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Mechanical Properties of Tank Car Steel at Flame Temperature and Modeling of Failure - A Review

Report No. WF_5792872

C. Hari Manoj Simha

January 2016

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by

C. Hari Manoj Simha

EXECUTIVE SUMMARY

A review of the mechanical response of two tank-car steel alloys, TC 128 Grade B, and ASTM 516 Grade 70, when exposed to high-temperatures during engulfing pool fires is presented in this work. In addition, this report reviews the state-of-the-art in Computational Fluid Dynamics (CFD) based modeling of pool fires and the state-of-the-art in failure modeling of tank car steels.

With regards to mechanical response at high temperatures, other than limited data on softening of strength as a function of temperature, no detailed and systematic studies were found in the literature. Accordingly, it is recommended that:

1. A comprehensive testing programme, per ASTM E21-09 standard, be carried out to systematically evaluate the tensile stress-strain response of the two alloys. It is also recommended that a judicious selection of new and ex-service samples be chosen for the testing. It is also recommend that for all of the samples, if feasible, the samples be machined from the cylindrical body of the shell after the forming operation; this will account for the work hardening of the forming operation. It is also recommended that some samples be selected from the head of the tank car as these are work hardened differently than the cylindrical part of the shell. Suggested temperature range is -40 ^{o}C to 800 ^{o}C.

2. A detailed microstructural evaluation of the tested samples be carried out and, if feasible, an evaluation of the high-temperature microstructure be carried out. A hot-stage in a Scanning Electron Microscope will be required for this purpose. One reason for this recommendation is to assess the microstructural changes associated with high temperatures. It is hoped that a study of the high-temperature microstructure may suggest modest modifications to initial alloy chemistry or processing that may lead to enhanced properties.

3. A comprehensive testing programme, per ASTM 139-11 standard, be undertaken to measure rupture times during creep of both the alloys. Again, a selection of new and ex-service samples should be chosen for testing. Suggested temperature range is 500 ^{o}C to 800 ^{o}C.

4. In all of the above testing, it is recommended that consideration be given to future potential for probabilistic models. Accordingly, based on an assumed confidence interval, a sufficient number of tests should be conducted so as to be able to construct probability distribution functions of the material properties.

With regard to CFD-based modeling, techniques for multi-physics modeling are being developed and are robust enough to admit application to study the problem under consideration. One of the main reasons for carrying out the CFD computations is to predict the magnitude, spatial and temporal extent of the flame (the thermal load), which is a function of the lading and other environmental factors. However, based on our experience, such models require significant computational power and involve computations which require solution times of days. It is therefore recommended that existing engineering models be calibrated using the results of the forthcoming experiments to be carried out at National Research Council (NRC). Alternatively, if the existing models are found wanting, validate CFD simulations using results of the forthcoming experiments and then develop engineering models using a limited set of CFD simulations to enhance the existing models (or develop newer ones).

The thermal load, in turn, serves as an input to the solid-mechanics computations which can be used to predict the failure event for the tank car. In this regard, based on the mechanical testing recommended above, it is possible to make predictions using the so-called damage-mechanics-based techniques. Again, it is recommended that existing engineering models such as the Insulation Defect Analyzer (IDA) be used to evaluate the failure times and model the failure event observed in the NRC tests. In the event that the predictions of IDA are overly conservative or un-conservative, the more involved damage-mechanics approaches may then be adopted.

LIST OF ABBREVIATIONS

AAR	Association of American Association of Railroads
AFFTAC	Analysis of Fire Effects on Tank Cars
BLEVE	Boiling Liquid Expanding Vapor Explosion
CFD	Computational Fluid Dynamics
IDA	Insulation Defect Analyzer
LNG	Liquefied Natural Gas
LPG	Liquefied Petroleoum Gas
MHIDAS	Major Hazard Incident Data Service
MPC	Materials Properties Council
NRC	National Research Council
PLG	Propane Liquefied Gas
PRD	Pressure Relief Device
RD	Rolling Direction
RT	Room Temperature
TD	Transverse Direction

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INTRODUCTION

Tank cars fabricated using medium-carbon, alloyed steels are routinely used to transport hazardous fluids. For flammable hydrocarbon ladings, such as crude oil, natural-gas condensates, ethanol or propane, during an accident (or derailment) there is potential for discharge owing to the failure of valves or puncture of the tank shell because of impact or impact with ruptured fragments. Accordingly, there is an increased risk of pool or jet fires. Instances of tank-car railroad accidents involving crude oil are in Lac-Mégantic, Quebec, Anon (2013b); Casselton, North Dakota, Anon (2013a); and Finland, Lautkaski (2009). In all of the cited accidents, a post-crash pool fire resulted. Furthermore, for instance, in the Lac- Mégantic accident, 47 lives were lost.

Statistics for the period of 1986 show that 16% of accidents involving freight trains conveying Liquified Petroleum Gas (LPG) in Great Britain resulted in a spill leading to fires, Lees (2012), As stated by D'Aulisa et al. (2014), analysis of tank-car accidents in databases such as Major Hazard Incident Data Service (MHIDAS), suggests that approximately 30% of accidents lead to Boiling Liquid Expanding Vapor Explosions. The MHIDAS, Anon (2003), is a international database of accidents and has been maintained since 1986 by the United Kingdom Atomic Energy Authority.

Pool fires, irrespective of whether the fire engulfs the car or is at distance from the car, subject the car to a thermal load (in addition to the internal vapor pressure). This load is more severe in the case wherein the tank is engulfed by the fire.

From the standpoint of risk assessments for tank car designs, regulatory purposes, or design reviews, computational methods involving Computational Fluid Dynamics (CFD) for the fire modeling, and finite element-based solid mechanics for the failure modeling of the tank car may be used. In parallel, under the auspices of Transport Canada, the National Research Council of Canada is carrying out a pool fire testing programme. For making failure predictions, mechanical properties at high temperature are crucial. Accordingly, Transport Canada has tasked CanmetMATERIALS, Natural Resources Canada to carry out a review and based on identified gaps make recommendations on mechanical testing required to make failure predictions.

