

# **THEORY**

# INDOOR DISPERSION

DATE: December 2023

INBU calculates effects due to the release occurring within a building. It modifies the source term to take into account mixing of air with the released material within the building. It calculates concentration build-up and decay with time. If the material is flammable it calculates vented indoor explosion effects and (following building failure) external explosion effects.

Reference to part of this report which may lead to misinterpretation is not permissible.







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#### **Prepared by: Digital Solutions at DNV**

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# <span id="page-2-0"></span>**ABSTRACT**

The indoor dispersion model INBU assumes a finite-duration constant release or an instantaneous release of hazardous material from a vessel or pipe within the building. Indoor dispersion calculations are carried out presuming ideal mixing conditions within the building. A constant vent volume flow rate is assumed from the building.

The INBU model also calculates the build-up and decay with time of the concentration within the building. The assumption of perfect ideal mixing within the building enables an analytical evaluation of the concentrations.

If the material is flammable, INBU also includes explosion calculations for two scenarios:

- The indoor confined explosion is based on the NFPA68 guidelines for vented explosions within buildings. Explosion overpressur es are calculated at 16 vent fractions (i.e. 1% - 16%) for buildings that cannot withhold an overpressure higher than 0.1 bar.
- If the building fails due to an indoor explosion, the initial confinement by the building would enhance the tendency for the material to detonate like TNT. INBU reports flammable mass and TNT explosion efficiencies at a range of concentrations reached in the building (between LFL fraction and UFL).



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# <span id="page-5-0"></span>**1 INTRODUCTION**

While emphasis of the Phast (Risk) program is on toxic and flammable effects felt outside buildings, the program does include an in-building model called INBU. This is because the release in the process plant is often confined by some kind of building as illustrated i[n](#page-5-2) 

[Figure](#page-5-2) 1. The program performs calculations to determine what effect the building has on the external release to atmosphere, and also potential explosion effects inside the building.

The in-building model described in this document primarily performs calculations to provide the initial specification of the cloud dispersing outside the building. However, it also performs supplementary calculations that do not affect the linked dispersion modelling:

- Calculate indoor concentration rise and fall from an instantaneous/ finite duration release in a building.
- Calculate external explosion data if building fails (TNT efficiencies for a number of standard concentrations if they are reached in the building)
- Calculate indoor vented explosion data according to NFPA68 (pressure rises for range of building vent areas)



**Figure 1. Illustration of an in-building release**

<span id="page-5-2"></span><span id="page-5-1"></span>The most important of the above calculations is the way the source term is modified prior to the dispersion model. There are four main options corresponding to permutations of natural versus forced ventilation and instantaneous versus continuous releases. There is also the possibility of removing the liquid part of the release entirely or partly from the material going into the cloud.

The assumptions being made are simplistic and they provide screening capability only. This is justified on the basis that more precise calculations are non-trivial (eg CFD) and beyond the scope of routine risk calculations.

The plan of this report is as follows. Chapter [2](#page-6-0) provides an overall brief overview of the INBU model including details of the linking between the Phast indoor discharge model, the Phast indoor dispersion model (INBU module INBU-CO) and the Phast outdoor dispersion models (model UDM without building-wake effects and model BWM including building wake effects). Chapter [3](#page-9-0) describes the INBU indoor dispersion logic in INBU, and Chapte[r 4](#page-13-0) describes the INBU explosion logic. [0](#page-20-1) includes guidance on INBU input and output data. This includes information on errors and warnings, which may be produced by INBU.



# <span id="page-6-0"></span>**2 OVERVIEW OF INBU MODEL**

# <span id="page-6-1"></span>**2.1 INBU sub-modules**

The INBU model includes the following sub-modules:

- **Dispersion** 
	- o Finite-duration constant release module INBU-CO from the building, used as input for subsequent dispersion calculations
	- o Time-varying indoor dispersion module INBU-TV, not used for subsequent outdoor dispersion calculations **Explosion**
	- o Vented explosion overpressure within the building calculated according to NFPA68 correlation
	- o External explosion modelling (if the building fails)
		- flammable mass
		- explosion efficiency

# <span id="page-6-2"></span>**2.2 INBU model input and output**

A detailed description of the INBU model input and output is given i[n 0,](#page-20-1) and a brief summary is given in the current section only.

The major INBU model input data are as follows:

- Material data [properties from Phast property database: DIPPR and additional non-DIPPR flammable/toxic data]
- Inbuilding vessel/pipe release data [post-expansion data obtained in Phast (Risk) from the discharge model]
	- o instantaneous/continuous flag
	- o duration (continuous only)
	- o mass (instantaneous) or mass rate (continuous)
- Final post-expansion data: temperature and liquid fraction
- building data:
	- o building dimensions: height, length, width
	- o vent data: natural ventilation (number of air changes) or forced ventilation (vent volume flow rate, exhaust diameter)
- Ambient data: temperature, pressure, humidity

The major INBU model output data are

- Discharge data from building
	- $\circ$  ventilation data: material and air volume vent rate (m<sup>3</sup>/s)
	- $\circ$  input data to outdoor dispersion model: material and air mass rate (kg/s), liquid fraction, droplet size, duration, velocity
- Indoor dispersion data
	- o concentration data in building as function of time: mass, volume concentration
	- o rise and fall times to concentration of interest
- **Explosion data** 
	- o Indoor explosion: pressure rises for range of vent fractions of building surface area
	- o External explosion (after building fails): TNT explosive masses and efficiencies for a range of indoor concentration levels

# <span id="page-6-3"></span>**2.3 Outdoor discharge from building (INBU-CO)**

The model INBU-CO includes simplistic logic which is used to calculate the outdoor discharge data from the building. Input to the model INBU-CO are vessel/pipe discharge data corresponding to either a finite-duration constant release of a continuous release or an instantaneous release (material name, mass flow rate or mass, post-expansion temperature and liquid fraction). The user specifies whether liquid droplets are (partly) trapped inside the building. INBU-CO presumes for the release from the building a finite-duration continuous release of a mixture of material and air. INBU-CO outputs release data from the building for input by either the building wake model BWM (including effects of building wake) or the Unified Dispersion Model UDM (excluding effects of building wake). INBU-CO output data for the release from the building include material and air release rates (kg/s), duration, and velocity. If droplets are not trapped, a very small value of the droplet diameter is input to the UDM (so rainout will not occur).



# <span id="page-7-0"></span>**2.4 Time-varying indoor dispersion (INBU-TV)**

The time-varying indoor-dispersion model INBU-TV calculates time-dependent indoor concentrations (volume fraction) following either a uniform finite-duration release or an instantaneous release within an enclosed ventilated module. It assumes ideal uniform perfect mixing within the building without stratification. As a result, it is most suitable for medium release rates where the exact spatial details of the concentration are not significant. The model is not applicable for very large release rates resulting in significant changes in pressure and ventilation (e.g. blowing out panels etc.). The model assumes either natural ventilation (prescribed volume changes per hour) or forced ventilation (prescribe ventilation rate,  $m<sup>3</sup>/s$ ). For a finite-duration release, the concentration increases during the duration of the release and subsequently decreases. For instantaneous releases, the concentration reduces after the release. Explicit analytical formulas are derived for the concentrations as function of time.

# <span id="page-7-1"></span>**2.5 Natural and forced ventilation**

The INBU model allows for both natural and forced ventilation as shown in [Figure](#page-7-4) 2.

