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A COMPUTER SIMULATION OF A DERAILMENT ACCIDENT: Part I - Model Basis

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ABSTRACT

A prototype computer program has been developed which is capable of simulating some of the consequences of a train derailment accident. The program is made up from a number of models which account for train derailment mechanics, flammable liquid spills, fire effects on remote targets, fire impingement on tank cars carrying dangerous commodities, explosion blast over-pressure and thermal radiation, and heavy plume and puff dispersion. Most of these sub-models have previously been developed and are available in the open literature.

The overall program consists of a pre-processor for inputting the surroundings data and train consist data, a simulation module containing the various models and a post-processor which presents the results of the simulation in graphical form.

The present paper briefly describes the overall organization of the program and the technical basis of the simulation models.

INTRODUCTION

In recent years there have been many studies performed to estimate the consequences of train derailment accidents. The consequences of particular interest are those that could potentially cause harm to people or property such as accidental releases of hazardous liquids or vapours, fires, and explosions. Many of these studies resulted in the development of models for predicting quantitatively the effects of these activities and some resulted in computer models. However, these models usually have remained as stand alone tools and many require detailed input which must be estimated from accident statistics or just guessed.

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The objective of the present study was to develop a prototype computer program for simulating the consequences of train derailment accidents. The program was to simulate what happens in a derailment accident starting from the time when the first car leaves the track to when the last tank car empties through its relief valve or explodes. The program was to be based on current methods of modelling the various processes taking place in such an accident. The first version of the program was to be a demonstration version and as such was to be limited in its capabilities.

The study involved a search for current models and techniques for estimating the consequences of the most significant accident related phenomena and in some cases the development of new models as required. These various models were then integrated into a single program. Pre-and post-processors were then developed for data input and results presentation.

The simulation program is called DERACS for Derailment Accident Simulation. The program is presently running on an IBM/AT compatible machine with run times in the order of one half hour, depending on the number of vehicles and the consequences involved.

This program is the prototype which is somewhat limited in scope. At present the program can handle up to forty cars in a train, and of these, up to eight can be tank cars carrying propane, chlorine or hexane. These commodities were chosen because they include a toxic gas, a flammable gas and a flammable liquid when released into the environment. Future versions of DERACS will be expanded to include more cars and additional commodities.

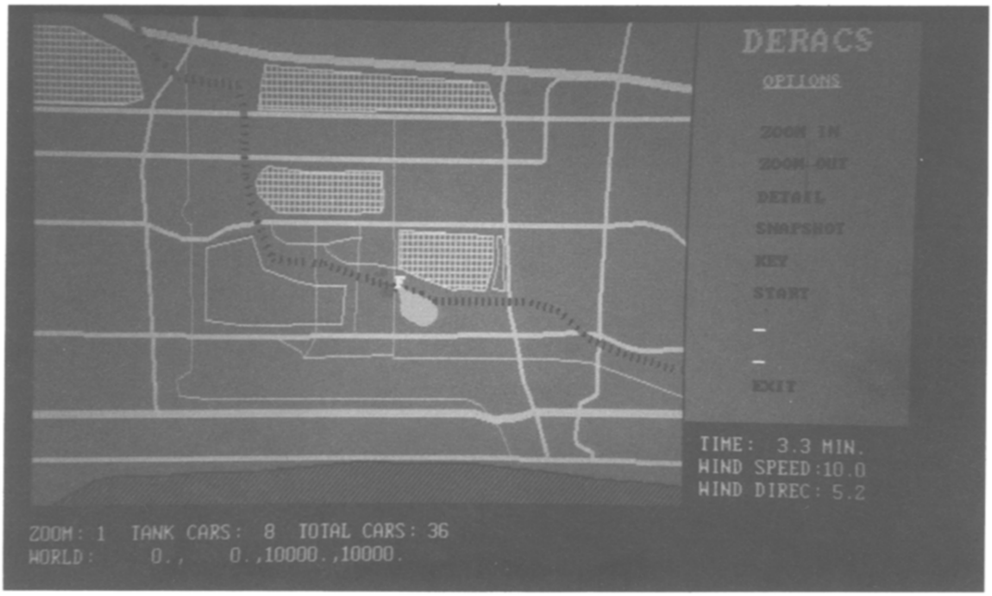

Figure 1 Example of Map Generated using DERACS Pre-Processor

The intended applications of the program include accident reconstruction, response team training and risk analysis. Because the simulation is based on current analysis techniques, it is possible that the simulation could be used as an on-site response tool and used as one input for response tactics. This latter application would only be possible after considerable additional development and validation.

PROGRAM ORGANIZATION

The overall program consists of the pre-processor, the simulation software, and the post-processor. The pre-processor is used to create the surroundings in which the derailment is to take place and also reads in the initial conditions of the train at the time of the derailment. The pre-processor will also allow the user to bypass the derailment mechanics simulation and input the locations of the derailed vehicles along with descriptions of punctures.

The pre-processor is a user friendly routine that allows the user with the aid of a mouse to draw a map including such things as: rivers and lakes, forests, roads of different sizes, single or double railway tracks, buildings, property boundaries, and elevation contour lines. The total map area is 10km by 10km and the user can input part or all of this area when creating the map. Figure 1 presents an example of a map created using the pre-processor and Figure 2 is a key to the symbols appearing on the map.

In addition, the pre-processor has the function of reading in all the other necessary information for the simulation, including environmental conditions, such as wind speed

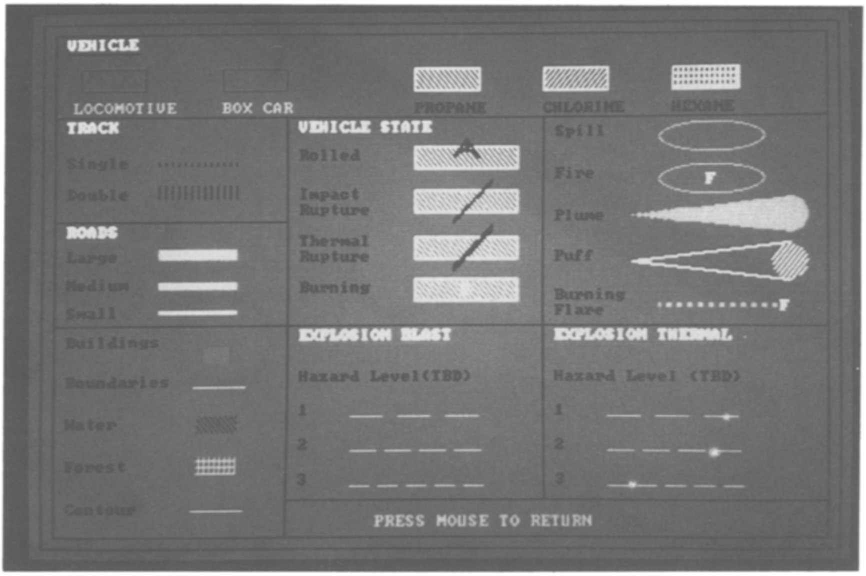

Figure 2 DERACS Key Page for Map Symbols

and direction, ambient temperature and atmospheric pressure, and train consist data such as car type, commodity, initial fill and temperature, etc.

