Improvement of modelling of LNG pool fires on water

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The aim of this study is to improve the validation of the models simulating LNG pool fires on water within the EVOLCODE 3.1 software developed by GDF SUEZ's Centre for Research and Innovation (CRIGEN), which is dedicated to the gas sector and new energy sources. This work relies on a detailed analysis of the validity of EVOLCODE 3.1 for this type of phenomenon. This analysis is based on experimental data currently available in scientific literature and, in particular, on tests recently carried out by the Sandia National Laboratory. EVOLCODE 3.1 is also compared to the 3D KFX software developed by ComputIT in an attempt to understand in detail the phenomena involved in these types of fires.

Introduction: Modelling of LNG pool fires on water- a challenge for LNG installations

With the development of the international LNG industry, the number of scientific studies on the safety of LNG installations has grown. Large scale tests on LNG pool fires carried out by the SNL [1] (Sandia National Laboratory), and financed by the DOE (Department of Energy), bear witness to the high level of interest on the part of the American administration in risk assessment of LNG pool fires.

LNG Installations are designed to avoid accidental leaks of flammable products; nevertheless, LNG pool fires are one of the scenarios included in hazard studies. In rare cases, an LNG pool can spread over a ground- or water surface as a result of loss of containment in an installation.

In 1987, in order to better predict the consequences of such an event, GDF SUEZ undertook numerous tests on LNG ground surface pool fires with diameters of between 2m and 35m, most notably at the Montoir-de-Bretagne site. However, until the recent SNL tests, very few experiments have been undertaken to quantify the consequences of an LNG pool fire on water (only those carried out by the US Coast Guard have been identified).

Since the 1990s, GDF SUEZ' CRIGEN (Centre de Recherche et d'Innovation sur le Gaz et les Energie Nouvelles - Centre for Research and Innovation on Gas and Renewable Energies) has been developing the EVOLCODE 3.1 software program, a tool for quantifying the consequences of hazardous phenomena associated with accidental releases from LNG installations. CORE is one of the software modules concerned with simulating liquid hydrocarbon pool fires [2].

CORE is essentially based on simplified models (solid flame) relying on experimental correlations. In parallel, for more complex configurations, the CRIGEN uses KFX software developed by ComputIT[3], which is a program used by the oil and gas industries for 3D digital simulation of fires.

The aim of this current study is to compare the EVOLCODE 3.1 tool and the KFX 3D simulation program with experimental data available in scientific literature. The KFX software is used elsewhere in order to gain a better understanding of the modelling of complex physical phenomena.

Methodology: Comparison of EVOLCODE 3.1 with available experimental data and with the CFD KFX Software

Experimental trials carried out by the USCG[4] and the SNL served as a basis for the validation of the models

There have been two campaigns of large-scale, public tests on LNG pool fires on water: tests carried out by the US Coast Guard in 1979 [4] and tests conducted by the Sandia National Laboratory in 2010 [1].

USCG Campaign, China Lake, 1979

The aim of these tests was to verify the applicability of models of heat radiation defining danger zones around an LNG pool fire on water. Seven pool fire tests were undertaken at the US Navy's Naval Weapon Centre at China Lake in the US using pool diameters of up to 15m. The diameter, height and radiative heat of the flame were measured for different spill mass flows (See Table 1).

SNL Campaign, Albuquerque, 2010

With the growth in the international LNG trade in recent years, the US government has financed a research programme focused on tests of large-scale (80-120m) LNG pool fires. The results of this experimental campaign show that the use of the solid flame model can be adapted for large scale pool fires [5] provided that the parameterization is good.

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[3] An outline of the KFX program is provided in appendix 1.
[4] US Coast Guard

Characteristics of the different tests

The following table indicates the experimental conditions for the various USCG and SNL test campaigns.

Table 1 : Experimental conditions for the USCG and SNL tests

Test no.	Discharge volume (m^3)	Discharge duration (s)	Flow rate = 10^{-2}x (m^3/s)	Mass flow (kg/s)	Air temperature (°C)	Relative humidity (%)	Surface wind speed (m/s)	Wind direction relative to ground (°)
USCG 1	5,3	254	2,09	8,7	29	34	0	0
USCG 3	4,2	49	8.57	36	29	52	0	0
USCG 4	4,2	248	1.69	7.1	31	32	2.2	80
USCG 5	3	32	9.38	39.4	21	54	0.9	180
USCG 6	5.7	52	10.96	46	24	42	2.6	95
USCG 12	5.7	81	7.04	29.5	22	27	0	0
SNL 1	60.5	570	12	50.4	4	32	4.8	331
SNL 2	198.7	144	190	798	-2	59	1.6	324

EVOLCODE 3.1 outline

CORE is a semi-empirical model based on the "solid flame" approach in which the flame is treated as a simple surface (an inclined cylinder or an inclined parallelepiped) which emits heat uniformly over its entire surface.

CORE allows the modelling of:

- fires in circular pools,
- fires in rectangular pools,
- fires in polygonal pools,
- the reduction of fire by foam
- the reduction of radiative heat by screens (walls, buildings)

Flame modelling

The geometric and radiative characteristics of a flame are calculated on the basis of correlations. They depend on the hydraulic diameter of the pool: D_h = 4 Surface / Perimeter.

