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## **DRA 08 - Tâche de fond relative à la validation des outils de modélisation**

Rapport d'auto-description de l'outil Boil-Over selon la  
procédure SAPHEDRA

MINISTERE DE LA TRANSITION ECOLOGIQUE

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# BoilOver – Prediction of thermal consequences of a boilover phenomena

## SAPHEDRA description

### A0 - Contact DATA

Name of Tool/model	BoilOver (BO)
Version of the tool	1.00
References of the last evaluation	First evaluation
Model developer contact information and references	Benjamin TRUCHOT <a href="mailto:Benjamin.truchot@ineris.fr">Benjamin.truchot@ineris.fr</a> +33(0)3 44 61 81 50

### A1 - Scientific assessment

#### A.1.1 Description of scope of application

The BoilOver (BO) model is dedicated to the prediction of thermal consequences of the boilOver phenomena that could happen on hydrocarbon tanks.

#### A.1.2 General flowchart of the tool and identification number of models

The BoilOver model is based on several computation. The calculation method, according the flowchart given on Figure 1, can be described through the following steps:

- evaluation of the hydrocarbon mass involved in the boil-over,
- computation of the fire ball characteristics,
- calculation of the radiative effect and induced consequences.

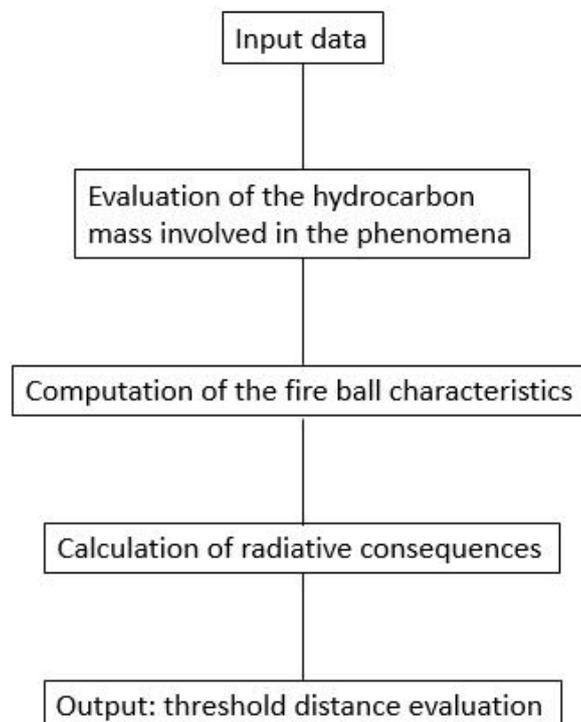


Figure 1: General flow chart of BoilOver model

### A.1.3 General description of databases

The BoilOver modelling tool uses values described in Table 1.

Grandeur physique	Fuel oil n°2	Light crude oil	Heavy crude oil
Boiling temperature (K)	544	535	621
Initial boiling temperature, 15% of the product evaporated (K)	453	348	368
Final boiling temperature, 85% of the product evaporated (K)	643	823	1047
Critical temperature (K)	929,8	686	810
Critical pressure (Pa)	$1,53 \cdot 10^6$	$1,86 \cdot 10^6$	$1,525 \cdot 10^6$
Liquid density at 288°K (kg/m3)	990	802	905
Gas density at 300°K (kg/m3)	11,65	6,686	9,7
Heat of vaporization at boiling temperature (J/kg)	$8,6 \cdot 10^5$	$2,92 \cdot 10^5$	$3,384 \cdot 10^5$
Heat of combustion (J/kg)	$4,01 \cdot 10^7$	$4,33 \cdot 10^7$	$4,184 \cdot 10^7$
Upper flammability limit (% volume)	0,055	0,055	0,055
Viscosity at 393 K (cSt)	10	2	5,2

Table 1: Material properties used in the BoilOver model

### A.1.4 Input and output visualization process

All input data are fulfilled using a dedicated GUI, in French, included in the EPHEDRA platform. A screenshot of this interface is reproduced Figure 2.