Additionally, after a review of the state-of-the-art of the CFD and solid-mechanics based failure modeling, recommendations for further modeling efforts were requested.

The present review is concerned with pool fires and the effects of the consequent thermal loads on the structural integrity of the tank car.

SCOPE AND OBJECTIVE

The scope of the present review is restricted as follows:

- Two materials: TC 128 Grade B, and ASTM 516 Grade 70, medium-carbon, alloyed steels.
- Only effects of pool fires on the mechanical and failure properties are considered. That is, effects of jet fires or failure due to impacts and rupture fragments are not within scope.

The tasks of the present review are:

- Review literature and identify gaps in mechanical testing and assessment of the two above mentioned steels with regards to carrying out finite element simulations of failure of the tank cars under pressure and thermal loading. A key output of the finite element simulations are predictions of the time at which failure will occur from the start of the thermal loading.
- Review literature on the Computational Fluid Dynamics (CFD) simulations that are used to model the thermodynamic evolution of the fluids (liquid + vapor) in the tank. It is the CFD based simulations that provide a thermal load (temperature history) which serves as an input to the solid-mechanics-based failure modeling.
- Review literature on the Solid Mechanics simulations that are used to model the high-temperature failure of the tanks shells. The items in the first task of the present review serving as inputs to these failure simulations.

- Make recommendations on a future course of action for the testing required for the solid-mechanics modeling, and a future course of action for the CFD and solid-mechanics modeling based on the above reviews.

POOL FIRE CHARACTERISTICS

In the event of a discharge of flammable lading from a tank car over water, land or snow, a pool forms and may ignite leading to a pool fire. A pool fire is defined as a “turbulent diffusion fire burning above a horizontal pool of vaporising hydrocarbon fuel, where the fuel has zero or low initial momentum.” – see www.hse.gov.uk/offshore/strategy/pool.htm.

Steinhaus et al. (2007) have reviewed recent research on and modelling of pool fires. They list the key physical characteristics that affect the burning behavior and consequently the resultant thermal loading :

- Pool geometry (diameter, depth, substrate. In the Canadian context, substrate includes snow)
- Fuel composition (lading mix)
- Ventilation conditions (wind models are characterized using the Froude number)
- Surrounding geometry (open air, proximity of structures)
- Emissivity of the fire

Depending on the above factors (a key dimensionless number in this context is the Froude number which is the ratio of the inertial force to the weight), it is possible to estimate the heat flux as a function of time and space using either engineering models (see, for instance, Fay (2006)) or using compressible CFD (see, for instance, the review by Steinhaus et al. (2007)). Thermal radiation effects of pool fire has also been studied; see Mudan (1984) or McGrattan et al. (2000), for a review

THERMAL EFFECTS OF POOL FIRE AND TESTING

In the event of a pool fire there are four possible scenarios with regards to interaction with tank cars. These scenarios are whether the fire is engulfing or non-engulfing and toppled (or upright) state of the tank. Whether the tank car is toppled or not is significant with regards to the location of the pressure-relief-device (PRD) relative to the vapor space, which in turn depends on the fill level of the tank. In the toppled case, the PRD may be in contact with the liquid and not function to relieve the pressure, in which case a Boiling Liquid Expanding Vapor Explosion (discussed later) may be unlikely, but a high temperature induced failure (heat induced tear) may result.

Whether a fire is engulfing or non-engulfing affects the rate and nature of thermal flux acting on the tank car; time and temperature then influence the failure and consequently a good estimate of the thermal flux history is central to accurate modeling of the failure of the tank.

Engulfing fire on an upright or toppled tank: The tank wall is heated through a combination of convection to the surface of the shell (or jacket in the event the tank has thermal protection), radiation in the vapor space and conduction into the fluid, which serves to take heat away from the shell of the tank with enhancement of heat transfer usually through film or nucleate boiling. In general, from experiments measurements of temperature in the vapor-wetted regions are between 550-750 ^{o}C and the liquid-wetted regions are below 130 ^{o}C (Manu (2008), has reviewed several relevant engulfing experiments).

It is also possible to prevent a failure or explosion in a fully engulfing fire if the tank becomes shell-full due to the thermal expansion of the lading as surmised in the accident in Finland, Lautkaski (2009).

In addition to the experiments reviewed in the thesis of Manu (2008), which include several scales, full-scale experiments with and without thermal protection of the cars were carried out using Liquid Petroleum Gas (LPG), see Anderson & Norris (1974) and Townsend et al. (1974). Metallurgical assessments from these tests led to the specification of plate and torch test which are embedded in standards for steels used in tank cars. These items are addressed later in the report.

It bears emphasis that most failure will occur in the vapor-wetted regions of the tank as the liquid-wetted regions are cooler and the mechanical strength in the former regions softens more than in the latter.

Another aspect of engulfing fires is the level of thermal protection of the tank. Tank cars may be protected by a layer of ceramic blanket (typically 13-mm thick) which in turn is surrounded by a steel jacket (typically 3-mm thick). Such protection may allow the tank car to survive up to a minimum of 100 min of engulfing fire, Birk (2000) but in the event that there are defects in the insulation, leading to increased heating of the wall, the time to failure of the tank will decrease. Birk et al. (2006b) and Birk et al. (2006b) experimentally studied the impact of insulation defects in propane tanks subjected to engulfing fires and found that even relatively small defects (approximately 8 -15% of the tank surface) located in the vapor-wetted region of the tank can lead to a tank rupture.