Depending on the options selected, the pre-processor will read in the location of the derailment point and the car number, truck number and axle number of the car which initiates the derailment.

The train speed and direction is also read in during the pre-processor session. If desired the user has the option of overriding the derailment mechanics simulation portion of the overall simulation. If this option is chosen, the user must specify the final placement and orientation of vehicles after the derailment, which cars are ruptured and what kind of ruptures have occurred.

The post-processor part of the DERACS software is one of the most important because it presents the results of the simulation to the user in a easily understandable fashion. The post-processor is used to read files that contain the results of the simulation and presents this information in graphical or text form to the user at the end of the simulation. By using the post-processor, the user can page through the simulation process and look at various instants in time during the simulation to see how the accident progressed.

The post-processor gives a plan view of the surroundings and shows placement of the vehicles after the derailment and the various events that are taking place such as spills, gaseous releases, fires, thermal ruptures, explosions, etc. The user can select any instant in time and print out a snapshot of the derailment scene. Figure 3 presents a typical image of an accident scene as shown using the post-processor. In this figure

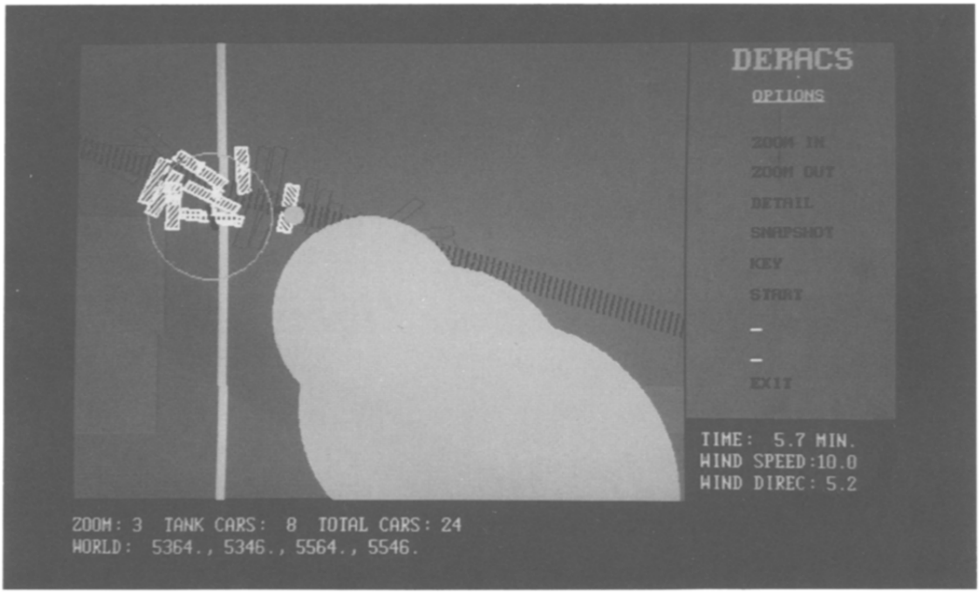

Figure 3 Post-Processor Image of Derailment Scene at One Instant in Time

we have zoomed in close to the accident location and we see the derailed cars, the location of a spill and the beginnings of a heavy gas plume.

The simulation module of DERACS carries out the time integration of the accident consequences starting from the time of the derailment to when the last car empties safely or BLEVE (boiling liquid expanding vapour explosion). The simulation module contains all the sub-models that are used to simulate the various processes taking place during the accident.

BASIC ASSUMPTIONS

To carry out the simulation a number of assumptions were necessary with regard to the consequence resulting from some actions. For example, when a tank car carrying propane is ruptured a number of things can happen, including:

1) Catastrophic failure of the vessel with resulting explosive release of the contents and subsequent ignition to form a fire ball.
2) Instantaneous release in the form of a toxic heavy gas puff with subsequent dispersion and possible ignition at some time.
3) Continuous release of the propane gas with possible ignition at some time.

Other consequences are possible. The exact consequences that occur are a complex function of many variables including the lading properties at the time of rupture, and the size, shape and location of the rupture. However, for the development of this first version of DERACS, it was necessary to assume simple relationships. For the ruptured propane car case, it is assumed a total loss of containment would result in an explosion and fire ball. In the event of a finite puncture it is assumed that a continuous release results in the dispersion of a cloud of propane. Eventual ignition of the propane cloud is not considered at present. In future versions of DERACS more sophisticated scenarios will be considered. Table 1 presents a summary of the most significant assumptions used in the present version of DERACS.

The DERACS simulation was developed around assumptions noted in Table 1, therefore the consequences shown by the simulation are limited to those noted.

TECHNICAL BACKGROUND

As stated earlier the simulation module of DERACS contains all the sub-models used to simulate the various processes taking place during the accident. The sub-models consider the following processes:

i) derailment mechanics
ii) derailment impact induced rupture of tank cars
iii) liquid and vapour release
iv) flammable liquid spill growth

v) plume and puff dispersion of heavy gases

vi) liquid pool fires and effects on surroundings

vii) fire impingement on tanks and thermal ruptures

viii) blast and thermal effects of explosions/BLEVES

Table 1 briefly describes the technical basis for the main sub-models. More complete technical descriptions can be found in Reference [1].

Action	Commodity	Consequence	DERACS Output
derailment	all	possible impact punctures of tank cars	punctured tanks identified
puncture/ rupture	chlorine	toxic release	plume extent
	propane	toxic release	plume extent
	hexane	flammable spill	spill diameter
total loss containment	chlorine	toxic release	puff extent
	propane	explosion/BLEVE	blast and thermal hazards
	hexane	flammable spill	spill diameter
flammable spill		pool fire	thermal radiation dose and, fire impingement of tank cars within spill region
tank car relief valve action	chlorine	toxic release	plume extent
	propane	burning flare	flare size
	hexane	burning flare	flare size
burning flare			fire impingement of tank cars within range of flare
explosion/ BLEVE		explosion and fireball with blast overpressure and thermal radiation	blast and thermal hazard distances
tank fire impingement		possible thermal rupture (total loss of containment)	tank and lading properties at time of failure

Table 1 Assumed Cause and Effect Relationships for Tank Cars and Commodities Considered in DERACS

Derailment Mechanics

The derailment mechanics sub-model involves the solution of the governing equations for rigid body motion of the vehicles allowing for four degrees of freedom (x, y, yaw, roll). These variables are defined in Figure 4 which also shows their relationship to the derailment point. This sub-model was developed specifically for DERACS and is unique in that it allows for vehicle uncoupling in the event of coupler breakage and vehicle roll. The only previous model (by Yang and Manos [2]) could not allow vehicle uncoupling and vehicle roll.

The vehicles are assumed to consist of a car body supported on two trucks, each having two wheel sets each. To limit the number of resulting differential equations, it has been assumed that the truck frames are fixed relative to the car body and the wheel sets are fixed relative to the truck frames.

The forces assumed to act on the vehicles include the inter car forces applied by the couplers, and the wheel/rail or wheel/ground forces.