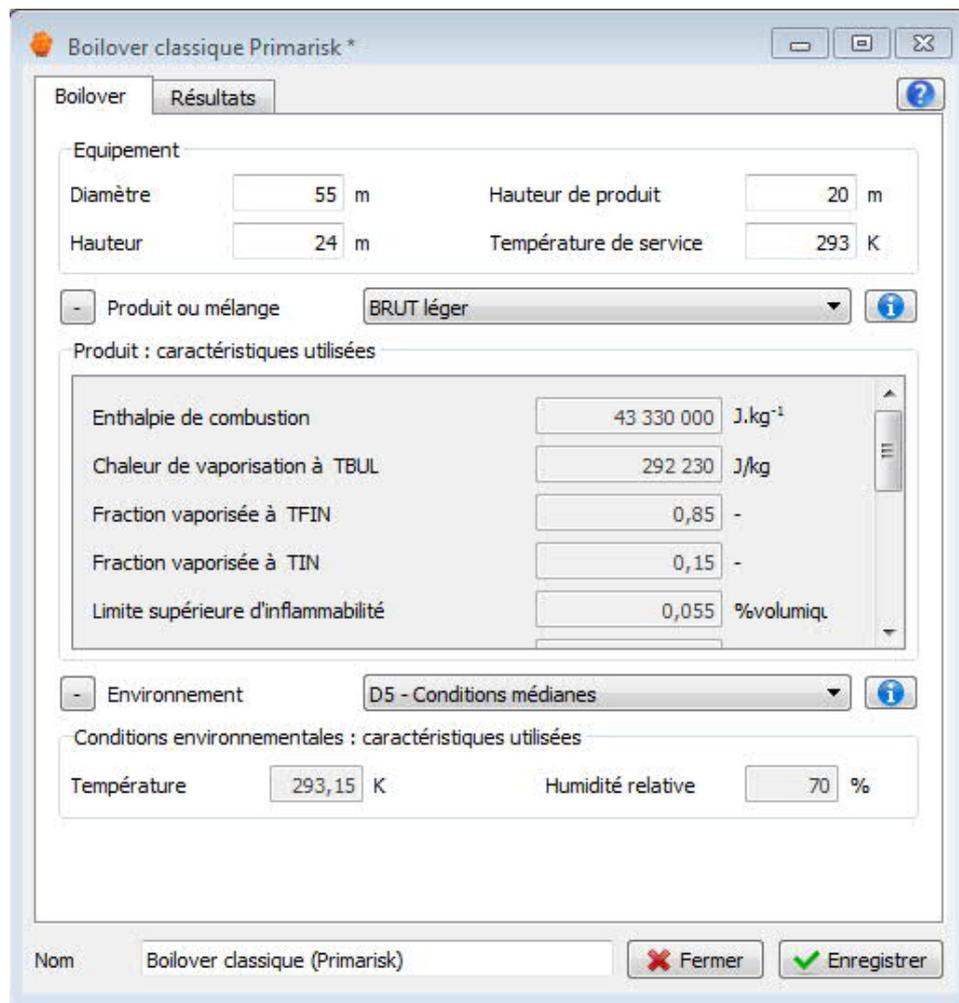


Figure 2: GUI screenshot (in French) for the BoilOver model in the EPHEDRA platform

The interface also enables visualizing the results in terms of a list of consequence distances.

## A.1.5 Detailed description of the theoretical approach of the models

Main characteristics of the physical models are detailed in following paragraphs.

### A.1.5.1 Evaluation of the hydrocarbon mass involved

Considering the initial quantity of product inside the tank, i.e. the initial height according to the input data, the hydrocarbon combustion rate is compared to the hot layer velocity. Obviously, the hot layer velocity should be higher than combustion rate to let the boilover possible. Both velocities are computed using the characteristics of the hydrocarbon on details of the storage. The combustion velocity,  $v_1$ , is computed by:

$$v_1 = 10^{-3} \frac{\left( \frac{\Delta H_c}{\rho_l(TM)} \right)}{TBUL + \int_{T_{SER}} C_p(T).dT}$$

This equation considers the hydrocarbon characteristic as heat of combustion,  $\Delta H_c$ , heat capacity,  $C_p$ , latent heat of vaporization,  $L_v$ , and density,  $\rho$ . The density is estimated at a mixed temperature,  $TM$ , mixed temperature computed as :  $TM=(T_{SER} \times TBUL)^{0.5}$ .  $T_{SER}$  is the temperature of the hydrocarbon in the tank,  $TBUL$ , its boiling temperature.

The hot layer velocity is based on the initial liquid height,  $HLIQ$ , and the estimated boilover time,  $t_{BO}$ :

$$v_2 = \frac{HLIQ}{t_{BO}}$$

with the boilover time calculated by;

$$t_{BO} = \frac{\rho_l(T_{SER}) C_p(T_{SER}) (T_{WAV} - T_{SER}) HLIQ}{\Phi}$$

In this equation,  $f$ , is the heat flux received by the pool surface, the value is fixed to 60 kW/m<sup>2</sup>.  $T_{WAV}$  is the hot wave temperature.  $T_{WAV}$  is estimated using the distillation curve of the product.

More details on the equations are given in the Ineris report □13<sup>1</sup>.

At the end of this first step, the resulting value is  $M_{vap}$ , the hydrocarbon mass that could be involved in the boilover phenomena.