Most of the testing in the literature, save the cited tests from the 70s, were small-scale and carried out using Liquefied Natural Gas (LNG) or propane. Consequently, selecting the test geometry, size of the PRD, and test conditions such that the results of the small-scale testing can be related to larger scales becomes an issue and has been addressed by Birk (1995) who emphasizes the need for a careful design of small-scale tests. Poorly designed small-scale tests will lead to dramatically different failure times and modes of failure for small and large scale tanks if the conditions are not similar.

Non-Engulfing fire on an upright or toppled tank:

It may happen that the tank will topple during an accident, in which case, it is likely that the PRD will be in contact with liquid and will not function as designed. However, though the shell wall is cooled by the liquid, due to increase in vapor pressure there is a risk of a confined explosion provided the fire lasts for a sufficiently long time. Here, explosion is used in the sense that strength of the steel decreases and the pressure in the lading increases; it is not used in the sense of a chemical reaction. From the standpoints of experiments and modeling, the non-engulfing case has not been as well studied as the engulfing case. In the case of a non-engulfing fire, tank (or thermal jacket) surface emissivity and radiation loads on the outer surface will affect the wall temperature.

BOILING LIQUID EXPANDING VAPOR EXPLOSION

In the case of Pressure-Liquefied Gas ladings a Boiling Liquid Expanding Vapor Explosion (BLEVE) is possible. If the vapor is heated up sufficiently leading to increased vapor pressure and the set pressure of the Pressure-Relief Device (PRD) is attained, the vapor is vented into the atmosphere, leading to a further drop in the liquid level as more of the liquid will continue to evaporate. This will also lead to a larger portion of the shell surface exposed to vapor which insufficiently cools those portions; this weakens the shell and possibly leads to failure.

When the shell fails, the liquid pressure suddenly drops to the atmospheric pressure. Owing to the liquid temperature being well above the boiling point at atmospheric pressure, the liquid abruptly evaporates leading to a violent expansion to a cloud that has a volume larger than that of the liquid volume by a factor on the order of magnitude of 1000; see article by Eckhoff (2014) for a review.

There are some debates in the literature about the exact conditions for the onset of a BLEVE with regards to the temperature of the liquid being at the “superheat limit temperature”. For a recent review of this issue and other details regarding BLEVEs the article by Eckhoff (2014) may be consulted.

As already suggested, owing to thermal expansion of the liquid, as the vapor is vented into the atmosphere, the tank may become shell full and in this case the risk of a BLEVE is mitigated, Lautkaski (2009). Birk & Cunningham (1994) proposed a map (see Figure **3**, the data are likely for propane) which has pressure as the ordinate and a product of the liquid temperature and fill level as the abscissa and found a well-defined boundary line demarcating tests in which a BLEVE occurred from the tests in which it did not.

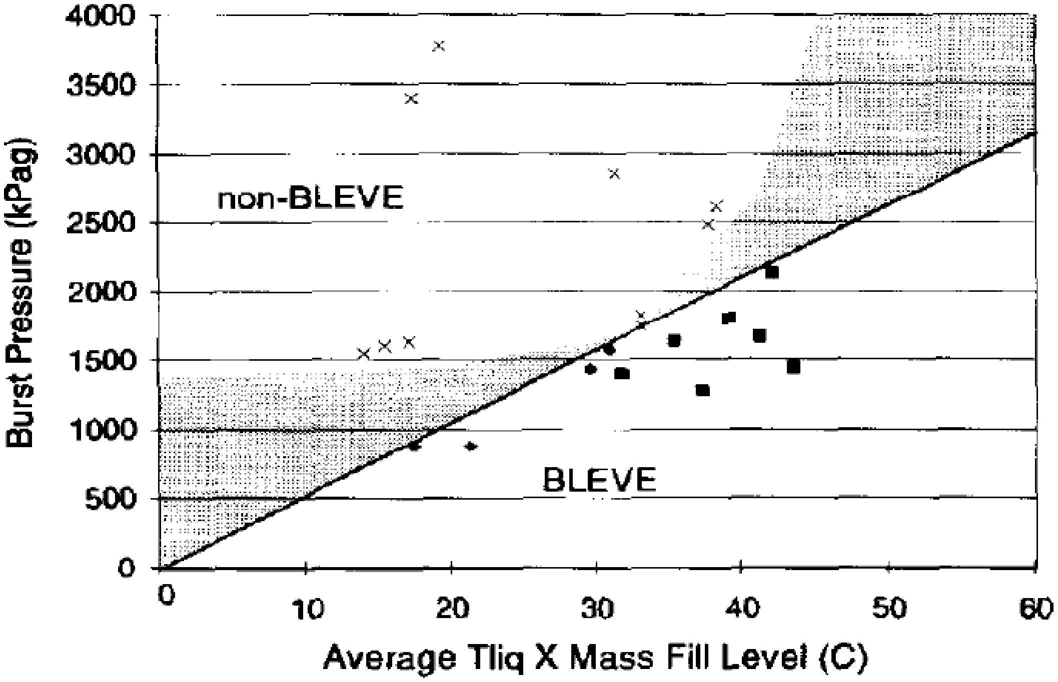

Figure 3 BLEVE map: (■) BLEVE; (◆) BLEVE in a weak tank; (×) non-BLEVE; (—) BLEVE boundary; (□) area of uncertainty

Figure 1: BLEVE map after Birk & Cunningham (1994).

Another mitigating factor in BLEVEs is stratification of temperatures in the tank. Isothermal liquid temperature is a convenient assumption and often adopted in modelling. In contrast, Birk & Cunningham (1996) reviewed experiments and found that the temperature of the liquid varies such that it is warmest in the layers in contact with the vapor, leading to stratification of temperature. The pressure in the tank was found to be governed by the warmest liquid in the tank and the pressure is higher than the pressure computed using isothermal liquid assumption. This means that if the PRD is activated and the tank fails, the resulting discharge will be less powerful if the temperature in the tank is stratified. Pressure in the tank being governed by the warmest layer and (not the average temperature), there will be less liquid energy when the liquid is stratrified.

