# A COMPUTER SIMULATION OF A DERAILMENT ACCIDENT PART II - SAMPLE SIMULATION

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# ABSTRACT

DERACS (Derailment Accident Computer Simulation) is a computer program developed to simulate some of the consequences of train derailment accidents involving fires and accidental releases of dangerous commodities. The present paper shows the results of two sample simulations that were performed using the prototype DERACS program. Technical details of the DERACS program are presented in Reference [1].

Because of the limitations of the prototype version of DERACS the sample simulations only approximate the Mississauga rail accident of November 1979. The results presented have not been validated in any way and should not be considered as accurate representations of the Mississauga accident. They were generated for discussion purposes only so that future applications of the DERACS program could be illustrated, and areas within DERACS requiring further development could be identified.

# INTRODUCTION

The DERACS computer program was developed as a tool for analysis of train derailment accidents where releases of commodities have resulted in fires, explosions and toxic plumes. The program was developed with the hope that it could become a valuable tool for analysis and training purposes, and possibly it could become an on-line tool for assisting response personnel in the future.

The organization and the technical basis for the various models in DERACS were described in Reference [1]. DERACS is based on a series of sub-models, all of which

is either available in the open literature or was developed for DERACS. These 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

The overall DERACS program consists of a pre-processor, a simulation module, and a post-processor. The pre-processor is used for data input which includes a map of the area surrounding the derailment, the derailment point, the train consist and its condition at the point of derailment, and any pertinent atmospheric data at the time of the derailment.

The simulation module carries out the time integration of the accident from the time of derailment to the time when the last tank has emptied safely or BLEVE'd (boiling liquid expanding vapour explosion). Further technical details of the various sub-models used in the simulation module can be found in References [1] and [2].

The post-processor is used to generate a graphic summary of the derailment accident simulation. This graphic summary shows a colour, plan view of the accident site including vehicle placement, vehicle puncture status, spills, fires, blast and thermal



Figure 1 Sketch of Mississauga Derailment Scene (from Ref. [3])

Derailed Car Number	Contents	Insulated	Punctured
1	toluene		
2	box car		
3	caustic soda	1	
4	caustic soda	l l	
5	caustic soda		
6	caustic soda		
7	chlorine	Yes	Yes
8	propane	Yes	Explosion
9	styrene		
10	styrene		
11	styrene	1	
12	propane	No	Explosion
13	propane	No	Explosion
14	propane		
15	toluene	1 1	Yes
16	toluene		?
17	propane		
18	propane		
19	propane		
20	propane		
21	propane		
22	propane		
23	propane		
24	toluene		

## Table 1 Summary of Derailed Cars and their Contents

hazard distances and toxic plume hazard distances. Further details of the pre-and post-processors can be found in Reference [2].

As stated earlier, the purpose of this paper is to present a sample simulation using the DERACS computer program. The specific example considered here is the Mississauga derailment of 1979. The results presented in this paper were generated using the prototype version of DERACS.

## THE MISSISSAUGA DERAILMENT

As reported in Reference [3], the Mississauga derailment occurred on November 10, 1979 and involved a train consisting of 106 cars. The derailment was initiated by the 33rd car in the consist and a total of 24 cars were derailed. A total of 21 were tank cars with 19 of these carrying dangerous goods including chlorine, propane, toluene, caustic soda, and styrene. The train speed was at the time of the derailment was not determined specifically but witnesses and estimates place the speed at between 70 and 100 km/hr. Figure 1 presents a sketch of the derailment scene from Reference [3]. Table 1 presents a listing of the derailed cars and their contents.

The 7th derailed car contained chlorine and this car suffered an impact or ferric chloride reaction inducted puncture 0.76m in diameter. As a result of this rupture,

chlorine was released into the environment. Other cars sustained impact induced ruptures resulting in the release of flammable liquids. Of the derailed cars, those cars with bottom fittings (all of the type 111 cars except car #24) had the fittings sheared off during the accident and their contents were released as a result.

