{C_i^{t+1} - C_i^t}{\Delta t}\right]$$

$$\left[\frac{\partial C}{\partial x}\right] = \left[\frac{C_i^{t+1} - C_{i-1}^{t+1}}{\Delta x}\right]$$

$$\left[\frac{\partial^2 C}{\partial x^2}\right] = \left[\frac{C_{i+1}^{t+1} - 2C_i^{t+1} + C_{i-1}^{t+1}}{(\Delta x)^2}\right]$$

5.2 Numerical solution for decaying contaminant species transport

The one-dimensional advective-dispersive equations in a semi infinite aquifer subject to a general non-linear sorption isotherm of the form

The one-dimensional advective-dispersive equations in a semi infinite aquifer subject to constant point source and linear biological or radioactive decay.

$$\frac{\partial C}{\partial t}-D\frac{\partial^2 C}{\partial x^2}+u\frac{\partial C}{\partial x}+aC=0$$

The above equation may be solved for a variety of boundary and initial conditions. However, the following boundary and initial conditions were considered.

B.C.

$$C(x=0,t>0)=C_0$$

$$C(x=L,t\geq 0)=0$$

I.C.

$$C(0<x\leq L,t=0)=0$$

Equation (1) can be discretized as follows by employing second-order accurate central difference approximation of the advective term

$$\frac{\partial C}{\partial t}=\frac{C_i^j-C_i^{j-1}}{\Delta t}$$

$$\frac{\partial C}{\partial x}=\frac{C_{i+1}^j-C_{i-1}^j}{2\Delta x}$$

$$\frac{\partial^2 C}{\partial x^2}=\frac{C_{i+1}^j-2C_i^j+C_{i-1}^j}{\Delta x^2}$$

Where C_i^j is contaminant concentration at i-th space step and j-th step, Δx is space step and Δt is time step.

So the 1-D advection-dispersion equation becomes, in FDM form:

$$\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}-u\frac{\partial C}{\partial x}-aC$$

So we have

$$(-k1-k2)C_{i-1}^j+(1+k3+2k2)C_i^j+(k1-k2)C_{i+1}^j=C_i^{j-1}$$

$$P*C_{i-1}^j+Q*C_i^j+R*C_{i+1}^j=C_i^{j-1}$$

Where $P=(-k1-k2)$, $Q=(1+k3+2k2)$ and $R=(k1-k2)$

Where i ranges from 2 to (n-1) [excluding the boundaries x=0 and x=n Δx].

In matrix form:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ P & Q & R & 0 & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & P & Q & R & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & P & Q & R & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & 0 & P & Q & R \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} C_1^j \\ C_2^j \\ C_3^j \\ . \\ . \\ . \\ C_{n-2}^j \\ C_{n-1}^j \\ C_n^j \end{bmatrix} = \begin{bmatrix} C_0 \\ C_2^{j-1} \\ C_3^{j-1} \\ . \\ . \\ . \\ C_{n-2}^{j-1} \\ C_{n-1}^{j-1} \\ C_n^{j-1} \end{bmatrix}$$

$$\left[M^F\right]\left[C^j\right]=\left[R^F\right]$$

The matrix $[M^F]$ is tridiagonal and is constant. At each time step, systems of equations are solved for concentrations at the nodes by forward and backward substitutions using Gauss Elimination Technique.