### A.1.5.2 Computation of the fire ball characteristics

Among the characteristics of the fire ball, the emissivity is first fixed to 150 kW/m<sup>2</sup> based on experimental data<sup>2</sup>. This hypothesis is used to compute the flame temperature,  $TFLA$ , and the gas density,  $\rho_g(TFLA)$  at this temperature using perfect gas relation:

$$TFLA = \left( \frac{\phi_0 + \varepsilon \cdot \sigma \cdot T_{AMB}^4}{\varepsilon \cdot \sigma} \right)^{1/4}$$

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<sup>1</sup> <https://www.ineris.fr/sites/ineris.fr/files/contribution/Documents/omega-13-eng-final-2-1425980693.pdf>

<sup>2</sup> Broeckmann et al, Boilover effects in burning oil-tanks - 7<sup>th</sup> International Symposium on Loss Prevention and Safety Promotion in the Process Industries, 1992

The mass concentration of hydrocarbon,  $C$ , is then computed assuming that the mixture is at the UFL (Upper Flammability Limit). Knowing the concentration and the total mass of hydrocarbon,  $MVAP$ , gives the fireball volume,  $V_{FB}$  and consequently its radius,  $r_{FB}$

$$V_{FB} = \frac{MVAP}{C}$$

$$r_{FB} = \left( \frac{3}{4\pi} V_{FB} \right)^{1/3}$$

The duration of this fireball is computed thanks to an experimental correlation<sup>3</sup>. This duration is then used to compute the height of the fire ball. More details are given in the Ineris □13 report.

### A.1.5.3 Calculation of radiative distances

The incident radiative heat flux in the surrounding is then estimated by computing the view factor, with an analytical formula since the fire ball is assumed to be a sphere and considering the atmospheric transmissivity using the Bagster<sup>2</sup> formulae.

### A.1.6 Detailed description of model calibration

Very few data exist for boilover phenomena, so calibration is not possible. The only calibration concerns the hypothesis made along the model as flame surface emitting power (SEP) or the UFL as a representative concentration. These hypotheses are based on scientific publications.

### A.1.7 Description of the mathematical approaches for models

The boilover model is mainly based on algebraic formulae that do not request specific numerical method.

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<sup>3</sup> Bagster, DF and PITBLADO, Thermal hazards in the process industry, CEP, pp. 69-75, 1989.

## A2 - Verification

### A.2.1 Description about development under quality assurance

The boilover model was developed under the Ineris internal quality procedure. Basic tests were achieved all along the development procedure to ensure that intermediate quantities are in accordance with expected values. Some comparisons were achieved for intermediate values.

### A.2.2 Description about mesh consistency tests

No mesh is used in the model.

### A.2.3 Management of interfaces between models

Exchanges between sub models are very simple. The first model computed the hydrocarbon mass involved in the phenomena. This mass is passed to the fire ball characteristics module that compute the radius of the ball, its duration and its height. Those three values are used to compute the radiative consequences.

### A.2.4 Tests about numerical approaches for the N models

Not relevant for the boilover tool. It does not require numerical models.

### A.2.5 Tests about comparison between numerical approaches for the N models versus analytical solution

This requirement is not relevant for boilover according that no PDE has to be solved.

## A3 - Sensitivity analysis

### A.3.1 Description of choice of range of values for varying parameters within the scope of application

The input parameters for the boilover model are the diameter of the tank, its height, the height of liquid inside the tank and the working temperature. The hydrocarbon product should also be chosen.

Varying parameters, description and variability ranges are presented in the table hereafter.

Parameter	Reference value	Variability range
<b>Tank characteristics</b>		
Tank diameter	60 m	20 to 100 m
Tank height	25 m	10 to 40 m
<b>Product characteristics</b>		
Name of the product	Fuel oil n°2	Both three products were testes
Height of the product	20 m	5 to tank height
<b>Service conditions</b>		
Service temperature	330 K	290 to 390 K

For sensibility study was also done regarding the product characteristics by varying all characteristics for fuel oil n°2.

### A.3.2 Detailed presentation of the results for each parameter (p) in order to be able to do the same modelling

Evolution of the 3, 5 and 8 kW/m<sup>2</sup> reached distance for varying above mentioned parameters are presented in the following graphs.

Detailed graphs are provided for 3 kW/m<sup>2</sup> distance and for fuel oil n°2. For other products and other thresholds, only some graphs are shown to illustrate the identical behavior.

