A DOSAGE BASED METHODOLOGY TO SIMULATE CROWD EVACUATIONS IN TOXIC ENVIRONMENTS

A Thesis

by

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ABSTRACT

For evaluating the consequences and planning for emergencies associated with toxic gas releases, the role of evacuation times is indispensable. In such a release scenario, evacuees may be subjected to varying doses of toxic gas which may result in various toxic effects and symptoms that may affect the ability to escape or take actions. Understandably, it is imperative to develop a methodology that accounts for the dosage-based effects of toxic substances on evacuees during the evacuation.

In this work, the previously proposed social force model for crowd evacuation is modified by introducing a dynamic dosage-dependent force term, Toxic Force, to account for the effects of various symptoms associated with toxic exposures. This force term is defined as a function of Toxic Load, which is an exposure-response based, level of injury estimation variable. The Toxic Load algorithm is put into effect to indicate the levels of injury due to multiple symptoms.

The existing Panic Simulator tool was modified in line with this novel methodology. A case study was conducted in which an evacuation of 51 people from a realistic geometry of an administrative building was simulated while subjecting them to different concentrations of hydrogen sulfide. The results of this study lent insights into the evacuation process. For instance, exit times of people who are farther from the exit exhibit significantly greater sensitivity to exposure concentrations than those of people closer to the exit. Such insights into the evacuation process can help implement more effective

mitigation methods, and help plan better emergency responses.

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NOMENCLATURE

AEGL	Acute Exposure Guideline Levels
COPD	Chronic Obstructive Pulmonary Diseases
ERPG	Emergency Response and Planning Guidelines
FDS+EVAC	Fire Dynamics Simulator and Evacuation
FED	Fractional Effective Dose
H_2S	Hydrogen Sulfide
IDLH	Immediately Dangerous to Life and Health
OSHA	Occupational Safety & Health Administration
TL	Toxic Load
WHO	World Health Organization

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1. INTRODUCTION

In the scenario of a toxic release, the events may progress in such a manner that human population near the release may be subjected to the hazards associated with the exposure to the toxic gas. The risks associated with such releases need to be analyzed and controlled. The role of emergency evacuation characteristics of facilities is indispensable in these analyses as this data helps in evaluating mitigation methods and evacuation strategies.

Evacuation models are used to simulate different evacuation scenarios to obtain an estimate of the evacuation times, however, most of the evacuation tools do not take into account the effects that the exposure to toxic gas might entail on the evacuation times. The models that do take into account the exposure, only do so to estimate the number of fatalities. In general, the effects of the symptoms associated with the exposure are not taken into account while the evacuation is simulated. This may lead to misleading results as the symptoms associated with the exposure impact the physical and psychological ability of the person to evacuate.

The severity and incidence of a toxic effect is a function of time and concentration called dosage. A dosage based implementation of the effects of the symptoms associated with the toxic exposure would mean that the effects are not being applied uniformly on all evacuees, but rather in accordance with their time and concentration of exposure.

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2. STATE OF THE ART

In order to undertake the task at hand, a review of the state of the art was conducted to gather the existing literature on relevant topics and establish the knowledge gaps. The results of these efforts are detailed below.

2.1 Crowd Evacuation Models

The purpose of evacuation of models is to simulate evacuation scenarios in order to lend an insight into the evacuation process by reproducing various phenomenon and factors associated with crowd evacuations. Evacuation models exist for scales ranging from evacuation of people from a small room all the way up to evacuation of cities through motor vehicles.

Crowd evacuation models are comprised of two parts, one, the geometry of the evacuation domain, and two, the evacuees, commonly known as agents. The evacuation models try reproduce real life phenomenon by modelling the interactions between the environment and the agents, and the interactions amongst agents.

A good evacuation model should be able to reproduce the various real-life observed phenomenon associated with evacuations. For example, in the case of an emergency evacuation from a building, the model should be able to reproduce phenomenon caused by panic like arching, clogging, and un-coordinated passing of exits.

Xiaoping et al. [1] reviewed and categorized crowd evacuation models with respect to six characteristic features, namely,

1. Approaches – the physics behind the formulation of the model

2. Types of Agents – if all agents are considered homogenous individuals or divided into groups on basis of age, gender, psychology etc.
3. Scale of model – if the models take a microscopic or macroscopic approach to the interactions
4. Space and Time – Discrete in space and time or continuous
5. Situations – if the design intent is for emergency situations or normal situations
6. Typical phenomena – the type of behavior intended to be reproduced, example, kin behavior (sticking close to a relative), arching at exits etc.

A total of 7 different approaches that can be used to model crowd evacuation were identified by Xiaoping et al. These approaches and some models based on those approaches are detailed below. It must be noted that none of the models mentioned below simulate evacuations in toxic environment.

2.1.1 Cellular Automata Models

Cellular automata are discrete idealizations of physical systems in which the physical quantities take discrete values. Cellular automata consist of a regular uniform lattice, usually infinite in extent, with a discrete variable at each site, called cell. The cellular automata evolve in discrete time steps with the value of variable in one cell being affected by the value in the neighboring cell. The change in value at these time steps is described by the 'local rules' which depend upon the nature of application [2].

The existing cellular automata models are either based on the interactions between agents and the environment or interactions among the agents.

For simulating emergency evacuations Zhao et al. 2006 [3] demonstrate the evacuation of a room. The room is discretized into the size of 0.4 by 0.4 m^2 (typical space occupied by and agent). The model is subject to set of local rules which govern the evacuation scenario. One of the rules governing the evacuation is that if the sum of number of agents to the 'Left' plus and the number of agents to the 'Right' is less than the sum of the number of agents 'Behind' and 'phi' ($L + R < B + \phi$), the agent will move to the empty cell he is facing, else he will stay at the current cell where phi is a measure of agent's level of anxiety or panic (eagerness to move).

The shifting of cells in the cellular automata models is as per the rule that cells move to a lower value. Varas at al. 2007 [4] used this approach by assigning some of the cells very high values to turn them into obstacles. He used this and a few other rules to study the effect of obstacles on evacuation.

Kirchner at al. used cellular automata models to study emergency behavior like competitive egress [5] and friction effects and clogging [6], by introducing two parameters - crowd density and a friction parameter.

Fang et al. 2003 [7] use the cellular automata approach to simulate bi-directional pedestrian movement.

2.1.2 Lattice Gas Models

Lattice gas models are a special case of cellular automata in the way that the agents in these models are live particles, whereas in cellular automata, the movement of agents is evaluated through the changes in cells. The agents are defined as points in a mesh consisting of empty sites to be occupied, and the agents move between these empty sites as per the local rules defined. The movement of the agents in these models is however more complex than the cellular automata models. The agents use the rules and surrounding environment to calculate the probabilities of movement in each direction and move to the site with the highest probability.

Tajima et al. 2001 [8] in their paper study the scaling and dynamic phase transition of the flow of agents exiting a hall with the help of Lattice gas model. They were able to demonstrate various patterns associated with evacuations, like arching and flattening and the time at which the transition from choked flow to decayed flow occurs.

Helbing et al. 2003 [9] used lattice gas model to simulate the evacuation of agents from a classroom setting. The agents in this model were represented on a square lattice with L*W sites to which movement is possible. A directional bias was introduced by using a variable called 'drift' which represents the haste the agent shows to reach the exit.

Song et al. 2006 [10] in his model combines the lattice gas approach with the concepts of social force (discussed below). He modifies the lattice gas model by assigning each agent with overlapable cells in addition to the regular cells, the social forces are applied when the overlapable cells are occupied by the overlapable cells of another agent, which decrease the probability of the agent to move in that direction.

2.1.3 Social Force Models

In social force models, the motion of agents is determined by the following main effects; the desire to reach a destination, desire to keep a certain distance from obstacles and walls, keeping a certain distance between oneself and other agent, and, (optionally) being attracted by other agents. The total effect is reflected in a force equation consisting of force terms reflecting each of these effects.

Using the idea proposed by Levin [11], that behavioral changes are guided by social fields or social forces as a motivation, Helbing published his first iteration of the social force model for pedestrian dynamics in 1995 [12]. In this publication, Helbing formulated three force terms that every agent is subjected to, one, representing the inherent nature of the agent to reach a destination, called as motivational force, the second is a repulsive force enforcing territorial effect for the agent, and lastly, the attractive force responsible for formation of pedestrian groups.

In his publication in 2000, Helbing et al. [13] improved upon the previously proposed social force model. The design intent of this model is to simulate the dynamic features of human behavior induced during panic situations, like people moving faster than normal, pushing and physical interactions between people, uncoordinated passing of bottlenecks, jams, arching and clogging at exits and tendency of mass behavior.

In this model, each agent is modelled as a circle and its motion is described by the differential equation shown below:

$$\boldsymbol{m_i}\frac{\boldsymbol{dv_i}}{\boldsymbol{dt}} = \boldsymbol{m_i}\frac{\boldsymbol{v_i^0(t)e_i^0(t) - v_i(t)}}{\boldsymbol{\tau_i}} + \sum_{\boldsymbol{j(\neq 1)}} \boldsymbol{f_{ij}} + \sum_{\boldsymbol{W}} \boldsymbol{f_{iw}} \qquad (1)$$

where, m_i - Mass of the agent

v_i - Velocity of the agent

v_i^0 - Desired velocity of the agent

$\boldsymbol{e}_i^0$ - Desired direction of the agent

τ_i - Characteristic relaxation time

$\boldsymbol{f}_{ij}$ – Agent-Agent interaction force

$\boldsymbol{f}_{iw}$ - Agent-Wall interaction force

The first term on the right is called the motivation force of an agent. This term determines the responsiveness of the agent to with which the agent will try to achieve the user-defined desired velocity ‘$v_i^0(t)$’. ‘$\boldsymbol{e}_i^0$’ is the vector pointing to the direction of the exit. The second term accommodates the agent-agent interactions and in addition to the previous model, in this iteration of the model, Helbing defined the third term which represents the interaction of the agent with walls.

The agent-agent interaction force and the agent-wall interaction forces are defined analogously and consist of three terms. They both contain a repulsive (first) term, which represents the psychological tendency to maintain a physical distance from walls and agents. The two other terms are inspired by granular interactions and come into effect when the agent collides with another agent or a wall. The first term counteracts body compression and is called 'body force', while the second term impedes the relative tangential motion, and is called 'sliding friction force'.

$$\boldsymbol{f_{ij}} = \left\{\boldsymbol{A_i}\,\mathbf{exp}\left[\frac{\boldsymbol{r_{ij}} - \boldsymbol{d_{ij}}}{\boldsymbol{B_i}}\right] + \boldsymbol{kg}\big(\boldsymbol{r_{ij}} - \boldsymbol{d_{ij}}\big)\right\}\boldsymbol{n_{ij}} + \boldsymbol{\kappa g}(\boldsymbol{r_{ij}} - \boldsymbol{d_{ij}})\boldsymbol{\Delta v^t_{ji} t_{ij}} \qquad (2)$$

$$\boldsymbol{f_{iw}} = \left\{\boldsymbol{A_i}\,\mathbf{exp}\left[\frac{\boldsymbol{r_i} - \boldsymbol{d_{iw}}}{\boldsymbol{B_i}}\right] + \boldsymbol{kg}(\boldsymbol{r_i} - \boldsymbol{d_{iw}})\right\}\boldsymbol{n_{iw}} - \boldsymbol{\kappa g}(\boldsymbol{r_i} - \boldsymbol{d_{iw}})(\boldsymbol{v_i} * \boldsymbol{t_{iw}})\boldsymbol{t_{iw}} \qquad (3)$$

where, A_i, B_i, k and κ are constants

r_{ij} – Sum of the radii of two agents under consideration

d_{ij} – Distance between the center of mass of two agents

d_{iw} – Distance between the center of mass of the agents and the wall

$n_{ij/w}$ – Normal direction to the agents or wall

$t_{ij/w}$ – Tangential direction between agents or wall

Δv^t_{ji} – Difference in tangential velocity of two agents

The social force model is used as a base for modeling other advanced behaviors. For example - Zheng et al. 2002 [14] used social force model proposed by Helbing et al. 2000 [13] in conjunction with neural networks to include two types of personalities. In this model, Zheng used the outputs of the behavior based neural network to affect the agent's desired velocity and direction.

Social force models successfully simulate most of the phenomenon associated with crowd evacuation, and achieve very realistic results [1]. However, in social force models, the repulsive force and attractive force accommodating interactions with agents and walls are based on granular interactions. This approach has been refuted by Henein and White [15] in their analysis, citing the fact that this behavior fails to account for the non-homogeneity of humans. They in-turn propose that the force be in the form of a dynamic field.

As previously discussed, Tajima et al. [8] studied the scaling and dynamic phase transition of the flow of agents. They point out that these phenomena are not accounted for in generalized force models like that of Helbing.

Xiaoping et al. [1] note that while models based on cellular automata and lattice gas are suitable for large-scale computer simulations, they do not take into account the high pressures generated during an evacuation like social force models do. These pressures due to crowd effects can help take into consideration the injuries caused due to these effects which would make the cellular automata and lattice gas approaches non-ideal if such studies are to be performed.

2.1.4 Fluid Dynamics Models

On the idea that, in a crowd, each person has a mass and velocity, the motion of crowds could be described by classical Maxwell-Boltzmann statistics. Henderson 1971 [16] developed equations for the probability density function for single fluctuating velocity component. He then observed three groups of homogenous crowds - students, pedestrians and children - and compared the measured distribution and Maxwell-Boltzmann distribution. He found a good agreement between both distributions in the cases of pedestrians and students which led him to conclude that pedestrian crowds behave similar to gases or fluids. This premise set by Henderson has led to the use of fluid dynamics models for simulating and studying crowd dynamics.

For example, Mnasri et al. 2016 [17] used fluid dynamics to simulate the flow of hajj pilgrims with the underlying assumption that there is a similarity between the flow of crowds and incompressible laminar fluids.

Hughes et al. 2003 [18] points out that initial fluid dynamics models did not consider the fact that crowds have an ability to think. However, this problem is being addressed by continuum modelling and development of new equations using the concepts of fluid mechanics and consultation from behavioral scientists.

2.1.5 Agent Based Models

Agent based models are computational models in which social constructs are built by specifying a set of rules that govern interactions among other agents. These models are suitable for providing valuable insights into the mechanisms and preconditions for panic and jamming by incoordination. This makes these models capable of reproducing complex human behavior like competition, queuing and herding. These models are capable of modelling complex human behavior arising due to different causes; however, it is a very challenging task to model human behavior.

Braun et al. 2005 [19] used Helbing et al. 2000 [13] model as the physical model and modified it by providing agents with behavioral attributes and individualities to account for their response to environmental changes, and analyzing their impact on the evacuation.

Pan et al. 2007 [20] used an agent based model to simulate social behaviors like competition, queuing and herding. They achieve this by modeling each human individual as an autonomous agent who interacts with a virtual environment and other agents according to an Individual Behavior Model and some global rules on crowd dynamics.

Agent-based models are computationally expensive when compared to the other models. The advantage agent-based models hold over other models is that they are the only ones that inherently address the heterogeneity of evacuees. This gives these models a unique feature of addressing the fact that human behavior is non-uniform.

2.1.6 Game Theoretic Model

An interactive situation, specified by the set of agents, the possible courses of action of each agent, and the set of all possible utility payoffs, is called a game. In a game, the agents assess all of the available options and select the alternative that maximizes their utility. Each agent’s final utility payoffs will depend on the actions chosen by all agents. The game theoretic model can be applied to single exit scenario, where it can represent the competitive behavior of agents during an emergency situation, but in the case of multiple exits, it can be used to simulate the dynamic exit selection behavior [21]. This approach ideally is suited for the analysis of how human reasoning and strategic thinking can affect evacuation behaviors.

Guan et al. 2016 [22] uses lattice gas models in conjunction with game theory to simulate evacuation. In this work, the agent calculates the probability of moving to the next site as per the rules of the lattice gas model, unless a conflict for the site arises with other agents, in which case, the probability of movement is calculated by utilizing game theory. This is done by making the probability a function of the game payoff matrix.

2.1.7 Approaches Based on Experiments on Animals

This is a new field of study and according to the Xiaoping et al. [1] two sets of experiments have been conducted. Saloma et al. [23] studied the behavior of mice under panic conditions by making them escape from water towards an exit. A comparative study between the observations and cellular automata model results was performed. Altusher et al. 2005 [24] performed experiments on ants with the aim of observing whether panic-induced herding at exits results in non-uniform use of exits. They observed that, for two symmetrically located exits, ants use both exits in approximately equal proportions in normal conditions, but preferred one of the exits if panic is created by adding a repellent fluid. According to Xiaoping et al. [1] the experimental findings coincide well with the theoretical predictions reported by Helbing et al. 2000 [13] for humans, and suggest that some features of the collective behavior of humans and ants are quite similar when escaping under panic.

However, Xiaoping et al. [1] also notes that humans have a stronger social consciousness compared to animals and exhibit social characteristics like kin behaviors unlike mice or ant.

Cellular automata and lattice gas models primarily consider the agents to be homogenous entities, which based on the applicability of the study can have significant impact on the outcomes. However, these approaches are computationally inexpensive.

Fluid Mechanics models are in general aimed at modelling and study of the flow of crowds as a whole. This approach is most suitable for modelling crowds with high densities as the assumption of considering the crowd as a continuum becomes questionable at low densities as pointed out by Hughes et al. 2003 [18].

The social force models are able to reproduce much of the characteristics of emergency evacuations, but the resultant human behavior is granular; which has been refuted. It is worth noting that social force models use force equations for every agent which provides these models the flexibility to introduce some amount of non-heterogeneity albeit not as advanced as constructing human behavior.

From the aforementioned descriptions, it can be concluded that, the approach that can account for the non-homogeneity of human behavior, the characteristics of evacuation under emergency situations while having the capability to construct human behavior is the agent-based approach. However, this approach is computationally expensive and difficult to model which makes these models non-ideal while developing new approaches.

2.2 Dosage

The incidence or severity of a toxic effect is a function of exposure concentration and time of exposure. This function of time and concentration is usually referred to as dosage. Due to an agent's movement during evacuation scenarios, it may be subject to a time and distance varying toxic plume, which deems it necessary to evaluate the exposure of the agent continuously. The monitoring of the exposure is crucial in order to be able to apply the effects of toxic exposure.

2.2.1 Modes of Toxic Exposure

The toxicant can enter the body through four routes,

1. Ingestion – Mouth
2. Inhalation – Mouth or Nose
3. Injection – Cuts in skin
4. Dermal Absorption – Skin Membrane

Injection and inhalational are usually the most effective methods for the delivery of toxicant to the blood stream. They both also usually result in the highest peak concentration of toxicant in the blood when compared with ingestion and absorption [25]. The most common mode of entry for gaseous toxicants is through inhalation.