6. Results and discussion

6.1 Contaminant concentration distribution for decaying species

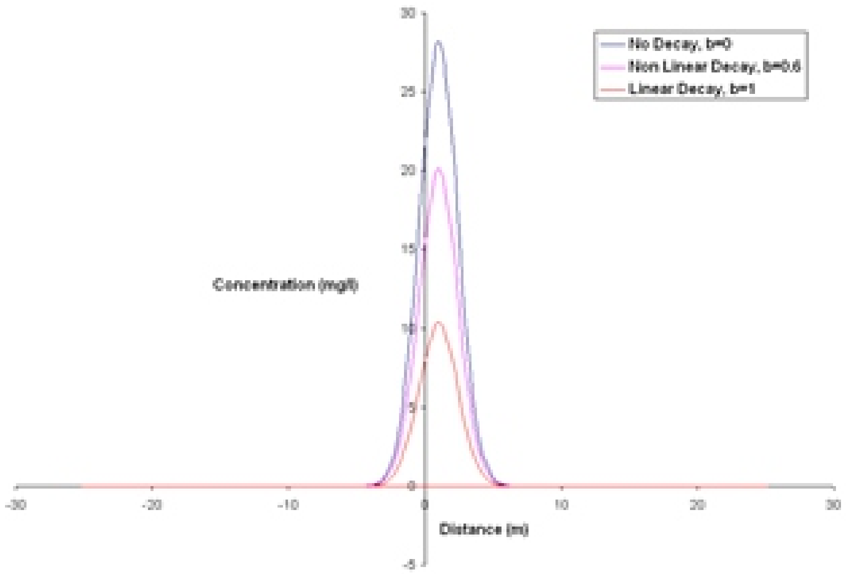

Figure 1 Contaminant concentration distribution subject to linear decay, non linear decay and no decay after an instantaneous spill

Figure 1 shows the concentration vs. distance profile at one month after the spill when no decay is present, according to equation (2); when linear decay is present, according to equation (2) setting b=1; and when non-linear decay is present, according to equation (4) setting b=0.6.

This comparison is quantitative and can be used to assess the effect of the non-linear parameter b, since the parameter a has dimensions affected by b. Yet, the graph shows the physical bounds of the plume.

In general, non-linear decay scales down the concentration profile, the degree of which is controlled by the magnitude of b. Since the concentrations are greater than 1 and b<1, most of the linear plume is scaled up with respect to the linear decay plume.