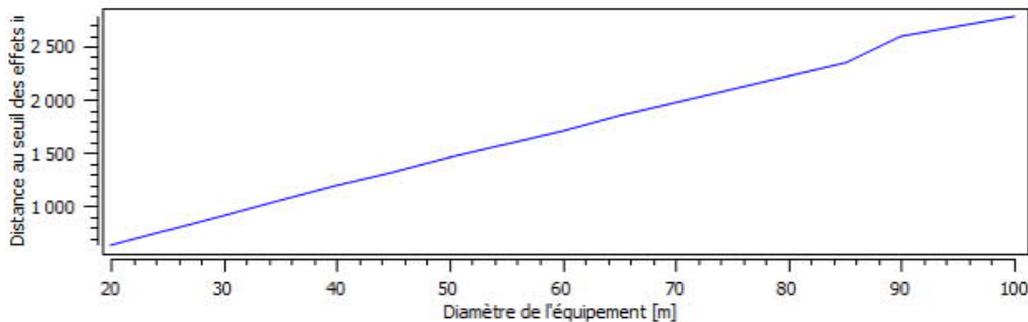


Figure 3: Influence of the tank diameter, evolution of the 3 kW/m<sup>2</sup> distance, HC volume from 6 000 m<sup>3</sup> (20 in-diameter tank with 20 m height of liquid) to 150 000 m<sup>3</sup> (100 m in-diameter tank, 20 m liquid height)

As expected, consequences rise when the diameter rise.

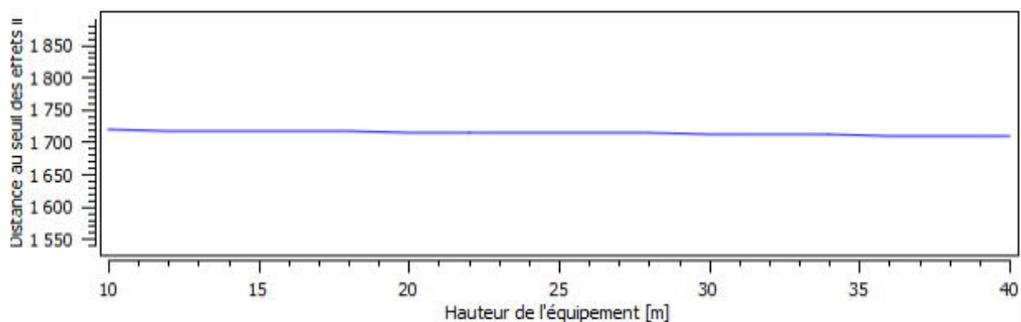


Figure 4: Influence of the tank height, evolution of the 3 kW/m<sup>2</sup> distance

The equipment height, for a given height of liquid does not really affect the computed distance.

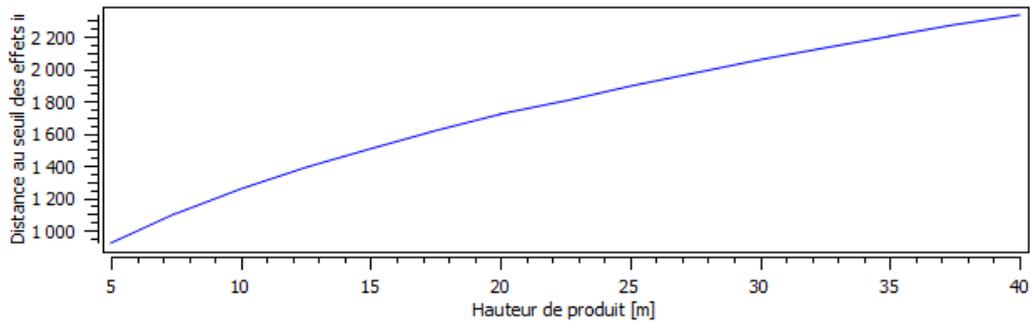


Figure 5: Influence of the liquid height, evolution of the  $3 \text{ kW/m}^2$  distance

This graph shows an expected tendency, more liquid is present when the fire starts, more fire is still here when the boilover is triggered. The tendency is confirmed when studying the  $5 \text{ kW/m}^2$  distance, Figure 6.

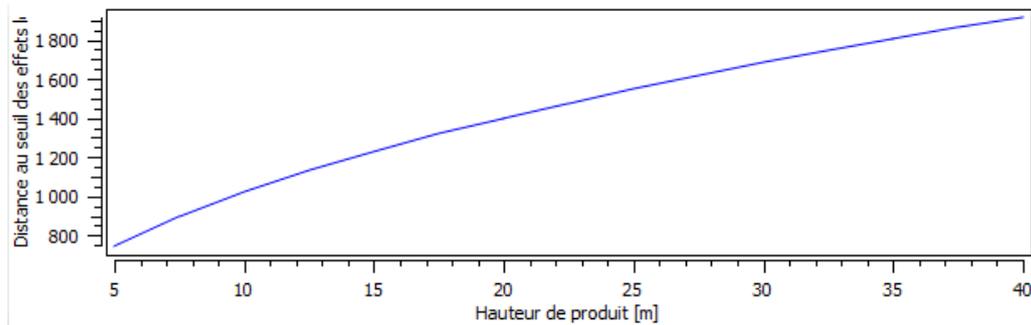


Figure 6: Influence of the liquid height, evolution of the  $5 \text{ kW/m}^2$  distance

Finally, the service temperature does not affect strongly the computed distances.