SHELL MATERIALS AND MECHANICAL PROPERTIES

TC128 Grade B: This is the most widely used shell material for tank car fabrication; as of 2005, 93.3% of tank cars were constructed using this steel, see Fig. 1-3 of the report by McKeighan et al. (2009). It bears emphasis that the preceding data are for pressure cars.

In the as-rolled condition, the pro-eutectoid ferrite and pearlite are “pancaked” in appearance and the pro-eutectoid ferrite and pearlite exist in layers; there is a layer of pro-eutectoid ferrite and then a layer of ferrite and this feature is termed as “banding”. After the mid-80’s regulations in the United States and Canada required the steel to be normalized, the steel is used in the normalized and stress-relieved condition. Normalizing, an added expense, is carried out after the rolling to reduce the banding and this leads to a marked improvement in the strength and impact properties (Charpy energy). Hicho & Harne (1991) provide more details regarding the microstructure of TC128B in the normalized and stress-relieved state.

At room temperature, in the normalized condition, per the Association of American Railroads (AAR) specification, the minimum yield strength of the material is 345 MPa and the minimum tensile strength is 560 MPa. Typical values for yield range between 344 MPa to 468 MPa and for strength range between 496 MPa to 627 MPa. See Table 4-2 of the report by Zahoor & Hicho (1998).

When subjected to thermal loading, the material softens; that is, the strength of the material decreases. Data on decrease in yield and ultimate strength of the material as a function of temperature have been reported in the following reports: Hicho & Harne (1991), Zahoor & Hicho (1998). Therein standard dog-bone shaped samples were subjected to uni-axial tensile loading. Remarkably enough, stress-strain curves for TC128B as a function of temperature were not found in the literature.

Typical yield strength and ultimate strength measured using the ASTM E 21-79 procedures for high-temperature measurements from Hicho & Harne (1991) are shown in Figure **2**. These tests were carried out at the stated temperatures for 30, 60, and 120 minutes. A high-temperature oven surrounds the sample whilst the test is being conducted. Special extensometers or optical instrumentation is required for these tests. Only the measurements in the rolling direction and a testing rate of 0.0127 cm/min are given here; the cited report gives data for both rolling and transverse directions and for two loading rates. As a point of reference, the minimum room temperature (RT) values of the yield and ultimate strength are shown as dotted and dashed lines, respectively in Figure **2**. The significant softening upon increase of temperature is apparent.

It is also useful to consider the reduction in area and elongation of the tensile specimens as a function of temperature. The latter two parameters, which are a measure of the ductility of the material, were found to increase continuously with temperature. From the standpoint of the microstructure, Hicho & Harne (1991) concluded that strain-aging effects could be discounted on account of the continuous decrease of the yield and strength even when the temperature was raised above the aging temperature of 316 ^{o}C. If dynamic strain-aging is playing a role, an increase in strength is expected.

Other room-temperature strength measurements in hoop and longitudinal direction (rolling and transverse) on TC128 Grade B of three vintages may be found in the article by Birk & Yoon (2006). The ASTM procedure called upon in the latter work was ASTM-E8M-98. They found that aging did not affect the mechanical properties of the steel.

Moreover, tensile testing carried out on TC128 B samples (40 shell and 21 head samples) machined from ex-service (pre and post 1989) cars showed that 82% of the samples met current yield and ultimate strength specifications.

From these two data source that report the mechanical strength of TC128 Grade B, we can gather together some observations on the mechanical response of this steel:

- The material displays anisotropy with differing yield stresses in the Rolling Direction (RD) and Transverse Direction (TD).
- The anisotropy is diminished or non-existent for the ultimate strength.
- The yield strength is rate dependent. However, ultimate strength displays only a modest rate dependence.
- For the uni-axial tension testing, the testing time does not appear to have a significant impact.

- Ex-service material appears to meet current yield and ultimate strength specification for the most part.