2.2.2 Exposure

Haber's Law states that the incidence or severity of a toxic effect depends on the total exposure, times the duration of exposure (see equation (4)). This formula was developed by a chemist called Fritz Haber. This approach along with some constraints has become the basis upon which exposure limits are set [26] [27].

$$k = Ct \quad (4)$$

The aforementioned equation however does not describe all cases of injury from chemical agent exposure. For exposure to irritant gases, it would usually underestimate toxicity at short exposures and overestimate toxicity for long exposure.

In order to account for the experimental data which was not represented accurately by the Haber's law, the concept of toxic load, which is an independent variable in terms of which toxic injury can be expressed was proposed by W.F. ten Berge in 1986 [28]. It is a form of injury factor and a more generalized term than dose [29]. For oral doses, it is equal to the dose (n=1), but for an inhaled gas, toxic load is a function of concentration and time, usually of the form [30];

$$Toxic\ Load = C^n t \quad (5)$$

where, C - Concentration

t - Time

n - Constant

It was demonstrated by ten Berge et al. (1986) [28] that Haber's rule seems not to be generally obeyed for exposure to gases by analyzing previously published experimental data of tests conducted on animals. The purpose for the introduction of 'n', also known as the ‘Toxic Load Exponent’ was to be able to account for the experimental evidence for dose-responses based on experimental data. W. F. ten Berge et al. (1986) also states that there is no general rule concerning the value of ‘n’ and that it should always be determined empirically through data from acute inhalation toxicity experiments in which both the concentration and exposure periods are available. The author also proposed that for continuously evaluating the exposure of an agent in a time varying concentration environment the following formula can be used.

$$Toxic\ Load = \int [C(t)]^n dt \tag{6}$$

This toxic load model is usually referred to as the ten Berge generalization of Haber’s law. This toxic load model however does not address the effect of detoxification done by the human body, which is more apparent when the toxic load is fluctuating or is zero in between high concentration exposures. Ride and Yee tried to address these problems by introducing new terms in their toxic load models [31] [32].

However, for time varying concentrations, only the applicability of the ten Berge model has been tested experimentally by Sweeney et al. [33], where the model showed good agreement with six out of the eight concentration profiles tested.

Boris et al. [34] proposed an algorithm to calculate toxic load for AEGL levels of gases from provided concentration-time points, using the model proposed by ten Berge et al. (1986) as a basis.

$$TL(t) = \int_0^t TL_{rate}(t')dt' \qquad (7)$$

$$where, TL_{rate}(t) \equiv \frac{dTL}{dt} = \frac{1}{t_b}[\frac{C(t)}{C_{t_b}}]^n \qquad (8)$$

where, $\boldsymbol{t_b}$ - Time corresponding to the upper limit of the band

$\boldsymbol{C_{t_b}}$ - Concentration corresponding to the upper limit of the band

$\boldsymbol{C(t)}$ – Instantaneous concentration

The algorithm uses pre-defined points of concentration and time to create a power function between those points. This power function is then used to calculate the Toxic Load rate for the requested exposure. This rate is then summed for the total period of exposure to obtain the Toxic Load. The algorithm returns values starting from 0 with 1 representing the onset condition.

The authors themselves point out a limitation of using this approach. Using the interpolations, the function sets the limits at the lower end and the higher end. These limits are based on a user defined time for the edges. For example, if the lower edge for one of the band was to be set at 30 seconds, and the extrapolated concentration corresponding to this time were to be 500 ppm. If the agent was to be subjected to a concentration of more than 500 ppm for 10 seconds, the function would for the exposure time provide a toxic load based on the maximum toxic load rate, which is 1/30 seconds, however an instantaneous exposure to 500 ppm will have delirious effects whether it is encountered at the beginning, middle or the end of the exposure, which will not be represented in the output.

2.3 Emergency Response

Emergency response to the consequences arising from toxic releases requires the assessment of strategies to be implemented in such scenarios. The two strategies available are either to evacuate the facility or shelter in place. To evaluate the applicability of each strategy usually the concentration or dose the people will be subjected to in each scenario is compared to some standard criteria. The concentration and dose criteria used for these evaluations are as discussed below.

ERPG is a set of exposure limits developed by the Emergency Response Planning Committee of the American Industrial Hygiene Association. They are based on animal toxicological data, human experience and existing exposure guidelines. ERPG concentrations are divided into three tiers as shown in Table 1 [35].

Table 1 - ERPG tiers and their physical interpretations

ERPG Tier	**Interpretation**
ERPG 1	The maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing more than mild, transient adverse health effects or without perceiving a clearly defined objectionable odor.
ERPG 2	The maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms which could impair an individual's ability to take protective action.
ERPG 3	The maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.

Acute Exposure Guideline Levels (AEGL) are a set of time and concentration values published by EPA (Environmental Protection Agency of the U.S.A.) that describe human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals [36].

AEGL consists of three levels and is provided for five time intervals – 10 minutes, 30 minutes, 1 hour, 4 hours and 8 hours – for each level. The interpretation provided by EPA for each level is shown in the tables Table 2.

Table 2 – AEGL tiers and their physical interpretation

AEGL Level	**Interpretation**
AEGL - 1	General population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic non-sensory effects
AEGL - 2	General population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape
AEGL - 3	General population, including susceptible individuals, could experience life-threatening health effects or death

The key difference between ERPG and AEGL is that AEGL is defined for multiple time limits, and also includes effects on susceptible individuals in its analysis.

National Institute for Occupational Safety and Health (NIOSH) publishes the Immediately Dangerous to Life and Health (IDLH) concentration for various chemicals, which are interpreted as safe levels for a 15-minute exposure.

AEGL limits can be used in a toxic load model, as multiple concentration and time values are provided for a particular toxic effect. These points can be used to establish the toxic load exponent, much similar in the way that Boris et al. have demonstrated [34]. However, Hawkins et al. [37] note that these guidelines are protective in nature and their use for predictive modeling can predict consequences orders of magnitude higher than those when toxicological concepts are used, they demonstrate this for the case of chlorine exposures. The authors state that only multidisciplinary techniques that use mathematical, statistical and toxicological concepts can ensure that predictive modeling provides proper guidance.

Probit equations are dose-response relationship equations of the form

$$Y = a + b * \ln(C^n t) \quad (9)$$

where Y is the probit value, which indicates the percentage of population that will be subject to the consequence corresponding to the dose ($C^n t$), and 'a' 'b' and 'n' are constants provided by CCPS and other similar organizations on the basis of toxicological studies [38]. It must be noted that for most toxic agents probit constants are available only for fatalities and no other effects/symptoms due to the exposure.

HSE proposed two levels of impact called Specified Level of Toxicity Dangerous Toxic Load (SLOT DTL) and Significant Likelihood of Death (SLOD). SLOT DTL is defined as the dose that results in highly susceptible people being killed and a substantial portion of the exposed population requiring medical attention and severe distress to the remainder exposed. SLOD is defined as the dose to typically result in 50% fatality (LD_{50}) of an exposed population.

The SLOT DTL and SLOD approaches extrapolate toxicity data to determine a dangerous toxic load that gives a specific level of harm for a certain received dose [39].

During the assessment of the consequences associated with toxic releases on the population, the aforementioned exposure levels are used as criterion for evaluating various mitigation and response strategies. However, it can be noted that for multi-level exposures like AEGL and ERPG, the effects of the exposures defined are very vague, which makes it hard to draw inferences about the specific effects that these exposure levels may have on the evacuation process.

2.4 Approaches for Simulating Evacuation in Toxic Environments

Fire Dynamics Simulator (FDS) and Evacuation (EVAC), commonly known as FDS+EVAC is a simulation module for FDS developed and maintained by VTT Technical Research Centre of Finland [40]. The evacuation model is an agent-based model. The model in addition to reproducing various psychological behaviors during evacuation also evaluates the dose-based impact on the walking speed of every agent due to smoke inhalation. The dose for every agent is calculated using Fractional Effective Dosage (FED) method and if the FED of the agent goes above 1, the agent is considered incapacitated. An impact on the velocity of the agent is also applied, but this impact is applied to account for reduced visibility and not the toxic effects. The effect on the velocity is applied in accordance with the experimental tests conducted on humans.

Durak et al. [41] used an agent based model to simulate the evacuation of a city in the case of a chlorine spill. The program they created models the drivers in an urban area and aims to optimize the timing of traffic lights in order to evacuate the drivers with minimum casualties. The design intent is to simulate various emergency scenarios ahead of time, so that corresponding traffic light timings can be planned.

The exposure of a driver to chlorine is based on the ingress of chlorine inside the vehicle assuming the air exchange rate of 7/hour inside the car. The ingress concentration is used to estimate the driver’s exposure, which is coupled with 'susceptibility' in order to obtain the exposure. Susceptibility is a defined property of an agent determining how prone the driver is to reaching an AEGL level. The model defines this property by randomly assigning each driver a number between 0.1 and 0.9 in a truncated normal distribution with mean 0.5 and standard deviation 0.2. For applying toxic effects, the model uses AEGL limits, and is programmed in such a way that AEGL-1 is the level at which 50% of people can detect the gas, AEGL-2 is the level at which 50% of people are affected by the gas and in some way disabled, and AEGL-3 is the point at which the gas is fatal to 50% of people.

The exposure model is used to affect driver behavior, with different consequences for AEGL-1, AEGL-2, and AEGL-3. At AEGL-1—detection—drivers become aware of the gas. They are more likely to turn on their radios and to learn more quickly about the instructions to evacuate. Drivers who reach AEGL-2 will stop their vehicles but they will continue to be exposed to gas in their stopped positions and their vehicles can block traffic. At AEGL-3, the person is considered a fatality.

Other features of the model include awareness; which is a factor causing a sense of urgency, capturing how stressed an individual is in response to a threat. This value is initially set to 0 and increases over time due to awareness, AEGL effects, and getting stuck in traffic.

Durak et al. in his methodology uses a dose based application for toxicity, he also couples this with distributed variables like susceptibility and awareness to induce the non-homogeneous response of human beings. However, the effects of symptoms that Durak et al. applies are very broad. He does not apply the specific symptom related effects of chlorine exposure. It must be noted that his study is based on a larger scale than that of a building evacuation and is applied to a highly specific activity like driving, which justifies his reasoning for applying the effects in such a way that only affects the driving capabilities.

Wan et al. [42] combined Gaussian Puff model (for toxic gas dispersion) with social force model (for evacuation) to simulate evacuation during a toxic gas release - terrorist event in a train station. Three areas called Lethal Area, Injured area and Flesh wound area, based on concentration and distance from the release source, were demarcated. The toxic effects were applied in the demarcated areas as follows; in the lethal area, the speed of the agent would be 0, in the injured area agent speed would be half its initial speed, in the flesh wound area the agent speed would be 90% of its initial speed and elsewhere it would be twice the initial speed due to nervousness. After running simulations for various scenarios, they made certain inferences about the case under consideration.

In this study two very important aspects of toxic exposure - time of exposure and the impact of specific symptoms associated with the exposure are not considered or only partially considered. The effects are applied in terms of decrease or increase in velocity; however, no scientific reasoning is provided for the suggested variations in speed.

Lovreglio et al. [43] highlight his methodology by simulating a case study of toxic gas release from a ship which gets dispersed to an area with people attending a concert, and their subsequent evacuation. Lovreglio uses a software called Pathfinder for evacuation simulations. The significant feature from Lovreglio et al's work is the calculation of each agent's dosage. Lovreglio et al. uses Haber's law as the basis ($Dose = C^n t$) for dose calculation. The authors in their methodology compares two approaches of calculating the dose and probability of mortality for the length of the evacuation firstly, using the static approach, in which a spatial analysis is performed and the mortality is calculated on the basis of final average total evacuation time secondly, a dynamic approach in which the dose is calculated through a curvilinear integral over the path of agent's evacuation. This is dose is then used in conjunction with probit relation to estimate the probability of his mortality. The static approach leads to a much higher amount of absorbed dose, and hence, higher probability of mortality when compared to the dynamic approach.

Lovreglio et al. use an approach to calculate the dynamic dose over the length of the evacuation; however, they do not calculate it during the evacuation to estimate and apply the effects of exposure, rather, they use post the evacuation simulation to estimate the probability of the agent's mortality if they were to evacuate through that path.

Liang et al. [44] showcase a methodology by simulating evacuation of people from a train station under a terrorist attack through a Sarin (Toxic Gas) release. The Gaussian dispersion model is used for the modelling of Sarin dispersion through the environment. For evacuation, an Agent-Based model is used where the behavior of every agent is modelled through a 'belief, desire, intention' paradigm. In order to account for the toxic effects, dosage is calculated using Toxic Concentration Time (TCt) and introducing a variable called 'Health Index' (H). H is the ratio of TCt to the Lethal Concentration Time (LCt) of Sarin. Based on the values of H obtained, the health of the agent is judged as follows: if H is between 0.5 and 0.8, the agent is seriously injured, if H is above 0.8 the agent is considered dead.

The authors use Haber's law for estimating the onset of an effect of toxic exposure, however, the authors only use this for applying the effect of mortality in the evacuation scenario. Also, the use of Haber's law is justified by experimental data for the toxic agent of choice – Sarin, which is not the case for other toxic agents.

2.5 Hydrogen Sulfide

The toxic agent of choice for this study is hydrogen sulfide as the hazards posed by its exposure are of prominent interest to the oil and gas industries**.** In addition to the oil and gas industry, hazards associated with the exposure to hydrogen sulfide are also relevant to pulp and paper industry, construction industry, sewage treatment plants and mining industry.

Hydrogen sulfide (H_2S) is a colorless gas with a distinctive odor. When found in atmosphere, it mostly has natural origins and is found near sulfur springs, lakes, and in air around geothermally active areas. The source of interest for this project and in chemical industries are mostly natural gas deposits, which can contain up to 42 percent hydrogen sulfide [45].

Hydrogen sulfide is classified as an irritant and a chemical asphyxiant. The gas' mode of exposure is through inhalation, from where it is absorbed in the blood stream through the lungs. Since the gas is heavier than air, it is rapidly absorbed by the lungs [46]. Odor of hydrogen sulfide is usually masked by the presence of propane or butane [30].

According to the toxicological review of hydrogen sulfide, submitted as a part of the IRIS report which is published by EPA, the exposure relationship for acute effects, particularly the ones related to the central nervous system and respiratory system can be very steep. There is also some data suggesting that children and neonates can be more susceptible to the neurological effects of H_2S [47].

According to air quality guidelines issued by WHO [45], major symptoms associated with hydrogen sulfide exposure are detailed as follows. At concentrations of 11 ppm and above conjunctival irritation occurs, due sulfide and hydrogen sulfide anions being strong bases. Serious eye damage occurs at a concentration of 50 ppm or higher. Above 150 ppm, hydrogen sulfide has a paralyzing effect on the olfactory perception so that the odor can no longer be recognized as a warning signal. At even higher concentrations, respiratory irritation is the predominant symptom, and at a concentration of around 287 ppm there is a risk of pulmonary edema. At very high concentrations there is strong stimulation of the central nervous system (CNS), with hyperpnoea leading to apnea, convulsions, unconsciousness, and death. At concentrations of over 1000 ppm there is immediate collapse. In fatal human intoxication cases, brain edema, degeneration and necrosis of the cerebral cortex and the basal ganglia have been observed.

T.L. Guidotti [48] has extensively studied the toxicology of hydrogen sulfide. The major inference from his studies is that the exposure-response curve for lethality is extremely steep for hydrogen sulfide, as can be seen from **Figure 1**, which implies that for hydrogen sulfide exposures, the concentration of exposure is a bigger factor than the duration of exposure. Guidotti (2010) [48] also claims that current models for risk assessment use the Toxic Load Exponent (TLE – ‘n’) value in a range between 1.36 and 4.36 but “empirical evidence strongly favors higher exponents”.

According to Guidotti [49], the major symptoms associated with hydrogen sulfide exposure and their corresponding concentrations are shown in Table 3.

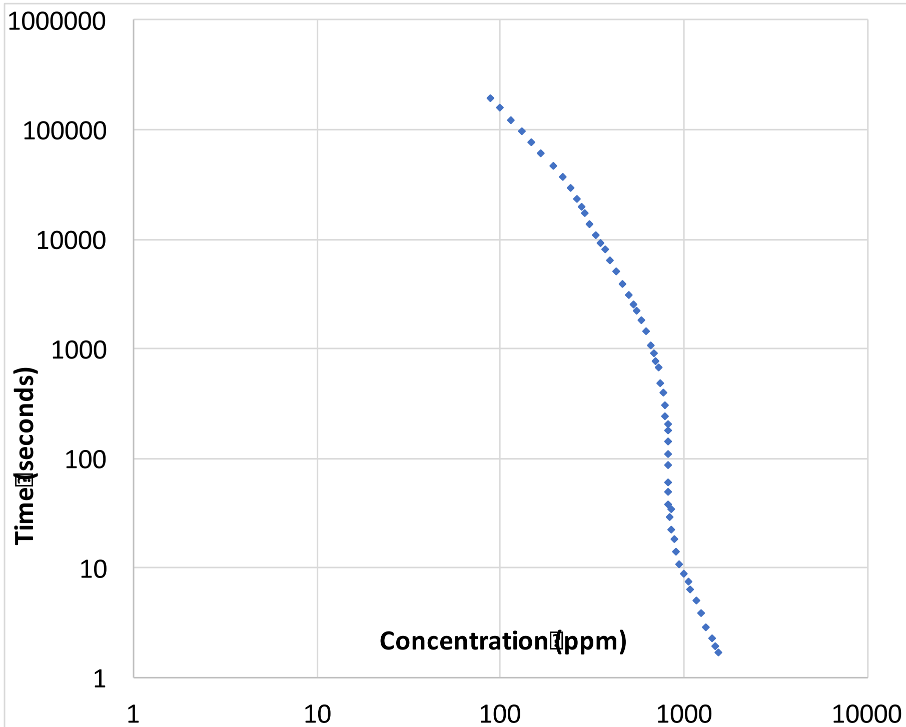

Figure 1 - Lethality Exposure-Response Curve for Hydrogen Sulfide adapted from [49]

Table 3 - Major Symptoms Associated with Hydrogen Sulfide Exposure adapted from [48]

Symptom	**Concentration (ppm)**
Odor Threshold	0.01 – 3
Eye and Lung Irritation	20 – 100
Olfactory Paralysis	100
Severe Eye and Lung Irritation	150 – 200
Pulmonary Edema	250 – 500
Knockdown	500
Breathing stops in one or two breaths	1000

Various standard exposure limits and emergency response guidelines for hydrogen sulfide used in the industry are shown below in Figure 2 and Table 5.