When the ventilation scheme is 'natural' [\(](#page-7-4)

[Figure](#page-7-4) 2a) the concept is that the material and ventilation air will leak out of the building from gaps around windows and doors. In effect the building boundary is porous. Also there is no specific location for the leak. In this case the user inputs the number of air changes n<sub>ac</sub>. Thus if the number of air changes n<sub>ac</sub> = 4 / hour, every 15 minutes the air in the building will be replaced; i.e. the duration of one air change  $t_{ac} = 1/n_{ac} = 900$  seconds. In case of natural ventilation, the release direction is presumed to be horizontal and the initial velocity is set to a minimum value, depending on the dispersion model being used (0.1m/s in the UDM).

When the ventilation scheme is 'forced' [\(Figure 2b](#page-7-3)) then the material and ventilation air will blow out of the building from a specific hole in the wall or roof. In this case, the user needs to specify the exhaust diameter *Dvent* (m) and the volume flow through the vent *v<sub>vent</sub>* (m<sup>3</sup>/s). The release direction is horizontal (wall vent) or vertical (roof vent).



<span id="page-7-4"></span><span id="page-7-3"></span>**Figure 2. Types of building ventilation** 

# <span id="page-7-2"></span>**2.6 Link between discharge, dispersion and jet fire models**

Link between discharge and dispersion models

 $\overline{a}$ 

The INBU model assumes either an instantaneous or a continuous vessel/pipe discharge inside the building.<sup>1</sup>

The release elevation is only input in Phast in case the INBU indoor dispersion model is linked with the outdoor dispersion model UDM. It is not input in case INBU is linked with the roof/lee release building wake dispersion model BWM. This should be set equal to the elevation height of the top of the building in case of roof vent releases, and the exhaust height in case of wall vent releases. In most cases, the building will be not buried and rest on the ground. In this case the elevation height equals the building height for roof vent releases. However in case of partly buried buildings, the elevation height is less than the building height, while for elevated buildings, the elevation height is larger than the building height.

The effect of in-building calculations upon the link between the discharge and outdoor dispersion calculations is to:

Theory | Indoor Dispersion | Page 6  $^{\text{1}}$  A warning is provided by the Phast (Risk) GUI in case the user selects 'multiple segments', and the method is changed to 'Average rate' over the release duration.



- 1) Calculate the release rate and release duration for the material. Here the instantaneous case is converted into a finite-duration, continuous release.
- 2) Set the liquid fraction to zero if the droplets are trapped.<br>3) Reset the drop size to very low if the droplets are not t
- Reset the drop size to very low if the droplets are not trapped. Thus the in-building model assumes that if the initial release is a gas-liquid mixture, the liquid in the resulting cloud is in the form of a mist (very small droplets) and the droplet size is set to the minimum size.
- 4) Provide an initial estimate of air mixed into the cloud before it emerges from the building (note that air is assumed to be at ambient conditions).
- 5) To provide a new discharge velocity and possibly the release direction

For calculating the temperature of the mixture of material and air released from the building, the material is presumed to be at the post-expansion temperature and the air at the ambient temperature.

#### Link between discharge and jet fire model

The above source term modifications also apply to the jet fire calculations. Jet fires are calculated only if the exit concentration exceeds the lower flammable limit and if forced ventilation is selected.



# <span id="page-9-0"></span>**3 INDOOR DISPERSION**

## <span id="page-9-1"></span>**3.1 Finite-duration constant release from building (INBU module INBU-CO)**

The section describes the model INBU-CO, which models the dispersion from the building as a finite-duration constant release. These release data are used in Phast as input for subsequent dispersion calculations (by Unified Dispersion Model UDM or building wake model BWM).

In version 6.7 additional changes were applied to this model to ensure fully consistent assumptions for the cases of continuous and instantaneous releases, i.e.:

- The release duration  $t_{out}$  is at least the duration of one air change  $t_{acc}$
- A maximum release duration  $t_{max}$  is applied for the release from the building
- All discharge mass (including liquid) is assumed to be released eventually from the building, unless the release duration is capped by the maximum release duration.

#### <span id="page-9-2"></span>3.1.1 Instantaneous discharge

First the case is considered of an indoor catastrophic rupture, where the entire inventory ( $M_{dis}$ , kg) is released instantaneously inside the building (with final post-expansion temperature  $T_{dis}$  and final post-expansion liquid fraction  $n_{dis}$ ).

#### Without trapped droplets

If option 'droplets are not trapped in the building' is selected, it is assumed that all released mass is released from the building during one air change with a constant release rate. Thus the release rate  $Q_{out}$ , the release duration  $t_{out}$ , and the release fraction ηout from the building are set as follows:

$$
Q_{out} = \frac{M_{dis}}{t_{ac}} \quad , \qquad t_{out} = \min \left( t_{\max} \, t_{ac} \right) \, , \quad \eta_{out} = \eta_{dis} \tag{1}
$$

Note that all discharged mass will not be released from the building in case the maximum release duration  $t_{max}$  is less than the duration  $t_{ac}$  of one air change.

#### With trapped droplets

If the option 'droplets are trapped in the building' is selected, it is assumed that part of the liquid remains in the building and is not released from the building. The remaining part of the liquid is released as pure vapour. Let r<sub>ligmass</sub> be the vapour mass fraction modification factor (default input 3). The release data from the building are now set as follows:

$$
Q_{out} = \min \left[ r_{liqmass}(1-\eta_{dis}), 1 \right] \frac{M_{dis}}{t_{ac}}, \quad t_{out} = \min \left( t_{max}, \frac{M_{dis}}{Q_{out}} \right), \quad \eta_{out} = 0 \tag{2}
$$

The formulation is in line with (but not identical to) logic currently used in Phast to set the flammable mass for BLEVE's and jet fires. In line with this the same default value  $r_{\text{liq} \text{mass}} = 3$  is chosen, instead of the less conservative value of rigmass = 2 suggested by the old Purple Book<sup>i</sup>. This would mean all mass would be released in case the initial liquid mass discharge fraction  $\eta_{dis}$  is less than 2/3. Note that for sub-cooled jets with 100% rainout, this option would lead to no mass released from the building; furthermore  $r_{liqmass}=1$  corresponds to all droplets trapped, and  $r_{liqmass} = \infty$  (and  $r_{dis} < 1$ ) to no droplets trapped.

### <span id="page-9-3"></span>3.1.2 Continuous discharge

Secondly the case is considered of an indoor constant finite-duration vessel/pipe release (flow rate  $Q_{dis}$ , kg/s; inventory  $M_{dis}$ ; duration t<sub>dis</sub>; final post-expansion temperature T<sub>dis</sub> and final post-expansion liquid fraction  $\eta_{dis}$ ).

The release rate  $Q_{\text{out}}$  and the release duration  $t_{\text{out}}$  from the building are first set as:

$$
Q_{out} = Q_{dis} , t_{out} = t_{dis} , \eta_{out} = \eta_{dis} , \text{ if not trapped}
$$
 (3)



$$
Q_{out} = \min \left[ r_{liqmass}(1-\eta_{dis}), 1 \right] Q_{dis} , \qquad t_{out} = \frac{M_{dis}}{Q_{out}} , \qquad \eta_{out} = 0 , \text{ if trapped}
$$
 (4)

Subsequently, if the value t<sub>out</sub> as calculated as above is smaller than the duration of one air change t<sub>ac</sub>, i.e. if t<sub>out</sub> < t<sub>ac</sub>, then the release rate is further modified such that the entire mass is released during one air change. Thus reset  $Q_{out} = Q_{out}$  (t<sub>out</sub>  $/t_{\text{ac}}$ ) and reset  $t_{\text{out}} = t_{\text{ac}}$ .

Finally if the value of t<sub>out</sub> is larger than the maximum duration t<sub>max</sub>, then reset t<sub>out</sub> = t<sub>max</sub>.