From the photographs shown in Reference [3], an intense fire was located at or near the 15th derailed car which contained toluene. This and other fires were likely the cause of the thermal ruptures of the 8th, 12th and 13th derailed cars which carried propane. The explosions of these propane cars resulted in extensive damage to neighbouring properties. At least one of the explosions occurred very early on, which leads to the conclusion that it was an impact-induced rupture. The explosions also resulted in large pieces of the tanks being thrown long distances (over 2km).

The above facts were used to formulate the input to the sample simulations performed using DERACS. Because of certain limitations of DERACS, some simplifying assumptions were required.

#### SIMULATION INPUT

At present DERACS is capable of simulating the derailment mechanics of up to 40 cars; where 8 can be tank cars carrying chlorine, propane or hexane. In order to perform a simulation of the Mississauga derailment, it was necessary to extract a subset of the actual accident. This subset was selected as a reasonable representation



Figure 2 Approximate Map of Mississauga Area Created by DERACS Pre-Processor

of the Mississauga accident while also fitting within the constraints of the present version of DERACS.

The Mississauga derailment occurred at Mavis Road in the city of Mississauga. An approximate map of the surrounding area (10 km by 10 km) was entered using the DERACS pre-processor and is shown in Figure 2. This map does not contain all of the details of the area but does show the approximate location of water, forest and inhabited areas as well as roads and rail lines. The DERACS pre-processor can be used to enter more detail than shown in the global view of Figure 2. Figure 3 shows the DERACS graphics key page which defines various symbols.

The wind speed was reported in Reference [3] to be 28 km/hr. This was entered with an assumed atmospheric pressure of 101.3 kPa and wind direction coming from the North West. An assumed air temperature of 10 deg C was used.

With DERACS, it is possible to predict the vehicle placement using the derailment mechanics simulation. By selecting the appropriate option, it is possible to bypass the derailment mechanics simulation and input the vehicle placement and rupture status directly. The bypass of the derailment mechanics simulation is practical for a response team at the site of an accident where the location of vehicles and punctures is known. In such a situation DERACS could be run to give a possible view of what to expect for the next few hours in the accident. However, before this can be done, significant further development and validation is needed.

VENICLE			
LOCOMOTIVE BOX	CAR . PROPANE	CHLORINE HEXAME	
TRACK	VENICLE STATE		
	Rolled		
	Impact Rupture	Plane	
ROADS	Thermal		
Large	Rupture	Puff	
Hedium -	Burning	Burning	
Small		Flare	
	EXPLOSION BLAST	EXPLOSION THERMAL	
	Hazard Level(TBD)		

Figure 3 DERACS Graphics Key Page

Two simulation cases were considered. The first case uses the derailment mechanics simulations while the second bypasses the derailment mechanics simulation.

# SIMULATION CASE 1

For Case 1 (derailment mechanics used to predict vehicle placement), a train consist of 36 cars was used including 8 tank cars. The consist was made up as shown in Table 2. In the sample simulation, the commodity hexane was substituted for toluene. This was necessary because the present version of DERACS can only consider chlorine, propane and hexane. Hexane was used as a substitute for toluene

Derailed Car Number	Simulation Car Number	Simulation Car Type	Protection
-	1	-	
1	2	-	
2	3	-	
3	4	-	
4 E	5	-	
5	5	-	
0	7	- - blavina	inculated
, ,	8	chionne	insulated
8	9	propane	Insulated
9	10	-	
10	11	-	
11	12	-	
12	13	propane	
13	14	propane	
14	15	propane	
15	16	hexane	
16	17	hexane	
17	18	propane	
18	19	-	
19	20	-	
20	21	-	
21	22	-	
22	23	-	
23	24	-	
24	25	-	
- 1	26	-	
-	27	-	
-	28	-	
-	29	-	
-	30	-	[
-	31	-	
	32	-	
	33	-	
-	34	-	
_	35	_	
_	36		
l			

 
 Table 2
 Summary of Consist Used in DERACS Simulation of Mississauga Derailment
 because, like toluene, hexane is a flammable liquid at atmospheric pressure. If hexane or toluene are spilled that could result in a pool fire. For all tank cars, it was assumed that they were filled to 90% capacity and their initial temperature was 10 deg C.

The derailment point was located at the intersection of Mavis Road and the rail line. The rail line was assumed to be straight track at the derailment point. The first truck of simulation car #4 was assumed to be the derailment initiator.