Classification	10 min	30 min	1 h	4 h	8 h
AEGL-1 (Nondisabling)	0.75 ppm (1.05 mg/m^3)	0.60 ppm (0.84 mg/m^3)	0.51 ppm (0.71 mg/m^3)	0.36 ppm (0.50 mg/m^3)	0.33 ppm (0.46 mg/m^3)
AEGL-2 (Disabling)	41 ppm (59 mg/m^3)	32 ppm (45 mg/m^3)	27 ppm (39 mg/m^3)	20 ppm (28 mg/m^3)	17 ppm (24 mg/m^3)
AEGL-3 (Lethality)	76 ppm (106 mg/m^3)	59 ppm (85 mg/m^3)	50 ppm (71 mg/m^3)	37 ppm (52 mg/m^3)	31 ppm (44 mg/m^3)

Figure 2 - AEGL Values for Hydrogen Sulfide reprinted from [36]

Table 4 - Basis used for defining AEGL levels for hydrogen sulfide adapted from [36]

AEGL Level	**Basis**
AEGL - 1	Based on a study conducted on three humans who were subjected to 2 ppm, and complained of headaches
AEGL - 2	Based on perivascular edema in rats
AEGL - 3	Based on the highest concentration causing no mortality in the rat after a 1-h exposure

Table 5 - ERPG Tiers for Hydrogen Sulfide adapted from [35]

ERPG Tier	Concentration
ERPG 1	0.1
ERPG 2	30
ERPG 3	100

National Institute for Occupational Safety and Health (NIOSH) publishes the Immediately Dangerous to Life and Health (IDLH) concentration for various chemicals, which are interpreted as safe levels for a 15-minute exposure. For hydrogen sulfide, NIOSH published the IDLH to be 100 ppm.

The toxicological review of H_2S leads to more information about the specific symptoms that are associated with the exposure when compared to the standard response guidelines. However, it can be seen that for the symptoms provided, the time of exposure is very rarely mentioned, and if mentioned, it is mentioned in a very vague language like “prolonged” exposure or “short” exposure, the meaning of which can be subjective. A clear exposure-response relationship for any of the symptoms of hydrogen sulfide was not found.

2.5.1 Effect on Evacuation due to Symptoms of Hydrogen Sulfide

To be able to model the various effects of exposure to hydrogen sulfide, it is pivotal to understand and evaluate the physical and psychological impacts of the symptoms arising from this exposure. These effects can then be translated into evacuation related properties, like walking speed, and be successfully implemented to reflect the effect on evacuation.

During the course of this study, no studies conducted on humans or animals that try to establish a direct correlation between evacuation (or its constituent characteristics) and concentration of H_2S or any of the symptoms associated with H_2S were found. However, Bhambhani et al. [50–54] conducted a series of experiments, in which they subjected humans to a concentration of up to 15 ppm, while they were exercising. The aim of these studies was to study the physiological implications of such an exposure on humans. The subjects were monitored using the appropriate apparatus and the collected data – Oxygen Consumption, Carbon dioxide production, Heart Rate, Expired Ventilation and Respiratory Exchange Ratio, Power Output and Lactate levels – were published. The power output data produced during these experiments could potentially be used to establish an approximate effect on the velocity of an agent. However, the power output was only published in one paper [52] which constituted the study in which the subjects were subjected to a concentration of up to 5 ppm. In this concentration range, no negative impact of the power output was found, rather, the subjects exhibited a higher power output when subjected to a concentration of 0.5 and 2 ppm, but not by a significant margin. In other studies that Bhambhani [50,51,53,54] published, the subjects were subjected up to

15 ppm of hydrogen sulfide concentration but no data was published for the power output or any other variable that could have been tangibly translated into an effect on velocity.

Fiedler et al. [55] systematically subjected 74 healthy non-smoking adults to concentrations of 0.05, 0.5 and 5 ppm of hydrogen sulfide to test the sensory and cognitive effects of acute exposure to hydrogen sulfide. He concluded that, humans showed a high level of anxiety when subjected to 5 ppm, when compared to 0.05 ppm and 0.5 ppm.

In medicine, people suffering with Chronic Obstructive Pulmonary Diseases (COPD) are subjected to standard 6-minute walking tests (6MWT). COPD is an umbrella term for diseases such as emphysema, chronic bronchitis, refractory asthma, and some forms of bronchiectasis. The aim of these tests is to test the pulmonary capabilities of patients. The test is standardized and is administered with a set of standard instructions.

Annegarn et al. [56] subjected 79 COPD patients and 24 healthy elderly subjects to a 6MWT. The walking characteristics of the subject were monitored through an accelerometer attached to the trunk of the subjects. It was noticed that COPD patients showed an altered walking pattern during the 6MWT compared to healthy subjects and these differences in walking pattern partially explained the lower 6MWD (6-minute walking distance) in patients with COPD. However, they concluded that the extent to which the patients show an altered walking pattern remains unclear. From the results published, the patients suffering from COPD travelled 26.2% less than the healthy patients over 6 minutes.

A point of contention for these studies is whether the test should be conducted on treadmills or in corridors. It has been noticed that people usually perform better in corridors they are familiar with. Stevens in 1999 [57] conducted this test on 21 subjects, male and female, split 3:4 on treadmill and in corridor. It was noticed that patients cover a significantly higher distance in corridors when compared to the distance covered on treadmills. Results from the three tests conducted in hallway and three tests conducted on treadmill were published. The average walking speed over 3 sets of tests conducted in corridor was 0.99 m/s. The average walking speed over 3 sets of tests conducted on treadmills was 0.8 m/s.

According to a study conducted on 11 patients (8 men, 3 women) by Pierre et al. [58], the author states that the tests conducted in corridor appear to be more effective and more efficient than the tests conducted on treadmills, making them a more suitable method to evaluate the exercise tolerance in patients suffering with COPD. The author hypotheses that this is due to the familiarity of the subject to the corridors.

Pulmonary edema is a condition in which excess fluid is built up in the lungs, which is collected in the air sacs. According to Akut et al. and Guidotti [46,48] pulmonary edema can be developed due to exposure to hydrogen sulfide immediately or up to 72 hours later. The symptoms of acute (sudden) pulmonary edema are [59]

1. Extreme shortness of breath or difficulty breathing (dyspnea) that worsens when lying down
2. A feeling of suffocating or drowning

3. Wheezing or gasping for breath

4. Anxiety, restlessness or a sense of apprehension

5. A cough that produces frothy sputum that may be tinged with blood

6. Chest pain if pulmonary edema is caused by heart disease

7. A rapid, irregular heartbeat (palpitations)

Mannan 2005 [30] notes that most of the deaths in case of chlorine exposures are diagnosed to be due to pulmonary edema, however T.L. Guidotti [48] notes that pulmonary edema is very rarely the cause of death in the case of hydrogen sulfide exposures, as at concentration high enough to onset pulmonary edema, usually death is caused due to the stimulation of the nervous system.

It can be seen that the symptoms associated with H_2S can have the potential of having a significant impact on the walking speed of the evacuee, however, in order to estimate the severity of the impact, links have to be drawn and inferences have to be made from the studies conducted for purposes other than evaluating the impact on evacuation capabilities while exhibiting these symptoms.

To summarize, it was found that there is a knowledge gap in accounting for the effects of toxic exposures while simulating evacuations. The guidelines used for decision making in evacuation scenarios do not provide specifics about the symptoms and specific inferences cannot be drawn about the effect on evacuation process from these. The toxicological data available for hydrogen sulfide details the symptoms associated with the exposure to hydrogen sulfide, however they do not provide a clear exposure response for those symptoms. The effects of the symptoms in terms of evacuation characteristics are non-existent, and links have to be drawn to studies conducted for other purposes to be able to make inferences about these effects.

3. MOTIVATION AND SCOPE OF WORK

While simulating of an evacuation under toxic conditions, it is crucial to be able to replicate typical human behavior exhibited during emergency evacuations, but in addition, a dynamic dose monitoring needs to be performed for every evacuee on the basis of which the effects of various physical and psychological symptoms associated with the exposure can be applied to each evacuee on the basis of his/her dosage. This would help analyze the effects of toxic exposures on the evacuation process.

In this work, the toxic load approach is used to indicate the level of toxic injury. The algorithm proposed by Boris at al. [34] is used to dynamically monitor the dose and modified to indicate the level of injury due to various symptoms associated with the exposure to hydrogen sulfide.

The physical effects of the symptoms associated with the exposure to hydrogen sulfide are translated into velocity deviations during evacuation with the help of various studies in the literature as a basis.

The social force model is used to represent the human behavior during evacuations. The effects due to the toxic exposure are applied by adding a dynamic dose-dependent force term which applies the effects corresponding to each evacuee by modifying its desired velocity.

4. METHODOLOGY

The aim of this project is to implement dose-based effects of toxic exposure on the evacuation process. In order to do so, firstly, the symptoms associated to the exposure and their exposure response were evaluated. In order to have a dosage-based implementation of the effects, a method to perform the dynamic monitoring of the dose was selected. The dose monitoring method was modified to indicate the onset of each symptom. The effects of these symptoms on the evacuation process were analyzed. These effects were then applied by making modifications to the exiting social force based evacuation model.

In order to test and observe the outcome of this methodology, a program in MATLAB was created for a single agent evacuation in one direction. After testing, this methodology was implemented into an evacuation simulation tool where it could be used to simulate representative evacuation scenarios with multiple agents in a ‘realistic’ geometry.

4.1 Toxicant, Symptoms, Toxic Load and Physical Effects

4.1.1 Symptoms and their Exposure-Response

The exposure-response relation for lethality in humans was published by Guidotti [49] as shown in Figure 1. The three levels of AEGL and their corresponding trend lines were plotted together with the exposure response for lethality provided by Guidotti [49] as shown in **Error! Reference source not found.**. It can be seen from **Error! Reference source not found.** that the exposure-response curves for the AEGL limits and the curve provided by Guidotti are of the same characteristic however, a massive difference in the concentrations was seen between the lethality curve and the AEGL-3 curve. Based on this inference, an assumption was made that the exposure-response relation is of the same characteristic for all symptoms associated with H_2S exposure.

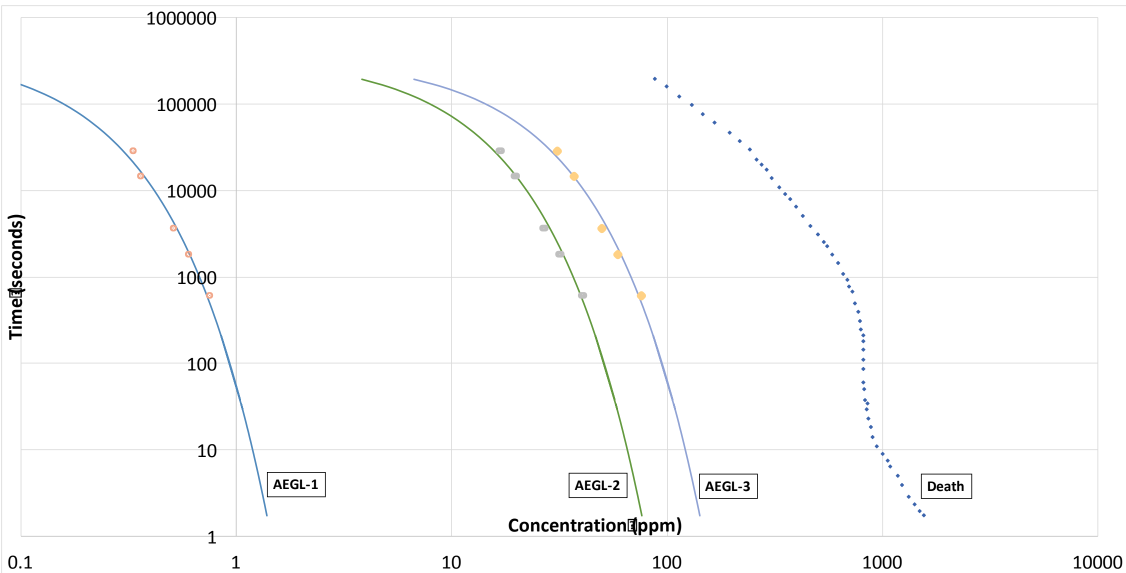

Figure 3 - AEGL limits and trend lines plotted with the exposure-response provided by Guidotti 1996 for lethality

The exposure-response curves for any of the symptoms associated with the exposure to hydrogen sulfide are not available in literature and hence it was decided to obtain the exposure-response curves for the different symptoms. This was done by using the assumption made earlier about the characteristic shape of the exposure-response curves of hydrogen sulfide exposure. Values for symptoms available in literature and those provided by public organizations, which provided a time value or some indication of time with exposure concentration were used to interpolate the data points for the symptoms' exposure-response relationships. The exact language and concentration from sources are shown in Table 6.

Table 6 – Concentration-time data for symptoms and their respective sources

Symptoms	**Concentration (Source)**
Odor becomes more offensive at 3-5 ppm	3-5 ppm (OSHA) [60]
Slight conjunctivitis ("gas eye") and respiratory tract irritation after 1 hour Throat irritation after 1 hour	50-100 ppm (OSHA) [60]
Pulmonary edema may occur especially from prolonged exposure	250-500 ppm (Guidotti 2010) [48]
Knockdown	500 ppm (Guidotti 2010) [48]

The characteristic exposure-response curve in the range of 10 seconds to 1000 seconds (~ 17 minutes) is almost a straight line. This had to be kept in mind while setting the limits of symptoms as most of the indoor evacuation scenarios will be in this time region. Keeping the aforementioned factors and the conclusion from the study by Fiedler et al.

[55] that humans show a higher level of anxiety when subjected to 5 ppm of H_2S, the point to scale down the curve for smell was taken to be 5 ppm at 10 seconds.

Considering the description that OSHA provides for eye, lung and throat irritation, and the concentration that Guidotti [48] provides for severe eye and lung irritation (150-200 ppm), the point for shifting the curve was considered to be 100 ppm for 45 minutes, as this also resulted in the 10 seconds to 1000 seconds region yielding the concentration values between approximately 150 and 180 ppm.

Since pulmonary edema could occur anywhere between 72 hours and immediately, and the definition of prolonged was not provided, it was decided to assume the highest value provided as a point of almost immediate onset of pulmonary edema. The interpolation points used in order to obtain the curves are shown in Table 7.

Table 7 - Interpolations used to scale down the lethality curve for symptoms

Smell	5 ppm for 10 seconds
Eyes & Lung Irritation	100 ppm for 45 minutes
Pulmonary Edema	500 ppm for 10 seconds

The curves obtained for various symptoms using the values in Table 7 are shown in Figure 4.

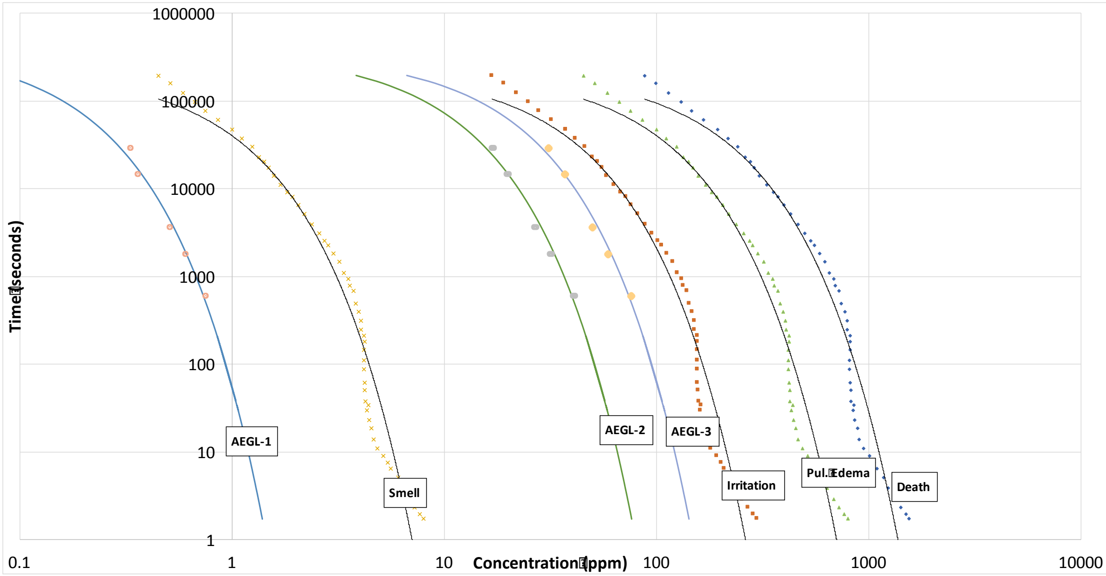

Figure 4 – Obtained Response Curves for Different Symptoms along with AEGL Curves for the 3 bands

From this figure, a very significant difference can be seen in the concentration levels of AEGL response curves and the symptoms' response curves. Both AEGL-2 and AEGL-3 level curves fall behind the irritation and pulmonary edema curves. The AEGL-3 curve is closer to the irritation curve, while the pulmonary edema curve is closer to the death curve. For the sake of this study, it was decided to continue with the obtained symptoms' exposure-response curves rather than the AEGL response curves due to the presence of the studies that link walking speed to the effects of these symptoms. It must be noted here that this is strictly an assumption, which was made due to lack of clear data and the results obtained by the use of this data are strictly for the purpose of demonstrating the methodology and in no circumstances are to be taken as representative of real scenarios. This methodology can be applied in a similar way for any exposure-response curve.

4.1.2 Toxic Load Algorithm and Modifications

The toxic load algorithm published by Boris et al. [34] calculates the rate at which a toxic injury is being approached – called the loading rate – at discrete time steps for the exposure-response provided. It then sums up these loading rates over the period of exposure to give the final toxic load which indicates the level of toxic injury. The algorithm has the ability to perform this calculation for different exposure-responses provided. Every exposure-response provided is called a band, and the output of the algorithm is discrete toxic load values for every 'band'. This gives the TL algorithm the ability to estimate level of toxic injury of different exposure-responses. This ability of the algorithm was used to calculate the level of injury for different symptoms, by defining the following bands.

1. Band 1 – Smell Exposure-Response – will henceforth be referred to as symptom 1
2. Band 2 – Severe Eye and Lung Irritation Exposure-Response – will henceforth be referred to as symptom 2
3. Band 3 – Pulmonary Edema Exposure-Response – will henceforth be referred to as symptom 3

In its native form, the TL algorithm would output one value of toxic load for each band. The value of interest is the values between 0 & 1 as it would indicate how close to the onset of a particular symptom an agent is (Toxic Load 1 indicates the onset condition). A modification to the output of the algorithm was made for ease of implementation into the evacuation model. This modification entails that the algorithm would not record the value of toxic load above the onset condition, making the maximum output for every band as 1.

The toxic load algorithm performs the following loop at every time step for every band:

1. Establish the concentration at edge time value of 30 seconds and 24 hours as per the exposure-response relation provided;
2. If concentration is between the two edge values, calculate the loading rate for the time step;
3. If concentration is below the value at 24 hours' edge, the loading rate is zero;
4. If concentration is above the value at 30 seconds' edge, the loading rate is 0.033 per second, which is the maximum loading rate.

The maximum loading rate is the same for all bands, which in practical terms would mean that if a concentration more than the highest concentration of all bands was to be provided, it would take the same time to reach the onset of every band, and that all the symptoms would onset at the same time.