### <span id="page-10-0"></span>3.1.3 Volumetric and mass ventilation rates; release speed

#### Volumetric ventilation rates

The ventilation rate *v<sub>vent</sub>* from the building (m<sup>3</sup> of material and air released per second) is user-specified in case of forced ventilation. In case of natural ventilation, it is calculated as follows,

$$
v_{vent} = n_{ac} \ V_{building} = \frac{V_{building}}{t_{ac}}
$$
 (5)

Here *nac* is the user-specified number of air changes in the building per second, and *tac* is the duration of one air change (s).

The material volumetric release rate is based on the material vapour density at the final post-expansion conditions (i.e. ignoring the liquid volume).

<span id="page-10-1"></span>
$$
v_{mat} = \frac{Q_{out}}{\rho_{VAP}}
$$
 (6)

Where the vapour density *ρVAP* is set as follows:

$$
\rho_{VAP} = \rho_{vap}(T_{dis}, P_{air}) \text{, if vapour release (Tdis > Tboil)}
$$
\n
$$
\rho_{VAP} = \rho_{sat}(T_{boil}, P_{air}) \text{, if 2-phase or liquid release (Tdis \le Tboil)}
$$
\n(7)

Here  $T_{\text{boil}}$  is the atmospheric boiling point of the discharged material and  $P_{\text{air}}$  is the atmospheric pressure.

Subsequently the air volumetric<sup>2</sup> and mass ventilation rates are set as follows

<span id="page-10-2"></span>
$$
v_{air} = v_{vent} - v_{dis}
$$
 (8)

$$
Q_{air} = \rho_{air}(T_{air}, P_{air}; r_H) \ V_{air}
$$
 (9)

Here  $T_{air}$  is the ambient temperature and  $r_H$  the relative humidity of the air.

#### Release speed

l

In case of forced ventilation, the release speed is obtained by dividing the total volumetric ventilation rate by the vent area,

$$
U_{out} = \min \left\{ U_{\max} , \frac{v_{vent}}{0.25 \pi D_{vent}} \right\}
$$
 (10)

Theory | Indoor Dispersion | Page 9 <sup>2</sup> An error is generated by the program in case the material ventilation rate *vmat* is larger than the total ventilation rate *vvent* volume rate of material from the building; see Appendix **Error! Reference source not found.**



INBU adopts a maximum release velocity *Umax* from the building, which is currently hardwired in the INBU code as 500 m/s. In case the above calculated velocity is larger than  $U_{\text{max}}$ , i.e. in case  $r_U = (U_{\text{out}}/U_{\text{max}})$  = 1, the maximum velocity is used to scale back the release from the building proportionately. Thus the data are reset as follows for this case:

$$
Q_{out} = \frac{Q_{out}}{r_U} , t_{out} = \min \{t_{\max}, r_U t_{out}\}, U_{out} = U_{\max} , \text{ if } r_U > 1 \tag{11}
$$

### <span id="page-11-0"></span>**3.2 Time-varying indoor dispersion (INBU module INBU-TV)**

The INBU indoor dispersion module INBU-TV calculates the time-varying indoor concentration, i.e. it sets the concentration rise and fall from an instantaneous/ finite duration release in a building.

The ideal mixing assumption is used to calculate one average concentration of released material in the building as it changes with time [see also Section 17.8.3 in Mannan<sup>ii</sup>]. The calculations vary according to the release specification – continuous releases will be treated differently to instantaneous releases.

The material mass  $M_{in}$  (kg) present in the building is set a function of the time t from the indoor concentration  $C_{in}$  (volume fraction) as

<span id="page-11-2"></span>
$$
M_{in}(t) = \rho_{VAP} C_{in}(t) V_{building}
$$
 (12)

with the vapour density defined by Equation (7).

The indoor dispersion model INBU-TV applies model theory similarly to the 'indoor concentration' model described in the TXCS theory manual<sup>iii</sup>. The latter model is used in Phast (Risk) to calculate the indoor concentration inside a building (with specified ventilation rate) resulting from a cloud passing the building.

#### <span id="page-11-1"></span>3.2.1 Continuous releases

The building (and 'building' could be any vessel enclosure) is treated as a perfectly mixed vessel (i.e. no stratification occurs) with two input streams and an output stream. For the mixing assumptions the materials are considered incompressible (which makes an analytic, rather than numerical solution possible). One input stream is the ventilation air which is assumed to flow in at a continuous rate. The other input stream is the released material once it has expanded from the storage pressure to the ambient pressure (volumetric flow rate  $v_{dis}$ , m<sup>3</sup>/s; duration t<sub>dis</sub>, s). These two streams are mixed in the building with the material already there and provide the output stream (mixture of material and air; vent volume flow rate  $v_{\text{vent}}$ , m<sup>3</sup>/s); see Figure 2.

Conservation of molar (volume) material, now yields

$$
V_{building} \frac{dC_{in}}{dt} = V_{dis} - V_{vent} C_{in} , \quad t \le t_{dis}
$$
  
\n
$$
V_{building} \frac{dC_{in}}{dt} = -V_{vent} C_{in} , \quad t > t_{dis}
$$
 (13)

Here V<sub>building</sub> is the volume of the building. This equation states that the increase of number of material moles inside the building equals the number of released moles from the discharge minus the amount of moles vented from the building.

The above equation can be solved analytically for concentration  $C_{in}$  as function of the time t since the start of the indoor vessel/pipe discharge:

$$
C_{in}(t) = \frac{v_{dis}}{v_{vent}} \left[ 1 - e^{-\frac{v_{vent}t}{V_{building}}}\right] = \frac{v_{dis}}{v_{vent}} \left[ 1 - e^{-\frac{t}{t_{ac}}}\right], \quad t \leq t_{dis}
$$
\n
$$
C_{in}(t) = C_{in}(t_{dis}) e^{-\frac{v_{vent}(t - t_{dis})}{V_{building}}} = C_{in}(t_{dis}) e^{-\frac{(t - t_{dis})}{t_{ac}}}, \quad t > t_{dis}
$$
\n(14)



#### <span id="page-12-0"></span>3.2.2 Instantaneous Releases

For instantaneous releases it is assumed that the initial expansion of material (expanded volume *Vdis*) displaces air from the building. This then defines the initial concentration in the building. Once the initial concentration is defined, the concentration decay is calculated. This is done analogous as for the case of the continuous release after the release has ended. Thus the instantaneous indoor concentration is set as follows:

$$
C_{in}(0) = \frac{V_{dis}}{V_{building}}, \qquad t = 0
$$
\n(15)\n
$$
C_{in}(t) = C_{in}(0) e^{-\frac{V_{van}(t - t_{dis})}{V_{building}}} = C_{in}(0) e^{-\frac{(t - t_{dis})}{t_{ac}}}, \qquad t > 0
$$

An improvement to the above treatment would be to relax the incompressibility assumption and employ a general thermodynamic treatment. A numerical scheme would then be required for the calculation of the concentration build-up with time. Pressure inside the building caused by the un-ignited release would also be predicted and the indoor calculations would be more compatible with the other Phast models. Such calculations have not been included in this model and are possibilities of further work.



# <span id="page-13-0"></span>**4 EXPLOSION**

Two explosion models are available to predict the explosion overpressures generated by the ignition of the build-up of flammable material in the building.

The first model is an indoor confined explosion model which predicts the overpressure inside the building given a certain level of venting. This model is based on NFPA68<sup>iv</sup> guidelines.

The second model is an external explosion model. It is an adaptation of the TNT external vapour cloud explosion if the building fails. This model calculates flammable mass and explosion efficiencies of TNT equivalency for a number of standard concentrations if they are reached in the building.