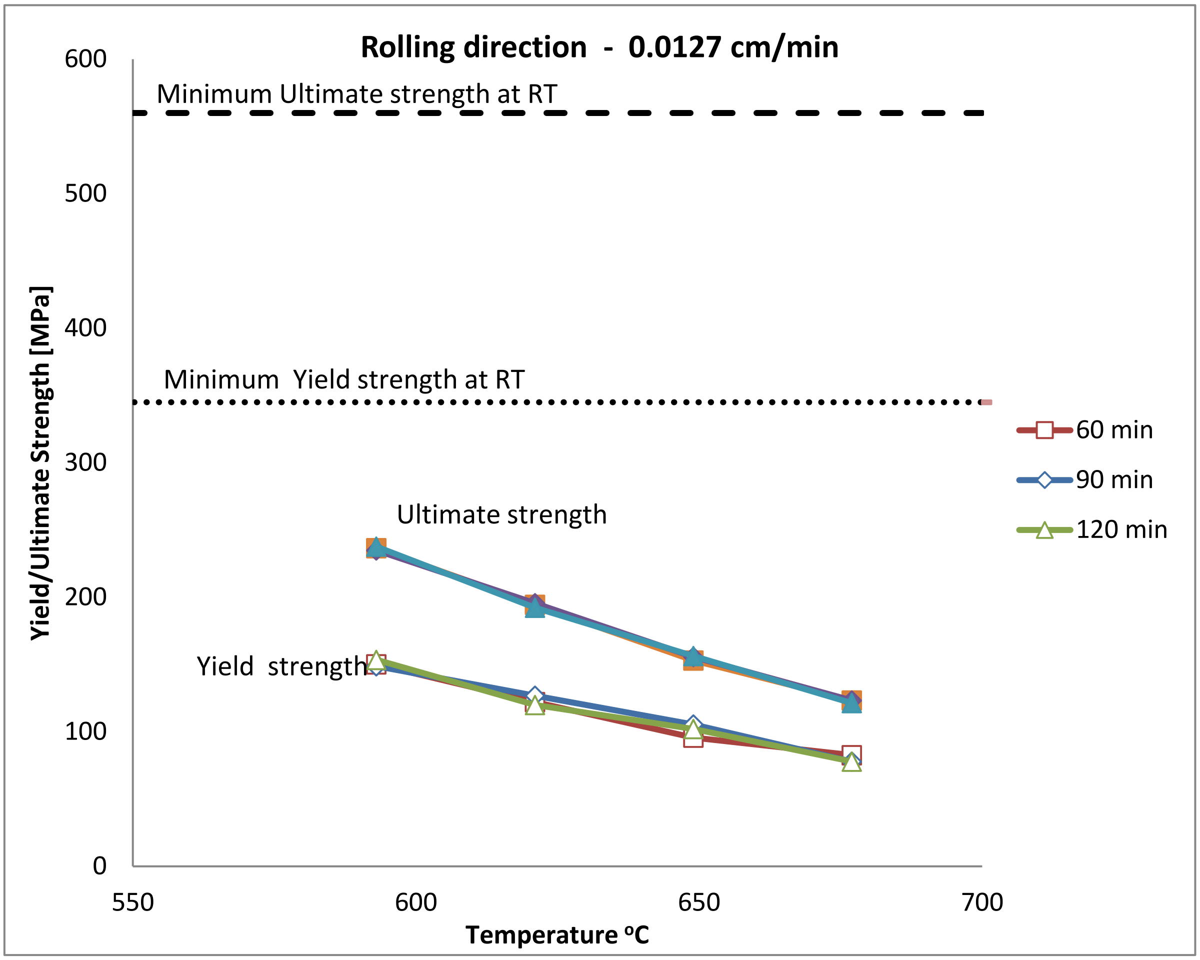

Figure 2: Quasi-static high temperature tensile testing data for TC128 Grade B; data after Hicho & Harne (1991). For reference, minimum yield and ultimate strength at RT are shown as dotted and dashed lines.

Temperature Bounds for TC128 Grade B: There are two key temperatures for this material, which emerged as a consequence of the assessment of the full-scale LNG test, designated as RAX201 and carried out in the 1970s, see Anderson et al. (1974). These are 427 °C and 630 °C. The former, according to Anderson (1982) is the threshold for the onset of microstructural change in TC128B, and the latter is the temperature at which the tank car failed in the RAX201 full-scale test. Consequently, 427 °C is the prescribed temperature for the plate to be heated up over a period of 13 minutes in the plate test, TP14877 (2013); the 13 minutes was the time taken in the RAX201 test for the shell to reach a temperature of 427 ^{o}C ; see also discussion in section 2.1.3 of the report by Birk (2000) wherein he recommends a time of 6 minutes based on heat transfer calculations.

Failure of the TC128 steel during pool fire loading: failure can occur through two different mechanisms:

1. Short-term overheating
2. High-temperature creep.

Short-term overheating is the result of the shell being exposed to excessively high temperatures over short time periods leading to material softening and then failure. In contrast, no yielding occurs during high-temperature creep but time, temperature, and load conspire together to lead to material failure; this is also called tertiary creep and is a time-dependent failure.

Failure due to short-term overheating usually leads to fracture surfaces that have a knife-edge like appearance and considerable wall thinning in the fracture edge. In contrast, failure surfaces owing to high-temperature creep will have a thick lips or edges and rough appearance; the appearance is due to the linkage of micro-voids and inclusions leading to fracture. For more discussion, the monograph by Viswanathan (1989) may be consulted.

In experiments with propane tanks, Birk et al. (2006b) noticed 50% of wall thinning and Manu (2008) has suggested that the action of both of the failure mechanisms could produce the resulting surfaces. That is, for very rapid failures (< 10 minutes) in which peak wall temperatures reached 720^{o}C or higher, knife edges were observed. For longer failure times and lower wall temperatures of 680^{o}C, displayed necking and rough failure edges. Additionally, metallurgical analysis of the propane tank accidents that involves a BLEVE in Truth or Consequences, New Mexico has shown that the failure was a consequence of a gradual elevated-temperature plastic deformation followed by stress rupture, Susan et al. (2005).

Short term heating is a yield phenomenon that can be accounted for in finite element simulations with high-temperature stress-strain data or in engineering models with formulas for thermal softening of the strength. These two items are addressed further in the report. High-temperature creep, on the other hand, requires specialized rupture testing.

Rupture Testing: In these tests, dog-bone shaped samples (usually cylindrical, but not necessarily) are placed in a high-temperature chamber and subjected to a constant load. The load is not high enough to cause yielding and is applied in a manner to prevent impulsive or shock loading. The relevant ASTM standard is E139-11. With time, due to creep deformation, the sample necks and the stress in the sample increases; eventually, due to significant necking the deformation is large enough to lead to rupture. Applied stress, temperature, and time-to-rupture are the results of the test. Birk & Yoon (2006) have carried out an extensive testing program to measure the rupture times in both the longitudinal and hoop direction of three different vintages of TC128 grade B steel. Typical rupture times for TC128 grade B steel are shown in Figure 3. For steel of vintage 1964 and earlier there appears to be a dependence of rupture times on direction; in contrast, for steel of later vintage there appears to be no dependence on specimen direction. As data in the figure shows, with increased temperature there is a decrease in both the rupture time and stress at which rupture occurs.

Probabilistic Methods: There is also an increasing trend in using probabilistic methods to predict failure. These methods require probability density function for material properties. If such methods are intended to be deployed, based on assumed confidence intervals, a sufficient number of tests can be conducted so as to construct probability density functions for the material properties.