The couplers are assumed to be infinitely strong for compressive loads but are assumed to release when a threshold load is exceeded. The assumed threshold load is 2.3 million N which is the elastic limit for the coupler shanks as reported by Wallace [3]. The couplers are modelled as a simple stiffness element. Once the couplers release, the cars are free to move apart. Because of the assumed use of shelf couplers, simple coupler release due to relative vertical motion is not considered.

Ground forces are assumed to act as a Coulomb type friction force, the direction being opposite to the vehicle velocity vector at the point of contact with the ground. The friction forces are assumed to act at the two truck centres for an upright car. The vehicle linear and rotational velocities are used to calculate the velocities at the two truck centres and these are used to determine the friction force directions and

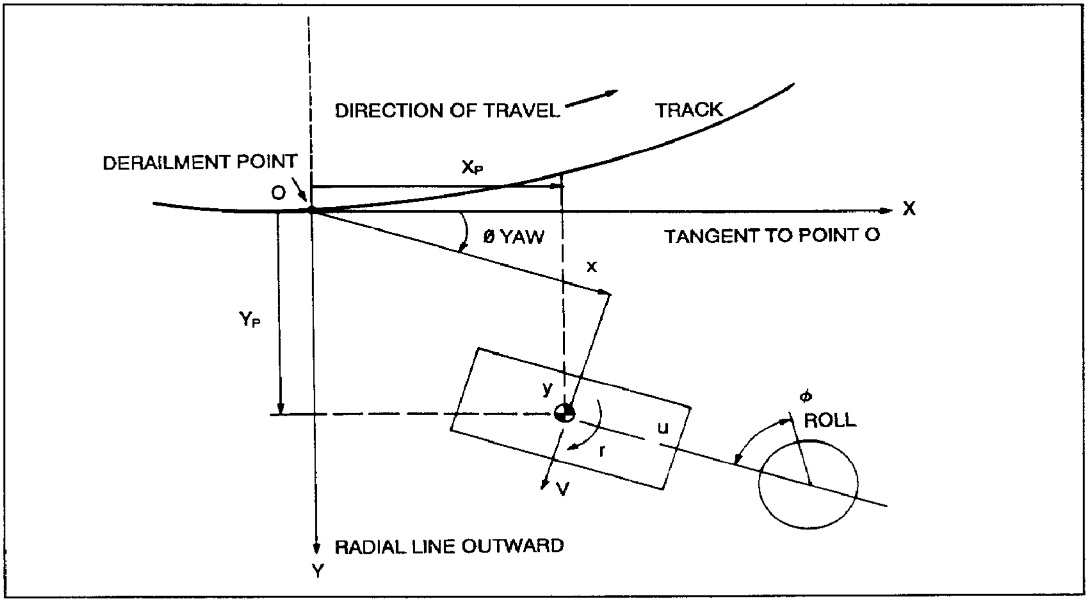

Figure 4 Definition of Degrees of Freedom of Car Relative to Derailment Point

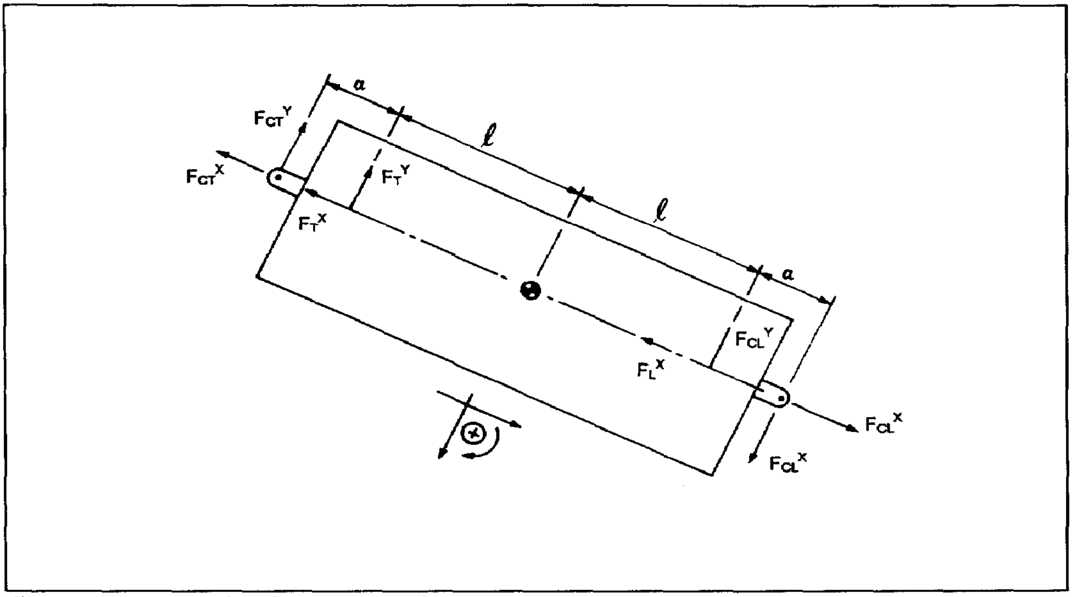

Figure 5 Free-Body Diagram of a Car

magnitudes assuming each truck supports half the car weight. Figure 5 shows the free body diagram for a car.

The equations of motion for the x, y and yaw degrees of freedom are as shown below:

longitudinal force balance: (1)

$$M(\dot{u}-Vr) = F_{CL}{}^{x}-F_{L}{}^{x}-F_{T}{}^{x}-F_{CT}{}^{x}$$

lateral force balance: (2)

$$M(\dot{V}+ur) = F_{CL}{}^{y}-F_{L}{}^{y}-F_{T}{}^{y}-F_{CT}{}^{y}$$

yaw moment balance: (3)

$$Ir = F_{CL}{}^{y}(a+l)-F_{L}{}^{y}(l)-F_{T}{}^{y}(l)-F_{CT}{}^{y}(a+l)$$

The model only allows roll of uncoupled tank cars (ie. coupler forces are assumed to assist in maintaining tanks in an upright orientation). Roll-over is considered imminent when either of the wheel normal forces approaches zero. It is assumed that the car losses its trucks and the tank becomes a rolling cylinder. If roll-over occurs the amount of roll is calculated using the following expression which was derived by using energy considerations. Because of the presence of a dome on the top of the tank car, the maximum roll angle is limited to 120 degrees.

$$\varnothing = \frac{S}{R} - \frac{V^2}{2\mu g R} \qquad (4)$$

where,

$\varnothing$ = roll angle

S = rolled distance

R = tank radius

V = velocity component in y direction

μ = friction coefficient

g = gravitational acceleration

The initiation of the derailment is an input and specifies the car and the truck that derails. The derailment point is the origin for all subsequent calculations as previously shown in Figure 4. It is assumed that all cars passing this point on the rail leave the rails and are from then on only guided by the soil interaction forces. Cars that have passed the derailment point ahead of the derailed car are guided by the rails. All cars are assumed to be engaging emergency braking.

The resulting second order differential equations are manipulated into first order ordinary differential equations. A variable run time Runge-Kutta Fehlberg [4] technique was used to solve the equations. Figure 6 presents an example of a predicted derailment scene.

