SIEMENS PROCESS SAFETY WHITEPAPER

Advanced Depressurization Analysis in gFLARE - Validation

SIEMENS

Executive Summary

Siemens is the recognized industry-leading provider of high accuracy analysis for blowdown, flare and relief system design. Our methodologies based on our gFLARE software enables a significantly more accurate quantification of risk than conventional engineering approaches. We have supported over 200 greenfield and brownfield projects in the last 15 years by providing safety consultancy services using gFLARE exclusively in-house. However, since 2021 we have commercialized gFLARE and it is now available to Operators, EPC's and consultants.

This Whitepaper reports the key features of gFLARE and its validation against experimental data.

Contents

1.Introduction

The process industry is quickly evolving in the face of several challenges including price uncertainty, increasing environmental regulations/responsibilities, and digital transformation. These challenges require an efficient delivery of projects with increasingly shorter schedules, whilst maintaining compliance with safety codes/ standards and minimizing the risk/cost of safety incidents. Model based safety analysis using specialized software has become important to meet the aforementioned challenges. Modern safety solutions require:

- Software that can cover multiple elements of safety design. This can improve workflow and reduce data handling errors.
- Earlier adoption of simulation tools, with fit-for-purpose models. Ideally, the same modeling environment can be used during the project lifecycle to:
  - Allow for early identification / elimination of risk during design phase enabling faster investment decisions.
  - Allow for optimization of design, minimizing the requirement for expensive materials, flare header sizes etc.
  - Serve as operator decision support during operations phase to perform 'what-if' analysis and operations planning.

1.1 Depressurization

A depressurization operation is designed to remove all combustible fluids during an emergency or for a planned shutdown in a controlled manner. It is intended to prevent the escalation of a leak or small fire into a major loss of containment event and potential explosions.
Typically, prior to depressurization a process plant is isolated into several independent systems. A full plant blowdown operation involves the simultaneous or staggered depressurization (blowdown) of all the pressurized gas (and/or liquid in some cases) in each system by routing it to one or more flare tips for controlled combustion.
The depressurization operation may itself be hazardous and several factors must be considered in the design of these safety systems. One particularly important risk is brittle fracture in process equipment and piping due to auto-refrigeration chilling during depressurization, which can lead to very low fluid temperatures and potentially low metal temperatures.
Hence, three main assessments need to be carried out during the design of depressurization systems:

1. Fire survivability assessment – To ensure depressurization is fast enough during a fire scenario to prevent vessel or pipe rupture or minimize the consequences of
2. Coldrupture blowdown assessment – To ensure the material of construction is adequate for minimum metal temperatures expected during cold blowdown.
3. Flare capacity / low temperature assessment – To ensure there is adequate flare capacity during simultaneous or staggered blowdown of process systems and that material selected for flare piping is adequate.

Our software solution addresses the above requirements. The key features of gFLARE are explained in Section 2, followed by its validation in Section 3.

2. Advanced Depressurization Analysis

gFLARE is set of safety model libraries that reside within gPROMS Process. It inherits all the capabilities of the gPROMS advanced process modelling and solution platform. This provides a desktop process modelling environment that includes all typical standard flowsheeting functionality.

gFLARE provides **a single fully integrated technical solution** that is compliant with the 7th edition of the industry standard API 521 guidelines for pressure relief and blowdown systems. The key features of gFLARE are:

1. **Validated, first principles models**:
   a. **Thermodynamics**
      i. Incorporate detailed mixture thermodynamics and rate-based modelling of the transient event. All standard cubic equations of state (EoS) models (e.g., Peng Robinson, SRK) are supported with exact definition of all components including hypotheticals and BIPs, if available.
      ii. Handle dense phase depressurization, where fluid crosses phase envelope from left of critical point.
      iii. Predict potential formation and equilibrium amounts of solid phases (e.g., hydrates and dry ice) during depressurization using appropriate thermodynamic models (GERG / SAFT).
   b. **Heat transfer** - Account for detailed heat transfer between:
      i. Equipment / piping wall and each of the fluid phases (gas, hydrocarbon liquid, non-boiling liquid) and internals (e.g., adsorbent packing)
      ii. Equipment / piping wall and ambient environment (air, sea, fire).
         1. The same model can be used for both fire survivability assessment and cold blowdown assessment.
      iii. **Fire survivability** – Rupture analysis.
         1. gFLARE models allow for application of the API analytical methodology (API 7th edition Appendix A) to determine precise heat loads into the system (vessel and piping)
         2. Integrated calculation of stresses during depressurization assessed against material ultimate tensile stress to determine risk of
2. **Flexible – Fit-for-purpose model configuration:**
   a. **Semi-Detailed Screening configurations** that represent the level of detail available during early stages of design (pre-FEED, FEED) including main vessels, representative lowpoints, blowdown lines and tailpipes.
      i. Early confirmation of design basis, number of blowdown orifices, confirm their impact on flare capacity and whether process sectionalization is adequate.
      ii. Identify minimum wall thicknesses to meet fire integrity and mitigate low temperature embrittlement.
      iii. Advise / explore potential piping layout issues and determine take-off location of blowdown orifices to minimize risk.
   b. **Detailed geometric configurations** that reflect the distributed nature of the blowdown segment based on detailed piping layout arrangement expected during EPC phase. All pipes and equipment can be explicitly modelled:
      i. Rigorously model the varying metal mass and heat transfer mechanisms in the different parts of system.
         1.Accurately determine fluid temperature upstream of restriction orifice and hence fluid temperature entering the flare network.
      ii. ii. Explicitly model all physical lowpoints in system with no limitation on number or location of lowpoints.
      iii. Explicitly model vessel nozzles / thermal sleeves if present.
      iv. Explicitly model shell and tube heat exchangers.

3. **Coupled process and flare representations solved simultaneously**
   a. gFLARE enables full assessment of the transient behavior of the flare system, yielding both highly accurate prediction of system capacity (Mach number, rhov2, backpressure) and precise view of cold front propagation into the flare system.
   b. A coupled representation allows full facility blowdown studies to be conducted where multiple segments are simultaneously depressurizing to flare system, allowing both staged (multiple sources from single blowdown segment) and staggered (where blowdown segments can be opened in sequence). This is important in capacity studies and low temperature studies, where multiple sources of cold fluid can lead to propagation of cold metal temperatures further down flare piping compared to single relieving source.
4. **Optimization**
   a. gFLARE inherits the powerful optimization algorithms in gPROMS that allow dynamic (or steady state) optimization including discrete / integer decisions and multiple
   b. Optimization of staged / staggered depressurization philosophy.
   c. Optimization of IPS response times / valve opening or closure times.
5. **Sequence of Events**
   a. The underlying gPROMS environment allow any sequence of events to be imposed on the model. These can be malfunctions / upsets where valves (say PCVs) fail open or closed. It can also be used to perform 'what-if' analysis.

Numerous publications over the years have detailed and highlighted the software's applications:

A. Hugo Rodrigues et al, "Design considerations for Pressurized Flare and Vent Systems for Efficient CO2 Management", ADIPEC, 2024

B. Hugo Rodrigues et al, "What is the Impact of Dynamic Flare System Design on Cost, Safety and Environment ?", Hazards 34, 2024

C. Hugo Rodrigues et al, "Practical examples and considerations in designing emergency depressurizing systems", Hydrocarbon Processing, 2023

D. Sathish Natarajan et al, "Depressurization of CO2 Rich Mixtures: Challenges for the Safe Process Design of CCS facilities and CO2 EOR Systems", 12th Global Congress on Process Safety, 2016

E. Apostolos Giovanoglou et al, "Optimal selection of materials of construction for gas processing facilities; Lessons learnt from a design case study", SPE Asia Pacific Oil & Gas Conference and Exhibition, 2016

F. Praveen Lawrence et al, "Using dynamic analysis for accurate assessment of pressure relief and blowdown system performance" Global Congress on Process Safety, 2014