The main correlations are outlined below:

- Rate of combustion ($kg.m^{-2}.s^{-1}$) (SHELL model) (D_h and L_m in m and m_{max} in $kg.m^{-2}.s^{-1}$)

$$\dot{m} = \dot{m}_{max}\left(1-e^{-D_h/L_m}\right)$$

- Flame length (m) (Thomas formula) (D_h and L in m, m in $kg.m^{-2}.s^{-1}$, ρ_a in kg/m^3, g in $m.s^{-2}$):

$$\frac{L}{D_h} = 42\left(\frac{\dot{m}}{\rho_a\sqrt{gD_h}}\right)^{0,61}$$

- Flame inclination (°) (Welker formula) (D_h in m, ρ_a in kg/m^3, g in $m.s^{-2}$, U_a in m/s, ν_a in m^2/s, g in $m^{-1}.s^{-2}$):

$$\frac{\tan\theta}{\cos\theta} = 0,7\left(\frac{U_a D_h}{\nu_a}\right)^{0,109}\left(\frac{U_a^{2}}{gD_h}\right)^{0,428}$$

- Flame Emittance ($kW.m^{-2}$) (D_h and L_m in m and E_{max} in $kW.m^{-2}$):

$$E = E_{max}\left(1-e^{-D_h/L_m}\right)$$

Where:

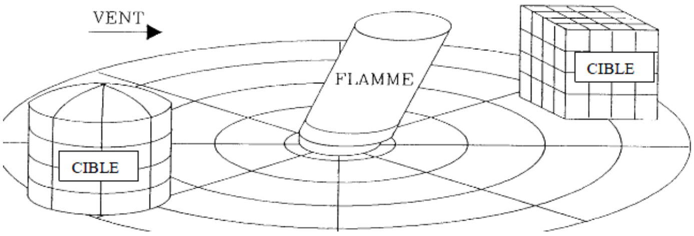
ρ_a= air density, U_a= wind speed, g = gravity, ν_a= kinematic viscosity of the air. The terms m_{max}, E_{max} and L are constants that depend on the nature of the fuel.

Modelling of the flow received by a target.

The flow (en kW/m^2) received by a target is expressed as $\phi = F.E.t_\alpha$ where:

- F is the shape factor, calculated on the basis of the shape of the flame as well as the distance between the target and the flame. The flame surface is meshed using triangular element on which the configuration factor is computed separately to improve accuracy in near field,
- E is the flame emittance,
- t_α is the atmospheric transfer coefficient. It accounts for the absorption of a portion of the radiative heat by water vapour, carbon monoxide and carbon dioxide in the air. Transmission factor of each species is estimated using the so called "spectral band method", transmission factor is estimated for each wavelength and is then integrated over the whole spectrum. To get the global transmission factor, one must consider energy point of view : the total amount of energy received by a target from a source is equal to the sum of all the contribution of individual wavelength. This approach has been developed with CORIA institute.

CORE has been validated on the basis of a relatively large number of LNG pool fires with various surface areas ranging from a few m^2 to 1000 m^2. The great diversity in validation elements allows CORE to be used for pool fires ranging in surface area from a few m^2 to several thousand m^2.



In 2011, a new feature has been added to CORE, which enables to simulate the effect of a dynamic pool fire. Basically, another module of EVOLCODE 3.1 called EVANUM which is used to evaluate the spilling and evaporation of a hydrocarbon pool is coupled to CORE: EVANUM return the diameter of the pool and CORE evaluate the flux received by the pool.

Pool spreading speed is evaluated assuming gravitational collapse of a column of fluid. The next relation has been established by Opschoor in 1979 :

$$\frac{dr}{dt} = \sqrt{2g\max\{0;h - h_{\min}\}}$$

When the thickness of the pool in less than h_{min}, friction and tension surface become more important than gravity and extension is stopped. h_{min} depends on soil nature and rugosity. Evolution of pool diameter is the controlled resolving the mass balance equation which can be expressed in volume since density is assume to be constant.

$$\frac{dV}{dt} = Q_{a\lim} - Q_{évap}$$

In the basic version of EVANUM convective heat transfer and radiation heat transfer are neglected in front of conduction heat transfer from the soil. EVANUM assumes liquid pool in boiling regime vaporization is directly proportional to heat flux received by the pool. Vaporisation speed reads :

$$v_{ébu} = \frac{q}{\rho_l L_v}$$

For a spread on soil, heat flux from ground is computed using conduction equation in semi-infinit medium

$$q = \frac{\lambda(T_{sol} - T_{ébu})}{\sqrt{\pi a t}}$$

With $a = \frac{\lambda}{C_p \rho}$ being the soil diffusivity. For a spreading on water, thermal heat flux is supposed to constant with value of qwater = 30 kW/m.

Gravitational collapse phase is identical, but when thickness of the pool is less than hmin, spreading is controlled by volume variation. In this phase, evaporation terme is assumed to be

$$Q_{évap} = \frac{\dot{m}}{\rho_l}$$

With $\dot{m}$ the combustion rate computed by CORE and ρ_l density of liquid pool. In our approach heat flux coming from water or ground are considered within radiation heat flux calculation of CORE.

KFX outline

KAMELEON is a three-dimensional dispersion calculation code for gas dispersion, fires and radiative heat which is used by the CRIGEN to calculate the consequences of a gas discharge. It is used in certain industrial safety studies of natural gas and LNG surface installations (estimation of gas jet dispersion, size and geometry of flames, heat flow in the environment and in structures).