This program has not been validated as yet and therefore results are presented for discussion purposes only.

Derailment Impact Induced Rupture of Tank Cars

For the overall derailment simulation, it is important to be able to predict impact induced ruptures. The impacts are occurring during the derailment due to coupler impacts on car shells. The impacts between the cars is modelled using the derailment simulation sub-model described earlier.

NO. OF CARS TOTAL = 36
NO. OF CARS DERAILED = 24
INTIAL TRAIN SPEED = 100 Km/hr
TRACK CURVATURE = TANGENT

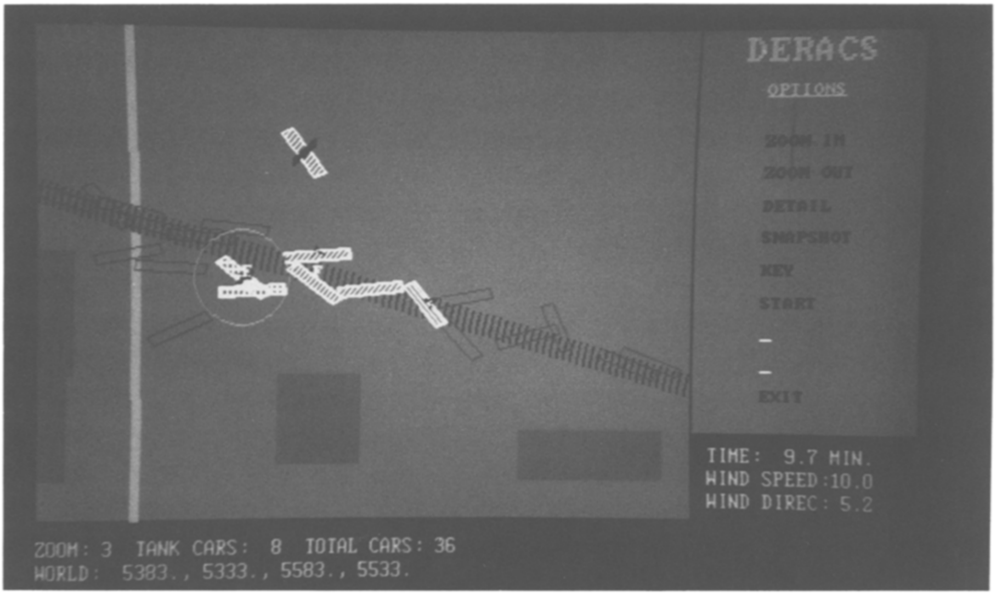

Figure 6 Typical Result of Derailment Mechanics Simulation

The prediction of impacts and impact induced ruptures is a very complex matter and the following analysis is a first attempt. Significant simplifications were necessary so that the program would run in a reasonable length of time on a micro computer.

In the present model, it is assumed that puncture will only occur when a free coupler comes in contact with a tank shell and the relative velocity between the coupler and the impacted tank is greater than 20 m/s. This type of puncture is assumed to be a round hole with a diameter of 0.3m and is assumed to be located at 0.5m above the bottom of the tank. If the relative velocity parallel to the tank axis is greater than 25 m/s, and the relative axial velocity is much larger than the lateral, then it is assumed that the puncture is a long tear resulting in a total loss of containment.

This simple impact rupture model is used to identify tank cars that have been ruptured. At present only the two cases above, namely the 0.3m diameter puncture and the total loss of containment, are possible. Future developments of DERACS will likely incorporate a more complex impact rupture analysis with additional possible outcomes.

Liquid and Vapour Release

Liquid and vapour release is of importance in the event of accidental rupture of tanks carrying dangerous goods. The rate of release and the phase of the released commodity determine whether a liquid pool will form or a toxic or flammable cloud will disperse into the atmosphere.

If a pool of flammable liquid forms then a pool fire is possible with resulting consequences including fire impingement on local objects and thermal radiation loading of remote targets. These effects will be discussed further in a later section. If a vapour is released, then an unconfined vapour explosion is possible (in the case of a flammable commodity) or a toxic plume (in the case of non-flammable commodity).

The rates of release of liquids and vapours are calculated using a modified version of the computer program LEAKR by Belore and Buist [5]. The LEAKR program can handle a number of different chemicals, tank shapes, and puncture sizes and geometries. Release rates can be predicted for both subsonic and sonic gaseous releases, single phase liquid releases or two phase subsonic releases.

LEAKR performs a time integration of the release of material from a tank and gives a prediction for the time required to empty the vessel. The calculation accounts for heat transfer effects between the tank lading and the ambient surroundings. As described by Belore and Buist [5], gaseous properties are calculated in the program using the Redlich-Kwong [6] equation of state and thermodynamic properties are calculated using the method of Balzhizer et al [7] and from Perry and Chilton [8]. The liquid state properties are calculated from Lyman et al [9] and Perry and Chilton [8]. For gaseous releases, the flow rates are based on relations for isentropic compressible flow with a discharge coefficient assumed to be 0.61. For single phase liquid releases where flashing is not taking place, the flow is treated as incompressible and the flow rate is

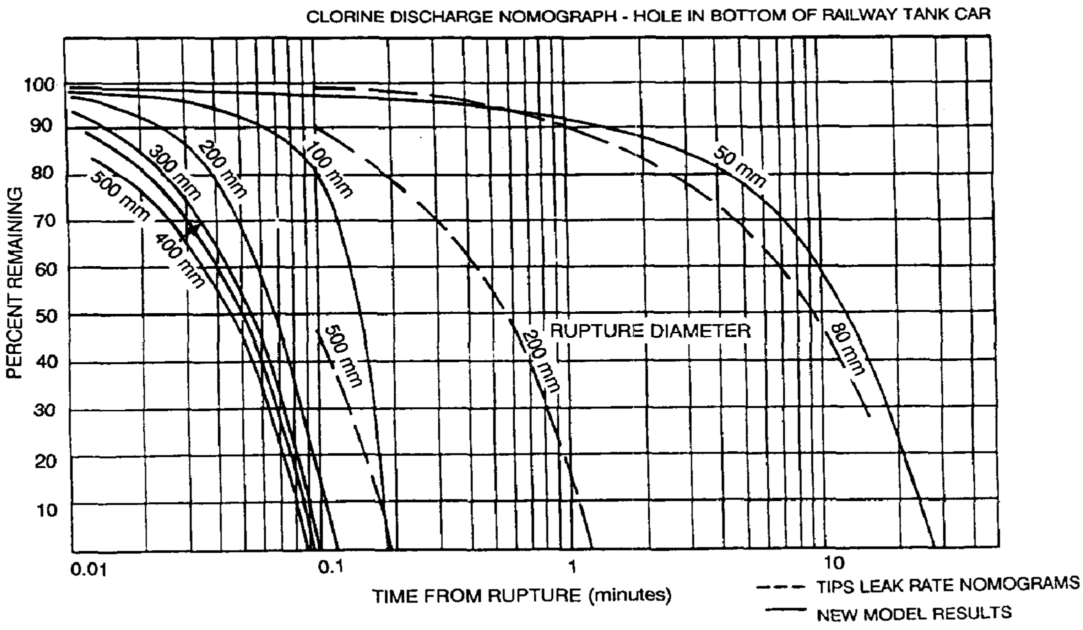

Figure 7 Comparison of LEAKR Results with TIPS Nomogram (from Ref. (5))

calculated from Dodge et al [10]. At very small pressure differentials, air ingestion is accounted for using the methods presented by Dodge et al [10]. When flashing occurs, the flow rates are calculated from Mayinger [11]. For choked two-phase flows the flow rates are calculated using the methods of Henry [12] and Delhaye [13]. The flow coefficients for both single-phase liquid and two-phase flows were taken from Dodge et al [10].