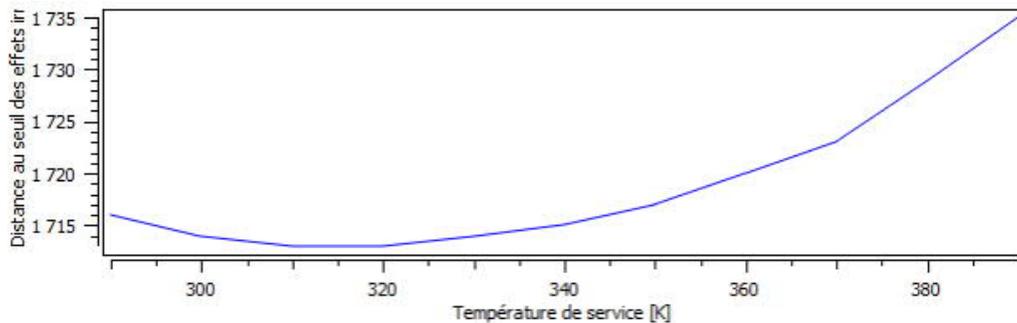


Figure 7: Influence of the liquid service temperature, evolution of the  $3 \text{ kW/m}^2$  distance

By modifying the product properties, for example initial and final boiling temperature, curves presented on Figure 8 and Figure 9 are obtained. Those curves were built for the reference conditions and keeping other properties of the product unchanged.

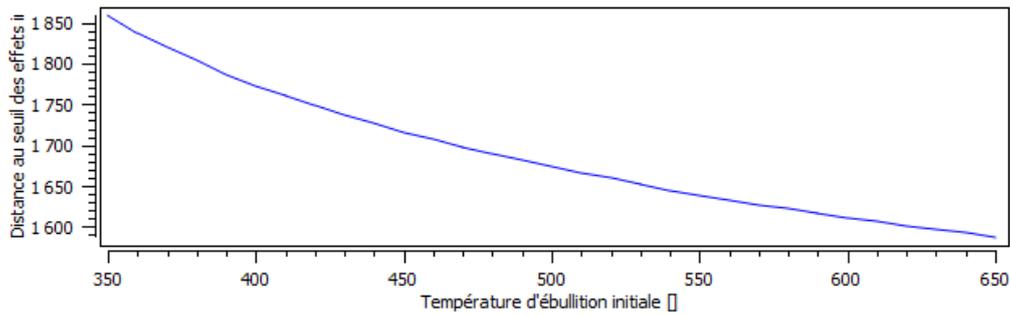


Figure 8: Influence of the initial boiling temperature, in K,, evolution of the 3 kW/m<sup>2</sup> distance

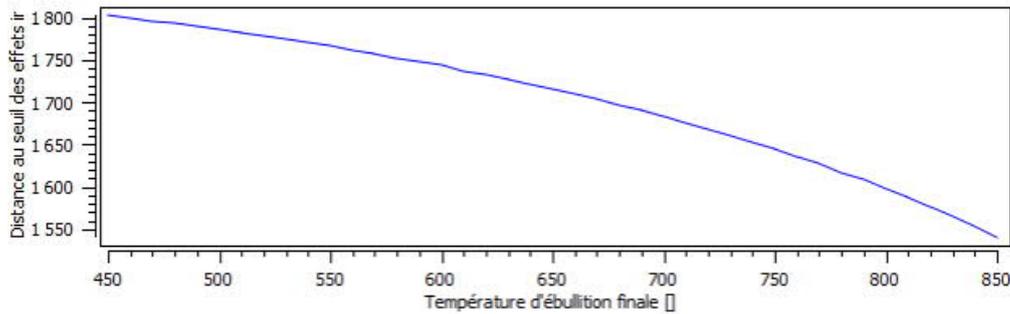


Figure 9: Influence of the final boiling temperature, in K, evolution of the 3 kW/m<sup>2</sup> distance

The influence of fuel viscosity, Figure 10. While it could appear surprising at first sight, it should be reminded that viscosity is only a criterion for the boilover to occur since if viscosity is not important enough, the liquid fuel is not pushed by vaporized water but water goes through the fuel. Then in the model, viscosity is not used to computed consequences, so zero influence is a normal situation.