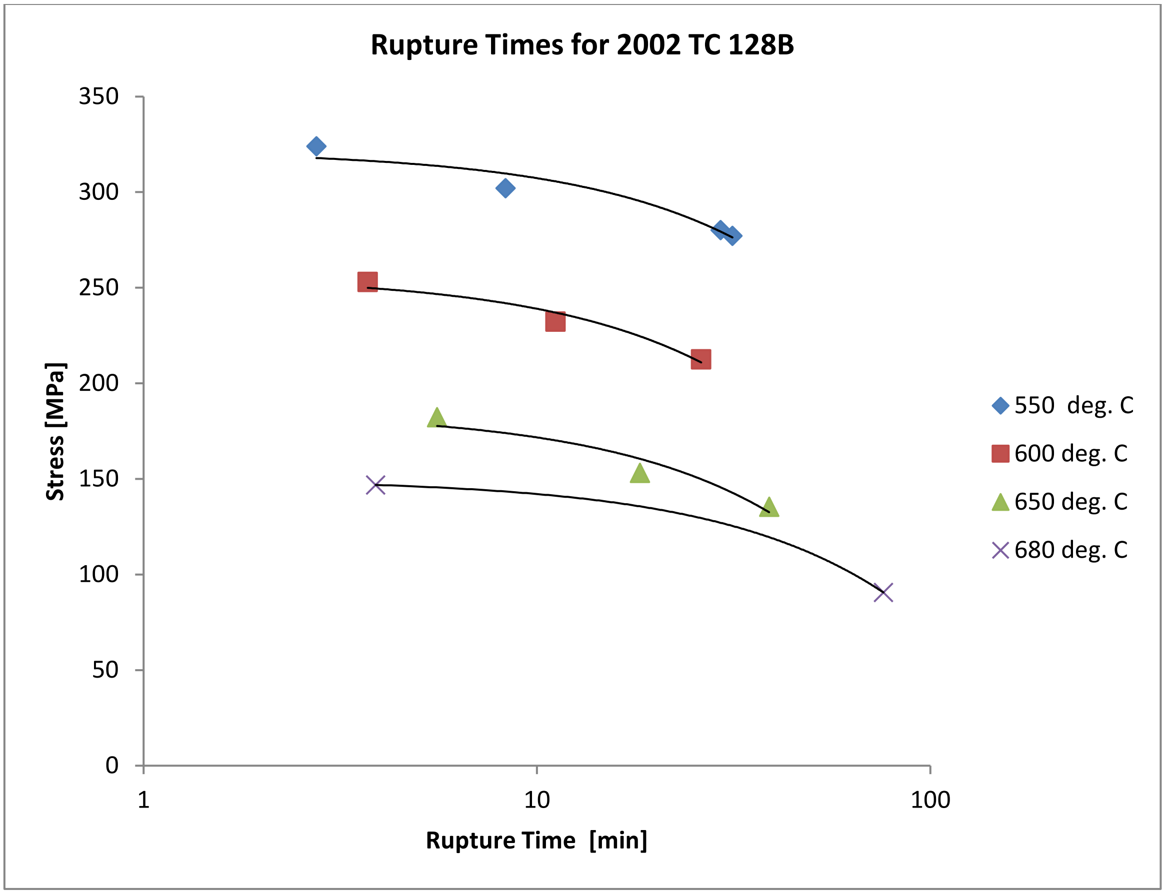

Figure 3: Rupture times for TC128 grade B steel of 2002 vintage. Specimens were machined from ex-service tanks in the hoop direction. Data after Birk & Yoon (2006).

ASTM 516 Grade 70: Ass of 2005, 0.3% of pressure tank cars were constructed using this steel, see Fig. 1-3 of the report by McKeighan et al. (2009). In many cases, the heads of the tank cars are constructed out of this steel, while the shell is fabricated from TC128 B.

The microstructure of ASTM 516 grade 70 in the normalized state is similar to that of TC128 B. It is composed of ferrite and pearlite with significant pearlite banding in the rolling plane Partin et al. (2010).

This is a commonly used material for pressure vessel applications. For that application the minimum yield strength is 220 MPa and the ultimate strength may lie between 415 MPa and 550 MPa. These strengths are lower than those of TC128 B (shown in Figure 2). However, no creep or rupture data were found during our literature search. Indeed, the material has been used for pressure vessels for low and moderate temperature operations and has good weldability. It is used in both the normalized and un-normalized form.

BACKGROUND ON CFD MODELING

From the standpoint of carrying out design reviews or risk assessment, modeling the failure of tank cars in pool fires becomes essential. At a general level, modeling approaches fall into two categories: engineering models that can be used for rapid assessments or detailed models that solve the equations of continuum mechanics. In the case of the fluid continuum, finite volume methods are commonly used; for the solid continuum, finite element methods are preferred.

Engineering Models for Pool Fires:

Engineering models are characterized by short run times (usually minutes or seconds) and provide results for rapid assessments. In general, they are based on solutions to simplified models and the solutions may be analytical or numerical. Alternatively, the model may be purely empirical and derived from fits to experimental data or results of simulation that have been partially validated. There are two types of models: models of the pool fires whose output is a thermal load as a function of time, or integrated models that use a simplified model of the tank car structure and the effects of the thermal load on the tank car including failure.

ENGULF: This computer model assumes a horizontal insulated tank in an engulfing fire, with liquid and vapor space. It predicts time for the response of the PRD, time to failure, water spray cooling, the pressures in the liquid and vapor space, and thermal response of the tank. Validation was carried out using engulfing fires of tanks containing propane and LPG, Ramskill (1988). The code uses a lumped parameter approach and computes temperatures due to heat transfer into liquid and radiation from inner surfaces, and pressure in the liquid and vapor space. Its outputs are pressure and temperature histories of the liquid, vapor, and tank wall. The pressure history allows prediction of failure of the tank car. Ramskill (1988) also suggests that the ENGULF code may be used to predict onset of BLEVE. Stratification was not modeled using this model and it has not been validated for complex hydrocarbons.