KAMELEON was developed in partnership with a Norwegian research laboratory (SINTEF) and with partners in the oil and gas industry (including GDF SUEZ). It is commercialized by ComputIT.

It is a complex calculation code, using a three-dimensional computational mesh capable of dealing with the dispersion (heavy or light gases of $C_xH_yO_z$ type), combustion (liquid hydrocarbon fires, also known as “pool fires”, and jet fires) and the radiative heat of a gaseous hydrocarbon turbulent diffusion flame.

KAMELEON can deal with transitory regimes and therefore allows the calculation of the temporal development of a plume or a flame for variable gas flow. It is specifically designed for the study of industrial safety issues.

In house, this code is applied to horizontal discharges, impacting discharges taking obstacles into account, i.e. discharges that cannot be dealt with using simple models. The study of such configurations is necessary in the areas of gas transport, underground storage (stations, well heads, compressor packages, above ground pipeline sections, etc.), distribution (discharge in urban environments, pressure reducing stations, etc.) and in the area of gas use (heating systems, for example).

KAMELEON deals with open environments (open air) or congested and confined area (buildings, offshore modules, etc.) and takes into account the geometry of obstacles. The representation of the environment is particularly important in the case of obstructed layouts where obstacles can perturb flows and form screens against radiative heat. The treatment of these obstacles involves the inclusion of heat exchanges between the flame and the obstacles. However, the mesh is orthogonal and the number of cells is limited (a limitation linked to the calculation time). Each object is, therefore, represented by a limited number of parallelepipeds and all details of a complex geometry cannot be represented. However, this type of mesh associated with porosity models is generally sufficient for resolving industrial safety problems and it greatly simplifies the geometric construction phase for the scenario.

The code has been validated by SINTEF on the basis of data available in the literature [11]. Furthermore, KAMELEON has been the focus of a validation campaign undertaken by several industrials using confidential tests.

Comparison between KFX, EVOLCODE 3.1 and the experimental tests

EVOLCODE 3.1 accurately reproduces the USCG and SNL trials

There are two possible methods for reproducing the pool fire tests for LNG spills using EVOLCODE 3.1:

- Dynamic (CORE DYN): used to directly simulate the evolution of the burning LNG pool(with the aid of “Dynamic fire” pre-treatment in CORE) ; in the case of a stationary flow, the pool size also reaches a steady-state stage albeit lower because of a higher evaporation rate due to the radiative heat from the flame. This approach is based on a new development in CORE as yet rarely used for the calculation of hazard zones.
- Stationary with a fixed diameter: Only the radiative phase of a stationary fire is simulated; the diameter is set at the value measured experimentally. This method provides an element of comparison so as to analyse the accuracy of the radiative heat model independently of the model for pool spread.

The following tables outline the comparison between EVOLCODE 3.1 and experimental values for dimensions, combustion rates and flame emittance. In each case, the experimental values are compared to the first method (EVANUM+CORE), the second method (CORE DYN) and the simulation using the actual experimental diameter (CORE).

Table 2: Experiment/EVOLCODE 3.1 comparison: Flame diameter

	Relative deviation (%)		
Test no.	Experiment	CORE DYN	CORE DYN deviation
USCG 1	8.5	8.5	0.0%
USCG 3	11.5	15	30.4%
USCG 4	9	7	-22.2%
USCG 5	12.8	16	25.0%
USCG 6	15	17	13.3%
USCG 12	14	14	0.0%
SNL 1	21.4	18	-15.9%
SNL 2	50.3	69	37.2%

The dynamic fire model provides a pool diameter with a ±30% accuracy in 7 out of 8 cases. The second SNL test is less accurately modelled because in this test not all of the pool ignited, leading to a significant discrepancy between the diameter of the flame (51m) and the diameter of the LNG pool (80m). The EVOLCODE 3.1 model assumes that both diameters are identical.

Table 3 shows that the combustion rate is practically the same regardless of the way in which EVOLCODE 3.1 is used. Nonetheless, it appears that EVOLCODE 3.1 estimates the combustion rate with less accuracy (ca ±50%) for USCG tests 3, 5 and 6. These discrepancies are interpreted as being the result of the interaction between the water surface and the LNG pool, which is greater in the case of impacting jets compared to free jets. Nevertheless, the remaining comparisons appear to show that it has limited consequences on the modelling of the intensity of hazardous phenomena.

Since the flame length is linked to the combustion rate, it can be seen from Table 4 that the discrepancies between calculated flame lengths and actual test values are more significant where the combustion rate is underestimated. The CORE and CORE DYN approaches tend to slightly underestimate flame height. The flame height indicated by EVOLCODE 3.1 corresponds to the height of a inclined cylinder in an attempt to reproduce the effects of a real flame, which tends to narrow towards its extremity. The accuracy for the flame height is itself relative but does influence the accuracy for emittance (see Table 5).

Table 3 : Experiment/EVOLCODE 3.1 comparison: Combustion rates.