### <span id="page-13-1"></span>**4.1 Indoor Confined Explosion Model**

The final pressure rise of a completely confined explosion can exceed 10 bar. In addition reflected pressure waves can drive local pressure values beyond this level. Such an overpressure will devastate buildings and plant. However, venting of the building limits pressure rise when the material does not detonate, but deflagrates (NFPA 68). NFPA 68 has two formulae to calculate this overpressure, one for low-strength enclosures which cannot withhold an overpressure higher than 0.1bar and the other for stronger enclosures. For low-strength enclosures with symmetrically distributed vent areas, the relationship between overpressure and ventilation area is given by:

<span id="page-13-5"></span><span id="page-13-4"></span><span id="page-13-3"></span>
$$
A_{vent} = C_{vent} \frac{A_{building}}{\sqrt{P}}
$$
 (16)

Here *Avent* is the ventilation area, *Abuilding* the internal surface area of the building, and *P* the overpressure developed inside the building (Pa). Phast assumes a cubic building with length *Lbuilding*, width *Wbuilding*, and height *Hbuilding*. Therefore the building volume and the building area are given by

$$
V_{building} = L_{building} W_{building} H_{building}
$$
\n
$$
A_{building} = 2L_{building} W_{building} + 2L_{building} H_{building} + 2W_{building} H_{building}
$$
\n(17)

The venting parameter*<sup>3</sup> Cvent* is defined as a function of the laminar burning velocity*<sup>4</sup> S<sup>L</sup>* of the indoor flammable material as equatio[n \( 18](#page-13-2) ) in NFPA 68 and shown in [Figure 3:](#page-14-1)

$$
C_{vent} = 1.57E^{-5}S_L^2 + 1.57E^{-4}S_L + 0.0109
$$
 (18)

Where the unit is bar<sup>1/2</sup> for *C<sub>vent</sub>* and cm/s for S<sub>L</sub>. Equation (18) can converted to SI units as:

<span id="page-13-2"></span>
$$
C_{vent} = 49.65S_L^2 + 4.96S_L + 3.45
$$
 (19)

Where the unit is Pa1/2 for *Cvent* and m/s for *SL*.

 $^3$ Based on an earlier version of NFPA68 the venting parameter was a constant value of 5.0 Pa<sup>1/2</sup> in previous releases of Phast which corresponds to a laminar burning velocity of 0.14 m/s. This is likely to cause underestimation of indoor overpressure.

Theory | Indoor Dispersion | Page 12 <sup>4</sup> Without accurate calculation of indoor temperature and pressure, the atmospheric temperature and pressure are used by INBU to estimate the laminar burning velocity of the indoor flammable vapor here.





<span id="page-14-1"></span>

Equatio[n \( 18](#page-13-2) ) is only recommended for material with laminar burning velocity up to 60 cm/s and corrections are needed to account for inertia of the vent panels. Use of this calculation helps design of ventilation systems that will vent sufficiently well to avoid serious structural damage or collapse of the building.

A separate correlation is given by NFPA 68 for enclosures that are capable of withholding overpressures higher than 0.1 bar, i.e. high-strength enclosures, and this has not implemented in the INBU model at present. Such models would require additional user-input, but would provide further resolution of the overpressure effects inside a building and are worth considering as future work.

# <span id="page-14-0"></span>4.1.1 Update to Indoor Confined Explosion Model (NFPA 68 -2013)

The NFPA 68 Guidelines for the venting deflagration of gas mixtures and mists were updated in 2013. The user will now have the option to select between the indoor confined explosion model described in section 4.1 (NFPA68 (version 2007)) and this new updated method (NFPA68 (version 2013)), with the Indoor explosion method flag. The NFPA68 (2007) method is the default method.

NFPA68 (2013) presents equations for choked and non-choked flow through the venting panel. The criterion for choked flow is vented overpressures greater than 0.5 bar. The current implementation of NFPA68 (2013) methodology only allows for non-choked flow through the vent. To predict vented overpressures for choked flow (i.e. greater than 0.5 bar) would require knowledge of the maximum overpressure developed in a contained deflagration of the same gas – air mixture (*Pmax*) which is a material specific property. At present, values for *Pmax* are not contained in our material property database and the values that are available in the NFPA68 (2013) guideline are only for a limited number of materials. Adding known values of *Pmax* to the property database and working out an approximate method to calculate them if not known is considered as future work.

This section contains the relevant equations for the calculation of the overpressure for non-choked flow subject to the following constraints:

- 1) Laminar burning velocity (*SL*) < 3 m/s
- 2) Maximum overpressure in a vented deflagration  $= 0.5$  bar
- 3) The maximum air velocity in the building prior to ignition is no greater than 5 m/s
- 4) The building is isolated from possible flame jet ignition and pressures caused by a deflagration
- 5) The aspect ratio of the building L/D is less than 5
- 6) Maximum overpressure developed in a contained deflagration by ignition of the same gas-air mixture (*Pmax*) = 10 bar

The relationship between overpressure and ventilation area is given by equatio[n \( 16](#page-13-4) ). The parameter *Cvent* is dependent on the laminar burning velocity, as well as on the total surface area of obstacles inside the building, the



height at which the vent is located, the aspect ratio (length to diameter) of the enclosure, the diameter of the vent, and the pressure rise (P).

$$
C_{vent} = 0.0223 \cdot \lambda \cdot S_L \tag{20}
$$

Where,  $C_{vent}$  is in units of (bar<sup>1/2</sup>), SL is in units of (m/s) and  $\lambda$  is the turbulent flame enhancement parameter, calculated according to:

$$
\lambda = \begin{cases}\n\lambda_1 & \text{if } \left( L_{building} / D_{he} \right) < 2.5 \\
\lambda_1 \left[ 1 + \left( \frac{L_{building} / D_{he}}{2.5} - 1 \right)^2 \right] & \text{if } \left( L_{building} / D_{he} \right) \ge 2.5\n\end{cases}
$$
\n(21)

Where  $D_{he}$  is the building hydraulic equivalent diameter, determined by:

$$
D_{he} = 4 \frac{A_{\text{eff}}}{P}
$$
 (22)

Where *P* is the perimeter and *Aeff* is the effective area:

$$
P = 2\left(W_{building} + L_{building}\right)
$$
 (23)

$$
A_{\text{eff}} = \frac{V_{building}}{H_{vent}} \tag{24}
$$

Where  $H_{\textit{vent}}$  is the height at which the vent is located and  $\,\lambda_{\!1}^{\phantom i}$  is calculated as:

$$
\lambda_1 = \begin{cases} \lambda_0 & \text{if } A_{obs} / A_s < 0.4\\ \lambda_0 (0.6 + A_{obs} / A_s) & \text{if } A_{obs} / A_s \ge 0.4 \end{cases}
$$
 (25)

With  $A_{obs}$  *A<sub>s</sub>* defined as the ratio of the total surface area of obstacles inside the building (m<sup>2</sup>) to the building internal surface area (m²); and  $\,{\lambda_{\scriptscriptstyle 0}}$  as the baseline turbulent flame factor.