To address this issue, the final toxic load output is the addition of the three bands, which is based on the on the assumption that if more advanced symptoms are to be exhibited, the highest symptom would be onset at the highest time and lower symptom would be onset at lower times. The outputs of the modified toxic load algorithm are shown in Table 8.

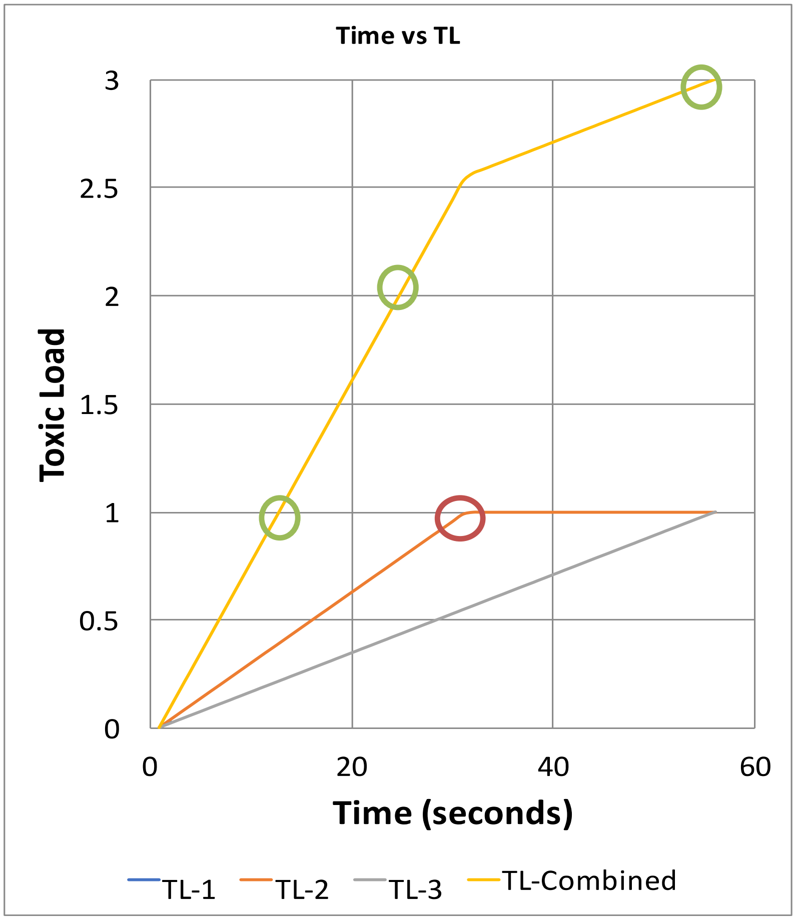

Figure 5 - Comparison of results of the combined TL approach and unmodified TL model

It can be seen from Figure 5 that when the concentration is high enough to onset the third symptom in 57 seconds, the first and second symptom would still be onset at 30 seconds, but for the modified algorithm with the combined TL, the first symptom would be onset at 12 seconds, the second symptom would be onset at 25 seconds, and the onset of the third symptom remains unchanged at 57 seconds.

Table 8 - Outputs of the modified toxic load algorithm

Symptom	**Toxic Load**
Smell	$0 < TL \leq 1$
Severe Eye and Lung Irritation	$1 < TL \leq 2$
Pulmonary Edema	$2 < TL \leq 3$

4.1.3 Physical effects of the Symptoms

On the basis of studies by Bhambhani and Fiedler [50–55], that were highlighted previously, the inference was drawn that due to the combination of an increased anxiety and no negative effect on the capability to perform physical exercise due to exposure of at least up to 5 ppm of H_2S, the agent will move faster when subjected to the characteristic smell of H_2S. Based on this the maximum achievable speed of the agent for this symptom is assumed to be 2 m/s which is almost midway between normal walking speed (1.35 m/s) and jogging speeds (less than 2.68 m/s) for average humans.

What is classified as the severe eye and lung irritation symptom actually entails coughing, throat irritation, lung irritation and eye irritation. The non-eye related effects can be associated with some of the symptoms that patients suffering from Chronic Obstructive Pulmonary Disorders (COPD) exhibit. Using the walking speed data published by Stevens [57] for 6 Minute Walking Tests conducted on patients walking in corridors as a basis, the maximum achievable walking speed of the agent exhibiting this symptom is assumed to be 1 m/s.

Due to the absence of walking speed or related data for patients suffering from pulmonary edema, noticing that the symptoms associated with pulmonary edema are quite severe when compared to other symptoms, and taking into account the observations made by Mannan 2005 and T. L. Guidotti [30,48], it was assumed that the onset of pulmonary edema would incapacitate the agent, making his velocity zero.

The velocity of the agent defined for every symptom are called symptom speed (v^{00}), and are summarized in Table 9 with respect to toxic load outputs.

Table 9 - Symptom speeds for respective TLs

Toxic Load	**Symptom Speed (v^{00})**
$TL = 1$	2 m/s
$TL = 2$	1 m/s
$TL = 3$	0 m/s

When evaluating the applicability of toxic loads on a population, their effects are usually applied on to the populace on the basis of toxic-load-response relationships. These relationships provide the percentage of the population that will be affected by the particular effect as a function of toxic load. This is done to enforce the fact that different members of the population will respond to the effects at different points, some before the onset and some after the onset condition, but the majority would experience the symptom very close to the onset condition. Due to the lack of toxic load-response data for the symptoms that the modified toxic load represents, and to accommodate this phenomenon, it was decided to start applying the symptoms at the beginning of the bands instead of the onset condition for each symptom in a continuous manner such that with the increased load, the severity of the symptoms will increase and the maximum effect of the symptom will be applied at the onset condition.

On the basis of these symptom speeds, continuous functions with respect to toxic load were developed and are shown in Figure 6.

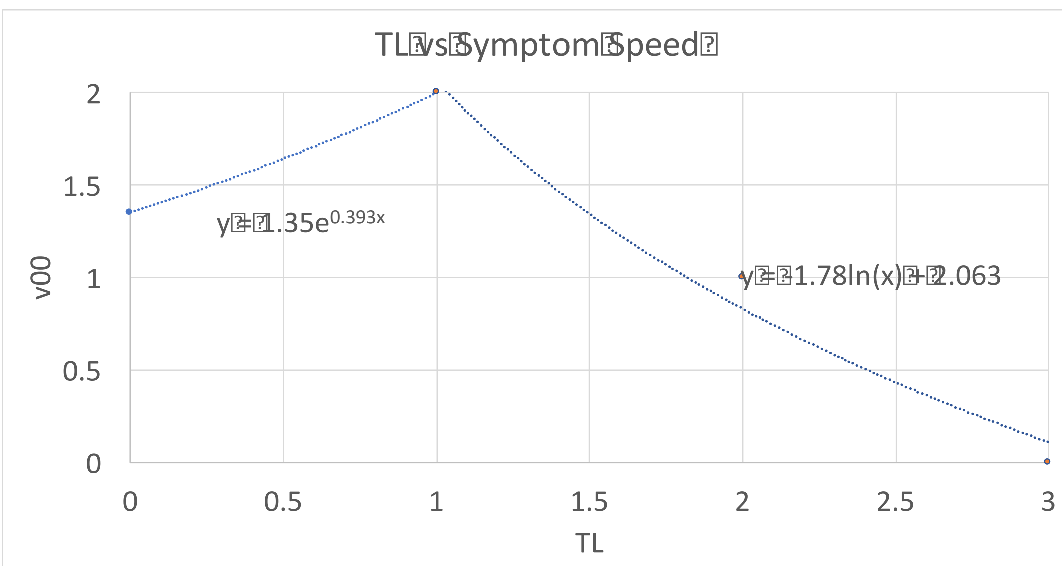

Figure 6 - Trendlines for v^{00} and TL function

The obtained continuous functions and their applicability is shown in Table 10.

Table 10 – Symptom speed functions for different Toxic Loads

Toxic Load	Symptom Speed (v^{00})
$TL = 0$	Unimpeded Desired Velocity
$0 < TL \leq 1$	$v^{00} = 1.35(e^{0.393*TL})$
$1 < TL \leq 2$	$v^{00} = -1.78 * \ln(TL) + 2.063$
$2 < TL < 3$	$v^{00} = -1.78 * \ln(TL) + 2.063$
$TL = 3$	0 m/s

These symptom speed equations as a function of toxic load mark the translation of the physical effects of the exposure to a property that is directly related to the process of evacuation.

4.2 Modifications to the Social Force Model

In order to implement the physical effects of the symptoms, a modification to the equation governing the evacuation itself had to be made. This was done by defining a new force term which would accommodate the effects of the symptoms.

The force term is defined in such a way that instead of subjectively pushing the agent toward the symptom speed, it would enforce the symptom speed as the property of the agent. The agent would not be able to achieve a speed higher than the symptom speed, but still be able to go slower depending on his environment, for example when he is in the crowd or faces a wall.

The force term does not interfere with the agent-agent interaction term and the agent-wall interaction term which helps in retaining their ability to reproduce evacuation related properties.

The new force term called 'toxic force' is added to the overall force equation and defined analogous to the motivational force. In toxic force, the velocity of the agent is replaced by the symptom speed, which is a function of the TL, and the desired velocity is multiplied by the vector pointing opposite to the desired direction vector. The representative functioning of the toxic force term is shown in Table 11

.

$$\boldsymbol{m_i}\frac{\boldsymbol{dv_i}}{\boldsymbol{dt}} = \boldsymbol{m_i}\frac{\boldsymbol{v_i^0(t)e_i^0(t) - v_i(t)}}{\boldsymbol{\tau_i}} + \sum_{j(\neq 1)} \boldsymbol{f_{ij}} + \sum_{W} \boldsymbol{f_{iw}} + \boldsymbol{f_t} \qquad (10)$$

$$\boldsymbol{f_t} = \boldsymbol{m_i}\frac{\boldsymbol{v_i^0(-e_i^0) - v^{00}(-e_i^0)}}{\boldsymbol{\tau_i}} \qquad \textbf{(11)}$$

Table 11 - Output of the force term for different TLs

Toxic Load	Symptom Speed (v^{00})	$f^{toxic} + f^{motiv}$
$TL = 0$	$v^{des} = v^{00}$	f^{motiv}
$0 < TL \leq 1$	$v^{00} = 1.35(e^{0.393*TL})$	$\boldsymbol{m_i \frac{-v^{00} e_i^0(t) - v_i(t)}{\tau_i}}$
$1 < TL \leq 2$	$v^{00} = -1.78 * \ln(TL) + 2.063$	$\boldsymbol{m_i \frac{-v^{00} e_i^0(t) - v_i(t)}{\tau_i}}$
$2 < TL < 3$	$v^{00} = -1.78 * \ln(TL) + 2.063$	$\boldsymbol{m_i \frac{-v^{00} e_i^0(t) - v_i(t)}{\tau_i}}$
$TL = 3$	0 m/s	0 N

As can be seen from the table above, the new toxic force term is able to modify the agent property of desired velocity as a function of the agent's dose. This marks the successful implementation of the dose based effects on the agent's evacuation.

4.3 MATLAB Implementation

In order to gain a better understanding of the modifications made to the social force model a small program was created in MATLAB. The program was designed for only one agent subjected to motivational force and toxic force moving in only one direction. This was done to visualize and inspect the effects of the newly introduced toxic force term.

The program consists of two parts, the calculation of Toxic Load and the solution of the second order differential equation. Initially the time limit, time step, characteristic relaxation time (tau), mass, desired velocity, initial velocity and the concentration as a function of coordinates had to be defined.

A loop is setup from the initial time up to the final time for every time step. The agent's TL, coordinates, velocity and force at every time step are calculated and everything except for his TL is stored for every time step. The final TL of the agent at the end of the loop is stored.

4.3.1 Toxic Load Calculation

A MATLAB function was created to define the concentration of the agent as function of distance. The concentration resulting from this function, the cumulative TL at the previous time step and time step is the input required for the calculation of TL. Once the TL is of the three bands is calculated, they are summed to obtain the TL of the agent. Based on the TL obtained, the symptom speed (v^{00}) of the agent is calculated.

4.3.2 Differential Equation Solution

For this methodology, finite difference approach was used to solve the second order ODE instead of using MATLAB's in-built ODE solvers. This was done due to the insight finite difference lends into the solution as in-built MATLAB solvers return the final solution, however solving the finite difference using a loop lends the ability to inspect the results at every time step for which the loop is set up.

Backward finite difference was used to solve the force equation due to the boundary conditions available. The two boundary conditions used for the solution were that the agent's distance at t=0 is zero, and that his velocity at t=0 is his initial velocity (0 m/s).

Using the finite difference equations and the boundary conditions the equation for x(t) obtained is as shown below.

$$x(t) = \left(\frac{\left(\left(x(t-1) * (2 * tau + h)\right) - \left(x(t-2) * tau\right) + \left((h^2) * v^0\right)\right) - \left((v^0 - v^{00}) * h^2\right)}{tau + h}\right) \tag{12}$$

Where,

x – Coordinate at respective time

h – Time step

t – Time

tau – Relaxation time

v^0 – Desired Velocity

v^{00} – Symptom Speed

using the newly obtained coordinates the velocity of the agent at time ‘t’ is calculated as

$$vel(t) = \frac{x(t) - x(t-1)}{h} \tag{13}$$

and using this velocity, the force the agent is experiencing at time ‘t’ is calculated as

$$force(t) = \frac{m(v^0 - vel(i))}{tau} - \frac{m(v^0 - v^{00})}{tau} \tag{14}$$

The values of the coordinates, velocity and force are stored for every time step and using the plotting tools available in MATLAB, the output of the program was defined to be a plot consisting of sublots of

1. Distance versus Time
2. Velocity versus Time
3. Total Force on Agent versus Time
4. Concentration versus Time

for the length of the solution.

Using this program, two test cases were created and studied in order to gain a better understanding of the methodology. The setup and results of these case studies are detailed in the next chapter.

It can be seen from the algorithm (Figure 7) that the test program calculates the toxic load of the agent at every time step based on the concentration that the agent is subjected to at that time step. The program then calculates the symptom speed for that time step which is then used in the force equation to obtain the new coordinates of the agent.

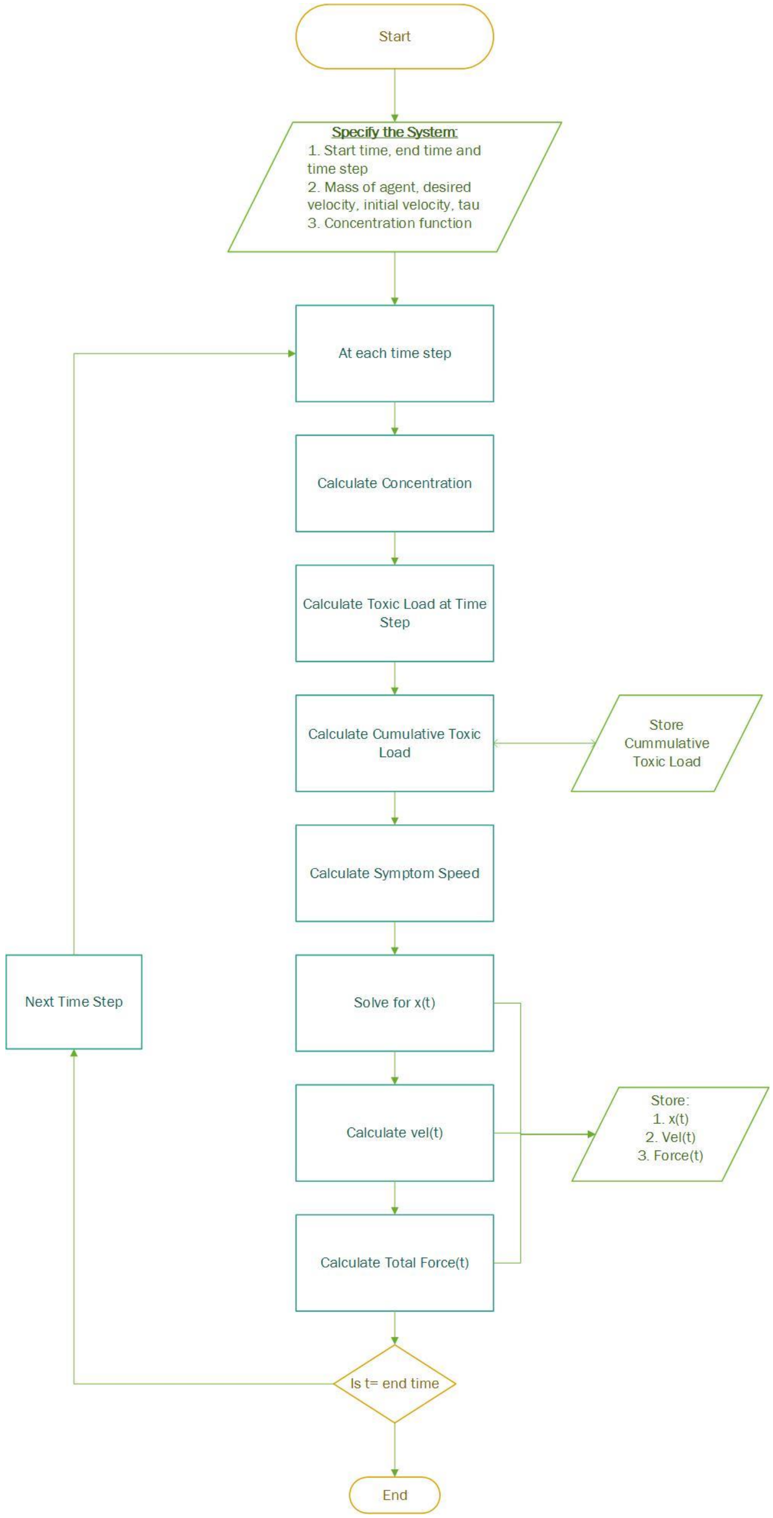

Figure 7 - Algorithm for the Test Case

4.4 Panic Simulator Implementation

Panic Simulator is a simulation tool created by Julian Schmidt and Alexander Spah using MATLAB, to simulate panic during evacuations. The tool is freely available at *(https://www.mathworks.com/matlabcentral/fileexchange/46849-panic-simulator)* and is free to use and/or modify.

4.4.1 Basis

The tool uses Helbing's social force model [13] as its basis. The model is implemented in its entirety into the simulator, which includes the use of three forces – the motivation force, the agent-agent interaction force and the agent-wall interaction force.

The simulator solves the differential equation for every agent simultaneously using MATLAB's in-built differential equation solver – ODE23. While solving the equation the model stores the time every agent exits the domain through the event record function of the ODE solvers.

The simulator also calculates the radial forces on the agents due to other agents and walls, which is then used to calculate the pressure applied on an agent (pressure divided by the surface area of agent) and is qualitatively displayed on the output simulation by changing of the color of the agent from green through yellow to red.