G. Apostolos Giovanoglou et al, "Process modeling requirements for the safe design of blowdown systems – changes to industry guidelines and how this impacts current practice", Global Congress on Process Safety, 2014

H. James Marriot, "Advanced hybrid modelling of separators for safe design in oil/gas production plants", HAZARDS 23, 2012

I. James Marriot et al, "A dynamic future for Flare design", Hydrocarbon Engineering, 2010

3. Validation

3.1 Low Temperature Cases

There are four available experimental cases in literature. These include two cases from Imperial College Experiments (Richardson and Haque) and two cases from Spadeadam Experiments[1]. The dimensions of the vessels used in these experiments are shown in Table 1.

Table 1: Vessel dimensions in the experimental cases

Specifications	Imperial College Experiments	Spadeadam Experiments
	I1 / I7	S9 / S12
Inside diameter (mm)	273	1130
Length (m)	1.524	2.25 (T-T)
Head Type	Flat	Torispherical
Vessel Orientation	Vertical	Vertical
Wall thickness (mm)	25	59

The test vessels used in Richardson and Haque [1]were smaller (like a 10in pipe) than standard industrial vessels encountered in many plants. On other the hand, the Spadeadam experiments were conducted using typical vessel sizes found in industry.

gFLARE temperatures are reported as average bulk temperature (gas, liquid or non-boiling liquid) which are considered uniform within the zone or fluid phase. Hence, wall temperatures are also uniform with the zone with variation in temperature across the thickness of the metal. In practice, the fluid temperatures vary, as is shown by the band of measurements in the subsequent plots. These variations are caused by significant natural convection within the vessel. The gas flow is expected to be an elongated toroidal motion corresponding to natural convection, superimposed on a weak axial motion as the gas leaves the process vessels, corresponding to forced convection.

gFLARE is configured to calculate the natural and forced convection heat transfer coefficients. We account for the additional internal velocities inside large diameter vessels that adds to overall heat transfer from just natural and forced convective heat transfer correlations alone.

With respect to the validation results shown here:

- gFLARE results were produced from the standard model configurations available to the user – there are no 'Tuning' factors used.
- Normally, it is the Minimum Metal Temperature which is of prime importance to the user, rather than the fluid temperatures, or any intermediate values. However, the temperature of the fluid exiting the vessel determines the temperature in outlet lines and blowdown lines. Hence, gas (fluid) temperature predictions in large vessels are also important.
- Note that in all experiments the grey shaded area of the graphical plots indicates the range of experimental values obtained.

The validation results are presented below.

3.1.1 Experiment I1 (pure N_2)

The starting conditions for this experiment in shown in Table 3.

Table 3: I1 Experiment starting conditions

Specifications	
Composition	100% N_2
Initial Pressure (bara)	150
Initial Temperature (K)	290
Orifice diameter (mm)	6.35
Back Pressure (bara)	1.01325
Ambient Temperature (K)	290
Orifice discharge coefficient	0.8

The results are shown in Figure 1 and Figure 2.

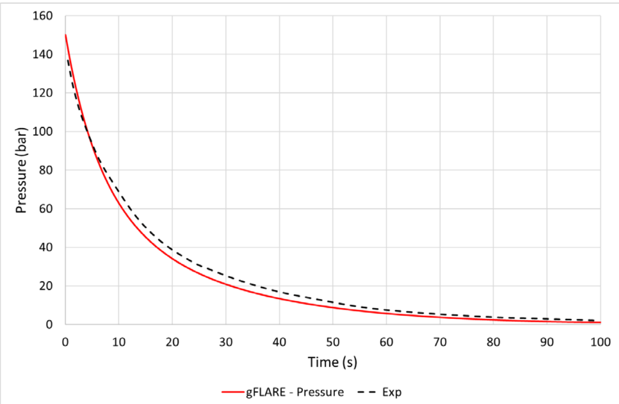

Figure 1: Pressure profile (I1 experiment)