As stated in Reference [3], the train speed at the point of derailment was not known for certain. As a result a number of simulation runs were performed using different train speeds. It was found that a train speed of 100 km/hr gave a reasonable derailment scene, with very good correlation, to the actual derailment scene. In this case it was considered important to be able to predict the correct number of derailed cars, and the total area covered by the derailed vehicles.

#### SIMULATION CASE 2

For this simulation case, the derailment mechanics simulation was bypassed and the placement of vehicles and their puncture status was input using the pre-processor.

Figure 4 presents the assumed vehicle placement as based on Reference [3]. As shown on Figure 1, 24 cars have been placed in positions which approximate the actual resting places of the derailed cars in the Mississauga accident. There were actually 21 tank cars among the derailed cars but, because of the present limitations of DERACS, only 8 tank cars are shown in Figure 4. For impact-induced ruptures, it was assumed



Figure 4 Assumed Vehicle Placement for Case 2: (derailment mechanics simiulation bypassed

that car 8 (chlorine) was punctured and cars 9 (propane), 16 and 17 (hexane) sustained total loss of containment.

# SAMPLE SIMULATION RESULTS

As stated above, two sample simulations were performed. The first case included a simulation of the derailment mechanics while the second case had the vehicle placement and ruptures as input. The results of these two simulations are presented separately.

### Case 1 - Simulation of Derailment Mechanics and Resulting Consequences

This case involved the simulation of the derailment mechanics as well as the simulation of the resulting consequences. Figures 5 and 6 shows a plan view of the derailment scene as predicted by the DERAIL module of DERACS. The DERAIL module is described in detail in Reference [3].

The important result to note is that the prediction shows that 24 cars have left the track which is in excellent agreement with the actual Mississauga derailment. The predicted total length of the track involved is approximately 140 m which is also in very good agreement with the actual accident.

As a result of the simulation, it was predicted that three impact punctures resulted including two of the propane cars and one of the hexane cars. This is indicated in Figure 6.



Figure 5 Predicted Vehicle Placement for Case 1: (zoom level 2)

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Figure 6 Predicted Vehicle Placement for Case 1: (zoom level 3)

Note that this simulation cannot account for the loss of bottom fittings which had a very significant effect in the Mississauga accident. The puncture of the hexane car results in a spill of flammable liquid and the propane car punctures result in heavy gas plumes. The present version of DERACS handles a leak of propane as a heavy gas dispersion problem and not as a local fire or explosion. For further details of the basic assumptions used in determining consequences, the reader is directed to Reference [1]. If a propane tank suffers a total loss of containment then it is assumed that an explosion will result. The simulation did not predict the puncture of the chlorine car which occurred in the actual accident. Following the derailment mechanics simulations, the DERACS main simulation program was used and the results can be summarized as follows:

The hexane spill resulted in a fire that engulfed one unpunctured propane car. Two plumes issued from the punctured propane cars. As the simulation progressed, the fire slowly burned itself out and the pool fire diameter decreased in size until the fire-impinged tanks were no longer impinged by fire. As a result, no thermal ruptures were predicted. The heavy gas plumes dispersed downwind. For this simulation the most significant event was the release of the propane gas as both an explosion and toxic hazard. Figures 7 to 11 show the derailment scene at various times during the simulation.

#### Case 2 - Input of Vehicle Placement and Simulation of Resulting Consequences

In this sample simulation, the vehicle placement was provided as input along with the location of punctures. Figure 4 shows the assumed placement and the assumed punctures were described in an earlier section. The DERACS simulation software was used to simulate the consequences of the assumed initial conditions. The results of this simulation can be summarized as follows.

The total loss of containment of the propane car resulted in an explosion and fire ball. Because the loss of containment occurred early on in the accident, the propane lading had not reached a high enough temperature for a BLEVE to be predicted. As a result, the total loss of containment resulted in a comparatively small explosion and fire ball. The resulting thermal and blast loads resulted in the destruction of nearby buildings as indicated by the hazard zones.