Figure 7 presents a graph from Reference [5] which shows a comparison between LEAKR and release rate calculations based on nomographs for chlorine published in the Environment Canada TIPS documents (see Reference [14]). For further details of these calculations and the LEAKR program the reader is directed to Belore and Buist [5].

For use in DERACS, the original LEAKR program has been modified such that it only calculates an instantaneous release rate given the commodity properties, the puncture type and location, and the commodity fill level. For release rate calculations in DERACS, only horizontal insulated or uninsulated, cylindrical tanks are considered and punctures are assumed to be round with random petals jagged in. The program no longer performs the time integration of the release with the prediction of the time to empty for the tank. The time integration function is performed by the DERACS simulation module using the results obtained from the modified LEAKR over a series of time steps during the accident simulation.

Flammable Liquid Spill Growth

Flammable liquid spills are important because of the fire hazard to neighbouring tanks and structures. For the present simulation it was desired to select a spill model that could be used to simulate fire induced ruptures of tanks as well as the thermal radiation hazards to remote targets.

Several models exist for predicting spill sizes as a function of time for any given release. For example Raj [15] developed a model for instantaneous spills. His model is based on the assumptions that the ground is flat, smooth and impermeable. This model tends to give large diameter, shallow pools and therefore is conservative for estimating pool sizes. However for large shallow pools, the fire durations will be short. For the present purposes, it was desired to have pools that burn for significant periods of time (20 to 60 minutes) because these are the fires that can lead to thermal ruptures of tanks later on in an accident. For example, full scale fire tests of unprotected rail tank cars carrying propane have been conducted by Phillips [16] and in these tests the tanks ruptured after 24 minutes of fire engulfment.

For time dependent spills Cline and Koenig [17] developed a model for transient pool growth. This model is based on mass conservation considerations and can account for ground seepage and other fuel consuming actions. However this model requires that a uniform pool depth be specified.

For the DERACS simulation a simple pool model was developed based purely on mass conservation effects. No account has been made for momentum considerations which affect pool spreading rates. The model is based on the assumption that the ground takes up a concave shape in the region of the spill. One radius of curvature is used to describe the shape of the surface. In the model, the size of the spill is calculated as a function of the mass of liquid currently in the pool. The following expression for mass conservation applies for the case of spilled liquid:

$$M = M_s - M_a - M_e \tag{5}$$

where,

M = mass of liquid in the spill

M_s = mass of liquid spilled

M_a = mass of liquid absorbed by the ground

M_e = mass of liquid evaporated (and burned)

The volume of liquid in the spill is

$$V = M/\rho \tag{6}$$

$$= \pi \left(Rh^2 - h^3/3\right) \tag{7}$$

where,

R = local radius of curvature of the ground

h = pool depth at the pool centre

ρ = average liquid density

For typical spills $h < R$ and therefore the pool volume can be simplified and resulting pool depth and radius can be calculated directly, as expressed below:

$$h = \sqrt{V/(\pi R)} \tag{8}$$

$$r = \sqrt{2Rh} \tag{9}$$

where, r = the liquid spill radius

The various mass terms in equation (5) are calculated separately using a simple Euler type integration scheme.

The spilled mass is based on the puncture release models described in the previous section. The mass flow rate of liquid calculated from these models is assumed constant over a single time step and the resulting mass of spilled liquid is calculated as the product of the release rate and the time interval. The mass of liquid absorbed by the ground must be specified by some method and in the present study this effect was neglected. The mass of liquid evaporated is based on a constant pool surface regression rate based on experimental results of Hottel [18] for large pool fires involving hydrocarbon fuels. A single constant surface regression rate of 0.000083 m/s is presently used in the model. The mass of liquid evaporated in one time step is then:

$$M_e = \rho V_s \pi r^2 \Delta t$$

where,

V_s = surface regression rate (10)

Δt = time step

At present a single constant ground curvature of 2000m has been selected. With this curvature a liquid spill of 50000kg of hexane will result in an initial pool diameter of 19.5m and the fire will burn for approximately 26 minutes. An unprotected tank car engulfed in such a fire is likely to suffer a thermal rupture.

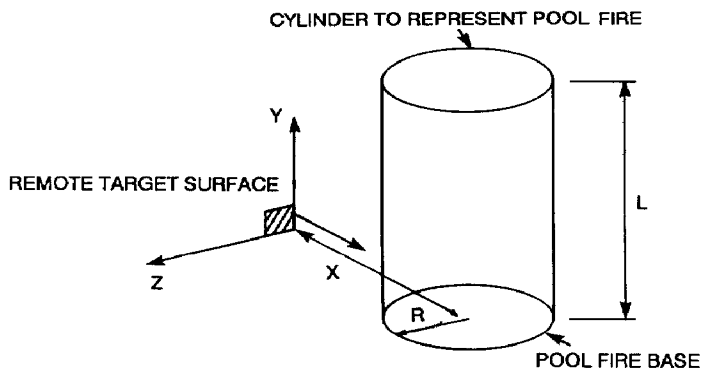

Figure 8 Model for Thermal Radiation from a Pool Fire to a Remote Target

Thermal Effects of Pool Fires

The thermal effects of pool fires are important because of the effect on objects that are impinged directly by the fire, and also on remote targets that are loaded by the thermal radiation emanating from the fire. In DERACS only direct fire impingement of tank cars is presently accounted for and this will be described in more detail in a later section. The model described here considers thermal radiation loads on remote targets.

Crocker and Napier [19] have shown that the thermal radiation from pool fires can be modelled by assuming the fire acts as a vertical right circular cylinder as shown in Figure 8. The radiation from the pool fire to the target can be calculated from the following expression for radiant exchange between surfaces separated by an absorbing intervening gas.

$$Q = F\,r\,E \qquad (11)$$

where,

Q = heat transferred by thermal radiation

r = atmospheric transmissivity

E = pool fire emissive power

F = surface to surface exchange factor

The pool fire emissive power is assumed to be 250 kW/m2 for pool fires greater than 50m in diameter. For smaller pool fires the emissive power is calculated by equation (12). This relation was based on data presented in Reference [20].

$$E = 250(1-e^{-.2Dp}) \qquad (12)$$

where,

Dp = pool fire diameter

An approximate expression for the atmospheric transmissivity was taken from Reference [21] and is shown below:

$$\tau = e^{(-7\times10^{-4}L)} \qquad (13)$$

where,

L = distance from the fire edge to the target (path length through air).