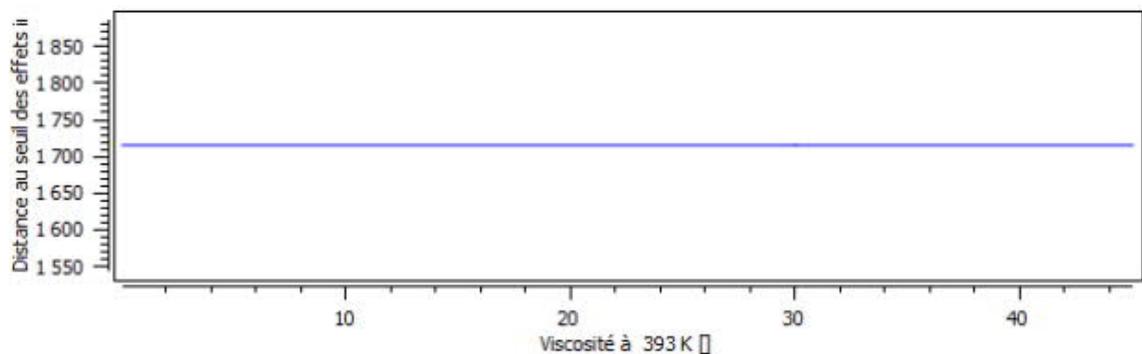


Figure 10: Influence of the fuel viscosity, in cSt, evolution of the 3 kW/m<sup>2</sup> distance

As an example, the influence of the tank diameter for heavy crude oil is plotted hereafter on Figure 11.

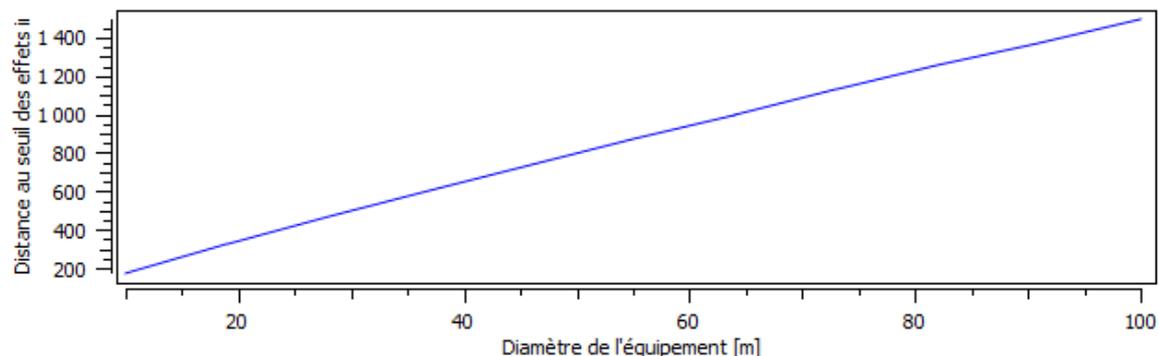


Figure 11: Influence of the tank diameter for the heavy crude oil, evolution of the 3 kW/m<sup>2</sup> distance

The curve confirms the results described previously for the fuel oil n°2.

### A.3.3 Interpretation of the results, and analyze results against expected physical behavior

The presented parametric study is in close accordance with expected physical phenomena.

## A4 - Validation

### A.4.1 Description of the choice of dataset (scope of application is covered)

While no reference data are available, no validation is possible for such a model. Only the physical behavior, through the parametric study was evaluated.

### A.4.2 Description of the choice of dataset (part that has been used for calibration)

As mentioned above, no reference data were available for calibration, hypothesis were done based on the available literature.

### A.4.5 Description of qualitative and quantitative comparison between experimental and numerical results

No comparison available since no experimental data were published. Some comparisons are proposed hereafter based on some accidents referenced in the BARPI database.

#### A.4.5.1 Milford Haven (UK – 1983)

In 1983, August the 30<sup>th</sup>, a 94 000 m<sup>3</sup> floating rood tank filled with light crude oil caught to fire. The tank diameter was about 78 m, the initial liquid height in the tanks is estimated knowing the initial mass, 47 000 t) to 12 m. During this accident, a boil-over occurred about 12 h after the fire ignition, the fireball was estimated to 90 m in diameter and reached 150 m in height. Before comparing with the model, it is important to note that the during the firefighting process, the crude oil was pumped out of the tank (about 1700 t/h). This reduce the liquid height to an initial theoretical value of 7 m. Both initial heights were computed to compare model predictions with observations, Table 2: Comparisons of observed and modelled values for the Milford Haven boilover

	Observed	Predicted – Initial height 12 m	Predicted – Initial height 7 m
Boilover occurrence delay	12 h	33 h	19 h
Fireball diameter	90 m	240 m	203 m (fireball center)
Fireball height	150 m	273 m	232 m (fireball center)

*Table 2: Comparisons of observed and modelled values for the Milford Haven boilover*

This comparison indicates that, the delay predicted by the model is overestimated, the boilover can occur, in reality, before the predicted delay. This is important to have this in mind when applying this model in emergency situations. It is also important to note that, without any detailed information, the service temperature was fixed to 330 K in the model, increasing this value lead to reducing the occurrence delay. Reducing it to 12 h remains however not possible based on the only initial temperature parameter.