4.4.2 Features

Domain – The simulator allows the user to define a domain by specifying length and width of the simulation area. The domain is represented as a mesh of 1m*1m squares. The domain needs to have an exit which can be placed anywhere in the domain, however, multiple exits are not supported. The domain is also where all the walls and agent are defined.

Agents – Every agent is allotted with the following properties – x and y coordinate, velocity in x and y coordinate and a radius. The radius of the agent can be changed, and the x and y coordinates are defined with respect to where the agent is placed in the domain. These properties are used to solve the force equation for every agent at every time step, after which the output becomes the new agent property. This is reflected through a live visualization of the evacuation scenario. The user is free to place the agent anywhere within the domain.

Walls – Walls, unlike agents are non-dynamic entities and treated as barriers. The position of the wall is used for the calculation of the agent-wall force. Like agents, walls can be placed anywhere in the domain, there is no limits on their length, angle or position, however their width is fixed.

Columns are modelled and in principal treated as walls, their radii can be user-defined.

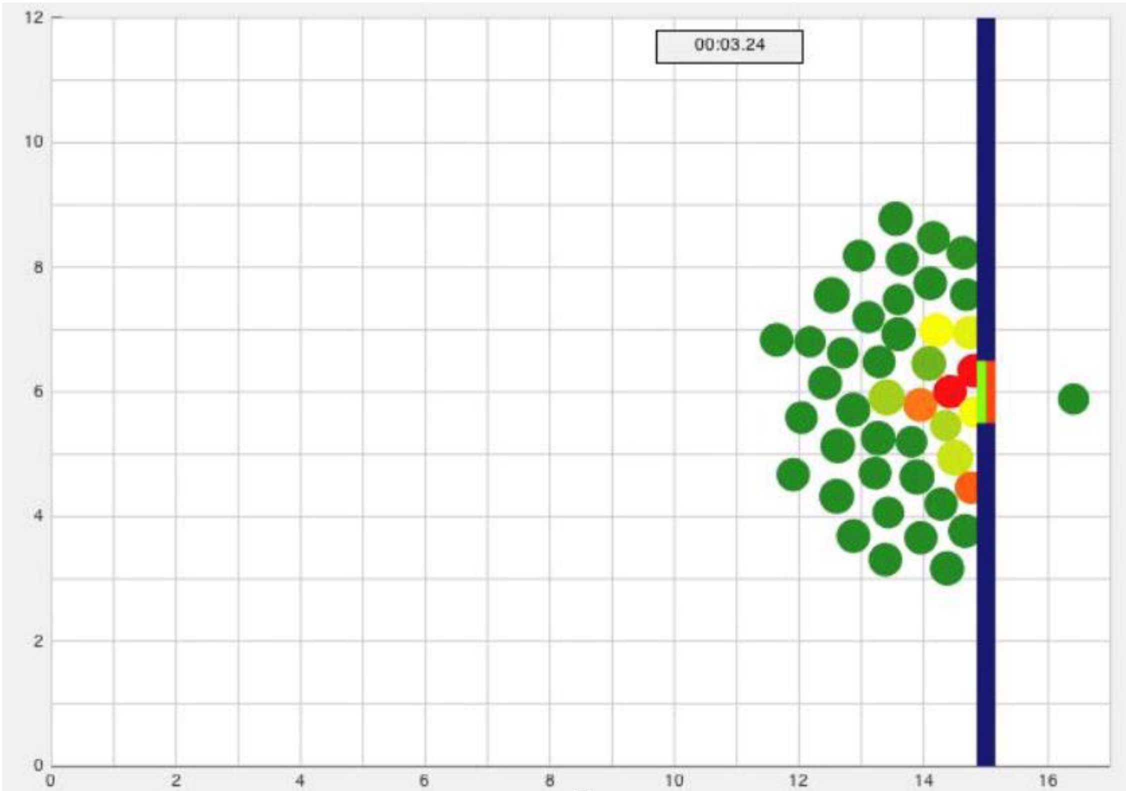

Figure 8 - A snapshot of the simulation being run in the Panic Simulator, the colors of the agents near to the door reflects the amount of pressure being exerted on them

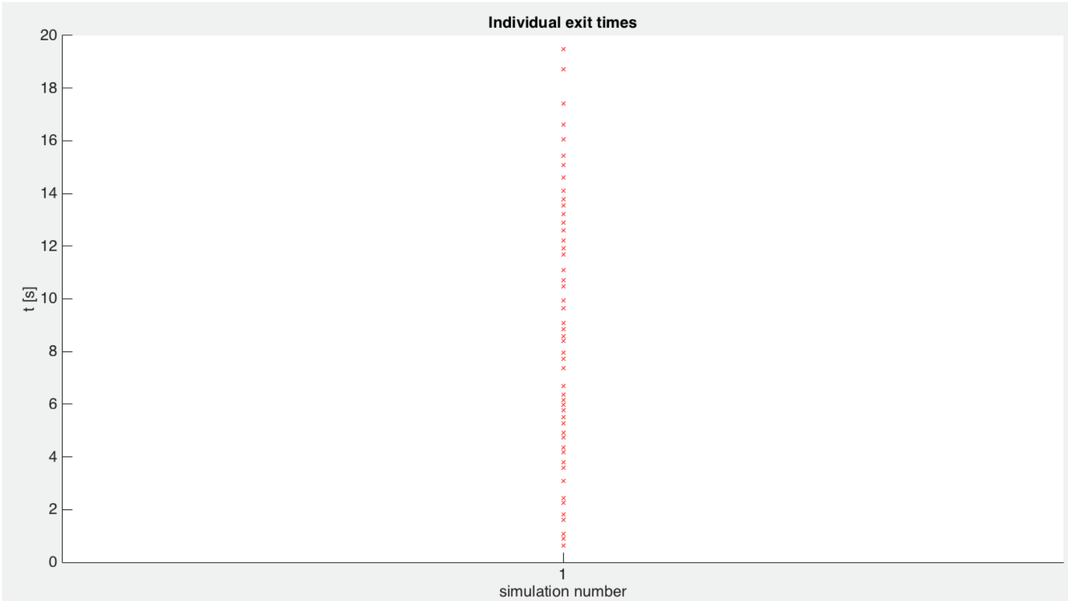

Figure 9 - A scatter of individual exit times obtained as a result of the simulation

Variables – Almost all the parameters of the evacuation can be user-defined. By default, all these parameters are kept at the values suggested by Helbing in his paper.

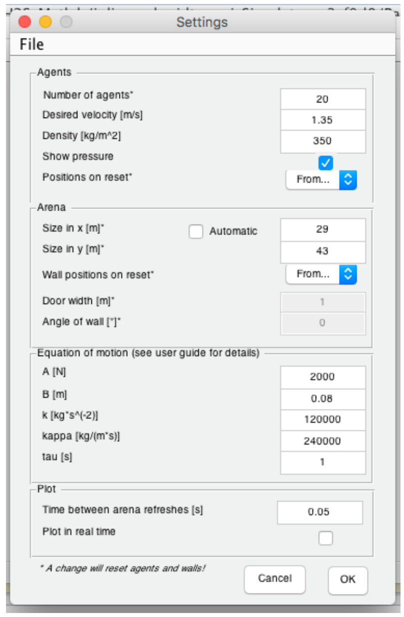

Figure 10 - Settings screen of PanicSim showing the variables that can be changed

Automate – The simulator has a statistical tool called the automate module, which allows for automatic changing of a variable and running multiple simulations. The inputs for the automate variable are the variable to change, the upper and lower limit of the variable, and number of averages to be taken at every value of variable. The module generates two plots as results, first, the graph of individual exit times at every run, and second the average evacuation time at every variable point considered.

Arena Editor – All the actions with regards to the placement of agents and walls can be carried out in the arena editor where, the agents, walls and columns can be placed in the domain at the user's discretion. The positions of the walls and the agents can be stored and can be loaded as either by default or when the user wishes to.

4.4.3 *Implementation of the methodology*

Concentration – As per the submission of this work, the implementation for only a constant concentration has been successfully completed. The concentration value is defined manually for the whole domain and applied throughout the length of the simulation. This concentration is used as an input for the TL calculation module.

Toxic Load – The three TL bands are defined for every agent as their property. This enables the simulator to calculate the TL and symptom velocity of every agent as per their exposure. The concentration is used as an input and the toxic load is calculated for every time step at which the ODE is solved.

Toxic Force – The toxic force is implemented in the panic simulator, in both x and y direction with the vector directions defined opposite to that of the motivational force. The toxic force is implemented in the function where all other components of the force equation are defined.

Automate – The automate module in the PanicSim was modified to include concentration as an automatable variable. The agent radius was modified in such a way that at the end of every run while in automate mode the radii of the agents would be re-allocated between a value of 0.24 and 0.29, in a normally distributed manner. The value of concentration can be varied from 0-1000 ppm. At the end of every run the automate module plots the evacuation time of every individual, and at the end of the sweep of all variable values, the average evacuation time at every value is plotted.

It can be seen from the algorithm (Figure 11) that there is a decision step for $t=t_{max}$, t_{max} was a new variable introduced to eliminate the simulation, as in its native form the simulation would terminate once all the agents left the domain, however, in case of agents becoming incapacitated the simulation to run indefinitely. To counter this, a new decision step was created after the ‘all agents exit’ decision step, due to which after a user defined time (t_{max}) the simulation would terminate irrespective of whether all agents have exited the domain or not. This time was set after observing the simulations in the high concentration regions, such that it would not end the simulation prematurely.

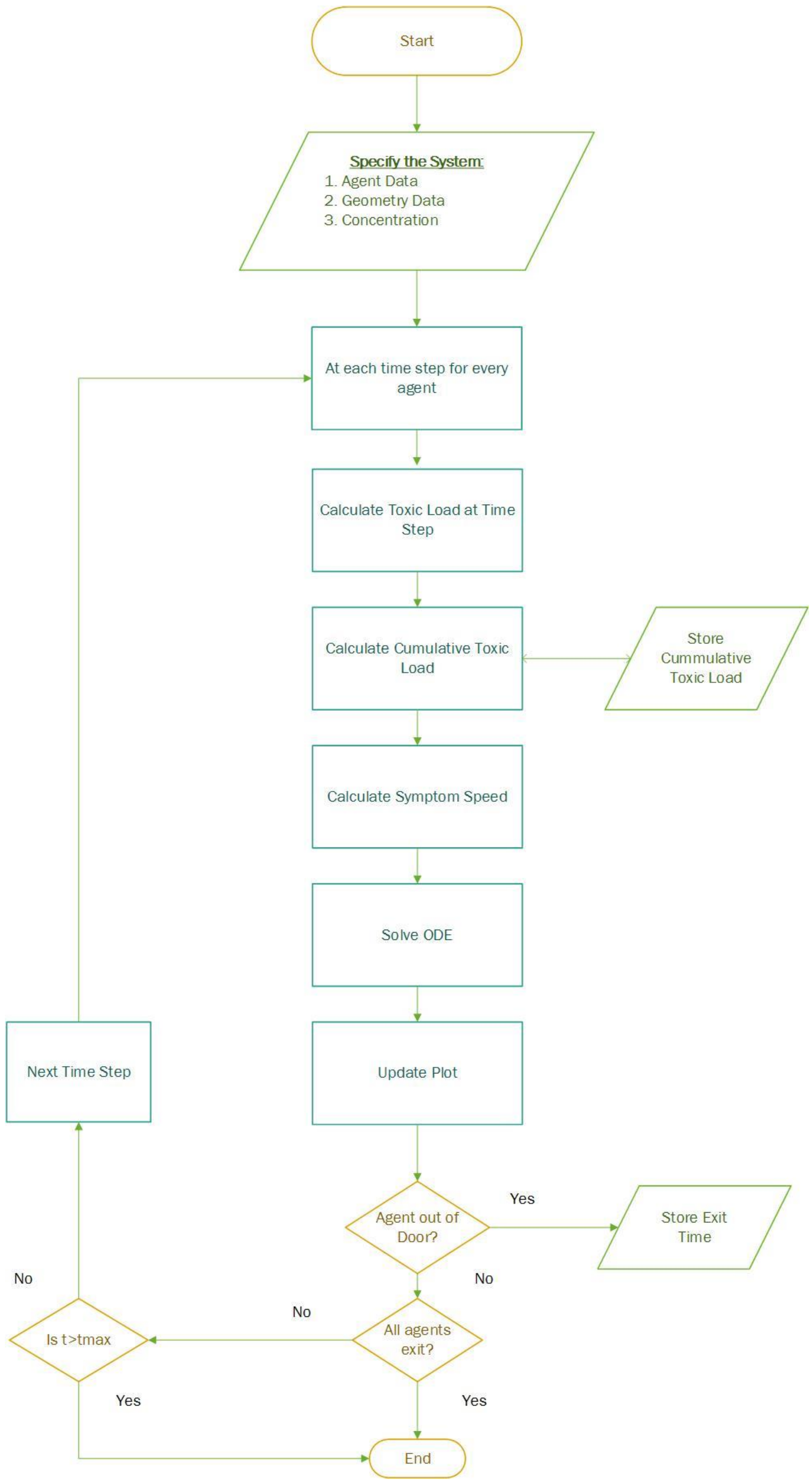

Figure 11 - Algorithm for Panic Simulator after Implementation

5. RESULTS AND DISCUSSION

In order to test and showcase the methodology detailed above, three case studies were conducted. The first two studies were conducted to test and visualize the methodology in its most basic form. The third study was conducted using the Panic Simulator tool to test the applicability of the methodology to realistic evacuation scenarios.

5.1 Case Study 1 – Fixed Time

The first case study created was to visualize the effects of the dose on the total force and velocity of the agent. Multiple runs were performed for the same time with different concentrations. The MATLAB program created for a single agent was used and the outputs at different concentrations are shown below.

The case was defined such that the agent has an unimpeded desired velocity of 1.35 m/s which he should obtain in 1 second (tau). The initial velocity of the agent is zero and the end time of the loop is 400 seconds.

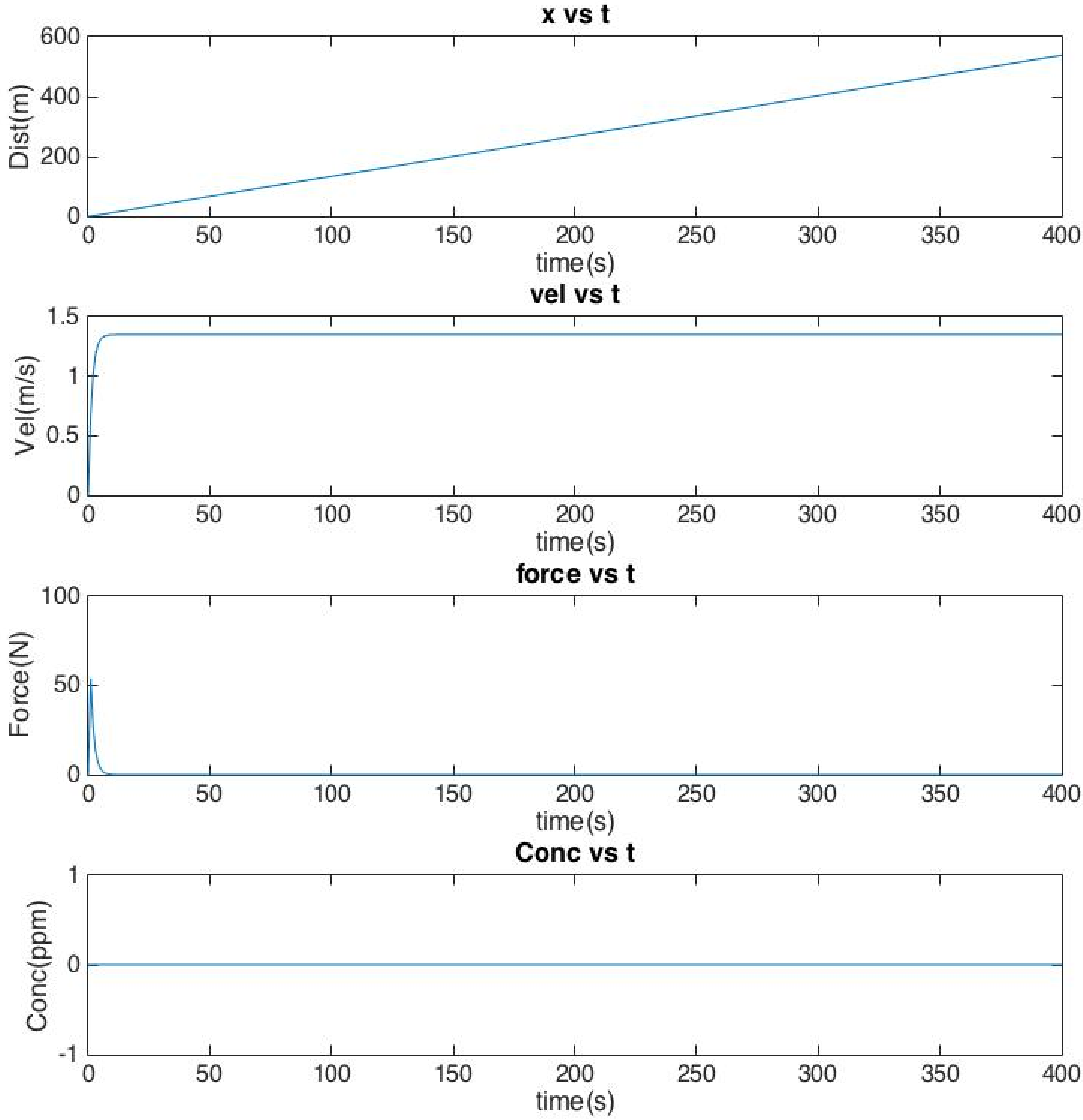

Figure 12 - The variation of velocity and total force during normal evacuation (0 ppm)

As can be seen from Figure 12, under normal conditions initially there is a massive spike in the total force value, which translates into a spike of velocity to the desired velocity of 1.35 m/s. The unimpeded desired velocity is achieved in one second, due to 'tau' being set as 1s. Once the agent achieves the desired velocity, the total force on the agent becomes zero. In this case, the response of the agent is only due to the motivational force.