	Combustion rate (kg/s.m²)			Relative deviation (%)	
Test no.	Experiment	CORE	CORE DYN	CORE deviation	CORE DYN deviation
USCG 1	0.19	0.1904	0.196	1.9%	4.9%
USCG 3	0.43	0.208	0.196	-52.0%	-54.8%
USCG 4	0.15	0.21	0.161	37.7%	5.5%
USCG 5	0.40	0.211	0.2	-47.7%	-50.5%
USCG 6	0.36	0.222	0.2	-38.8%	-44.9%
USCG 12	0.22	0.218	0.192	-1.9%	-13.6%
SNL 1	01.5	0.21	0.2	40.0%	33.3%
SNL 2	0.15	0.214	0.21	42.7%	40.0%

Table 4 : Experiment/EVOLCODE 3.1 comparison – Flame length

	Flame length (m)			Relative deviation (%)	
Test no.	Experiment	CORE	CORE DYN	CORE deviation	CORE DYN deviation
USCG 1	24	27	27	12.5%	12.5%
USCG 3	47.2	26	44	-44.9%	-6.8%
USCG 4	25.5	20	24	-21.6%	-5.9%
USCG 5	55	28	46	-49.1%	-16.4%
USCG 6	42	33	50	-21.4%	19.0%
USCG 12	44	31	41	-29.5%	-6.8%
SNL 1	70	57	50	-18.6%	-28.6%
SNL 2	141	106	132	-24.8%	-6.4%

Lastly, Table 5 compares the corrected experimental flame emittance with the flame emittance calculated by EVOLCODE 3.1. The corrected experimental flame emittance corresponds to the emittance of a radiative cylinder with a diameter and height corresponding to modelled flame and emitting the same heat flux as real flame at the experimental measurement points. This comparison is more representative than a direct comparison with the average emittance because the flame model used in EVOLCODE 3.1 is that of a solid, cylindrical flame.

It is therefore clear that there is **a good agreement between experimental values and the emittance values calculated by the EVOLCODE 3.1 model** (accuracy of ca ±30%), **regardless of the method used**.

Table 5 : Experiment/EVOLCODE 3.1 comparison – Flame emittance

	Flame emittance (kW/m²)			Relative deviation (%)	
Test no.	Corrected experimental value	CORE	CORE DYN	CORE deviation	CORE DYN deviation
USCG 1	–	139	139	-	-
USCG 3	207	190	174	-8.2%	-15.9%
USCG 4	200	192	130	-4.0%	-35.0%
USCG 5	187	194	183	3.7%	-2.1%
USCG 6	185	207	181	11.9%	-2.2%
USCG 12	224	203	170	-9.4%	-24.1%
SNL 1	191	187	181	-2.1%	-5.2%
SNL 2	169	195	194	15.4%	14.8%

The following figure shows a comparison between the heat flux measured in the two SNL experiments and those calculated by EVOLCODE 3.1 using the different methods. The use of the stationary fire model with the experimental diameter value (CORE module alone) shows a high level of agreement with the experimental data. The use of the dynamic fire model overestimates heat radiation levels by approximately 40%; this is principally due to the fact that the model assumes that the entire pool ignites while in the experiment only a portion of the LNG pool did in fact ignite.

Almost 74% of the measurement points are ±40% accurate when CORE alone is used (fixed diameter). This result can be explained by the fact that the shape of the pool differs from the circular model used in CORE: in fact, the model was calibrated using fires whose dimensions were controlled, which is not the case for a free-spreading pool as in the case of the SNL tests. In addition, the model provides an upper bound in 87% of cases.

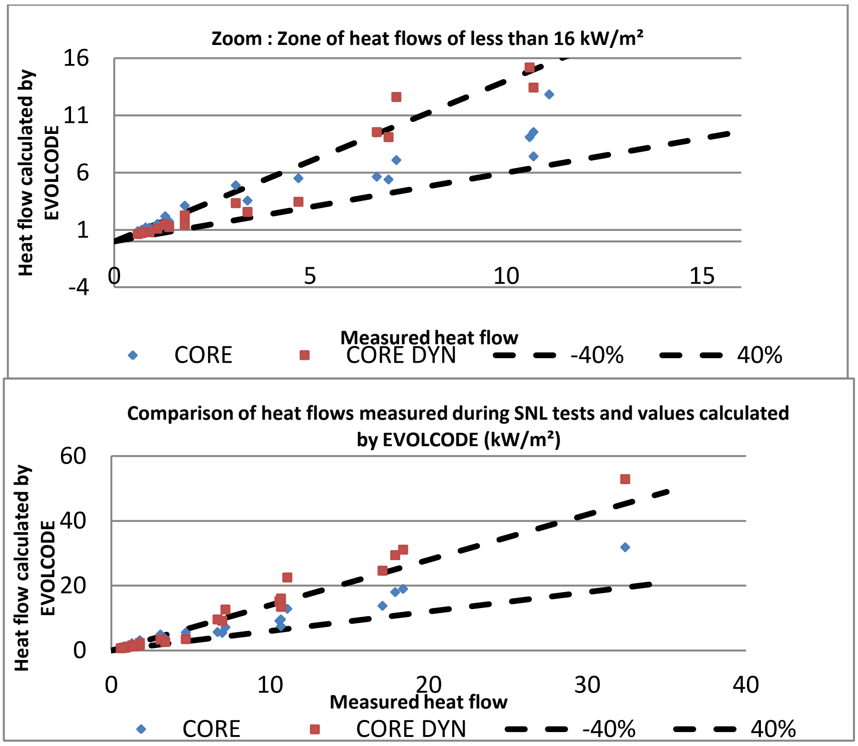


Figure 1 : The use of EVOLCODE 3.1 with the dynamic fire model allows the SNL experiments to be fairly accurately described.

Table 6 : EVOLCODE 3.1 allows correct description of the SNL experiment.