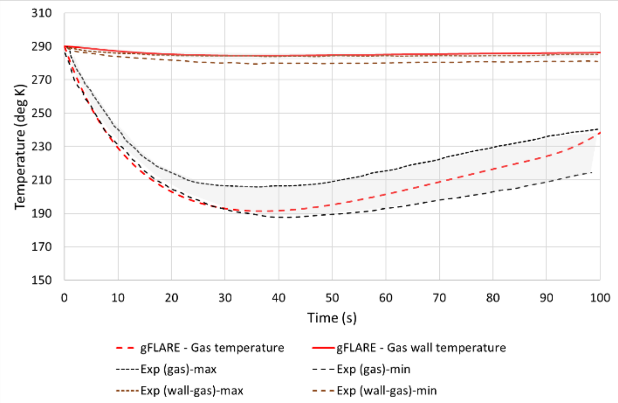

Figure 2: Gas and Gas-wall temperature profile (I1 experiment)

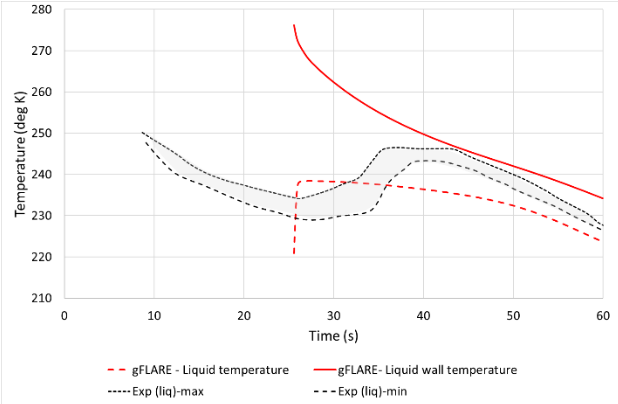

Figure 4: Liquid and Liquid-wall temperature (I7 Experiment)

As shown in Figure 1, the blowdown profile is matched by gFLARE, which for this simple gas system validates the orifice model equations. The difference in recorded pressure may be due to the estimated instrument accuracy of +/-0.2bar and some measurement lag.
The fluid and wall temperature predicted in gFLARE is a good fit to experimental data (Figure 2).

3.1.2 Experiment I7 (N_2 and CO_2)

The starting conditions for this experiment in shown in Table 4.

Table 4: I7 Experiment starting conditions

Specifications	
Composition (mol%)	70% N_2 and 30% CO_2
Initial Pressure (bara)	150
Initial Temperature (K)	290
Orifice diameter (mm)	6.35
Back Pressure (bara)	1.01325
Ambient Temperature (K)	290
Orifice discharge coefficient	0.8

The results are shown in Figure 3 and Figure 4.

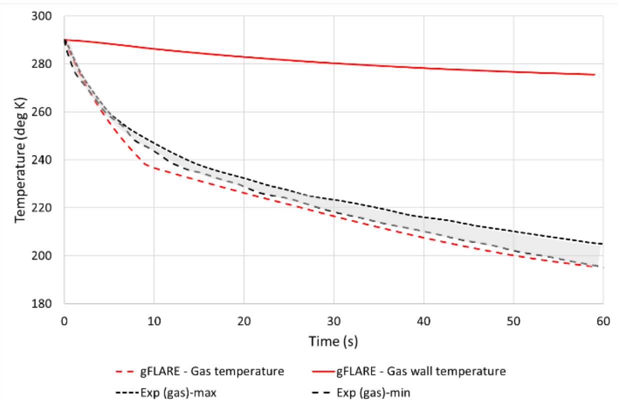

Figure 3: Gas and Gas-wall temperature profile (I7 experiment)

The following are the main findings:

- Phenomenon – During depressurization, the gas expands inside the vessel and cools. gFLARE predicts that the fluid crosses the phase envelope at 10 seconds but predicts that nucleation occurs for another 15 seconds before liquid droplets pool at the bottom of the vessel. When this cold liquid hits the warm metal at the bottom of vessel, then the liquid temperature increases sharply, while the temperature for the wall in contact with this liquid drops sharply. As depressurization proceeds, more liquid is condensed and accumulated at the bottom of vessel and this boils and cools as the pressure
- Gas temperature – gFLARE prediction of gas temperature is aligned with measured data.
- Liquid temperature – gFLARE predicts formation of a bulk liquid phase 25 seconds into depressurization based on standard nucleation settings. Subsequently, the liquid temperature predictions of gFLARE are close to measured data.