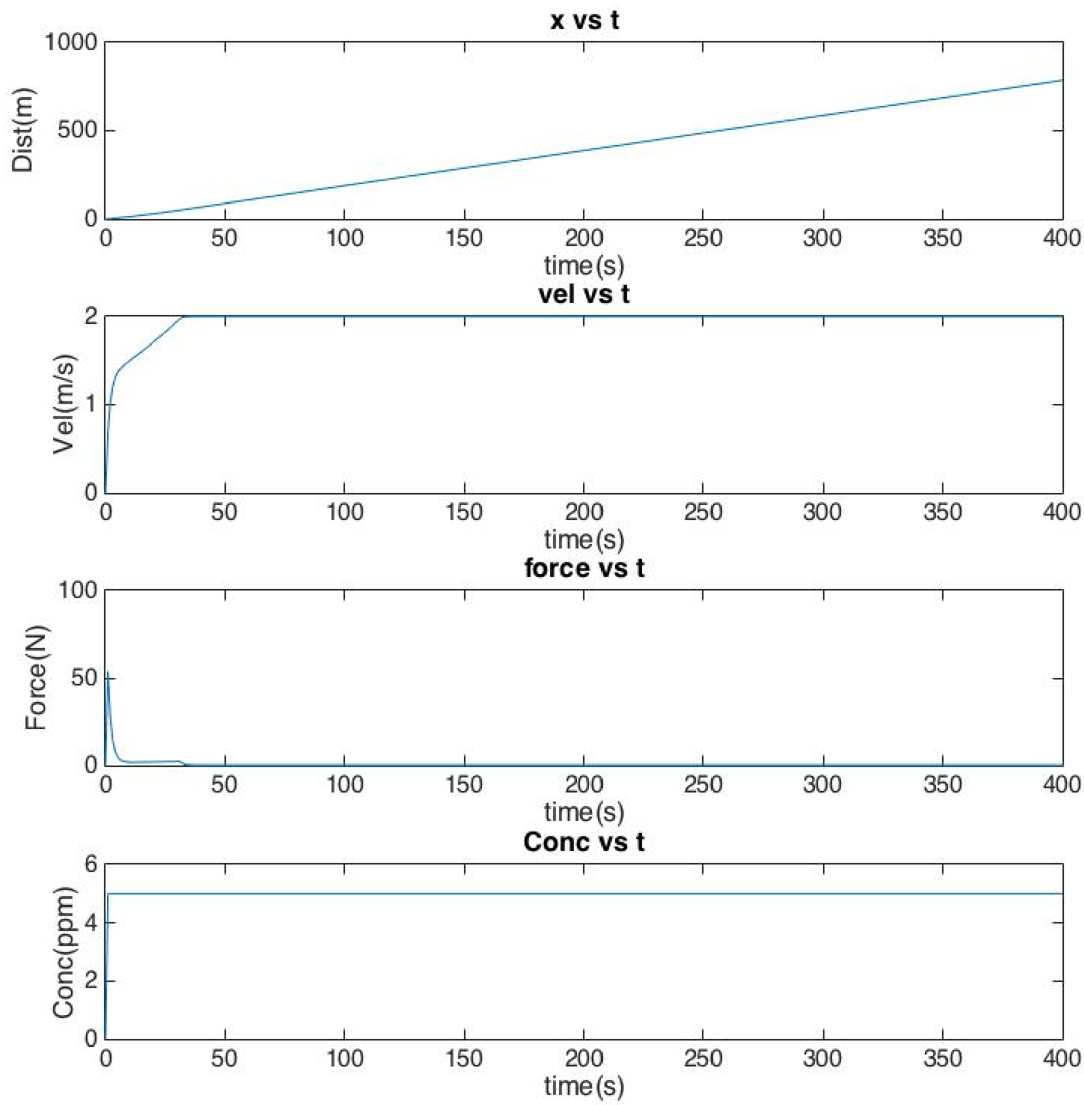

Figure 13 - The variation of velocity and total force when subjected to 5 ppm H_2S

Figure 13 shows the output for the case in which the agent is subjected to a concentration of 5 ppm for 400 seconds. It can be seen from the figure that initially the agent achieves the unimpeded desired velocity of 1.35 m/s, but due to the presence of H_2S, the agent's toxic load increases which results in his velocity moving towards 2m/s. Once the symptom speed of 2m/s is achieved, the force value becomes zero. It must be noted here that, the agent is subject to the H_2S concentration from the onset of the problem, however he does not begin to show the full effect of the symptom till almost 40 seconds, this is due to the dose-based application of the symptoms, highlighting the main difference between a concentration based and dose based application of the symptoms.

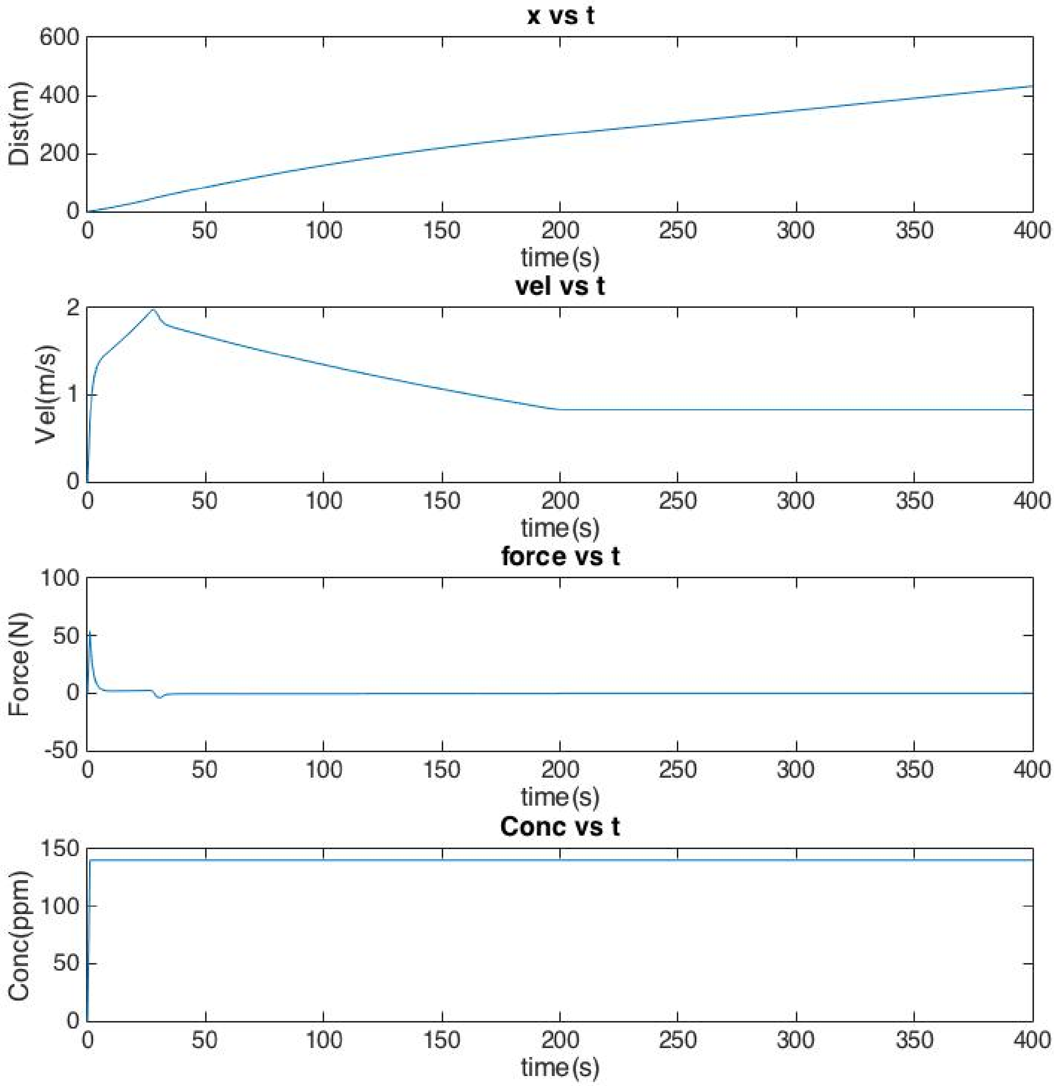

Figure 14 - The variation of velocity and total force when subjected to 140 ppm H2S

Figure 14 shows the output for the case in which the agent is subjected to a concentration of 140 ppm for 400 seconds. It can be observed from the figure above that at higher concentrations, initially the agent first achieves the unimpeded desired velocity of 1.35 m/s, and later due to the effects of symptom 1 the agent accelerates to 2 m/s similar to the previous case, but as his toxic load increases and reaches above a value of 1 due to continued exposure, the agent's speed starts tapering off towards the symptom speed at TL value of 2. The total force in this case is applied in the opposite direction at the onset of symptom 2 to decrease the agent's speed to the symptom speed. In this case, it could be seen that the agent still does not exhibit any effects of symptom 3. This case is also a representative of how a dose based application of effects of toxic exposures can vary from a concentration based application of effect as the agent is subjected to a constant concentration of 160 ppm from the onset of the problem, however he does not show the full effects of the major symptom associated with that concentration till 200 seconds.

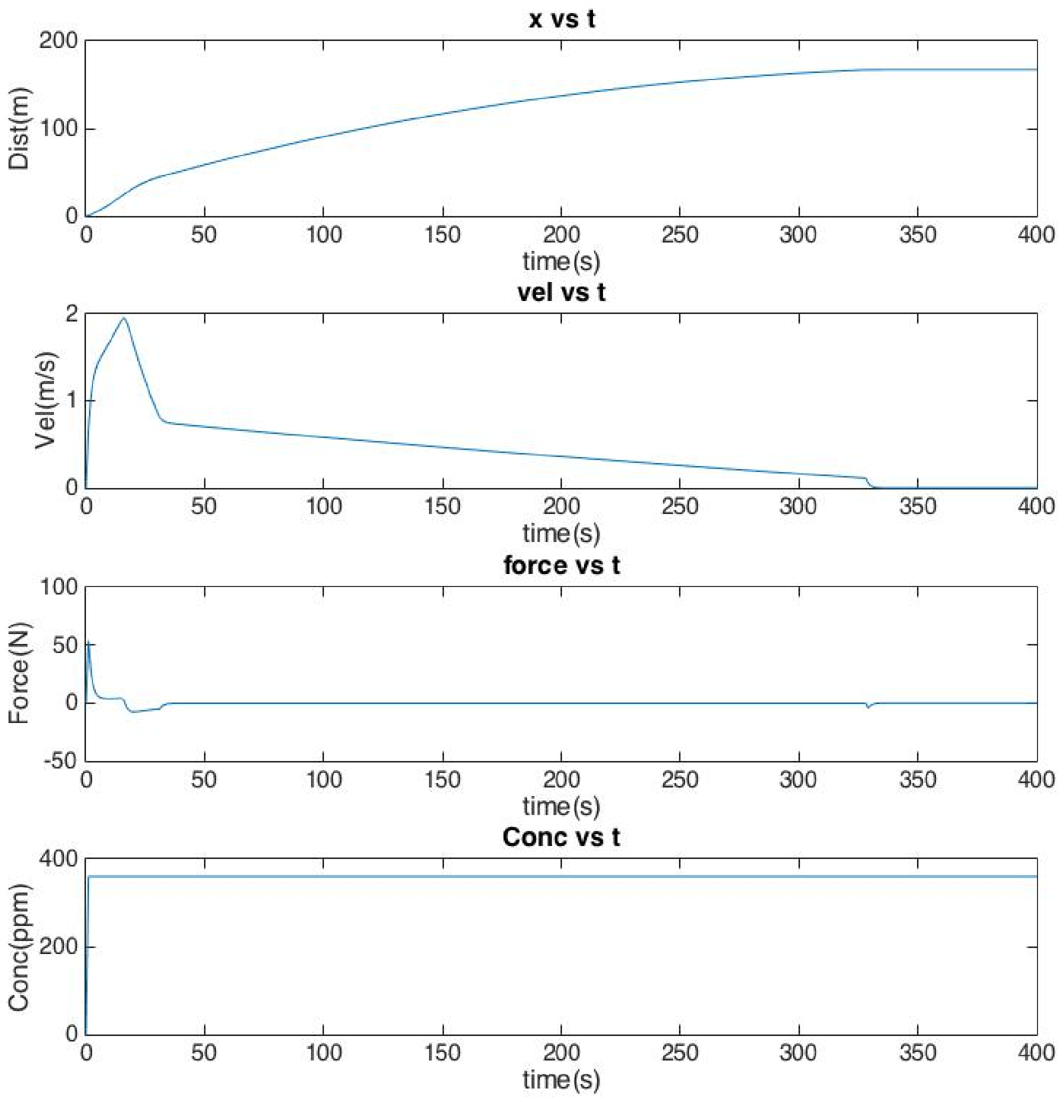

Figure 15 - The variation of velocity and total force when subjected to 360 ppm H2S

Figure 15 shows the output for the case in which the agent is subjected to a concentration of 360 ppm for 400 seconds. The case showcases the effects of all three symptoms on the agent. Initially it can be seen that the agent achieves the symptom speed of symptom 1 after which his velocity starts decreasing to below 1 m/s and then slowly drop off to near zero, at which point he reaches the toxic load of 3 and is incapacitated. It also illustrates the implications of the addition of the outcomes of the toxic load bands. The concentration that the agent is subjected to in this case is above the threshold concentration for both band 1 and band 2. If the resultant TL was not obtained by the addition of TL bands, the output would be that the agent would exhibit both symptom 1 and symptom 2 at 30 seconds, since the addition of TL bands is done, the agent's onset of symptom 1 occurs first and then the onset of symptom 2 followed by the effect of symptom 3. The addition of the TL bands to obtain the TL of the agent ensures that the onset of smaller symptoms at higher concentrations is sooner than the advanced symptoms when the concentration is beyond the threshold concentration for the smaller symptoms.

5.2 Case Study 2 – Fixed Distance

A second test case for the evacuation of a person from a long corridor was created. The scenario setup was such that the agent starts from a stationary position (initial velocity = 0 m/s) and has an unimpeded desired velocity of 1.35 m/s. The agent is to walk 400 m only in x-direction where the exit is located. The agent will be subjected to a concentration of hydrogen sulfide from 6 meters onward till the end of his path. This scenario was created to see visualize the real-world use of this methodology –the impact on the evacuation time due to the dose based effects on evacuation. The MATLAB program created was used to evaluate this scenario.

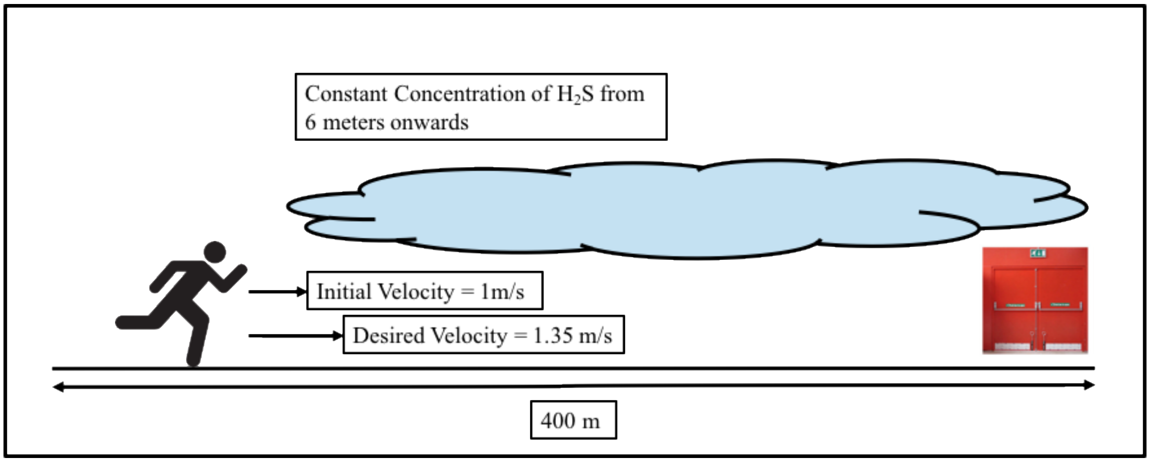

Figure 16 - Visualization of the Test Case

The results obtained when the agent is subjected to 5 different concentrations are shown in Figure 17. The red line at the top of the Figure 17 indicates the exit, and the blue, green, yellow and brown lines represent the distance the agent travels versus time for each case.

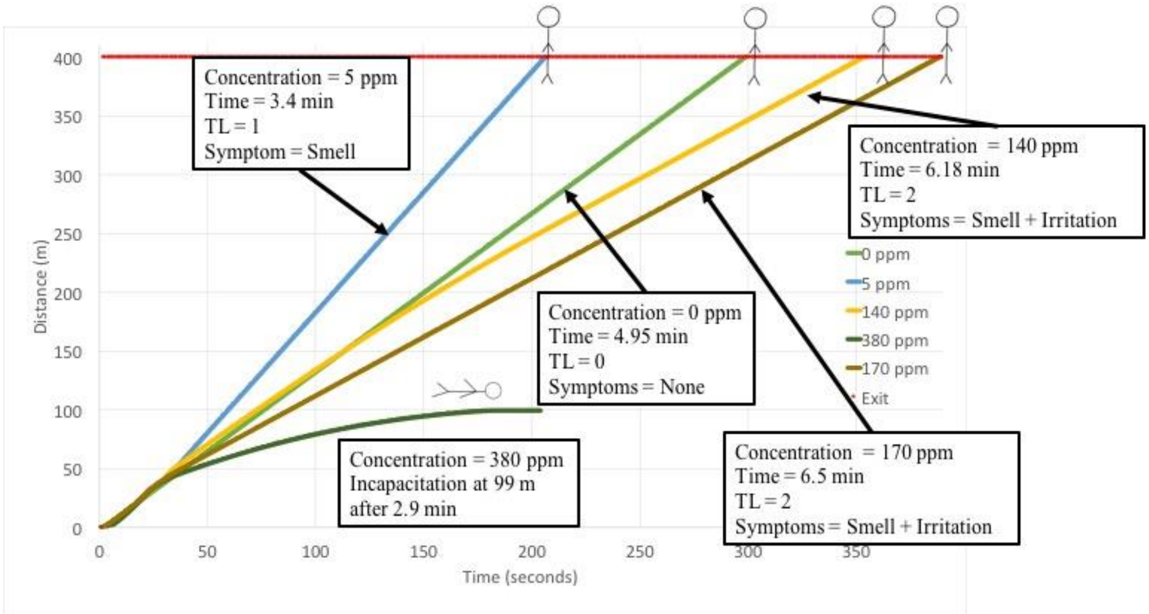

Figure 17 - Results from the Test Case at various Concentrations of H_2S

As can be seen from Figure 17, the agent takes 4.95 minutes to evacuate with an unimpeded velocity of 1.35 m/s when he is not subjected to any hydrogen sulfide. However, on the introduction of 5 ppm H_2S the agent takes about 31% less time to reach the exit. It should be noted here that, this might not necessarily be true for crowd evacuations, as agents moving faster may evacuate slower due to crowd effects like, physical contact and clogging which is commonly referred to as the 'faster is slower' effect.

When the agent is subjected to higher concentrations, it experiences symptom 2 in addition to symptom 1, due to the effects of which he evacuates slower. It can be noted that the agent travels the same distance faster when subjected to 140 ppm concentration when compared to 170 ppm concentration even though the cumulative TL in both cases is 2.

This is a perfect example to showcase the use of the TL approach – due to a higher concentration, the dosage or the rate of toxic loading of the agent will be higher and hence the onset of the symptoms will occur sooner having an effect on the overall evacuation time.