For this configuration the radiant exchange factor was compiled by Howell [22] and for the present case has been simplified to the following expression:

$$F = \frac{1}{S}\left\{1-\frac{1}{\pi}\left(d_1-\left(\frac{(H^2+S^2+1)}{\sqrt{B^2+4H^2}}\,Hd_3+Hd_2\right)\right)\right\} \qquad (14)$$

where,

x = distance from the pool centre

R = pool fire radius

L = pool fire height

$S = x/R$

$H = L/R$

$A = H^2-S^2+1$

$B = H^2+S^2-1$

$d_1 = \mathrm{acos}(A/B)$

$d_2 = \mathrm{acos}(1/S)$

$d_3 = \mathrm{acos}(A/SB)$

With these expressions it is possible to estimate the heat flux from the pool fire at different distances from the fire centre. In the present application it was desired to use these equations to estimate distances to specified levels of danger. Table 2 presents three levels of steady state fire damage reported in Reference [19] and used in the present model for describing pool fire thermal radiation hazard levels.

In the DERACS simulation graphical output, pool fire sites are shown with three levels of fire hazard as described in Table 2. These hazards are displayed as concentric rings centred at the pool fire centre.

HAZARD LEVEL	STEADY STATE HEAT FLUX	HAZARD DESCRIPTION
1	4.7 Kw/m^2	Human Pain
2	12.6	Wood Building Ignition after some time
3	37.8	Damage to other vessels

Table 2 Steady State Fire Damage Levels Used In DERACS

Plume and Puff Dispersion of Heavy Gases

At present DERACS can consider chlorine and propane and both of these are heavy gases. In the event of a puncture as a consequence of a derailment, it is important to show the extent of the dispersing gases that are released. In the event of a total loss of containment of a tank car, an instantaneous release will occur and a puff type dispersion model is needed. For a continuous type release, a plume model is needed.

The present simulation is a time integration through a derailment event. During this time integration, the release sources are varying in strength and therefore it was desired to use time dependent models for tracking plume and puff type releases of heavy gases.

Numerous dispersion models are available in the open literature. These various models range in complexity from simple Gausian type models to those which involve the solution of the 3-dimensional continuity, momentum and energy equations including the effects of turbulence. For the present purposes it was desired to have a time dependent type model that can run quickly on a micro-computer. For this reason the Box type model was selected, which is accurate for the near field of a release of heavy gas.

In a Box type model, the heavy gas cloud is modelled as a vertical cylindrical box of radius R and height H as shown in Figure 9. This cylinder is assumed to contain gas of

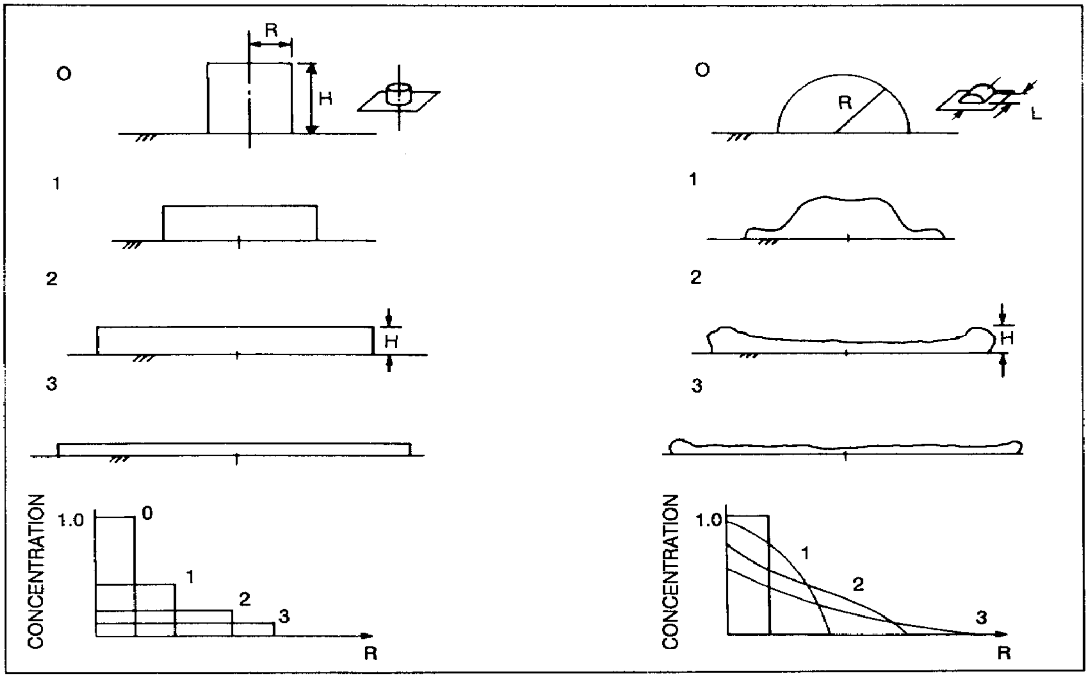

Figure 9 Sketch Showing box Model of Dispersing Puff in Comparison with Properties of Actual Puff (from ref. [23]).

uniform concentration. As the box moves down wind, its dimensions change due to air entrainment, gas expansion and gravitational slumping. As air is entrained, the gas concentration in the box is reduced. Air is entrained through the top and sides of the box. The gas cloud is also assumed to have heat transfer interaction with the ground and the surroundings.

At present both plume and puff releases are modelled in DERACS using the Box Puff Model of Meroney [23]. For a puff type release, the application of the Box Puff Model is straight forward. For a continuous release, a series of simple puffs are used. Each puff represents the quantity of gas released in one simulation time step (20 seconds). It should be noted that this type of approach is not very accurate and is likely to over estimate the rate of gas dispersion. Box Puff Models are developed based on the assumption that air is entrained through the sides and top of the cylindrical box. However, air entrainment for plumes is effected by the reduced air/gas interface area.

For the present version of DERACS, this inaccuracy in the modelling of plume dispersion has been accepted. This weakness in the model will be corrected in future versions of DERACS.

In DERACS, plumes and puffs are displayed as a coloured patch on the map. The size of the patch indicates the size of the area where the gas concentration exceeds some preselected value. For chlorine this level is the 0.000075kg/m^3 which is immediately dangerous to life and health. For propane the concentration was arbitrarily selected to be 0.06 kg/m^3.

Fire Impingement on Tanks and Thermal Ruptures

Fire impingement on tank cars is handled using the tank thermal computer model TANKCAR developed by Birk [24]. The tank car thermal model can simulate a long cylindrical tank filled partially with liquid and partially with vapour exposed to either an engulfing type fire, such as caused by a burning pool, or a torch type fire, such as that caused by a relief valve flare from a neighbouring tank. The model can account for the effects of a number of thermal protection devices such as pressure relief valves, thermal insulation, radiation shielding, temperature sensing relief valves, and novel internal protection devices including heat dissipating matrices. The model can simulate the effects of roll and pitch of the tank.

The overall thermal model is made up of a series of sub-models which represent the various processes taking place within the tank.