3.1.3 Experiment S9 (Methane, Ethane, Propane)

The starting condition for this experiment is shown in Table 5.

Table 5: S9 Experiment starting conditions

Specifications	
Composition (mol%)	85.5% C1, 4.5% C2 and 10% C3
Initial Pressure (bara)	120
Initial Temperature (K)	303
Orifice diameter (mm)	10
Back Pressure (bara)	1.01325
Ambient Temperature (K)	293
Orifice discharge coefficient	0.9

The results are shown in Figure 5, Figure 6 and Figure 7.

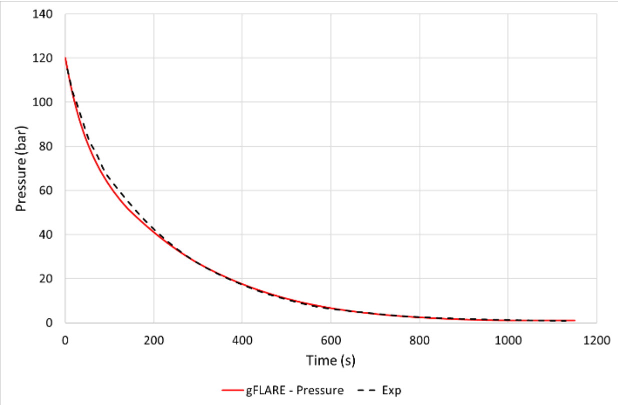

Figure 5: Pressure profile (S9 experiment)

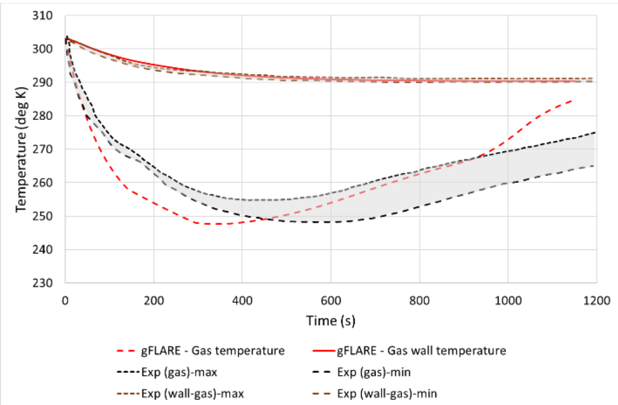

Figure 6: Gas and Gas-wall temperature profile (S9 experiment)

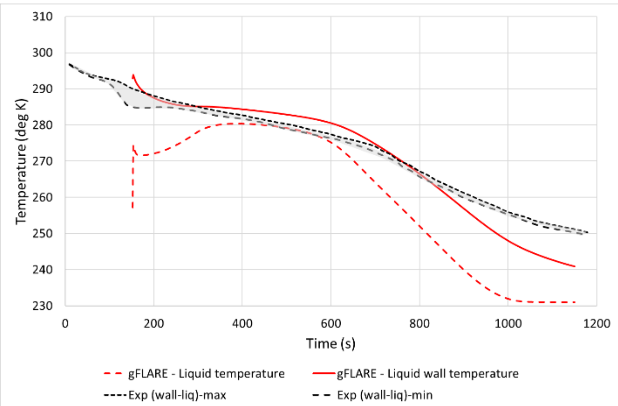

Figure 7: Liquid and Liquid-wall temperature profile (S9 experiment)

The following are main findings:

- Gas temperature – The minimum gas and gas-wall temperature predicted in gFLARE matches the experimental results.
- Liquid temperature
  - It appears that liquid may have been present in the vessel from start of depressurization which was not noted in the experiment. From Figure 7 above, the measured data starts at 297K. this is different to initial wall temperature measurement which is at 303K in Figure 6.
  - gFLARE predicts formation of bulk liquid phase 160 seconds into depressurization and much colder liquid and wall in contact with liquid temperatures. The profile of the liquid temperature curve is much steeper indicating the composition must be different.