HEATUP: This computer model is similar to ENGULF and validation again is restricted to engulfing fires of propane and LPG tanks.

Other models that may be instanced are simple empirical models of thermal loads due to pool fires, Fay (2006) and radiation loads to pool fires, Mudan (1984). A comparison of the various models of radiation may be found in the article by Rew et al. (1997), and this motivated them to develop a radiation model POOLFIRE6. Although they concluded that the model performed adequately, they emphasize the need for validation data in the case of large-scale, wind-blown tank fire data and measurements of incident radiation at locations close to the flame surface.

A critique of engineering models is that liquid-phase expansion and temperature stratification due to buoyancy effects on fuel in contact with the heated walls are not modeled; however, there has been some effort in including these effects in engineering models Gong et al. (2004). The importance of incorporating stratification in modeling efforts has been pointed out by Birk & Cunningham (1996).

Computational Fluid Dynamic Models of Pool Fires:

Computational Fluid Dynamics (CFD) is a general technique that incorporates constitutive assumptions and solves the conservation equations (conservation of mass, momentum, and energy) incorporating finite volume, finite difference, or finite element methods. In general, popular commercial codes such as ANSYS and Star-CCM+ use the finite volume method. Constitutive assumptions may be incompressibility in the case of gasses, compressibility for fluids, turbulent flow, multiphase flow for vapor, and boiling. Owing to the transient nature of the engulfing fire, implicit unsteady schemes are used for the time integration of the momentum equations, and explicit schemes for time integration of faster events such as the BLEVE.

As in the case of the engineering models, CFD computations are used for both modeling pool fires alone or including their effects on the thermodynamic conditions in the tank as a consequence of the engulfing pool fire. However, for features such as temperature stratification in the tank, or the complex fluid flow leading to the BLEVE, CFD is suitable. Note that in the case of a BLEVE the simulation will have to account for the dynamics of the opening of the PRD which involves coupling a continuum simulation with the response of system-level model of the PRD. The latter has not been attempted yet, D'Aulisa et al. (2014)

Instances of pool fire models using CFD incorporating wind effects, turbulence, soot, heat feedback (due to radiative and convective components) to the fuel, and phase change from liquid to vapor are reviewed by Steinhaus et al. (2007). The preceding, and other studies, Novozhilov & Koseki (2004), for instance, focus on methanol or LPG as fuels, complex hydrocarbons such as crude oils have not been studied. This point is also emphasized in the annexe of Phase I report from the National Research Council, Lam et al. (2015).

A second class of CFD models includes the tank car in the simulation and compute wall heat up times, stratification of temperature, radiation inside the tank from the vapor-wetted regions, and thermal expansion of the liquid phase. A noteworthy recent work is modeling of a propane fire engulfing a tank car using user-developed functions incorporated into the CFD solver FLUENT in ANSYS, D’Aulisa et al. (2014). One particular feature of this study was the modeling of stratification and thermal expansion of the liquid phase, which are difficult to incorporate in an engineering approach. However, the preceding CFD simulations required implementation of user subroutines for condensation-evaporation and special equations of state. They also point out that a shortcoming in their approach is the neglect of the PRD, the inclusion of which will complicate the modeling due to mixing and consequent impact on stratification. It is noteworthy that each of the simulations required 44 hrs of run time for a two-dimensional simulation carried out on four cores.

BACKGROUND ON SOLID MECHANICS MODELING

Failure of the tank is modeled using the principles of solid mechanics. Again, models may be classified into engineering and finite element-based methods. In the engineering approach, the yield strength is softened per some model as a function of the temperature and the corresponding internal pressure at which the hoop stress exceeds the threshold yield is the failure pressure. A shortcoming of the engineering technique is the neglect of the time-dependence of failure at high-temperature, and this is partially alleviated by the use of rupture models for creep.

In finite element –based models, the three-dimensional equations of conservation of momentum, are solved as a function of time. The material is modelled as an elastic-plastic material with hardening (and softening as a function of increased temperature) and the failure is modeled using the principles of damage mechanics. Damage mechanics appears to be the preferred method for the detailed modeling of time-dependent failure; however, owing to the wide unavailability such models have to be implemented as user subroutines in commercial finite element packages.

AFFTAC

AFFTAC stands for Analysis of Fire Effects on Tank Cars and is the most widely used software program for qualifying and evaluating thermal protection systems for tank-cars. It relies on simplified engineering models to model the fire conditions, external and internal heat transfer, the PRV action, thermodynamic model, and failure model. The assumption of isothermal liquid properties (not stratified) is the most significant source of modeling deficiencies in this program, Birk (2000).

The failure model accounts for thermal softening of the steel but not for the time-dependent rupture properties of the steel. A simplified model for the thermal softening is used to estimate the pressure corresponding to the liquid temperature at which the vessel will fail. This is another significant approximation in the AFFTAC code.

For a comprehensive review of the AFFTAC code and recommendations for improvement the review by Birk (2000) may be consulted. Droste & Schoen (1988) have also used softening yield to study failure of LPG cylinder in engulfing fires of LPG storage tanks.

Insulation Defect Analyzer (IDA, also called Tank2004)

Largely, to rectify the shortcomings of the AFTAC model, the IDA program was developed by Birk (2005). This model includes the following:

- Three-dimensional geometry of the tank was accounted for by discretizing it into zones
- Thermal model for lading included stratification of temperature and its impact on pressure
- Owing the three-dimensional geometry, defect location was accounted for
- A realistic PRD model including effects such as spring softening
- Liquid entrainment into the PRD at high fill levels
- Robinson's life fraction rule (Viswanathan (1989)) for modeling high-temperature stress rupture

This program has been validated by predicting the failure event in engulfing and non-engulfing propane fires, Birk et al. (2006b). One limitation is that thermal stratification in the vapor phase (when PRD is closed) is not taken into account. A criticism of this program is that the failure prediction times are early when compared with experimental results, especially if the hot spot area in the tank is small. Along these lines, Manu (2008) argues that three-dimensional finite element simulations could be used to improve the predictions.