The puncture of the chlorine car resulted in the release of chlorine gas into the environment. This plume drifted downwind for some distance at lethal concentrations. The total loss of containment of the hexane car resulted in a large pool fire that initially



Figure 7 Case 1 Simulation Results at 0.3 min. (zoom level 3)



Figure 8 Case 1 Simulation Results at 3.3 min. (zoom level 2)



Figure 9 Case 1 Simulation Results at 3.3 min. (zoom level 1)



Figure 10 Case 1 Simulation Results at 9.7 min. (zoom level 1)



Figure 11 Case 1 Simulation Results at 20.7 min. (zoom level 1)

engulfed or partially engulfed several propane cars. As the fire burned itself out, the pool fire diameter decreased and slowly the number of tank cars impinged by fire were reduced. However at 24 minutes into the simulation, one of the uninsulated tank cars experienced a BLEVE. This BLEVE caused thermal and blast loads to a large area. Figures 12 to 16 present views of the simulation at different times.

## DISCUSSION

The previous examples show some of the capabilities of the prototype version of DERACS. As expected, there are differences between reality and simulation. However, considering the limitations of the present version of DERACS, the results are very interesting. The derailment mechanics simulation was very accurate at predicting the total number of cars derailed and the length of the track region affected by the derailed vehicles. This was a function of the assumed train speed at the time of the derailment. However, the predicted final resting place of the vehicles were not in very good agreement with the actual accident. The actual cars were spread out farther and this would result in less interaction between the cars during the remainder of the simulation. Reasons for these discrepancies are not clear at this time and it is evident that the derailment mechanics simulation model requires further development and validation.

The derailment mechanics routines were not very successful at predicting the location or the numbers of punctures and this resulted in predicted consequences that differed considerably from those observed in the Mississauga derailment. For example, there was no predicted release of chlorine and no predicted thermal ruptures for the simulation including the derailment mechanics. It should be noted that the present impact rupture routines are very crude such that they could run quickly on the IBM/AT machine. The impact rupture routines require further development as do the derailment mechanics routines if more accurate and realistic results are to be obtained in the future.

When the vehicle placement and puncture locations were entered as input the simulation was more realistic. This is an obvious result since adding more information as input naturally results in better output. However, it should be recalled that only the vehicle placement and locations of punctures were input. No data pertaining to release rates, or pool fire sizes were input. All of these variables were handled using the DERACS sub-models.

It should also be remembered that only 8 tank cars were included in this simulation, accounting for the small numbers of spills, fires, explosions and releases. As DERACS is developed, it will be able to handle a larger number of tank cars and the number of events occurring in the simulated accidents will increase rapidly because of the larger number of possible vehicle interactions. Future versions of DERACS could also include more commodities and additional tank types.



Figure 12 Case 2 Simulation Results at 0.3 min. (zoom level 3)



Figure 13 Case 2 Simulation Results at 0.3 min. (zoom level 2)



Figure 14 Case 2 Simulation Results at 0.7 min. (zoom level 2)



Figure 15 Case 2 Simulation Results at 5.7 min. (zoom level 2)





A prototype derailment accident computer simulation program has been developed. The program has been used to simulate parts of the Mississauga train derailment.

The derailment mechanics module was able to predict the number of vehicles derailed and the approximate track area affected by the derailment. It was not able to accurately predict vehicle placement or the location of impact-induced ruptures. As a result the remaining simulation of the accident consequences did not agree well with the Mississauga accident. However, the results were not unrealistic. Further development is required if accurate predictions of vehicle placement and rupture are to obtained in the future.

As a predictive tool, DERACS gave better results when the derailment mechanics routines were bypassed. The resulting consequences were in close agreement with the actual Mississauga accident. The simulation results included a toxic chlorine cloud, an explosion of a ruptured propane car, pool fires and a thermal rupture of a propane car resulting in a BLEVE. The number of events was smaller than the actual accident because only 8 tank cars could be considered by the present version of DERACS.

The results of this development work indicate that the DERACS concept is feasible. As a minimum, DERACS can be used as a derailment accident simulator. Such a simulator could be valuable for the purpose of response team training. It could also prove useful in creating accident scenarios which could be used to test response procedures or future accident response expert systems.

# REFERENCES

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