▪ gFLARE predicts that all the methane and ethane in the liquid phase evaporate, vigorously after the first 10 minutes, and the liquid phase left at the end of depressurization is pure propane.

▪ Extending the simulation for longer period will cause liquid wall temperature ultimately to also reach -42°C.

- Equation of State used:
  - Using CSMA instead of PR78A will predict liquid phase formation at around 130 seconds in gFLARE. This is due to minor differences in the phase envelope between CSMA and PR78A for this composition.
  - This does not have a big impact on minimum observed temperature.

▪ Again, gFLARE predicts that liquid left at the end of depressurization is pure propane.

- Initial liquid phase present in vessel
  - Our explanation for the difference between experimental data and predicted gFLARE values is due to presence of heavier hydrocarbon liquid at the start of blowdown as a residue from say past experiments.
  - A test was performed assuming 1E-3 m^3 of Hexane (liquid) is present at the start of the experiment inside the vessel. The results from this run are shown in Figure 8. Results are similar for CSMA and PR78A.

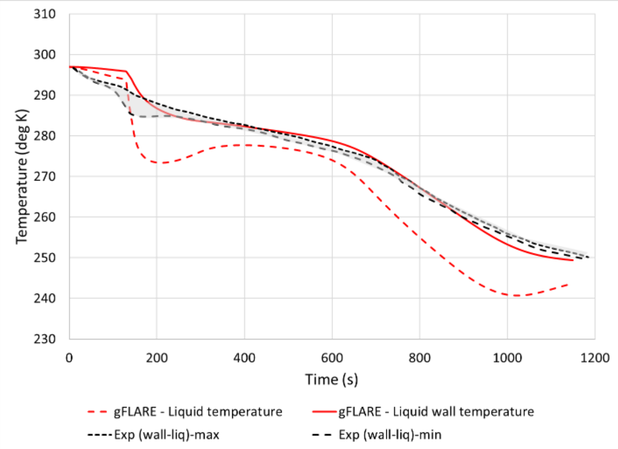

Figure 8: S9 experiment with small amount of Hexane present at start of experiment

3.1.4 Experiment S12 (Methane, Ethane, Propane)

The starting conditions for this experiment in shown in Table 6.

Table 6: S12 Experiment starting conditions

Specifications	
Composition (mol%)	66.5% C1, 3.5% C2 and 30% C3
Initial Pressure (bara)	120
Initial Temperature (K)	290
Orifice diameter (mm)	10
Back Pressure (bara)	1.01325
Ambient Temperature (K)	293
Orifice discharge coefficient	0.9

The results are shown in Figure 9, Figure 10 and Figure 11.

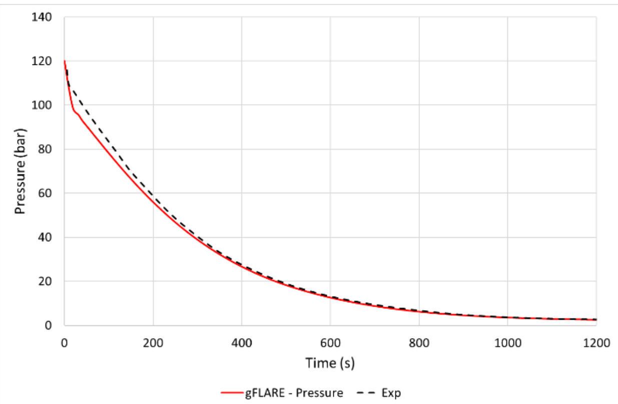

Figure 9: Pressure profile (S12 experiment)

- The fluid is in dense phase initially. The experimental data also drops sharply initially, but levels off faster. Delays in gFLARE model of a few seconds (to account for nucleation) before liquid forms causes pressure to drop faster for longer.