The flame-to-tank heat transfer sub-models can account for either an engulfing pool fire or a two-dimensional torch. The pool fire model accounts for thermal radiation and convection. The thermal radiation is calculated as a function of the circumferential position on the tank by accounting for the typical shape of large pool fires in the absence of cross wind effects. The convection calculations are based on empirical relations for convection to horizontal cylinders in a cross-flow. The torch sub-model is based on empirical relations for a jet impinging on a flat plate.

The temperature distribution in the tank wall and associated coverings is calculated using finite difference techniques. The finite difference solution accounts for pure conduction through the tank wall and insulating layers. The finite difference solution also accounts for the heat transfer from the fire to the tank outer surface, and from the tank inner surface to the lading. The inner surface heat transfer sub-models account for convection and radiation in the vapour space, and convection and boiling in the liquid region.

The thermodynamic process sub-model treats the lading as three distinct regions: the vapour space, the liquid boundary, and the liquid core. It is assumed that the vapour and liquid boundary (near wall and free surface) are in thermodynamic equilibrium and saturated. The core is assumed to be sub-cooled initially, but after some period of venting it reaches equilibrium with the liquid boundary and vapour space.

The pressure relief valve sub-model accounts for both the mechanical action of a relief valve and the fluid mechanics. Valve cycling effects on flow rates are accounted for by a steady state valve model which assumes the valve to be partially open, representing the reduced flow capacity during cycling. The valve flow sub-models can account for dry vapour flow and for frozen liquid flow.

The wall stresses are calculated at the point on the wall circumference which experiences the highest temperature, and includes pressure induced (hoop) stress and stresses due to radial temperature gradients in the tank wall. The tank failure analysis is based on the maximum normal stress theory of failure. Degradation in the wall material strength with increases in temperature is accounted for using available data for tank car steels.

The computer model is capable of predicting the tank internal pressure, mean lading temperatures, wall temperature distribution, relief valve flow rates, liquid level, tank wall stresses and tank failure, all as functions of time from initiation of the fire impingement. The model has been extensively validated (see Reference [24]) by comparing its predictions with the results of numerous fire tests involving full and fifth-scale rail tank cars exposed to engulfing fires. Figures 10 to 13 present one example of validation results showing comparison between TANKCAR predictions and actual test results for full scale fire tests. The Fire test data shown is from Reference [16].

Thermal Effects of Explosions/BLEVES

In the event of a thermal rupture or total loss of containment of a tank containing propane, DERACS assumes a fire ball type explosion will result. In the DERACS

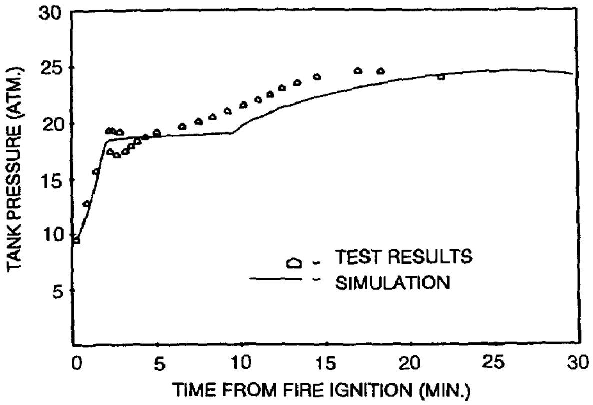

Figure 10 Predicted & Meas. Tank Pressure vs Time for Full Scale Tank Car, Propane, Engulfing Fire

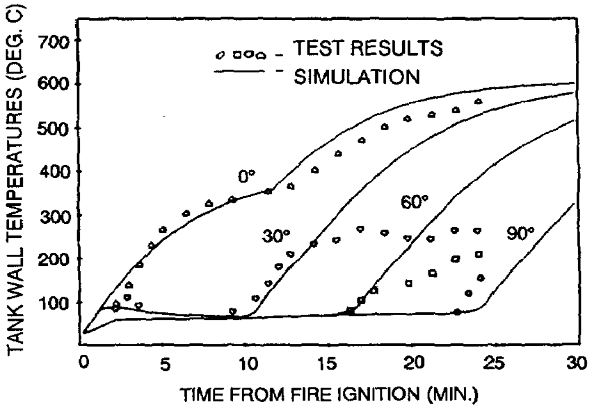

Figure11 Predicted & Meas. Tank Wall Temp. vs Time for Full Scale Tank Car, Propane, Engulfing Fire

simulation the resulting fire ball will have both blast and thermal effects of the surroundings. This section describes the techniques used to estimate the thermal effects of the explosion.

As discussed in Reference [25], the consequences of a total loss of containment of a pressurized flammable liquid depend on the conditions at release. The consequences range from a slow burn-off to a violent explosion and fire ball.

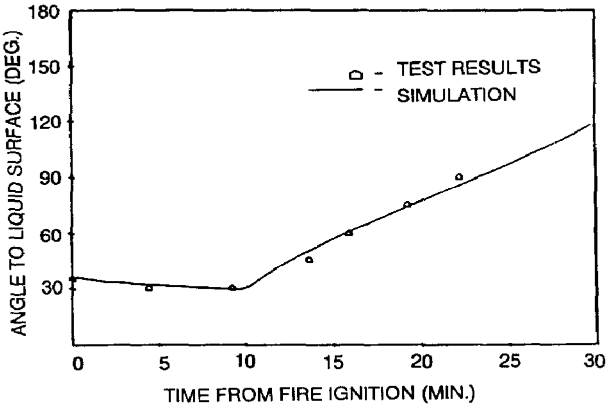

Figure 12 Predicted & Meas. Liquid Level vs Time for Full Scale Tank Car, Propane, Engulfing Fire

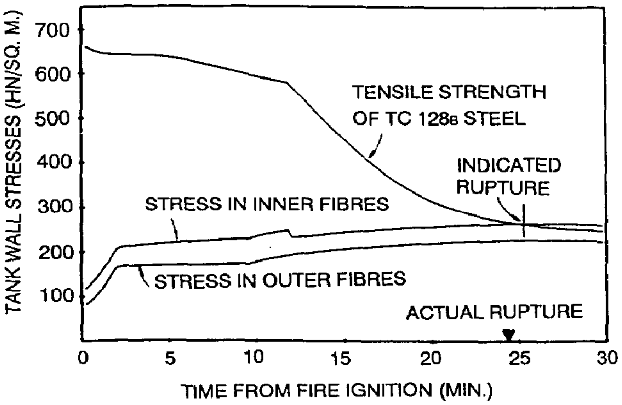

Figure 13 Predicted Tank Wall Stresses & Strength vs Time for Full Scale TankCar, Propane, Engulfing Fire

For the case of a car containing a commodity such as propane, a total loss of containment will result in a very rapid boil-off of part of the contents. The rapid flashing and the high exit velocities result in significant liquid droplet entrainment. In the case of a BLEVE (boiling liquid expanding vapour explosion), the boil-off is so rapid it acts like an explosion. The resulting cloud of vapour and entrained liquid droplets usually result in a large fire ball.