It can also be observed that when the concentration is high enough, the agent is incapacitated due to the onset of pulmonary edema, however it can be noted that the rate at which the agent initially travels is almost identical to other cases but as his dose increases, the agent's rate of travel decreases ultimately resulting in incapacitation due to pulmonary edema.

The MATLAB program was used to test the applicability of this methodology to time varying concentration.

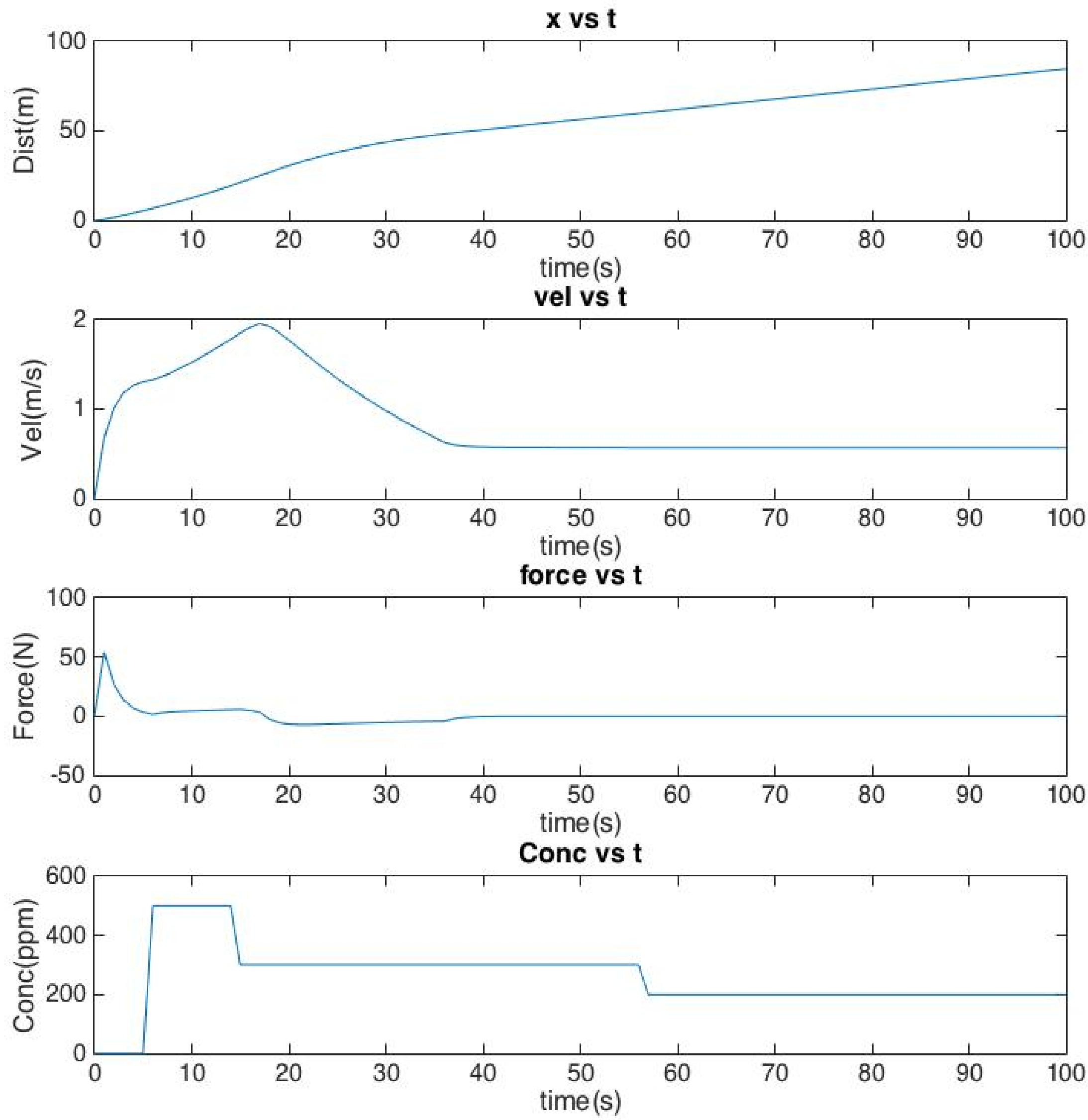

Figure 18 - The variation of velocity and total force when subjected to varying concentration of H_2S

This case illustrates the reasoning behind using a dose based application of exposure Initially the agent is subjected to a 500-ppm concentration of hydrogen sulfide for a short amount of time, a dose based implementation ensures that even if this is the case, the agent will not show advanced symptoms unless his dose warrants it, unlike concentration based application of effects. This also illustrates the practicality of the implementation of this methodology as during an evacuation the agent will be subject to varying concentrations.

5.3 Case Study 3 – Realistic Scenario in Panic Simulator

5.3.1 Geometry

A part of a real administrative building's geometry was reproduced in the Panic Simulator as reasonably as possible. The result was a representation of the building rooms and their respective walls. The building geometry used was adopted from the work of Argyropolous et al. 2017 [61] as shown in Figure 19. In this study, a simplified geometry of the area highlighted with red boundaries was used. The domain is 19 meters wide and 41 meters long. The part of the building under consideration has 7 big and 12 small occupied rooms (offices and non-machinery rooms). The exit for the building is located in the west side, 15 meters above the south most part of the building and is 2 meters wide. There are two paths leading to the exit, a corridor stretching from the south west most corner and a corridor stretching from the exit to the east side of the building.

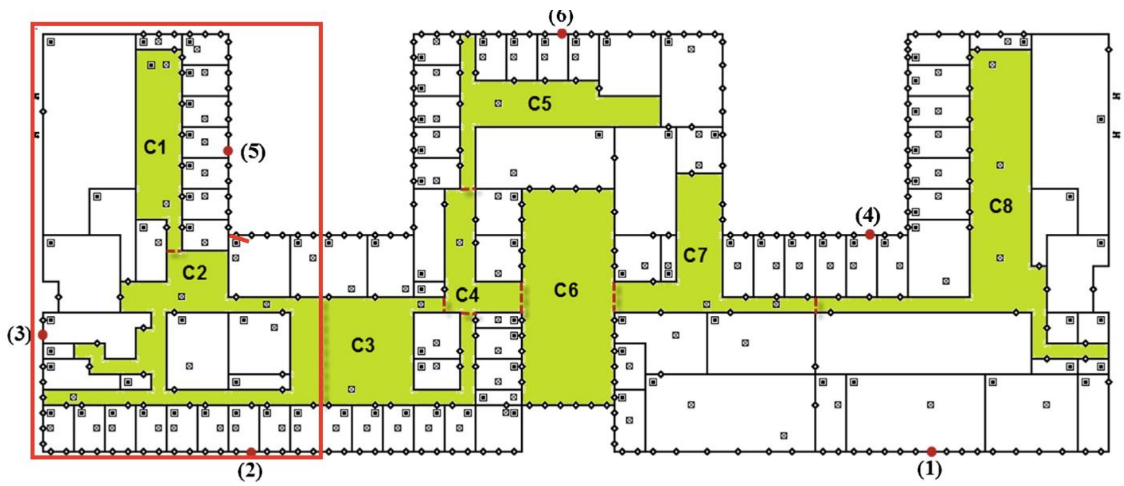

Figure 19 - Building Layout

5.3.2 Agents

The big room towards the west side is the bathroom complex and contains 6 people, the longer room on the east side is the combined mail room and store room and also contains 6 people. The shorter room above the mail room is a meeting room and contains 4 people. The rest of the rooms in the building are offices. The agents were placed in the offices on the basis of the following criteria – the larger offices would contain 3 people and the smaller offices would contain 2 people.

The agents are defined in such a way that at the end of every run they are assigned a radius between 0.24 and 0.29 meters, which in the FDS + EVAC manual [40] are the minimum radii of females and maximum radii of males respectively. Every agent has an initial velocity of 0 m/s, an unimpeded desired velocity of 1.35 m/s and tau of 1 second.

5.3.3 Simulation Parameters and Constants

Evacuation scenarios at different concentrations were simulated. The simulations run from 0 to 10 ppm were run at a difference of 1 ppm, and from 10 ppm to 500 ppm were run at a difference of every 10 ppm. At every concentration, the simulation was repeated 10 times in order to obtain a distribution of evacuation times. At the end of every run, only the radii of the agents were reset, as discussed above, while all the other parameters remained unchanged. All the values of the constants of the agent-agent interaction forces and agent-wall interaction forces were taken to be the same as they were suggested by Helbing in his paper [13].

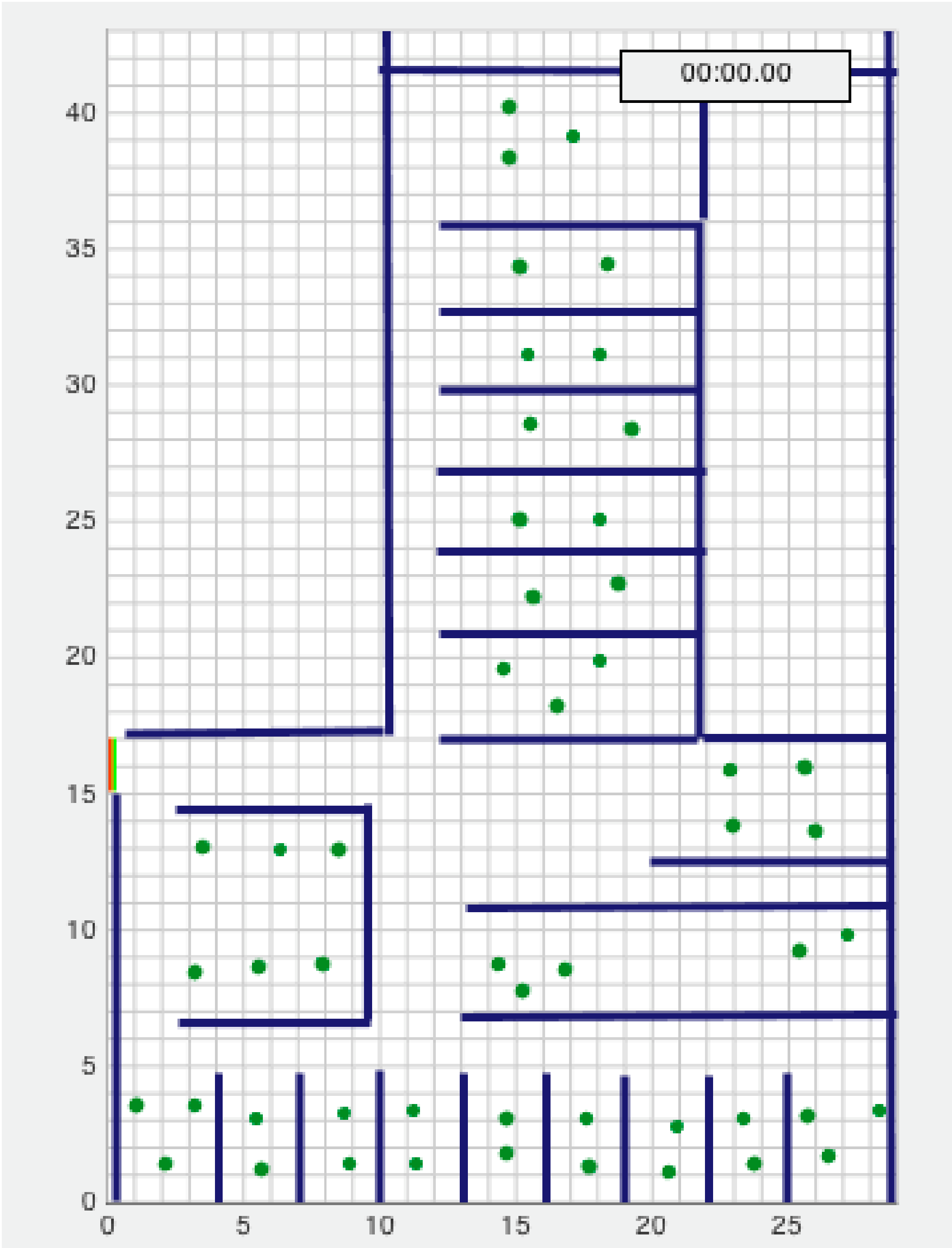

Figure 20 - The simulation domain showing the layout of walls and the position of the agents at the beginning of the simulation

5.3.4 Results and Discussion

The Figure 21 show the position of the agents at 30 seconds for 0, 5, 180 and 410 ppm of hydrogen sulfide respectively.

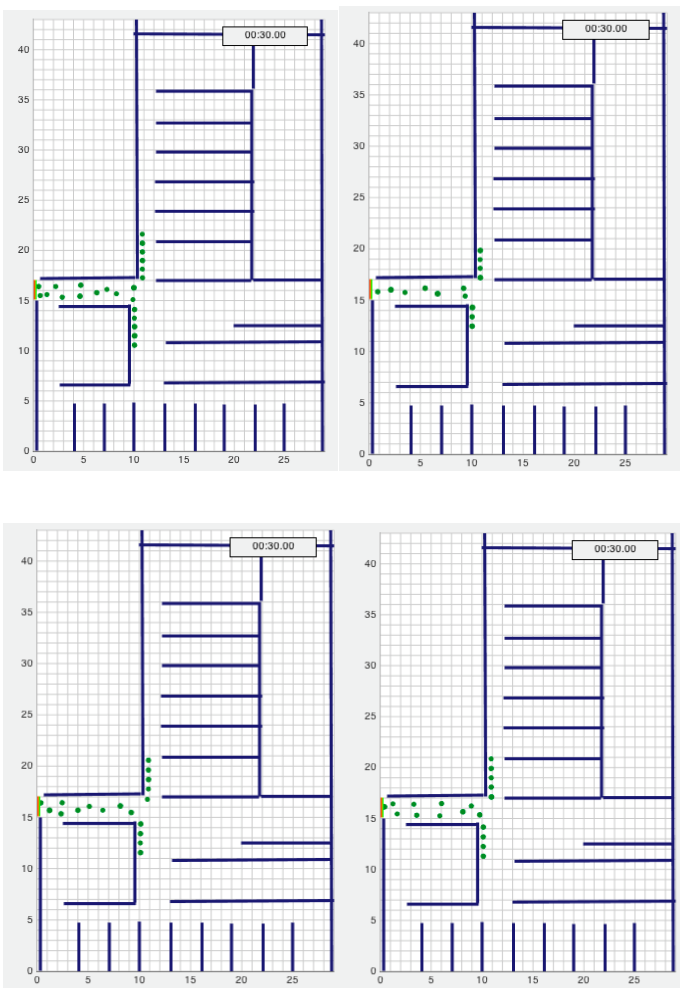

Figure 21 - Position of agents during simulation when subjected to different concentrations, in clockwise manner; 0 ppm, 5 ppm, 180 ppm and 410 ppm

It could be seen from Figure 21 that more agents were able to evacuate in 30 seconds when subjected to any of the above concentrations of hydrogen sulfide when compared to the scenario in which agents were not subjected to hydrogen sulfide. However, from Figure 22 it can be seen that when subjected to a concentration high enough more than half the agents become incapacitated.

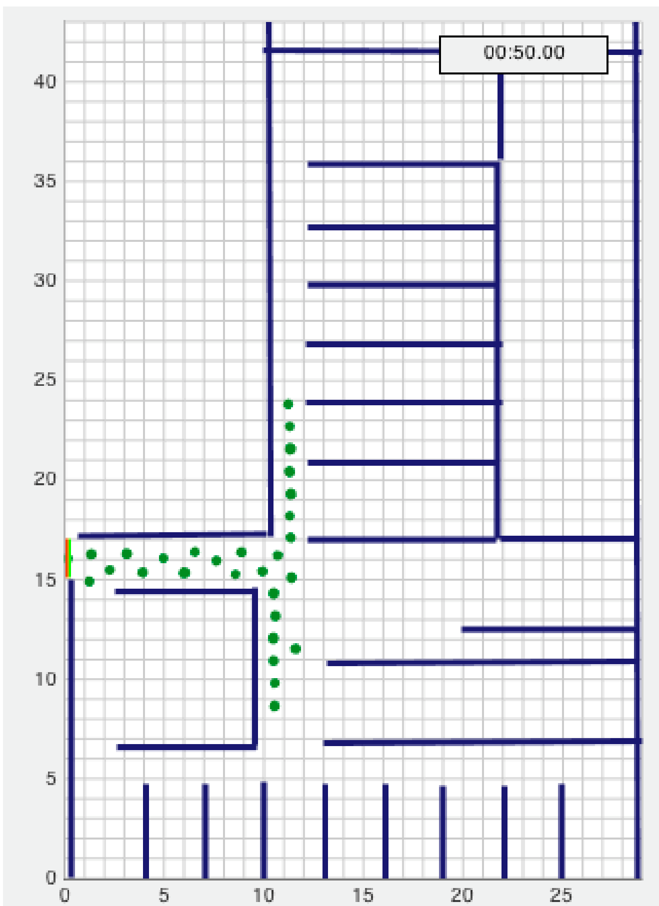

Figure 22 - Position of agents after 50 seconds when subjected to 450 ppm, the agents seen are incapacitated

In order to conduct an in-depth analysis of the evacuation process the time at which every agent exits the domain was recorded (building evacuation time). These exit times were analyzed to draw inferences about the case under consideration and about the methodology.

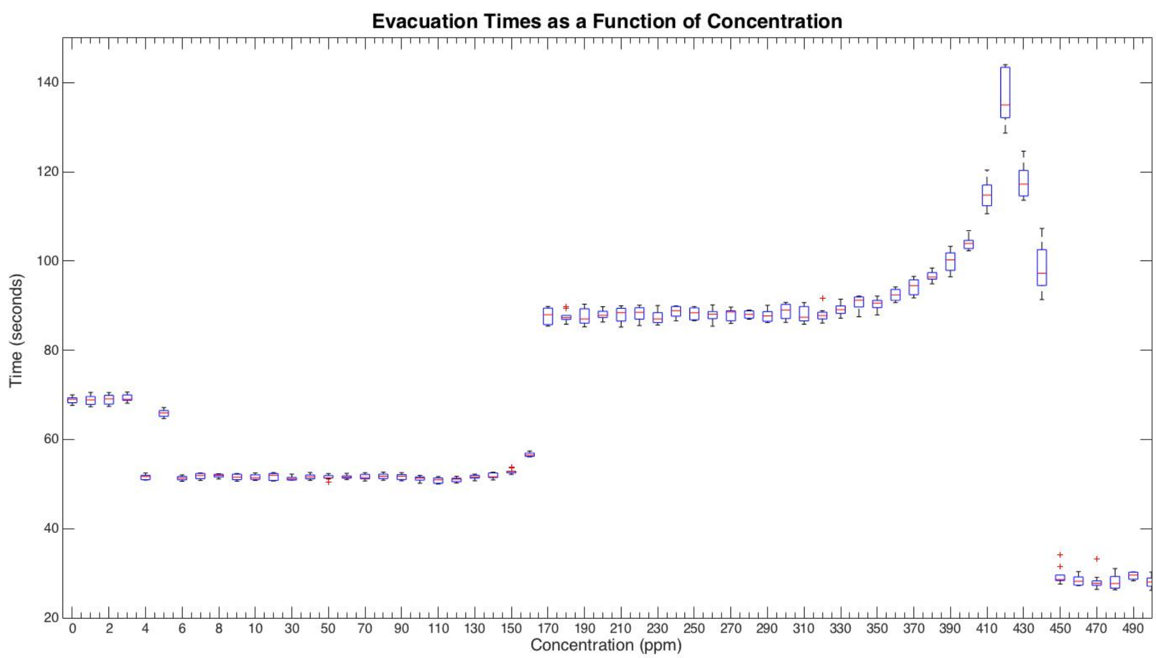

Figure 23 - Building evacuation times a function of hydrogen sulfide concentration

Figure 23 shows the distribution of building evacuation times (exit time of the last agent) over the range of concentration of hydrogen sulfide under consideration.