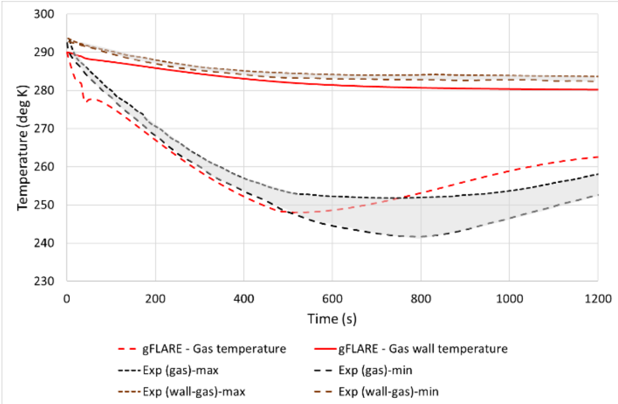

Figure 10: Gas and Gas-wall temperature profile (S12 experiment)

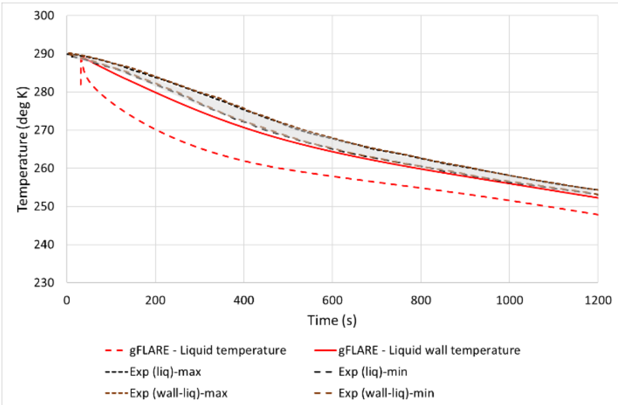

Figure 11: Liquid and Liquid-wall temperature profile (S12 experiment)

The following are the main findings:

- Liquid wall temperature is colder than the gas wall – gFLARE predictions of gas and wall in contact with gas temperatures are consistent with data and predictions are conservative.
- Liquid wall temperature – gFLARE predictions match measured data and are conservative.
- Note that significantly larger quantities of liquid are formed in S12 as compared to S9 due to the greater amount of propane present.
    - However, the liquid phase left at the end of depressurization is again approaching pure propane.
    - The experiment was stopped at approximately 1.0 barg. If simulation is continued for longer and pressure drops closer to atmospheric, then minimum of 231K (-42°C) is expected here as well.

3.2 Fire Case

The Federal Institute for Materials Research and Testing (BAM) of Germany performed a pool fire test in 1999 to investigate the effect on a partially filled rail tank car containing LPG[2], [3]. This tank car was constructed from low-temperature carbon steel and the dimension of this vessel is shown Table 7.

Table 7: Vessel dimensions / Initial conditions used in BAM

Specifications	BAM Experiment
Inside diameter (mm)	2900
Length (m)	5.95
Head Type	2:1 Ellip
Vessel Orientation	Horizontal
Wall thickness (mm)	14.9/ 17
Composition	100% Propane
Liquid volume (m^3)	10

The pool fire was partially confined because there was a U-shaped embankment adjacent to the rear and sides with a height of 6m. This was a well-instrumented experiment with fire and wall temperature measurements in several locations. Significant variations in fire and consequently wall temperatures were observed around the vessel due to partial confinement. There was no depressurization or PSV protecting the vessel and rupture occurred during the experiment after 17 minutes.

Due to the significant variability in the fire temperature and fluxes around the vessel, a single set of values will not fit the data for the three main locations reported. API 521 7th Ed. (Table C.5) has published one of set of values that can be used. We have used these values in gFLARE simulations as summarized in Table 8. Scandpower Type 235 LT properties were used for the material of construction.