Accurate point number/Total point number	With a 0% to +30% accuracy	With a +30% to 50% accuracy	With a >+50% accuracy	With a -30% to 0% accuracy	With a -50% to -30% accuracy	With a <-50% accuracy	With a -30% to +30% accuracy	With a -40% to +40% accuracy	With a -50% to +50% accuracy
CORE	30.4%	13.0%	21.7%	30.4%	4.3%	0.0%	60.9%	73.9%	78.3%
CORE DYN	34.8%	21.7%	21.7%	21.7%	0.0%	0.0%	56.5%	60.9%	78.3%

KFX accurately simulates the SNL tests; comparison with the USCG tests was not performed due to incomplete data.

The KFX program developed by ComputIT allows the simulation of the spread, dispersion, and ignition of an LNG pool. This digital simulation software (CFD) numerically solves the basic equations of fluid mechanics, thermodynamics and turbulence. CRIGEN has already carried out a comparison of KFX with experimental tests on pool fires and pool spread on a ground surface [5]. This study showed that KFX could be used to accurately simulate large scale LNG pool fires.

The KFX simulations require that a large number of parameters be considered. Due to a lack of data concerning the USCG series of experiments, KFX modelling proved to be impossible. As a result, in this section only the SNL tests, for which a full dataset is available, were subjected to KFX modelling.

Two approaches were adopted in the use of the software:

- The simulation of an LNG pool with a fixed diameter equal to the experimental diameter. This approach validates the relevance of the software only for the simulation of fire.
- The simulation of a spreading pool ignited from the onset (the moment of ignition corresponds to the start of the spill). This approach allows the ability of the software to simulate the entire phenomenon (pool formation + fire) to be tested.

The following tables compare the geometrical characteristics of the flame simulated by KFX to experimental data. It appears that KFX reasonably reproduces (±40%) the geometry of the flame whether by setting the diameter to the experimental value or by allowing the calculation of spread to determine the diameter.

Table 7 : Experiment/KFX Comparison – Flame diameter

	Flame diameter (m)		Relative deviation (%)
Test no.	Experiment	KFX Spread	KFX/EXP deviation
SNL 1	21.4	20	-4%
SNL 2	50.3	44*	-12.5%

*The flame is not circular at its base; the reported diameter represents the equivalent diameter corresponding to the same surface averaged over several simulation instants.

Table 8 : Experiment/KFX Comparison – Flame length[5]

	Flame length (m)			Relative deviation (%)	
Test no.	Experiment	KFX Spread	KFX fixed diameter	KFX Spread/EXP deviation	KFX fixed diameter/EXP deviation
SNL 1	70	50	44	-28%	-37%
SNL 2	141	150	200	6%	+40%

It is also interesting to note that the second test simulation reproduces the incomplete ignition of the pool as illustrated in Figure 2 below.

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[5] Flame length was calculated on the basis of the KFX RGBA output, which combines local temperature and the soot mass fraction so as to determine the shape of the flame. Because the flame fluctuates during simulation, the average over several simulation instants was used for the calculation.

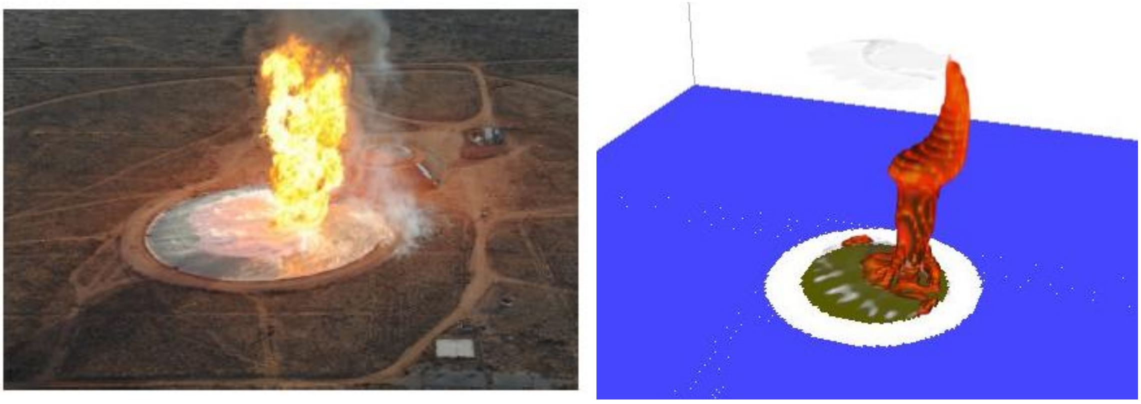

Figure 2 : KFX allows the incomplete ignition of the pool, observed experimentally, to be reproduced.

Figure 3 compares the heat flux measured during the SNL tests with those calculated by KFX using the different methods. There is a good agreement with experimental data when the software is used with the experimentally measured diameter, but the simulation using the free spread gives even closer results[6]. Table 9 shows that the results are less accurate than with EVOLCODE 3.1. However it is important to keep in mind that EVOLCODE 3.1 relies on correlations provided by numerous LNG pool fire tests, while KFX is a generic code based on numerical simulation. It is therefore more difficult to obtain a result which is close to reality using this software. Nonetheless, the results indicate that KFX can reproduce, with a high degree of accuracy, the behaviour of LNG pool fire phenomena and can therefore be used to supplement experiments where needed.