In the figure, the red line inside the box indicates the median of the data, the top and bottom box edges represent the 25th and the 75th percentile, respectively, and the whiskers at the bottom and top indicate the minimum and maximum time recorded for that scenario, respectively.

At 4 ppm, a gradual drop in evacuation times can be noticed, which culminates into a sudden drop of almost 30% at 5 ppm. This behavior can be attributed to the effects of the first symptom due to which the anxiousness of the agents rises, prompting them to walk faster. It was expected that an increased agent velocity in an enclosed area would lead to significant clogging and jamming and increase evacuation times. To the contrary it was noticed that the building exit size, layout and corridors significantly accommodate these effects.

The evacuation times remain constant till 120 ppm, after which a slight rise can be noticed leading up to a massive jump in evacuation times at 170 ppm. This behavior is due to the effects of symptom 2 – severe eye, throat and lung irritation – due to which the agent's ability to evacuate is impaired and it can only walk at a maximum velocity of 1 m/s.

The evacuation time remains unchanged till 320 ppm, after which a slight increase in evacuation times can be noticed. This rise becomes more dramatic as the concentration increases leading to evacuation times reaching almost twice as high (at 420 ppm) when compared to evacuation times at 0 ppm. This increase is attributed to the third symptom – pulmonary edema, due to which the agent's walking speed drops slowly towards zero, as a function of their TL.

After 420 ppm, a drop in the evacuation times is seen, this is due to the fact that from 430 ppm onwards some agents become incapacitated and are unable to evacuate. The figure displays the evacuation time of the last agent that was able to evacuate. The drop in the evacuation time is due the fact that more agents start becoming incapacitated and are unable to evacuate with the increase in concentration. At 450 ppm and above, the evacuation time is 30 seconds. This is due to the fact that these concentrations are above the threshold concentrations of symptom 3's exposure-response, which makes the onset condition for the highest symptom to be achieved in 30 seconds.

It can be seen by observing the box sizes that with increase in evacuation times the variations in the evacuation time also becomes more prominent and with the decrease in evacuation time, the variations in evacuation times decreases.

Individual exit times for every agent were analyzed from a concentration of 400 ppm to 500 ppm in order to gain more insight into the effects of the final symptom. The number of agents incapacitated versus the agents able to evacuate when subjected to concentrations between 400 ppm and 500 ppm were plotted in Figure 24.

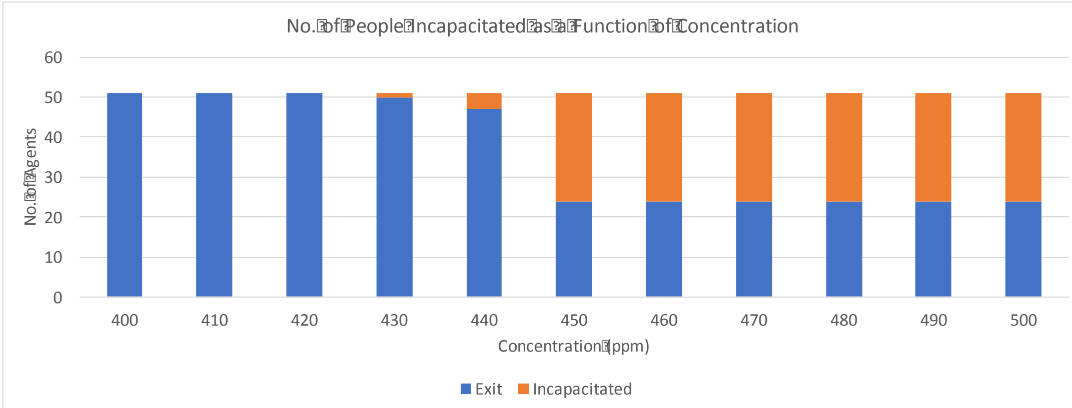

Figure 24 - Number of agents incapacitated versus agents that are able to evacuate as a function of concentration

The figure shows the number of agents (out of 51 agents) that are incapacitated with increasing concentration. At 430 ppm, the data indicates that there is only one agent that will be subjected to a dose high enough to be incapacitated and the remaining 50 agents are still able to evacuate. This number of agents increases to 3 with an increase of 10 ppm in concentration (440 ppm), and 48 agents are still able to evacuate. The number of agents incapacitated rises significantly at 450 ppm and stays that way all the way to 500 ppm. At 450 ppm and beyond, 53% of the agents are unable to evacuate the building. In this particular case, 47% of the agents are positioned in the building in such a way that even when subjected to 500 ppm of concentration, they will not experience a dose high enough to inhibit them from evacuating the premises.

In order to gain more insight into the complete evacuation process for this case, a distribution of the exit times for every agent at every concentration were plotted.

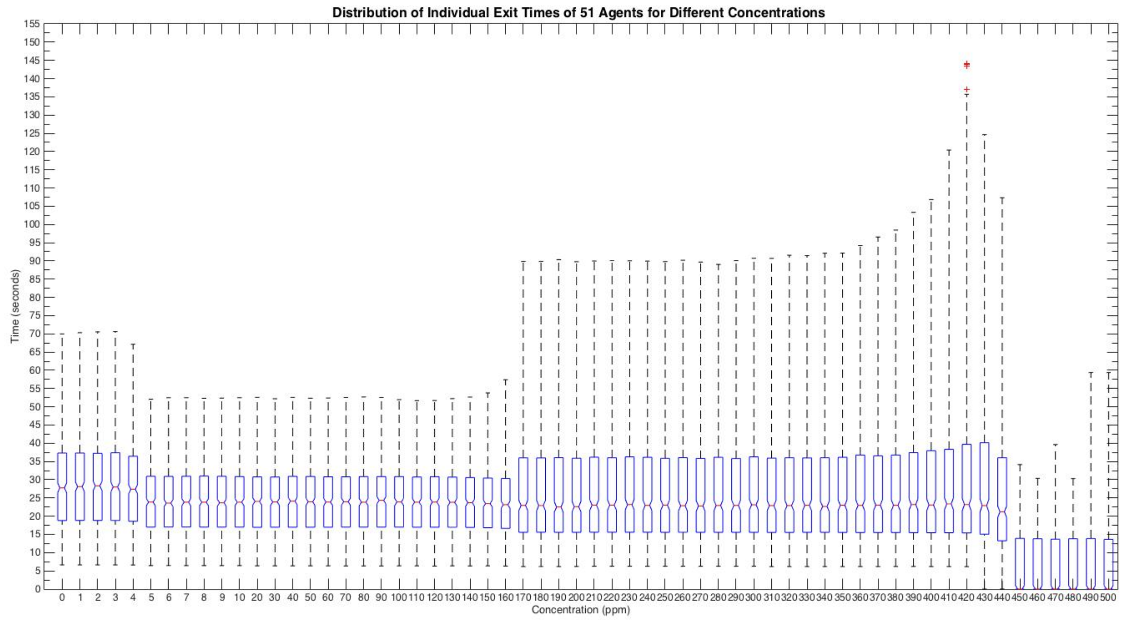

Figure 25 – Distribution of individual exit times of 51 agents for different concentrations

In Figure 25, at every concentration the input is the individual exit times of all agents for the 10 simulation runs at that concentration, this data is analyzed and plotted as one boxplot for that concentration, in which the bottom whisker represents the lowest individual exit time recorded for an agent, and the highest whisker represents the highest individual exit time recorded for an agent. The red bar indicates the median individual exit time and the edges of the box represent the 25^{th} and 75^{th} percentile individual exit times respectively.

The top whiskers represent the evacuation time of the building (evacuation time of the last agent) and are consistent with the observations made in Figure 23, that there is a significant effect on the evacuation time of the last agent throughout the range of the concentration.

By observing the bottom whiskers it can be seen that, there seems to be a negligible effect on the evacuation time of the first agent across the range of concentration.

There is a noticeable difference in the 25th percentile times across the concentration, but the changes are less pronounced when compared to the variations of the 75th percentile times. Two other noteworthy observations are that, throughout the range of the plot, the 25th percentile mark moves only in the negative y-direction denoting that the evacuation time of at least the first 12 agents only decreases throughout the range of concentrations and that for concentrations ranging from 400 ppm and above, the variation of the 75th percentile time is not as pronounced as the jump in the evacuation times of the agents. From these observations, it can be fair to say that, the first 25% of the evacuees, do not experience the second symptoms at all, or do not experience it for enough time to have a negative impact on their evacuation times. Also, up to 430 ppm, 75% of the evacuees (first 38 agents to evacuate) are affected less negatively by the symptoms of exposure when compared to the last evacuee.

It must be noted that the data from 430 ppm to 500 ppm is not truly representative of the scenarios as the evacuation time of the agents that that are incapacitated is recorded as 0 which makes the analysis for these concentrations skewed. The only inferences that should be taken from these bar plots are that these are the concentration where some of the agents will not be able to evacuate, and the exit times of the last agent who is able to evacuate.

The observations from this figure paint a fairly complete story of the scenarios and ring true to the reasoning behind implementing dosage based symptoms in evacuation simulations. It re-enforces the reasoning behind this work that during an evacuation, the exit times of agents and the evacuation time will depend upon the dosage rather than just the concentration that they are subjected to, even when a toxic agent like H_2S is considered whose exposure-response curves are very steep.

A more in-depth chronological analysis of the scenarios was conducted to gain more insight into the evacuation process.

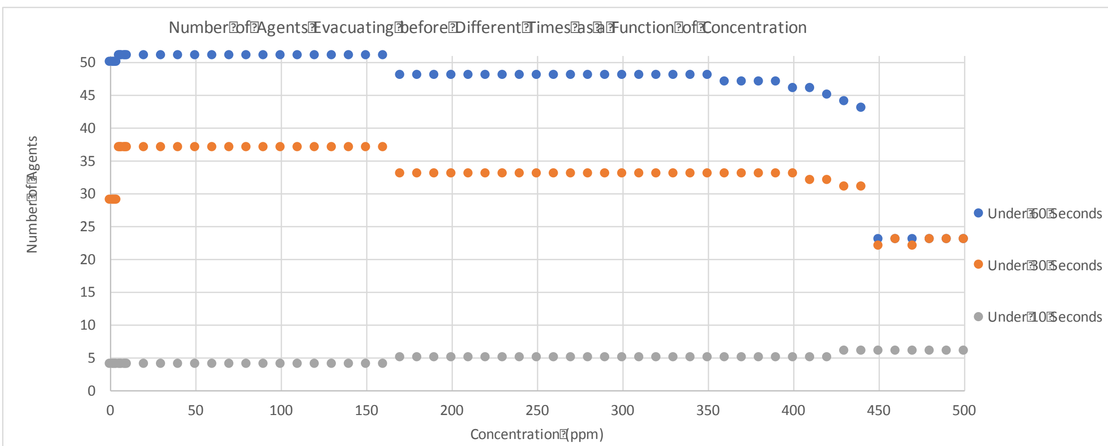

Figure 26 - Number of agents evacuating in under 60, 30 and 10 seconds as a function of concentration

From Figure 26 it can be seen that only one agent is unable to evacuate before 60 seconds when subjected to no, or very low concentrations of hydrogen sulfide, however all agents evacuate in under 60 seconds when subjected to concentration between 5 ppm to 160 ppm. The number of agents evacuating in under 60 seconds slowly drops as the concentration is increased, however, the drop in the number of agents begins again at 350 ppm in a very gradual manner and goes on till 430 ppm. This is the range when the agents start experiencing the effects of symptom 3. Almost 85% of the agents are able to evacuate in under 60 seconds even when subjected to 430 ppm of hydrogen sulfide. This explains the previous observation that the 75th percentile time does not show a variance as high as the evacuation time. The drop in the number of agents after 430 ppm is due to the agents not being able to escape at all.

The number of agents that are able to evacuate in under 30 seconds increases significantly when the agents are subjected to a concentration between 5 ppm and 160 ppm. There is drop in the number of people being able to evacuate when subjected to a concentration of 170 ppm to 400 ppm, but it is not as pronounced as the rise in the number of agents that is seen at 5 ppm. This lends an insight for case under consideration that some agents are able to evacuate faster in a highly toxic environment than they would in a non-toxic environment. This is due to the application of the effects of the first symptom first and then the second symptom.

With the increase in concentration, the number of agents evacuating before 10 seconds' increases. This is consistent with the previous observation about the exit time for 25% of the evacuees keeps decreasing as the concentration increases. The agents that are able to evacuate in this time period do not stay in the domain long enough to experience the effects of the second and the third symptom.

One of the factors determining the exit time of an agent is its position with respect to the exit. Based on the simulations, some trends with regards to agent position were observed and these trends are shown by the demarcations made in the simulation domain, as shown in Figure 27;

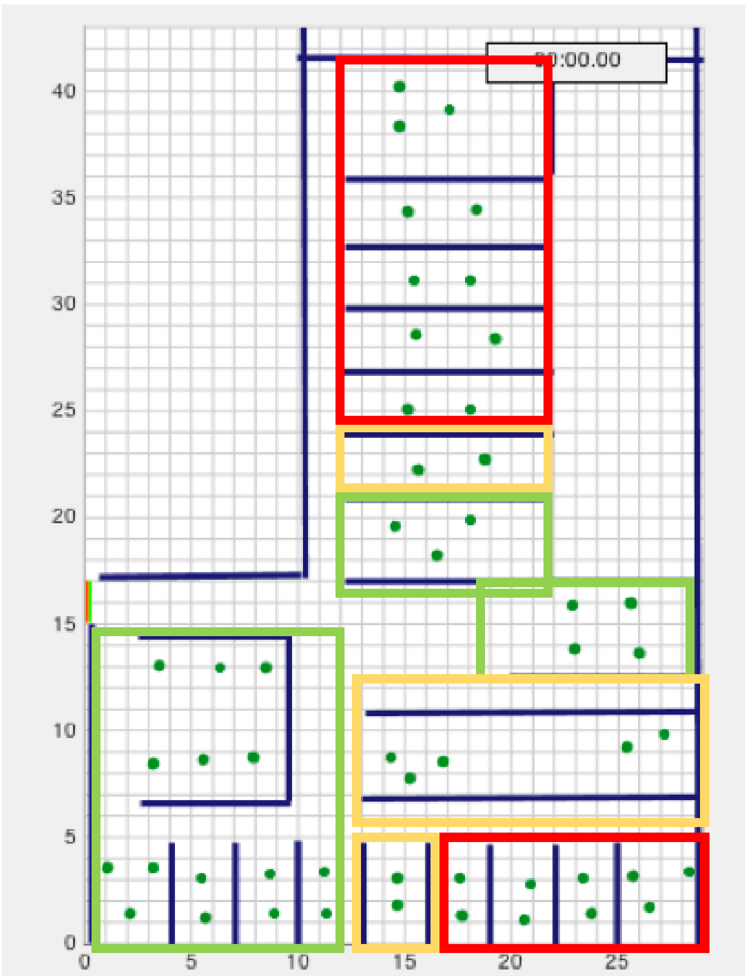

Figure 27 - Area demarcation for agents on the basis of evacuation times and evacuation trends

From all the data gathered and by visually observing the scenarios while simulations were being run, it was established that;

1. The agents in the green area are able to successfully evacuate the premises irrespective of how high the concentration is. This is due to their close proximity to the exit, which enables them to exit the domain before 30 seconds. They account for almost 43% of all agents.
2. The agents in the yellow region, if subjected to a concentration high enough, are unable to evacuate. But when they are able to evacuate, they show a peculiar property that their evacuation time is always either less than or equal to the evacuation time when they are not subjected to any toxic environment. They account for 18% of the agents.
3. The agents in the red region, are the ones that experience the most prolonged exposure to the toxic agent due to their distance from the exit. These agents are the last ones to exit and their exit times in some scenarios are as high as twice the exit time when they are not subjected to a toxic environment. They account for 39% of all agents.

The results from studies like this can help improve the assessment of mitigation and emergency response strategies. For example, in this case, one could observe that emergency doors close to the red regions can help mitigate the consequences, as the agents from those regions would be able to exit sooner. Alternatively, the agents in the red and yellow regions could be trained and provided with self-contained breathing apparatus to help decrease the exposure.

6. CONCLUSION AND FUTURE WORK

In this work, a dosage based level of injury variable was used in conjunction with a social force model to introduce the effects of toxic exposures during evacuation. This methodology was implemented in an evacuation simulation tool and demonstrated through a case study.

Through the case-study it was revealed that a dosage based approach to applying various effects on evacuees can lead to different evacuation patterns for different concentrations and different building regions. It was seen that for a toxic agent like H_2S which has a very steep exposure-response curve, if the effects are applied in a dosage based manner, the effects are not exhibited uniformly when the concentration is constant throughout the domain for the length of the evacuation. This methodology is also applicable for simulating evacuations with time and distance varying toxic plumes.

This methodology is independent of the exposure-response data used in this work and is applicable for any type of exposure-response relationship for any toxic agent. The concept of the toxic force term devised in this study is applicable to any social force evacuation model, or agent-based evacuation model that uses the social force model as its basis. The application of the effects can be improved upon by using the toxic load not only as a function of severity but also a measure of proportion of population affected by implementing Toxic Load – Response relationships. More variables that enforce the non-homogeneous behavior and response of humans during evacuation situations and to toxic exposure can be implemented.

The major challenges and knowledge gaps seen during the course of this study was the lack of dose-response relations for the symptoms associated with the toxic agent. The concentration data for symptoms in toxicological data are usually provided in wide ranges with vague time definitions, if any. There is also a knowledge gap in the understanding of the physical and psychological implications these symptoms can have on the evacuation process. Due to these factors, various assumptions had to be made for this study.

In its current form, this methodology can provide only a superficial understanding of how toxic environments will affect the evacuation process. It must be noted that simulating realistic evacuations was not the aim of this work. In order to simulate scenarios to obtain realistic results firstly, a better understanding of the toxicological aspects and their implications on the evacuation process needs to be obtained, which can then be used to improve the dosage and effect part of this methodology, this methodology would then have to be implemented into more advanced evacuation tools that have been experimentally validated.

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