Consequences seems over-estimated with the model since the fireball diameter is twice the observed one and, according the height comparison, the predicted life duration of the fireball seems larger than the observed one, that also contributes to increase the radiation effect.

#### A.4.5.1 Tocoa (Venezuela - 1982)

The second case of boilover that could be used in the Tocoa one. This boilover occurred on a heavy fuel oil (FO) 40 000 m<sup>3</sup> tank initial filled at 40%. The tank height was 17 m, its diameter about 55 m. The initial liquid height is estimated to 6.5 m. Comparison of available data is proposed hereafter in Table 3.

	Observed	Predicted
Boilover occurrence delay	6 h	10 h
Fireball diameter	No information	276
Fireball height	300 m	364 m (fireball center)

*Table 3: Comparisons of observed and modelled values for the Tocoa boilover*

As for the previous case, the predicted occurrence delay is larger than the observed one, with the same comment regarding the service temperature, fixed to 330 K in the model, if the real one is higher, the occurrence delay would be reduced. To get a predicted delay of 6 h, the initial temperature should be set to 420 K (150°C).

The prediction of the fireball characteristics seems one more time overestimated, that is positive for safety prediction.

#### A.4.6 Explanation of the validity of the tool when there are no data to compare (information recorded during accident or/and numerical data)

The evaluation of the model was achieved by estimating the physical behavior thanks to the parametric study.

#### A.4.7 Synthesis of all the comparisons

The model requires a more rigorous experimental comparison as soon as experimental data will be published.

## A5 - User-oriented assessment

### A.5.1 Description of user-oriented documentation

A brief documentation mainly focused on the description of the input parameter is provided in the Ineris [13 report](#).

### A.5.2 Description and analysis of ergonomic criteria

The GUI was developed in the EPHEDRA platform.

The screenshot shows a software window titled "Boilover classique Primarisk" with a "Résultats" tab. The interface is organized into several sections:

- Equipement:** Contains input fields for "Diamètre" (60 m), "Hauteur" (25 m), "Hauteur de produit" (20 m), and "Température de service" (330 K).
- Produit ou mélange:** A dropdown menu showing "FO n°2".
- Produit : caractéristiques utilisées:** A table listing physical properties:

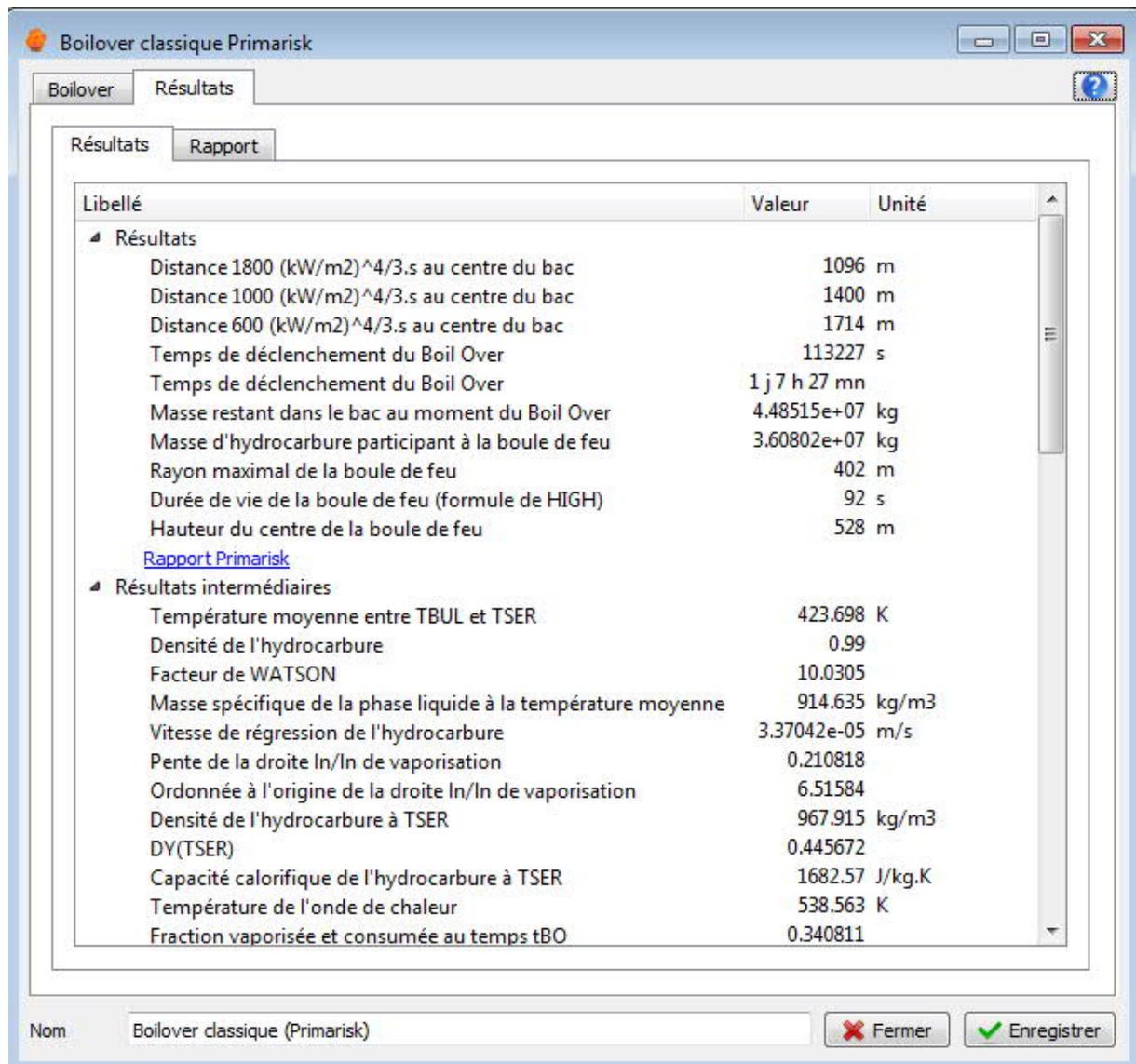
Température critique	929,8 K
Température d'ébullition finale	653 K
Température d'ébullition initiale	453 K
Température d'ébullition-TBUL	544 K
Viscosité à 393 K	10 cSt
- Environnement:** A dropdown menu showing "D5 - Conditions médianes".
- Conditions environnementales : caractéristiques utilisées:** Contains input fields for "Température" (293,15 K) and "Humidité relative" (70 %).

At the bottom, there is a "Nom" field with the value "Boilover classique (Primarisk)" and two buttons: "Fermer" (with a red X icon) and "Enregistrer" (with a green checkmark icon).

Figure 12: Example of the EPHEDRA embedded GUI

### A.5.3 Analysis of clarity and flexibility of output results

The main result available in the GUI is the distance reached for the different radiative flux thresholds, Figure 13. Several intermediate values are given in the results table to let the user aware of the physical behavior of the product during the boilover phenomena and enable him to achieve a critical analysis.



Libellé	Valeur	Unité
↳ Résultats		
Distance 1800 (kW/m2) <sup>4/3</sup> .s au centre du bac	1096	m
Distance 1000 (kW/m2) <sup>4/3</sup> .s au centre du bac	1400	m
Distance 600 (kW/m2) <sup>4/3</sup> .s au centre du bac	1714	m
Temps de déclenchement du Boil Over	113227	s
Temps de déclenchement du Boil Over	1 j 7 h 27 mn	
Masse restant dans le bac au moment du Boil Over	4.48515e+07	kg
Masse d'hydrocarbure participant à la boule de feu	3.60802e+07	kg
Rayon maximal de la boule de feu	402	m
Durée de vie de la boule de feu (formule de HIGH)	92	s
Hauteur du centre de la boule de feu	528	m
<a href="#">Rapport Primarisk</a>		
↳ Résultats intermédiaires		
Température moyenne entre TBUL et TSER	423.698	K
Densité de l'hydrocarbure	0.99	
Facteur de WATSON	10.0305	
Masse spécifique de la phase liquide à la température moyenne	914.635	kg/m3
Vitesse de régression de l'hydrocarbure	3.37042e-05	m/s
Pente de la droite ln/ln de vaporisation	0.210818	
Ordonnée à l'origine de la droite ln/ln de vaporisation	6.51584	
Densité de l'hydrocarbure à TSER	967.915	kg/m3
DY(TSER)	0.445672	
Capacité calorifique de l'hydrocarbure à TSER	1682.57	J/kg.K
Température de l'onde de chaleur	538.563	K
Fraction vaporisée et consommée au temps tBO	0.340811	

Figure 13: Example of the results visualization in the EPHEDRA embedded GUI for boilover

### A.5.4 Description of assistance in the input data setting, computational aspects

The tool is dedicated for Windows and works on 32 and 64 bits machines.