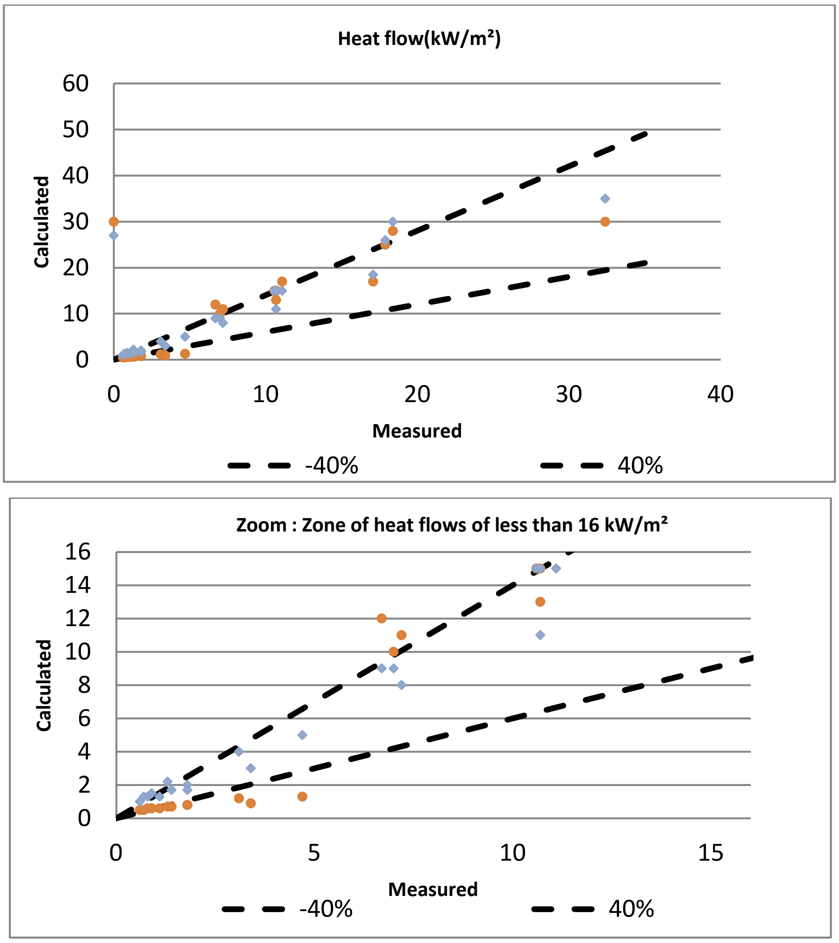

Figure 3 : The use of KFX with the dynamic fire model allows the SNL test to be accurately reproduced.

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[6] Towards the end of the simulation (after 120s of a 150s simulation), it can be seen that the ignited portion of the pool tends to increase, leading to an increase in the radiative heat level. The flow values reported in this document correspond to a period during which the simulation is practically stationary (between 70s and 120s).

Accurate point number/Total point number	With a 0% to +30% accuracy	With a +30% to 50% accuracy	With a >+50% accuracy	With a -30% to 0% accuracy	With a -50% to -30% accuracy	With a <-50% accuracy	With a -30% to +30% accuracy	With a -40% to +40% accuracy	With a -50% to +50% accuracy
KFX fixed diameter	4.3%	17.4%	17.4%	21.7%	17.4%	21.7%	26.1%	34.8%	60.9%
KFX free spread	43.5%	21.7%	26.7%	8.7%	0.0%	0.0%	52.2%	60.9%	73.9%

Table 9 : KFX allows the SNL experiment to be accurately reproduced.

In addition, the grid sensitivity was tested for one of the simulated cases: the calculations were performed with a 2m cell-size grid in the zone close to the spread, amounting to approximately 700 000 calculation cells. A finer mesh with cells 1m in size in the cubic zone, amounting to 5 000 000 calculation cells, was tested for only one of the simulation cases (Test 2 with fixed pool diameter).

Figures 4 and 5 illustrate the evolution of the heat flow for the two simulations at the level of two measurement points. These calculations show that sensitivity to the mesh persists, with no clear possibility to identify a direct link between the mesh and the accuracy of the results.

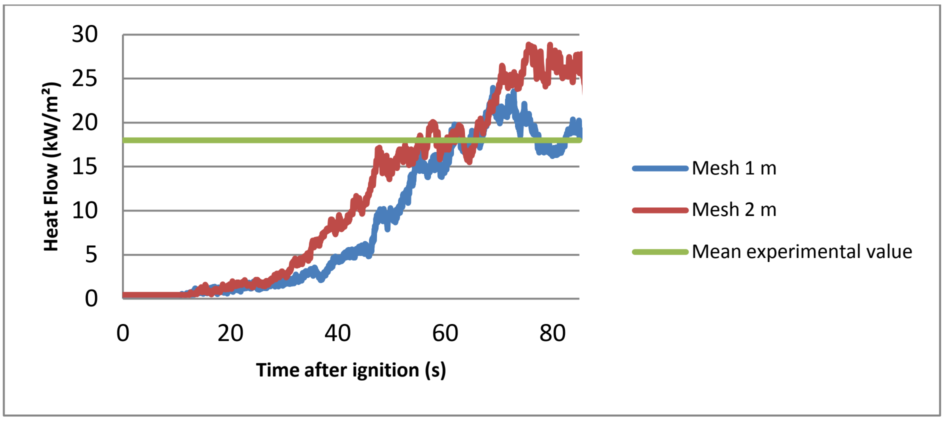


Figure 4 : Evolution of heat flow at a height of 55m and 110m north of the spill location