Damage-Mechanics Based Approaches:

Herein, defects in the material that initiate and evolve owing to the high temperatures are abstracted as a damage variable and used to degrade the strength of the material. It is in the initiation and evolution laws that the damage models differ. The literature on the application of damage mechanics to prediction of tank-car failure is light. The most significant contribution appears to be in the thesis of Manu (2008) and the articles by Manu et al. (2009a) and Manu et al. (2009b).

They used the Materials Properties Council (MPC) model developed by Prager (1995), calibrated it using the rupture testing, implanted it in the Abaqus finite element package and used it to model the failure of ASME S 455 tanks of several sizes exposed to propane fires. They concluded that the MPC model was appropriate and gave reasonably good predictions of failure times. For engulfing failure of 500 US gallon pressure vessel failure, the MPC model at 650 ^{o}C the model predicted a failure time of 12.1 min which compared well with experimental failure times of 10-15 min; engulfing pool fire experiments using these tanks are reported by Birk et al. (2006a). For more detailed comparison of the MPC model with other damage-mechanics based approaches, the thesis of Manu, 2008 may be consulted. The author of the current report has also used damage-mechanics-based approaches for modeling failure of pipeline steels Simha et al. (2014) and is of the opinion that this is a promising approach for failure prediction.

We were unable to find a coupled multi-physics failure assessment of tank-cars. Herein, a three-dimensional model of the tank would be subjected to a transient thermal load and the equations of structural deformation would be concurrently solved. The computational technology to carry out such simulations exists, but the computing resources and computational time would be significant.

SUMMARY AND RECOMMENDATIONS

A review of the mechanical response of two tank-car steel alloys, TC 128 Grade B and ASTM 516 Grade 70, when exposed to high-temperatures during engulfing pool fires is presented in this work. In addition to the mechanical response this report reviews the state-of-the art in Computational Fluid Dynamics (CFD) based modeling of pool fires and the state-of-the art in failure modeling of tank car steels.

With regards to mechanical response at high temperatures, other than limited data on softening of strength as a function of temperature, no detailed and systematic studies was found in the literature. Accordingly, it is recommended that:

1. A comprehensive testing programme, per ASTM E21-09 standard, be carried out to systematically evaluate the tensile stress-strain response of the two alloys. It is also recommended that a judicious selection of new and ex-service samples be chosen for the testing. It is also recommend that for all of the samples, if feasible, the samples be machined from the cylindrical body of the shell after the forming operation; this will account for the work hardening of the forming operation. It is also recommended that some samples be selected from the head of the tank car as these are work hardened differently than the cylindrical part of the shell. Suggested temperature range is -40 ^{o}C to 800 ^{o}C.

2. A detailed microstructural evaluation of the tested samples be carried out and, if feasible, an evaluation of the high-temperature microstructure be carried out. A hot-stage in a Scanning Electron Microscope will be required for this purpose. One reason for this recommendation is to assess the microstructural changes associated with high temperatures. It is hoped that a study of the high-temperature microstructure may suggest modest modifications to initial alloy chemistry or processing that may lead to enhanced properties.

3. A comprehensive testing programme, per ASTM 139 standard, be undertaken to measure rupture times during creep of both the alloys. Again, a selection of new and ex-service samples should be chosen for testing. Suggested temperature range is 500 ^{o}C to 800 ^{o}C.
4. In all of the above testing, it is recommended that consideration be given to future potential for probabilistic models. Accordingly, based on an assumed confidence interval, a sufficient number of tests should be conducted so as to be able to construct probability distribution functions of the material properties.

With regard to CFD-based modeling, techniques for multi-physics modeling are being developed and are robust enough to admit application to study the problem under consideration. One of the main reasons for carrying out the CFD computations is to predict the magnitude, spatial and temporal extent of the flame (the thermal load), which is a function of the lading and other environmental factors. However, based on our experience, such models require significant computational power and involve computations which require solution times of days. It is therefore recommended that existing engineering models be calibrated using the results of the forthcoming experiments to be carried out at National Research Council. Alternatively, if the existing models are found wanting, validate CFD simulations using results of the forthcoming experiments and then develop engineering models using a limited set of CFD simulations to enhance the existing models (or develop newer ones).

The thermal load, in turn, serves as an input to the solid-mechanics computations which can predict the failure event for the tank car. In this regard, based on the mechanical testing recommended above, it is possible to make predictions using the so-called damage-mechanics based techniques. Again, it is recommended that existing engineering models such as the Insulation Defect Analyzer be used to evaluate the failure times and model the failure event observed in the NRC tests. In the event that the predictions of IDA are overly conservative or un-conservative, the more involved damage-mechanics approaches may then be adopted.

The crux of Transport Canada’s experimental and modeling effort is focussed on the capacity to make informed decisions and choices for the transport of crude oil, condensates, and ethanol. The consultant report which forms an appendix to the Lam et al. (2015) states that the limitations of the engineering style model are because they “…do not adequately address the thermal gradations through the liquid and vapor phase, nor are they able to model more complex hydrocarbon mixtures, such as crude oils." Solid-mechanics-based failure approaches depend on an accurate transient thermal load. So the second shortcoming stated by the consultant becomes crucial. With regards to the first, as our review indicates, the IDA only suffers from lack of stratification in the vapor phase. Consequently, we advocate a two-step approach.

Based on the results of the planned testing at NRC, calibrate existing engineering models to develop fire source models. Thereafter, use the fire source models as thermal loads in the existing IDA program to predict failure times.

If the predictions are overly conservative (or non-conservative) when compared with the experimental failure times, adopt the more involved damage-mechanics based approach as this has shown to be the most promising technique.

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