6.2 Results obtained by numerical model

6.2.1 Contaminant concentration distribution species for decaying and sorbing species at different time

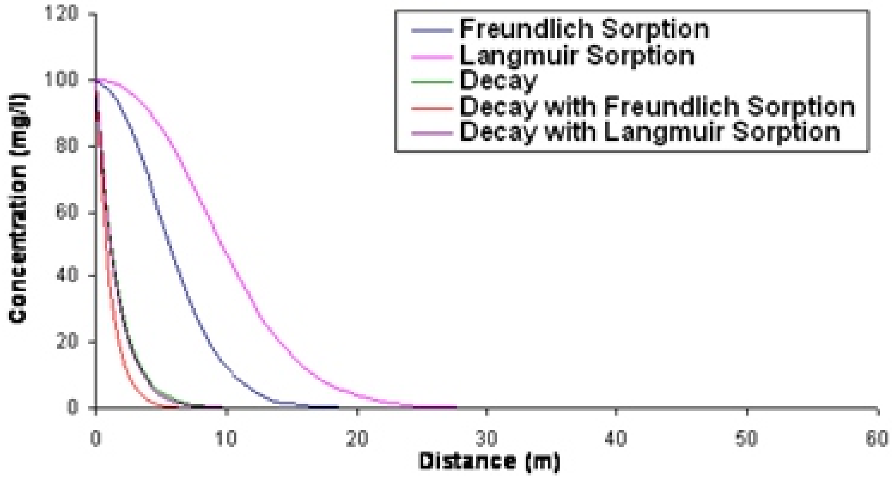

Figure 2 **Concentration Distribution at 10 month**

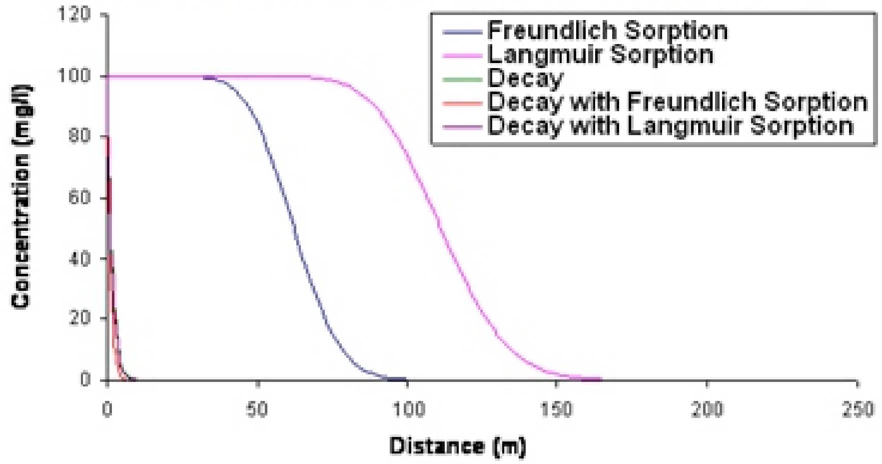

Figure 3 **Concentration Distribution at 120 month**

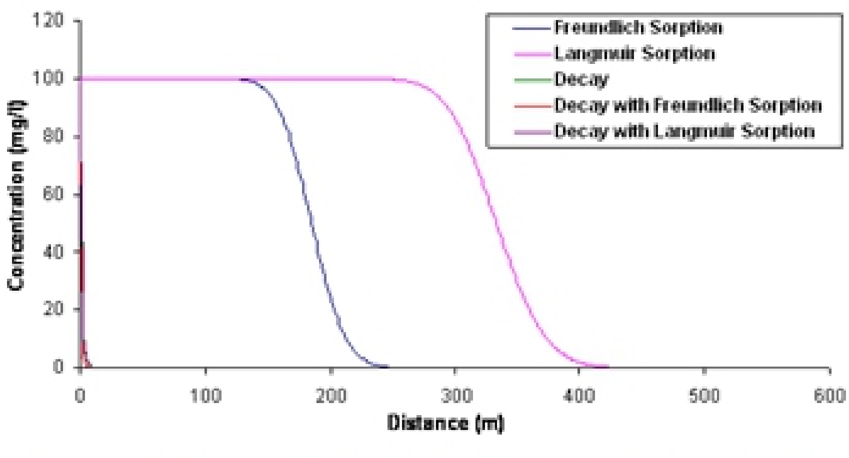

Figure 4 **Concentration Distribution at 360 month**

Figures 2,3 and 4 shows concentration distribution of contaminant species at different time in longitudinal direction.

It is observed that at initial time contaminant species rapidly reduces in domain due to sorption and decay. Contaminant specie dose not travel more distance As time increases plot clearly difference between decay, Freundlich sorption and Langmuir sorption. Contaminant species diminish due to decay. In case of Freundlich sorption and Langmuir sorption solute particle travel long distance in the direction of ground water velocity and slowly reduces its movement and existance. Because of high value of Freundlich retardation factor contaminant species velocity less than velocity of species due to Langmuir sorption.

At the initial few months it is observed that front of concentration distribution curve is smooth and concentration slow decrease. However, as time increases front become sharp. It indicates that after traveling certain distance in long time concentration reduces rapidly.

6.2.2 ***Contaminant concentration distribution species for decaying and sorbing species at different distance***