Parameter	Specification	Rear-Center	Rear-Left	Rear-Right
ϵ-fire	Hydrocarbon flame emissivity	0.6	0.6	0.6
ϵ-surface	Equipment emissivity	0.5	0.65	0.4
α-surface	Equipment absorptivity	0.5	0.65	0.4
h	Convective HTC	20 W/m^2/K	20 W/m^2/K	20 W/m^2/K
T-gas	Temperature of combustion gases	1000°C	800°C	800°C
T-fire	Fire temperature	1000°C	800°C	800°C

The wall temperature predictions of gFLARE are shown in Figure 12. As observed, there is a good match between gFLARE predictions for wall temperature with API predictions based on assumed parameters and BAM experimental data.

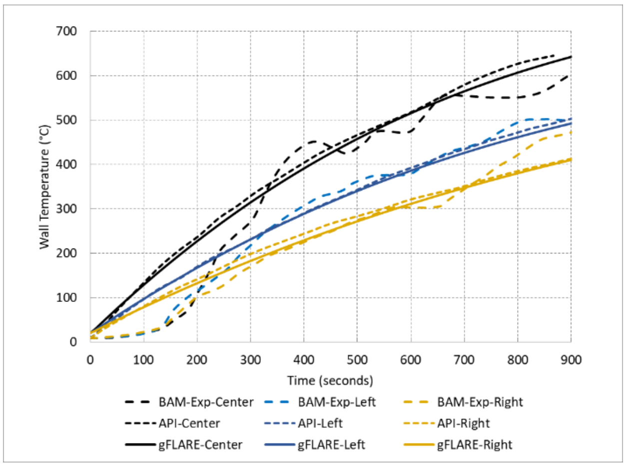

Figure 12: Wall temperature predictions BAM experiment

The following are the main findings / comments:

- gFLARE has the capability to model different fluxes in different sections of the wall as it happened in reality during this experiment. This level of flexibility is not usually warranted and hence the current release of gFLARE does not offer this feature and uniform fluxes are applied to all the walls of the vessel.
  - The curves shown in Figure 12 correspond to Rear-Center, Rear-Left and Rear-Right evaluated as three separate simulations in gFLARE.
  - The effect of this is that when Rear-Center parameters are used, greater heat reaches the liquid inside vessel than in reality and likewise when Rear-Right parameters are used, lower heat reaches liquid inside vessel.
- The gFLARE predictions of rupture time are shown in Figure 13 using Rear-Center parameters. Rupture was predicted to occur at 13 minutes.

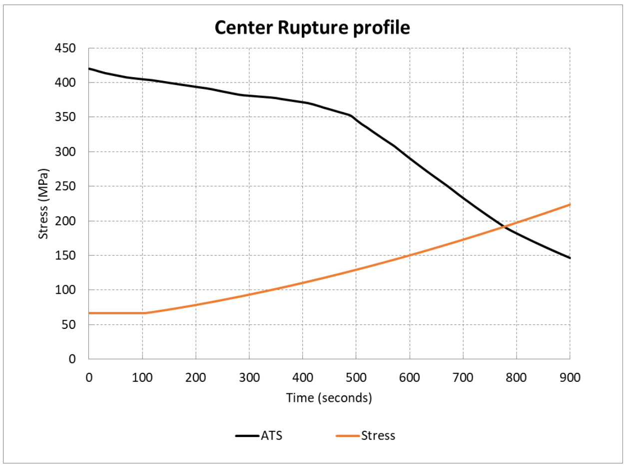

Figure 13: Rupture profile using Rear-Center parameters

4.References

[1]. Haque, M.A., et al. "Blowdown of Pressure Vessels: II. Experimental Validation of Computer Model and Case Studies." Trans IChemE, Vol.70, Part B (1992)

[2]. C. Balke, W. Heller, R. Konersmann, and J. Ludwig, "Study of the Failure Limits of a Railway Tank Car Filled with Liquefied Petroleum Gas Subjected to an Open Pool Fire Test", Federal Institute for Materials Research and Testing (BAM), Berlin, Test Report III.2/9907, September 13, 1999

[3]. J. Ludwig and W. Heller, "Fire Test with a Propane Tank Car", Federal Institute for Materials Research and Testing (BAM), Berlin, Test Report III.2/9907, 1999