The baseline turbulent flame factor is given by the following equation:

$$
\lambda_0 = \varphi_1 \varphi_2 \tag{26}
$$

Where  $\,\varphi_{_{\!1}}\,$  is given by:

$$
\varphi_1 = \begin{cases} 1 & \text{if } \text{Re}_f < 4000 \\ \left(\frac{\text{Re}_f}{4000}\right)^{0.39} & \text{if } \text{Re}_f \ge 4000 \end{cases}
$$
 (27)

with

$$
\text{Re}_f = \frac{\rho_u S_L (D_{he}/2)}{\mu_u} \tag{28}
$$

Where  $^{\rho_{u}}$  is the mass density of unburned gas-air mixture (kg/m3) = 1.2 for flammable gases with stoichiometric concentrations less than 5 vol%, and an initial temperature of 20 oC; SL is the laminar burning velocity;  $^{\mu_{u}}$  is the unburned gas mixture dynamic viscosity (kg/m.s) = 1.8 x 105 for gas concentrations less than 5 vol% at ambient temperatures

 $\varphi_2$  on the other hand is calculated by the following set of equations:

$$
\varphi_2 = \max\left(1, \ 1.23 \left(\frac{\text{Re}_{v}}{10^6}\right)^{0.0487/S_u}\right) \tag{29}
$$

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Where,

$$
\text{Re}_{v} = \frac{\rho_{u} u_{v} (D_{v}/2)}{\mu_{u}}
$$
 (30)

 $D_{_{\cal V}}$  is the vent diameter (m) determined as (4 x  $A_{\rm vent}/\,\pi)^{0.5}$  and  $\mu_{\rm v}$  is the vent velocity given by:

$$
u_{\nu} = \sqrt{\frac{200000 \, P}{\rho_u}}\tag{31}
$$

#### <span id="page-16-0"></span>**4.1.1.1 Calculation procedure**

The calculation of the venting parameter Cvent, as it is dependent on the overpressure (P), is done iteratively until the desired level of convergence is reached. The procedure is the following:

- 1. Guess an initial value of the venting parameter (*Cvent\_try*)
- 2. Calculate the overpressure solving equation [\( 16](#page-13-4) ) for *P*
- 3. Calculate the venting parameter *Cvent* using the pressure rise obtained in step 2)
- 4. Calculate the difference  $C_{vent}$   $C_{vent\_ty}$ <br>5. If the difference is less than the toleran
- If the difference is less than the tolerance value exit with the calculated P
- 6. Otherwise update the value of  $C_{vent\_try} = C_{vent}$  and repeat the procedure from step 2)

# <span id="page-16-1"></span>**4.2 External Explosion Model**

If the building fails to confine the explosion (a likely scenario) significant overpressure levels could be experienced outside the building. The initial confinement of the explosion would enhance the tendency for materials to detonate like TNT and lead to high overpressures relative to those experienced in unconfined vapour clouds. This external explosion model of INBU estimates flammable masses, using equation [\( 12](#page-11-2) ), and explosion efficiencies for a number of standard concentrations if they are reached in the building, and they can be used as input to the TNT equivalent model of Phast to calculate overpressure levels around the explosion and the risk caused by it

<span id="page-16-2"></span>The highest overpressure caused by vapour cloud explosion in confined spaces is normally found for slightly rich mixtures, i.e. slightly higher concentration than the stoichiometric concentration which is 9.5% for methane and 6.54% for ethylene<sup>y</sup>. The correlation used by INBU to estimate the explosion efficiency follows a similar trend shown in [Figure 4](#page-17-0) for methane given by Kuthta<sup>vi</sup>. The efficiency, which is treated as the fraction of the maximum pressure, is assumed to be a function of the indoor concentration *Cin* of the flammable mixture and is approximated by two parabolas as explained below.



<span id="page-17-0"></span>The two parabolas intersect at concentration *Cin=CX*, as given in equatio[n \( 32](#page-17-1) ). The parabola for *Cin>C<sup>X</sup>* has a minimum  $f(C_{in})=C_2=0.7$  for  $C_{in}=A_2=UFL$  fraction. Furthermore the parabola for  $C_{in} < C_{\chi}$  has a maximum of  $f(C_{in})=C_1=1.0$  for  $C_{in} = A_1 = 1.15C$ <sub>st</sub>. Thus it can be found that the parabolas are given by

$$
f(C_{in}) = C_1 + B_1(C_{in} - A_1)^2 , C_{in} < C_X
$$
  
= C\_2 + B\_2(C\_{in} - A\_2)^2 , C\_{in} \ge C\_X (32)

By imposing f(LFL fraction) = 0.01, and imposing continuity of  $f(C_{in})$  and  $df(C_{in})/dC_{in}$  at  $C_{in}=C_x$ , one can solve for  $B_1$ ,  $B_2$ and  $C_X$ :

<span id="page-17-1"></span>
$$
B_1 = \frac{0.01 - C_1}{(LFL\,fraction - A_1)^2}
$$
  
\n
$$
C_x = A_1 + \frac{C_1 - C_2}{B_1(A_1 - A_2)}
$$
  
\n
$$
B_2 = B_1 (1 - \frac{A_1 - A_2}{C_x - A_2})
$$
  
\n(33)

[Figure 5](#page-18-0) compares the estimated explosion efficiency by the INBU correlation, i.e. equatio[n \( 32](#page-17-1) ), against the fraction of the maximum pressure by Kuthta for methane<sup>[vi](#page-16-2)</sup>. The agreement is good when the indoor concentration is lower than  $A_1$ i.e. 1.15C<sub>st</sub>, and the prediction is generally conservative at higher concentrations<sup>5</sup>.

 $\overline{a}$ 

Theory | Indoor Dispersion | Page 16 <sup>5</sup> The UFL and LFL fractions of methane given by DIPPR database are slightly different from that used by Kuthta.



<span id="page-18-0"></span>**Figure 5. Comparison of estimated explosion efficiency by INBU against data by Kuthta for methane[vi](#page-16-2)**



# <span id="page-19-0"></span>**5 FUTURE DEVELOPMENTS**

Additional verification and testing could be considered for the existing INBU model. This could include a sensitivity study to study the effect of parameter variations to further ensure correctness and robustness of the model.

Extensions of the current in-building dispersion model could be considered such as more sophisticated indoor droplet/rainout modelling, more rigorous thermodynamics of indoor mixing of material and air, inclusion of stratification, etc. Furthermore the time-varying dispersion model INBU-TV could be applied to determine the time-varying release from the building. Thus it could be linked with the time-varying outdoor dispersion model UDM or the building wake model BWM.

The INBU indoor explosion model could be further extended to include the separate correlation given by NFPA 68 (2013) for choked-flow. This will additionally require adding known values of *Pmax* to the property database and working out an approximate method to calculate them if not known.



# <span id="page-20-0"></span>**APPENDICIES**

### <span id="page-20-1"></span>**Appendix A: Guidance on INBU input and output data**

#### <span id="page-20-2"></span>*A.1* Input data

A list of the input data for the building wake model is given b[y Figure 6.](#page-22-1) These data are split into the following categories:

- 1. Input data (always to be specified by the users)
	- 1.1. Vessel/pipe release data (indoor discharge)
		- 1.1.1. Type of release: instantaneous or continuous
		- 1.1.2. Name of released material (name as in Phast Risk GUI)
		- 1.1.3. Release duration, s (not used for instantaneous release)
		- 1.1.4. Material mass flow rate, kg/s (continuous) of released material mass, kg (instantaneous)
		- 1.1.5. Material post-expansion data (following depressurisation to ambient): temperature (K) and liquid mass fraction
	- 1.2. Building data: height H<sub>building</sub> (m), length L<sub>building</sub> (m), width B<sub>building</sub> (m)
		- 1.2.1. Vent location  $(0 = \text{Wall vent}; 1 = \text{Root vent})$ <br>1.2.2. Vent height measured from the ground to
		- Vent height measured from the ground to the upper edge of the vent (m). If the vent location is "Roof vent" the vent height is set to the height of the building.
		- 1.2.3. Ratio of surface area of obstacles inside the building to building surface area. The surface area of obstacles inside the building include: Piping, tubing, and conduit with diameters greater than  $1/2$  in; structural columns, beams, and joists; stairways and railings; equipment with a characteristic dimension in the range of 2 in. to 20 in.  $(5.1 \text{ cm to } 51 \text{ cm})$
	- 1.3. Ambient data: temperature  $T_{air}$  (K), pressure p<sub>air</sub> (Pa), and relative humidity  $r_H$  (fraction). The temperature and pressure are taken at the reference height as specified in the Phast GUI.
	- 1.4. Termination criterion and output control
		- 1.4.1. Termination criterion
			- 1. risk-based run; termination is based on material/result type:
				- if flammable, run stops when the maximum concentration falls below the minimum concentration c<sub>min</sub>
				- if toxic, run stops when the maximum concentration falls below the concentration corresponding to the minimum probability of death  $p_{min}$ . For toxic mixtures, the toxic calculation method specifies whether to use the probit functions provided for the mixture, to use the most toxic component, or to combine doses from components. This calculation is also dependent on the parameter 'maximum release duration'.
				- if both flammable and toxic, the run stops after both the minimum concentration  $c_{\text{min}}$  and the minimum probability of death p<sub>min</sub> have passed
				- if inert, risk-based run is not allowed
			- 2. concentration and distance based run: run stops when both concentration is below  $c_{min}$  and maximum distance  $x_{\text{max}}$  have passed
			- 3. distance-based run: run stops when maximum distance  $x_{max}$  has passed.
			- 4. concentration based run: run stops when concentration is below  $c_{min}$

The run will be terminated earlier in case either the absolute maximum distance  $x_{\rm max}$ <sup>abs</sup> has been passed, or the maximum centre-line height  $h_{\text{max}}$  has been achieved. The run will also be terminated earlier if the maximum number of output steps  $n_{max}$  has been achieved.

The user can specify that the stopping criterion for cloud dispersion calculations relates to the calculation of "Concentration Based Risk" – (Stop Mode 4). In this case the explosion related calculations are not wanted even if the material is flammable. Where the material is both flammable and toxic, the user can specify that flammable only, toxic only or both sets of results are calculated. Where toxic results only are specified, the explosion related results are not wanted.

- 1.4.2. concentration of interest  $C<sub>int</sub>$  (volume fraction)
- 1.4.3. fraction of LFL to finish<br>1.4.4. CAS number of compor
- CAS number of component to monitor
- 1.4.5. Flam/Toxic/Both results flag; 0 both results, 1 flam results only, -1 toxic results only, -2 material inert



- 2. Parameters (input data to the changed by expert users only)
	- 2.1. Release from building
		- 2.1.1. droplets trapped (conservative) or not trapped (less conservative assumption)  $2.1.2$ . vapour multiplier  $r_{liqmass}$  of post-expansion material vapour fraction  $(1-r_{dis})$
		- 2.1.2. vapour multiplier rliqmass of post-expansion material vapour fraction (1-ηdis) to calculate amount of material released from the building during one air change. For more precise use, see Section [3.1](#page-9-1)
		- 2.1.3. minimum droplet size (do not change), m
		- 2.1.4. maximum duration of release from building  $t_{\text{max}}$ , s
	- 2.2. Explosion data
		- 2.2.1. TNT explosion efficency
		- 2.2.2. Venting equation constant C<sub>vent</sub> (used by NFPA68 indoor explosion correlatio[n \( 16](#page-13-4) ))
		- 2.2.3. Use the NFPA68 2013 vented explosion model? ( $0 =$  False;  $1 =$  True). This flags toggles between the old NFPA68 and NFPA68 2013 indoor vented explosion model
	- 2.3. Ambient data: molecular weight, kg/kmol

The above input data are derived from the generic spreadsheet for the INBU model as shown i[n Figure 6.](#page-22-1) The first part of the input data should always be specified by the user (vessel/pipe release data, building data, ambient data, termination criterion and output control). The second part of the input data correspond to the values of the input parameters (release from building, explosion, ambient data), which should be changed by expert users only. For each input parameter a brief description of the meaning of the parameter is given, it unit, and its lower and upper limits. The 'Default' column contains a complete list of input data corresponding to a continuous release of chlorine. The subsequent columns include examples for continuous/instantaneous releases with forced or natural convection. These only contain values that are changed with respect to the default values.