As discussed in Reference [25], it is difficult to estimate the amount of remaining liquid after the boil-off period. Reference [25] states that, if more than 35% of the lading flashes, it is likely that all of the contents will be consumed in a fire ball. If less than 35% flashes then some liquid will remain and will burn-off slowly. In DERACS it is assumed that all of the liquid contents will be consumed in the fire ball. The resulting fire ball diameter is calculated from Reference [20] using the following expression:

$$D_{max} = 5.33m^{0.327} \tag{15}$$

where,

m = fuel mass (kg)

D_{max} = the maximum fire ball diameter

This relation is based on experiments for fuel masses ranging from 3 - 31kg but the validity has been verified for much larger masses [20].

The fire ball will have a growth stage and a shrink stage and these stages will take some finite time to develop. The fire ball's effective duration as described in [20] can be estimated from the following expression:

$$t_a = 0.923m^{0.303} \tag{16}$$

where,

m = fuel mass (kg)

t_a = time (sec)

During the development of the fire ball, the diameter grows and the fire ball rises due to buoyancy. In the present situation it is desired to calculate a thermal radiation dose resulting from the fire ball. Therefore it has been assumed that the fire ball has a diameter Dmax and is located with its centre at ground level. The fire ball duration is assumed to be t_a.

The emissive power of the fire ball is calculated for Reference [20] using the following expression:

$$E = E_{max}(1-e^{-bD_s}) \tag{17}$$

where,

E_{max} = 469 kW/m^2

b = .18 m^{-1}

D_s = fire ball diameter

The flux reaching a remote target can now be easily calculated from the following:

$$Q = E\,r\,F \tag{18}$$

where,

r = atmospheric transmissivity
F = radiant exchange view factor

As with the case of the pool fire radiation, the atmospheric transmissivity is calculated from Reference [21] using the following expression:

$$r = e^{(-7\times10^{-4}x)} \tag{19}$$

where,

x = distance from the fire edge

The radiant exchange view factor was based on a sphere radiating to an object oriented towards the fire ball at ground level and as reported in Reference [21]. This expression is shown below:

$$F = \frac{(H/D_s+0.5)}{4\{(H/D_s+0.5)^2+(R/D_s)^2\}^{3/2}} \tag{20}$$

where, R = radial distance of target from point directly below fire ball

H = height of fire ball centre

The radiation dose is calculated from the simple expression:

$$\text{Dose} = Qt_a \tag{21}$$

As with pool fires, three hazard levels are calculated for thermal radiation from fire balls. Table 3 presents the dose criteria used for the displayed hazard levels. Dose levels and their effects were taken from Reference [19].

Blast Effects of Explosions/BLEVES

When an explosion or BLEVE occurs, a pressure disturbance will propagate outwards from the blast centre. This pressure disturbance or over-pressure is followed

HAZARD LEVEL	DOS kJ/M^2	DESCRIPTION
1	375	Third Degree Burns
2	250	Second Degree Burns
3	125	First Degree Burns

Table 3 Thermal Hazard Levels for Fire Ball Thermal Radiation

by a rush of high velocity air. The combination of the over-pressure and air can be very destructive to property and life. In DERACS, if an explosion occurs the level of the blast hazard and the distance from the centre of the explosion are estimated.

In the explosion calculation, the initial mass of the explosive is assumed to equal the total mass of lading in the tank. This mass is then converted to an equivalent mass of TNT using data from Reference [26]. Table 4 contains a partial listing from the above reference.

The equivalent TNT mass is then reduced by multiplication of an explosion efficiency for unconfined vapour cloud explosions. As discussed in Reference [27], this explosion efficiency varies widely for unconfirmed vapour cloud explosions. As shown in

COMPOUND (1kg)	EQUIVALENT TNT MASS (kg)
methane	11.95
ethane	11.34
propane	11.07
butane	10.91
ethylene	11.26

Table 4 Conversion Factors for TNT Equivalency (from Ref. [26])

Reference [27], the range of efficiencies is between 0.05 and 0.65. The efficiency of the blast is determined by the vapour cloud conditions at the time of ignition.

In DERACS, it is assumed that, if a BLEVE occurs, the explosive efficiency will be high (ie. = 0.65) while if a BLEVE is unlikely, the efficiency will be low (ie. = 0.10). These explosion efficiencies are used to estimate explosion hazards.

Based on the TNT equivalent mass and the explosive efficiency, it is possible to estimate the free field over-pressure as a function of distance using the following empirical relation from Reference [26]:

For display of explosion hazards DERACS uses three preselected free-field over-pressures to calculate hazard distances from the centre of explosion.

$$\frac{P_o}{P_a} = \frac{808\,[1+(Z/4.5)^2]}{\sqrt{1+(Z/.048)^2}\;\sqrt{1+(Z/.32)^2}\;\sqrt{1+(Z/1.35)^2}} \qquad (22)$$

where, P_o = fire field overpressure

P_a = ambient pressure

Z = scaled distance

$$= \left[\frac{P}{P_o}\right]^{0.333} \left[\frac{T_o}{T}\right]^{0.333} \frac{d}{W^{.333}}$$

and, d = actual distance

W = TNT equivalent mass

T_o and P_o = reference atmospheric temperature and pressure

TYPE OF DAMAGE	OVER-PRESSURE (mbars)
Windows shattered, plaster cracked; minor damage to some buildings	35-75
Personnel knocked down	70-100
Failure of wooden or asbestos siding for conventional homes	75-150
Failure of walls constructed of concrete blocks or cinder blocks	125-200
Self-framing paneled buildings collapse	200-300
Oil storage tanks ruptured	200-300
Serious damage to buildings with structural steel framework	300-500
Eardrum rupture	350-1000
Reinforced concrete structures severely damaged	400-600
Railroad cars overturned	400-600
Probable total destruction of most buildings	700-800
Lung damage	2000-5000
Lethality	7000-15000

Table 5 Blast Damage—Side on Over-Pressure Correlation (Large Explosion)

Over-pressure levels and their associated damage estimates are presented in Reference [26]. A partial listing from Reference [26] is summarized in Table 5.

Presently, in DERACS, the three levels of damage selected are: Lethal (7000m bar), Destruction of Buildings (700m bar), and Storage tank ruptured (200m bar). When an explosion is indicated (total loss of containment of a tank containing propane), the lading mass is converted into an equivalent TNT mass and an explosion efficiency is determined based on the temperature of the lading at the time of containment loss. DERACS then determines the three distances to the above stated hazard levels and these are displayed using the post-processor.

CONCLUSIONS

A prototype computer simulation program (DERACS) has been developed for predicting some of the major consequences associated with train derailment accidents where dangerous commodities are involved. The simulation sub-models are based on models that have been previously published in the open literature.

The present version of DERACS is limited in scope and is intended for demonstration purposes. Possible applications include risk studies, accident reconstruction, response personnel training and tactics development and possibly on-site tactical assistance. However, before the program can be used for any applications, significant further development is required.

The next phase of development will involve sub-model testing and refinement. Depending on the targeted applications, some sub-models will be replaced with more sophisticated approaches, and some new sub-models will be added for consequences that are presently not accounted for, such as tank rocketing.

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