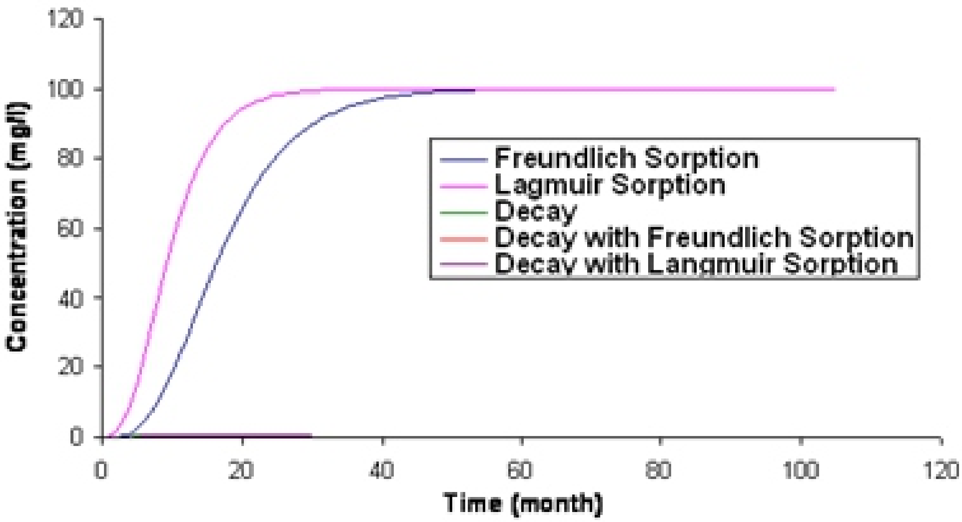

Figure 5 **Concentration Distribution at 1 meter**

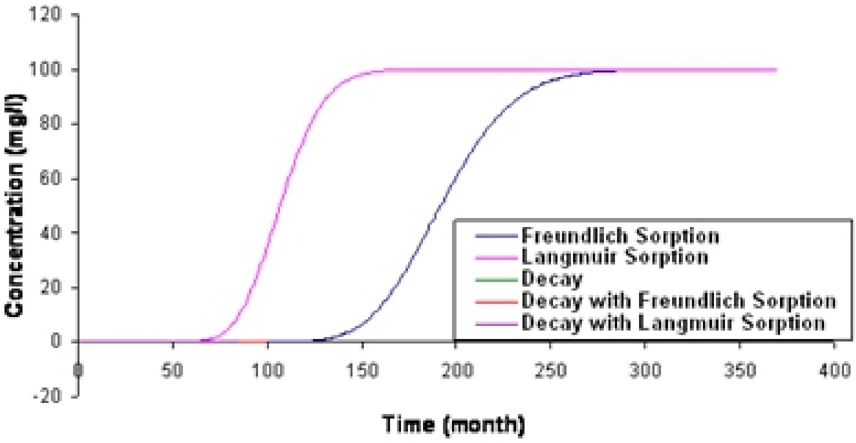

Figure 6 **Concentration Distribution at 100 meter**

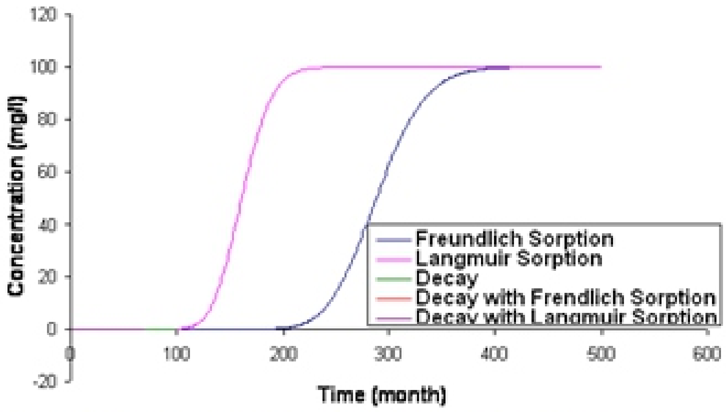

Figure 7 **Concentration Distribution at 150 meter**

Figures 5, 6 and 7 shows concentration distribution of contaminant species at different distance for continuous time.

It is observed that plume of contaminant species reaches early period in case of Langmuir sorption, shows that contaminant species velocity in the longitudinal direction of ground water is high. In case of Freundlich sorption, plume takes more time to reach at particular distance than Langmuir sorption. It indicates that contaminant species velocity more affected due Freundlich sorption than Langmuir sorption.

Contaminant species almost diminishes due to decay. When we take combine effect of decay and sorption, decay is always dominant than sorption. Because of that species concentration reduces rapidly in aquifer.

7. Conclusions

Using the method of decomposition, series solutions were constructed for the advective–dispersive transport equation in aquifers subject to nonlinear decay, non-linear Freundlich sorption, or nonlinear Langmuir sorption. Using the concept of double decomposition, the series were used to obtain analytical simulant solutions, which are closed-form expressions of part of the parent series. The analytic simulants were tested for numerical accuracy with respect to the parent non-linear series solution with an excellent agreement.

Plumes undergoing non-linear decay experience a profile re-scaling with respect to that of linear decay, the degree of which is controlled by the magnitude of the non-linear parameter b. The direction of the scaling (scaling up or scaling down with respect to the linear decay plume) is controlled by the magnitude of b (whether greater or less than 1). When values of $b<1$ produce plumes that experience less decay (i.e., are scaled up) than that of the linear decay, whereas values of $b>1$ produce non-linear plumes that experience more decay (i.e., are scaled down) than that of the linear decay.

However, the approximate analytical models presented here are not capable of predicting the form of a contaminant plume when the initial concentration is large and at the same time $\underline{a}$is large, or when $> Ci$. More research is needed on the identification of simple solutions for the later conditions.

The FDM predictions were found to be in excellent agreement with analytical solutions for a wide range of field conditions with regard to dispersion and source definition. The new developed numerical model can be used for the forecasting of contaminant dispersion under non-linear reactions, or for the quantitative description of the effect of non-linearity in the sorption parameters, on the time-space distribution of the contaminant. The solution for numerical values of state variable only at specified points in the space and time domains defined for the problem. The above FDM model solved by using implicit scheme is unconditionally stable. The proposed models are flexible, stable, and could be used for laboratory or field simulations at early or prolonged contamination scenarios.

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