| <b>Inputs</b>  |  |  |            |                        |                | DNV INDOOR DISPERSION MODEL INBU |                  |
|--|--|--|------------|------------------------|----------------|----------------------------------|------------------|
| Input  |  | <b>Description</b>   |            | Limits                 |                | Cont_Natural_Tox                 | Inst_Forced_Flam |
| Index  |  |  |            | Lower                  | <b>Upper</b>   |                                  |                  |
|  |  | <b>VESSEL/PIPE RELEASE DATA</b>  |            |                        |                |                                  |                  |
| IN   |  | 1 Instantaneous/Continuous Flag (1=inst 2=cont)<br>Material name   |            | $\mathbf{1}$           | $\overline{2}$ | <b>CHLORINE</b>                  | <b>PROPANE</b>   |
|  |  | 3 Release duration (continuous)  |            | 0.00                   |                | $6.00E + 02$                     |                  |
|  |  | 4 Mass flowrate kg/s (continuous) or Mass kg (instantaneous)   | kg/s or kg | $1.E-06$               | $1.E+09$       | $1.06E + 00$                     | 1000             |
|  |  | 5 Post-expansion temperature   | Κ          | 1                      | 900            | 2.39E+02                         |                  |
|  |  | 6 Post-expansion liquid fraction   |            | 0.00                   | 1.00           | 8.08E-02                         |                  |
|  |  | <b>BUILDING DATA</b>   |            |                        |                |                                  |                  |
|  |  | 7 Building height  | m          | 0.001                  | 500            | $5.00E + 00$                     |                  |
|  |  | 8 Building length<br>9 Building width  | m<br>m     | 0.001<br>0.001         | 500<br>500     | $1.00E + 01$<br>$1.00E + 01$     |                  |
|  |  | 10 Natural or Forced ventilation Flag (0=natural, 1=forced)  |            | $\mathbf 0$            | $\mathbf{1}$   | $\sqrt{ }$                       |                  |
|  |  | 11 Number of air changes (input for natural ventilation only)  | Hz         | $\mathbf 0$            | 10             | 1.11E-03                         |                  |
|  |  | 12 Exhaust diameter (input for forced ventilation only)  | m          | 0.01                   | 100            | $1.00E + 01$                     | $1.00E + 01$     |
|  |  | 13 Volume flow through vent (input for forced ventilation only)  | m3/s       | 0.00                   | 500            | 5.56E-01                         | 5.56E-01         |
| A  |  | Vent location ( $0 =$ Wall vent; $1 =$ Roof vent)  |            | 0.00                   |                | $1.00E + 00$                     |                  |
|  |  | Vent height - measured from the ground to the upper edge of the vent   |            |                        |                |                                  |                  |
|  |  | (m)  | m          | 0.00                   |                | $0.00E + 00$                     |                  |
|  |  | Ratio of surface area of obstacles inside the building to building   |            |                        |                |                                  |                  |
|  |  | surface area   |            | 0.00                   |                | $0.00E + 00$                     |                  |
|  |  | <b>AMBIENT DATA</b>  |            | 200                    | 350            | 2.83E+02                         |                  |
|  |  | 14 Atmospheric temperature<br>15 Atmospheric pressure  | Κ<br>Pa    | 50000                  | 120000         | $1.01E + 05$                     |                  |
|  |  | 16 Atmospheric humidity  |            | 0.00                   | 1.00           | 7.00E-01                         |                  |
|  |  | <b>TERMINATION CRITERION AND OUTPUT CONTROL</b>  |            |                        |                |                                  |                  |
|  |  | Dispersion termination criterion: 1 - min. prob. (toxic) and/or min.   |            |                        |                |                                  |                  |
|  |  | conc. (flammable), 2 - min.conc. and max.dist., 3 - max.dist., 4 -   |            |                        |                |                                  |                  |
|  |  | 17 min.conc. [no flammable results for option 4]   |            | 1                      |                |                                  |                  |
|  |  | 18 concentration of interest, fraction   |            | 0.00                   | 1.00           | 3.00E-05                         |                  |
|  |  | 19 Fraction of LFL to finish   |            | 0.01                   |                | 5.00E-01                         |                  |
|  |  | 20 CAS number of component to monitor  |            |                        |                | 7782505                          |                  |
|  |  | Flam/Toxic/Both results flag; 0 - both results, 1 - flam results only, -1<br>21 toxic results only, -2 - material inert  |            | $-2$                   | 1              | 0                                |                  |
|  |  |  |            |                        |                |                                  |                  |
|  |  | PARAMETERS (values to be changed by expert users only)   |            |                        |                |                                  |                  |
|  |  | <b>RELEASE FROM BUILDING</b>   |            |                        | $\mathbf{1}$   |                                  |                  |
|  |  | 22 Are droplet trapped in building? 0: false, 1 (or non-0): true<br>23 Vapour multiplier   |            | $\overline{0}$<br>0.00 |                | $\overline{2}$                   |                  |
|  |  | 24 Minimum droplet size (UDM input if droplets not trapped)  | m          | 0.00                   | $1.E-03$       | 1.00E-08                         |                  |
|  |  | 25 Maximum duration of release   | S          |                        | $0.00$ 1.E+08  | $3.60E + 03$                     |                  |
|  |  | <b>EXPLOSION</b>   |            |                        |                |                                  |                  |
|  |  | 26 TNT Explosion Efficiency (external explosion model)   |            | 0.01                   | 1.00           | 1.00E-01                         |                  |
|  |  | 27 Venting equation constant (NFPA68 indoor explosion correlation)   | Pa         | 0.00                   |                | 2.48E+01                         |                  |
| A  |  | Use the NFPA68 2013 vented explosion model? ( $0 =$ False; $1 =$ True) $\vert \cdot \vert$   |            | 0.00                   | 1.00           | $1.00E + 00$                     |                  |
|  |  | <b>AMBIENT DATA</b>  |            |                        |                |                                  |                  |
|  |  | 28 Molecular weight (of air)   | kg/ kmol   | 10.00                  | 100.00         | 2.90E+01                         |                  |
| Figure 6.<br>Input data for model INBU   |  |  |            |                        |                |                                  |                  |
| A.2<br>Model run and output data   |  |  |            |                        |                |                                  |                  |
|  |  | The output data are listed by Figure 8. The output data are split into the following categories:   |            |                        |                |                                  |                  |
| Building data: building area Abuilding and building volume Vbuilding. These are calculated from the building dimensions;<br>1.<br>see Equation (17). |  |  |            |                        |                |                                  |                  |
| 2.   |  | Release from building [continuous model INBU-CO; see Section 3.1].   |            |                        |                |                                  |                  |
|  |  |  |            |                        |                |                                  |                  |
|  |  | 2.1. Volumetric ventilation rates (m <sup>3</sup> /s) for material ( $v_{dis}$ ), air ( $v_{air}$ ) and total ( $v_{vent}$ ); see Section 3.1.3<br>2.2. Mass release rates (kg/s) for material $(Q_{opt})$ and air<br>2.3. Liquid data: liquid mass fraction $\eta_{\text{out}}$ and droplet diameter $d_{\text{out}}$<br>2.4. Release duration tout<br>2.5. Release velocity U <sub>out</sub> |            |                        |                |                                  |                  |
| 3.   |  | Indoor concentration data [time-varying model INBU-TV; see Section 3.2].   |            |                        |                |                                  |                  |

**Figure 6. Input data for model INBU**

#### <span id="page-22-1"></span><span id="page-22-0"></span>*A.2* Model run and output data

- 1. Building data: building area Abuilding and building volume Vbuilding. These are calculated from the building dimensions; see Equation (17).
- 2. Release from building [continuous model INBU-CO; see Section [3.1\]](#page-9-1).
	- 2.1. Volumetric ventilation rates (m<sup>3</sup>/s) for material ( $v_{dis}$ ), air ( $v_{air}$ ) and total ( $v_{vent}$ ); see Sectio[n 3.1.3](#page-10-0)
	- 2.2. Mass release rates (kg/s) for material  $(Q_{opt})$  and air
	- 2.3. Liquid data: liquid mass fraction  $\eta_{\text{out}}$  and droplet diameter  $d_{\text{out}}$
	- 2.4. Release duration tout
	- 2.5. Release velocity U<sub>out</sub>
- 



- 3.1. Indoor dispersion arrays versus time. The data are produced in incremental times until the maximum time  $t_{\text{max}}$ . For instantaneous releases the concentrations will decay. For continuous releases the concentration rise until time  $t_{dis}$  and subsequently decay. The arrays are as follows:
	- 3.1.1. Time t since start of indoor vessel/pipe release, s
	- 3.1.2. Material mass M<sub>in</sub> in building, kg
	- 3.1.3. Concentration C<sub>in</sub> (of component to monitor), mole fraction
- 3.2. Number of concentrations of interest (maximum of 8). The program calculate rise times and fall times for the following potential concentrations levels [depending on material being toxic, flammable or both; and depending whether a concentration of interest  $C<sub>int</sub>$  (volume fraction) is specified as input]:
	- Concentrations for specified CAS component i of the released material
		- $\circ$  ERPG concentrations for component i (volume fraction):  $C_{ERPG1}^i =$  ERPG1\*10<sup>-6</sup>/y<sub>i</sub>,  $C_{ERPG1}^i$  = ERPG2\*10<sup>-6</sup>/y<sub>i</sub>, C<sub>ERPG3</sub><sup>i</sup> = ERPG3\*10<sup>-6</sup>/y<sub>i</sub>; here y<sub>i</sub> is the mole fraction of component i of the released material; and ERPG1, ERPG2, ERPG3 are the ERPG concentrations in ppm o Concentration of interest for component i:  $C_{int}^i = C_{int}/y_i$
	- LFL fraction and LFL for released material
	- Concentrations for released material
		- $\circ$  1.15  $*$  C<sub>st</sub>, where C<sub>st</sub> is the stoichiometric concentration
		- o min(UFL, C<sub>in</sub>max) for released materal, where C<sub>in</sub>max is the maximum indoor concentration [obtained at time  $t=0$  for an instantaneous release and time  $t = t_{\text{dis}}$  for a continuous discharge]
- 3.3. Rise times to concentration of interest. This is the time  $t_{rise}$  when the concentration of interest  $C_{int}$  is reached while the concentration is rising, i.e. when the indoor concentration  $C_{in}(t_{rise}) = C_{int}$  width  $dC_{in}/dt > 0$ ; see [Figure 7.](#page-23-0)
- 3.4. Fall times to concentration of interest. This is the time t<sub>fall</sub> when the concentration of interest  $C_{int}$  is reached while the concentration is falling, i.e. when the indoor concentration  $C_{in}(t_{fall}) = C_{int}$  width d $C_{in}/dt$ <0; see [Figure 7.](#page-23-0)