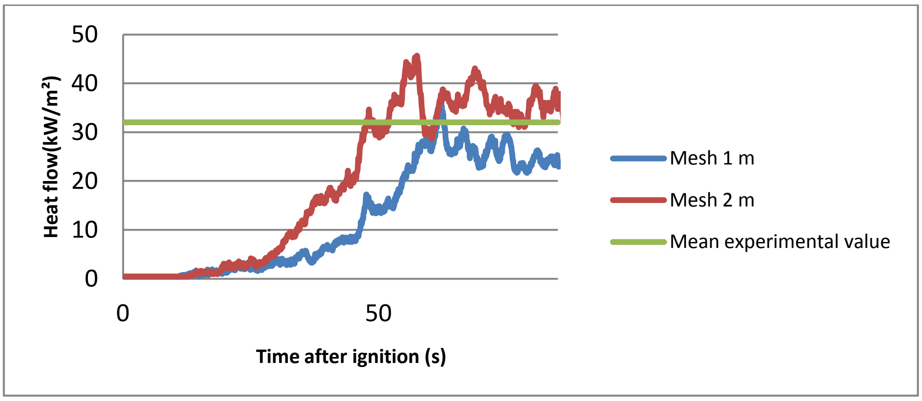


Figure 5 : Evolution of heat flow at a height of 55m and 110m south of the spill location

Overview of comparisons: EVOLCODE 3.1 and KFX allow LNG pool fires on water to be adequately simulated.

The comparisons performed show that EVOLCODE 3.1 allows the large-scale experimental tests on LNG pool fires to be simulated in an acceptable manner (74% of measurement points are accurate within ±40%). Moreover, the model provides an upper bound in 87% of cases.

The KFX software appears equally adequate to model these phenomena and to try to define the physical tendencies (comparable validation: 62% of measurement points accurate within ±40%) and therefore better understand the associated physical phenomena.

In the case of EVOLCODE 3.1, these results are all the more satisfactory because the physics of the phenomena involved are complex and the. The EVOLCODE 3.1 models thus provide upper bound modelling in most cases with a degree of overestimation limited to +40% in the case of radiative heat levels mainly due , in the case of test no.2, to the non-consideration of the partial ignition of the LNG pool.

KFX succeeds in providing an acceptable estimate of the levels of heat flow in the two SNL tests; in addition, the program manages to reproduce the incomplete ignition of the pool in the case of test no.2. The use of the spread module upstream produces acceptable results for estimating flame geometry and heat flow levels.

Analysis of smoke screen formation capable of limiting overestimation of flows

It has been observed in other instances of hydrocarbon fires that an increase in pool diameter triggers an increase in the production of soot, which in turn can create a screening effect on the flame by the smoke. In [9], P. Raj suggests a modification of the standard model for LNG pool fires in order to take into account this phenomenon, which can lessen fire intensity. However, the 2010 SNL experiment did not confirm the formation of a smoke screen capable of lessening the radiative heat intensity as had been anticipated by the researchers. In fact, very little smoke was observed during the SNL experiment, less than was produced during the tests undertaken by GDF SUEZ at Montoir-de-Bretagne in 1987 (35m diameter fires) as can be seen in Figure 6.

Figure 6 : The Montoir LNG pool fire tests (left) show a greater production of smoke than the SNL experiment (right).

According to the research team, the main reason for this discrepancy lies in the presence of water around the LNG pool fire [8]. Several studies quoted in [8] indicate that the presence of water vapour generally has the effect of reducing the production of soot: The presence of water can lower both the fuel- and combustion air partial pressure thereby disrupting the chemical equilibrium. It can also have an impact on the thermodynamic and radiative balance of the flame and finally it can be chemically active.

The various phenomena described above can be taken into account by KFX except for the chemical aspects, which would require a modification of the combustion model. Sensitivity studies have been carried out using this program in order to verify whether the numerical simulation can reproduce experimental observations and provide certain hints so as to better understand the reduced presence of soot in the SNL tests.

Several parameters which can influence soot formation have been the subject of KFX tests:

- Scale effect: the larger the fire diameter, the greater the formation of soot is expected to be.
- The presence of water around the pool fire: according to the experimental researchers, the latter ought to reduce the presence of soot.
- Wind speed during the phenomenon: this aspect has not been mentioned by the SNL researchers, but it constitutes an additional difference between the SNL and the GDF SUEZ tests.

Scale effect:

Several calculations were performed using KFX where the diameter of the flame was varied. As can be noted in Table 10 below, KFX reproduces quite well the increase in soot level with increasing diameter. It is also clear from Figure 7 that the soot is located at the centre of the flame where, in the context of experiments, unburnt hydrocarbons are found due to lack of oxygen.

Table 10 : Evolution of soot mass fraction maximum calculated as a function of diameter.

Pool diameter (m)	Soot mass fraction maximum
10	0,011
30	0,018
60	0,02
90	0,023
120	0,027
150	0,03

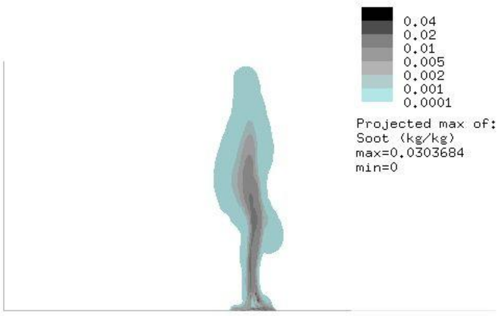


Figure 7 : Soot is located at the centre of the flame where some of the gas remains unburnt.