- <span id="page-23-0"></span>**Figure 7. Rise times and fall times to indoor concentrations of interest** Figures shows the case of an indoor continuous release with release duration  $t_{dis}$  and maximum duration  $t_{\text{max}}$  for discharge from building;  $t_{\text{rise}}$  and  $t_{\text{fall}}$  are the rise and fall times for the concentration of interest Cint.
- 4. TNT external explosion data [see Section [4.2\]](#page-16-1). These data are only provided for a flammable material with concentrations exceeding the LFL fraction.
	- 4.1. These data are given for all flammable concentrations of interest (C<sub>in</sub> = LFL fraction, LFL, 1.15C<sub>st</sub>, min(UFL,  $C<sub>in</sub>$ <sup>max</sup>). These data are as follows:
		- 4.1.1. Explosive mass (kg):  $M_{in} = \rho_{VAP}C_{in}V_{building}$ , kg; see Eq. (12)
		- 4.1.2. Corrected explosive masses, i.e. *Min f(Cin)*. Explosion efficiency *f(Cin)* is calculated as given by Eq[. \( 32](#page-17-1) ).
		- 4.1.3. TNT explosion efficiency, i.e. *f(Cin* )*fTNT.* The latter efficiciency is obtained from the property database (if specified in the database) and otherwise obtained from the TNT explosion efficiency parameter.
	- 4.2. Worst-case (largest) corrected explosion mass
- 5. Indoor explosion data [see Section [4.1\]](#page-13-1). These data are only provided for a flammable material with concentrations exceeding the LFL fraction. These data are as follows:
	- 5.1. Critical vent area. This is 1% of the total building surface area Abuilding.



5.2. Vented explosion arrays (see Equation [\( 16](#page-13-4) ):

- 5.2.1. Vent area *Avent(i) = (i/100) \* Abuilding*; i =1,2,…16
- 5.2.2. Vent fractions *Avent(i)/ Abuilding*
- 5.2.3. Pressure rises  $P(i) = C_{\text{ven}}^2 [A_{\text{vent}}(i) / A_{\text{building}}]$



<span id="page-24-0"></span>**Figure 8. Output data for indoor dispersion model INBU.**



The above output data are derived from the generic spreadsheet for the INBU model BWM. The output data are included in the output columns on the right-hand side of the above figure (one column for each run). Output data for the dispersion array data are not included in this figure.

#### <span id="page-25-0"></span>*A.3* Detailed information on INBU errors and warnings

Below information on errors and warnings are given, which can currently be produced by the INBU model.

#### Error messages

INBU 13 "Instantaneous release volume %1%Volume% exceeds building volume"

This error is reported if the release volume *Mdis/ρVAP* [see Eq. [\( 8](#page-10-2) )] after an instantaneous discharge within the building has a volume that exceeds the building volume *Vbuilding*. In this case the building could possibly be destroyed by the overpressure. The user must make a decision on how to model such a release. A conservative assumption would be to model the release as an outdoor dispersion. Otherwise he could take other measures, e.g. increase the size of the building or reduce the pipe/vessel mass inventory.

INBU 14 "Continuous release volumetric rate %1%VolumeFlow% exceeds building ventilation rate"

This message is reported for instantaneous releases, if the material volumetric flow from the building *vdis* is larger than the total ventilation rate *vvent*. In this case, the user could model the release as outdoors or take other measurements (e.g. change the ventilation specification).



# <span id="page-26-0"></span>**NOMENCLATURE**

Indoor discharge of hazardous material (post-expansion state after depressurisation to ambient)

- *ddis* Droplet Sauter Mean diameter (m)
- *Qdis* Mass flow rate for case of continuous discharge (kg/s)
- $v_{dis}$  Volume flow rate of case of continuous discharge (m $3$ /s)
- *M*<sup>dis</sup> Mass inventory prior to start of discharge (kg)
- $V_{dis}$  Volume inventory prior to start of discharge (m<sup>3</sup>)
- *tdis* Release duration for case of continuous discharge (s)
- *tac* Duration of one air change of the building (s)
- *Tdis* Final discharge temperature (K)
- *ηdis* Liquid mass fraction of hazardous material released into building

Building ventilation Specification

D<sub>vent</sub> Vent diameter (m)

*v*<sub>vent</sub> Vent volume flow rate (m<sup>3</sup>/s)

#### Initial state for outdoor dispersion from building (INBU-CO)

- $\alpha_{out}$  Angle from horizontal (rads)
- *Cout* Concentration (volume fraction)
- *dout* Drop diameter (m)
- *ηout* Liquid mass fraction
- *zout* Vertical height above ground (m)
- *Qout* Mass release rate (kg/s)
- *tout* Release duration (s)
- *Tout* Temperature (K)
- *U*<sub>out</sub> Release velocity (m/s)
- $U_{\text{max}}$  Upper limit for the release velocity (m/s) *tmax* Maximum release duration (s)
- Others (INBU-TV)
- V<sub>building</sub> Volume of building (m<sup>3</sup>)
- $C_{\text{in}}(t)$  Indoor concentration (volume fraction)<br>  $M_{\text{in}}(t)$  Indoor material mass (kg)
- $M_{in}(t)$  Indoor material mass (kg)<br>
t ime since start of indoor w
- time since start of indoor vessel/pipe discharge (s)

#### Others - Explosion

- $A_{building}$  Total internal surface area of building  $(m<sup>2</sup>)$
- 
- *A<sub>vent</sub>* Explosion ventilation area<br> *C<sub>st</sub>* Stoichiometric concentrati *Cst* Stoichiometric concentration fraction
- P Overpressure developed inside the building (Pa)
- *S<sup>L</sup>* Laminar burning velocity of flammable material (m/s)

#### Parameter

rliqmass Multiplier on the material mass vapour fraction (1-ηdis) to increase the mass emitted from the building if liquid trapped option is chosen

# Subscripts<br>dis

dis discharged material (post-expansion state after depressurisation to ambient)

air air

- out released from building (initial state of outdoor dispersion)<br>vent ventilation from building
- ventilation from building



#### **About DNV**

We are the independent expert in risk management and quality assurance. Driven by our purpose, to safeguard life, property and the environment, we empower our customers and their stakeholders with facts and reliable insights so that critical decisions can be made with confidence. As a trusted voice for many of the world's most successful organizations, we use our knowledge to advance safety and performance, set industry benchmarks, and inspire and invent solutions to tackle global transformations.

### **Digital Solutions**

DNV is a world-leading provider of digital solutions and software applications with focus on the energy, maritime and healthcare markets. Our solutions are used worldwide to manage risk and performance for wind turbines, electric grids, pipelines, processing plants, offshore structures, ships, and more. Supported by our domain knowledge and Veracity assurance platform, we enable companies to digitize and manage business critical activities in a sustainable, cost-efficient, safe and secure way.



# <span id="page-28-0"></span>**REFERENCES**

<sup>i</sup> Committee for the Prevention of Disasters. "Guidelines for Quantitative Risk Assessment. – Purple Book, CPR 18E, Den Haag, SDU (1999)  $\overline{a}$ 

ii Mannan (editor), "Loss Prevention in the Process Industries: hazard identification, assessment and control", Third Edition, Butterworth-Heinemann, Oxford (2005)

iii "TXCS Theory Manual (Model for Toxics Calculations)", Part of Phast Technical Documentation available on Phast Reference CD, DNV, London (2006)

iv NFPA 68 – standard on explosion protection by deflagration venting, National Fire Protection Association, Edition 2007; available via website [www.nfpa.org](http://www.nfpa.org/)

<sup>v</sup> Bjerketvedt, D., Bakke, J.R. & van Wingerde, K., Gas Explosion Handbook, GexCon, CMR

vi Joseph Kuchta, An investigation of fire and explosion accidents in the chemical, mining and fuel-related industrials: a manual. Bulletin 680, Bureau of Mines, United States Department of the Interior (1985).