Influence of water on pool combustion:

The presence of water is taken into account by adding a water vapour source term around the LNG pool. The input rate was calculated by estimating the vaporisation of water following absorption of radiative heat from the flame[7]. In addition, a heat exchange flow from water surface of 30kW/m^2 was integrated into the simulation in line with standard EVOLCODE 3.1 practice. Figure 8 shows that water vapour is drawn in at the base of the flame and thus ends up in the combustion zone.

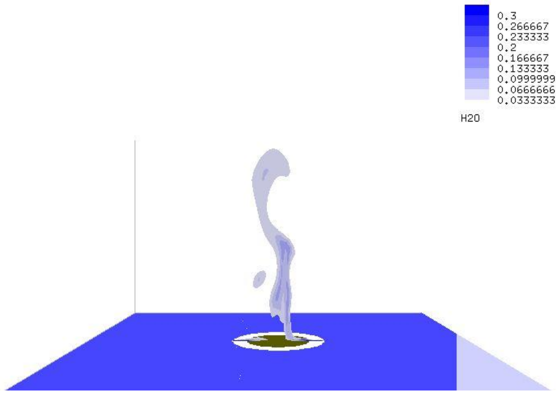
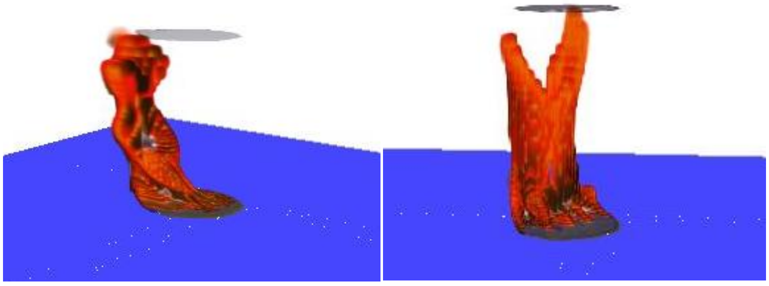


Figure 8 : Fluid motion draws in water vapour at the base of the flame

For this simulation, taking water into account reduces the formation of soot by 25% compared to a simulation which omits water. The figure 9 shows the shape of the flame calculated by KFX with and without the presence of water. This reduction in soot, which is hardly discernible in the figure, is not very significant and does not entirely explain the marked difference between the 1987 GDF SUEZ tests and those carried out by the SNL in 2010.

Influence of the wind:

Another difference between the SNL tests and the GDF SUEZ tests is the intensity of the wind, which was low at the time of the SNL tests and high during the GDF SUEZ tests. An additional simulation was carried out using a wind speed of 5 m/s at a height of 10 m from the ground (it should be remembered that previous simulations had a near-zero wind speed). It is evident from the shape of the flame that the formation of smoke increases, in particular in the upper part of the flame, a situation which corresponds to experimental observations. In addition, the formation of soot is almost 50% greater in this case.



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[7] For a heat flow value of 100 kW/m^2 absorbed by water (corresponding to typical flow values measured in the Sandia experiment), a surface evaporation rate of 0.045 kg/s/m² is obtained.

Figure 9 : According to KFX simulations, an increase in wind speed increases soot formation (Left: Flame with a wind speed of 5 m/s. Right: flame with wind speed of 1 m/s at 10 m from the ground).

It appears therefore that KFX can reproduce the weaker formation of soot observed in experiments and provides a means of studying flame behaviour under different conditions. In addition, the simulations highlight the role of the wind in the formation of soot, which had not been identified experimentally. A possible explanation is that the recirculation of unburnt fuel leads to the further formation of soot. Further tests are needed in order to confirm these predictions.

Taking into account the screening of the flame by smoke could lead to a reduction in the overestimation of danger zone extents by standard models. However, since the soot production phenomenon is very complex, it cannot be easily integrated into EVOLCODE 3.1 except by means of an empirical correlation. Numerical simulation using a CFD program such as KFX might help in the development of such a correlation but it would have to be further validated, which would require that additional, large-scale tests be carried out.

Conclusions: EVOLCODE 3.1 and KFX allow LNG pool fire tests to be simulated correctly.

The comparisons carried out indicate that the EVOLCODE 3.1 and KFX programs allow large-scale tests of LNG pool fires to be simulated adequately.

In the case of EVOLCODE 3.1, these results are all the more satisfactory because the physics of the phenomena involved are complex and the models used to describe them are relatively simple. The EVOLCODE 3.1 models thus provide upper bound modelling in most cases with a degree of overestimation limited to +40% in the case of radiative heat levels mainly due , in the case of test no.2, to the non-consideration of the partial ignition of the LNG pool.

KFX succeeds in providing an acceptable estimate of the levels of heat flow in the two SNL tests; in addition, the program manages to reproduce the incomplete ignition of the pool. The use of the spread module produces reliable results for estimating flame geometry and heat flow levels.

Taking into account the screening of the flame by smoke could lead to a reduction in the overestimation of danger zone extents by standard models. However, the soot production phenomenon is extremely complex and it can only be simulated using a CFD program such as KFX (provided it has been validated for this domain).

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