



CHEF implementation @ dsm-firmenich

Dispersion/explosion effect distance calculations

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dsm-firmenich 

Introduction

Pier-Jan Hettema

- Chemical Engineer – TU Eindhoven – Netherlands
- 14 years operations – Dupont, Shin-Etsu
- 5+ year consultant in Reliability Engineering and Process Safety
- 10 years Process Safety Expert – ADM, dsm-firmenich

- EPSC Board member since 2021



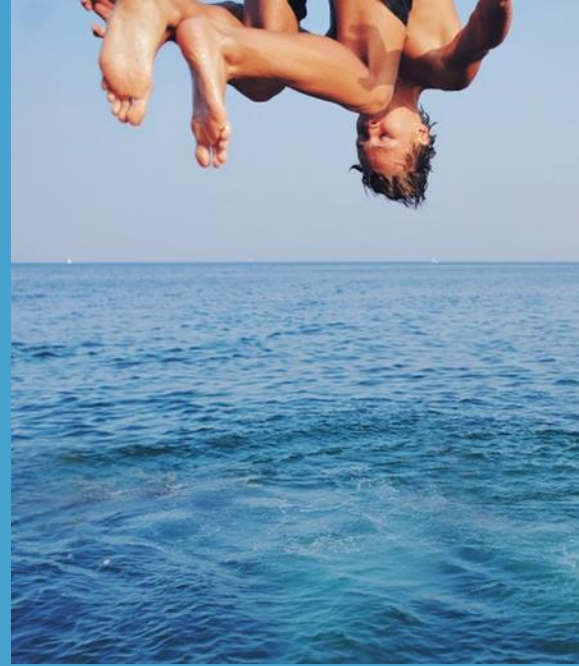
Innovators in nutrition, health and beauty



Perfumery
& Beauty



Taste, Texture
& Health



Health, Nutrition
& Care



Animal Nutrition
& Health

Three dynamic markets, two iconic names, one foundational purpose

dsm-firmenich: we bring progress to life

We're a trusted partner to global companies operating in high-growth and resilient markets. We're innovators in nutrition, health, and beauty

~30,000

passionate, talented, and diverse people in our global team

150+ years

of combined scientific discovery and innovation heritage

€12+ bn

combined revenue

- Ken First retires at DOW – RAST is donated to EPSC and CCPS
- 2017 RAST introduction into EPSC
- EPSC work group (Dow, BASF, Dupont, DSM, ...)
- Aware of CHEF → same formulas but simplified → better fit

- Focus on CHEF as supporting tool
- Internal training in technical background and use of CHEF
- Mandatory now for HAZOP and OBRA scenarios

The tool

Excel V4.3 via CCPS →

The screenshot shows a webpage titled "RAST Manual and CHEF Aid" with a breadcrumb trail "Home / Risk Analysis Screening Tool (RAST) and Chemical Hazard Engineering Fundamentals (CHEF)". The page is dated "Last updated February 15, 2023". It lists three manuals available for RAST users: "RAST USER MANUAL V4.2", "RAST USER MANUAL (CHINESE)", and "CHEF CALCULATION AID V4.3". Below this, there is a link to "contact us" for questions, comments, or suggestions. At the bottom, there are navigation links: "Download and Install", "up", and "Frequently Asked Questions (FAQs) →". On the right side, there is a "Table of Contents" menu with links to "RAST Overview", "CHEF Overview", "Case Studies", "Terms and Conditions", "Download and Install", "RAST Manual and CHEF Aid", "Frequently Asked Questions (FAQs)", "RAST Development History", and "CHEF Guide".

Home / Risk Analysis Screening Tool (RAST) and Chemical Hazard Engineering Fundamentals (CHEF)

RAST Manual and CHEF Aid

Last updated February 15, 2023

The Following Manuals are Available for RAST Users:

- RAST USER MANUAL V4.2
- RAST USER MANUAL (CHINESE)
- CHEF CALCULATION AID V4.3

Questions? Please [contact us](#) with questions, comments, or suggestions about RAST. |

[RAST User Manual V4.2](#)

[CHEF Calculation Aid V4.3](#)

← Download and Install up Frequently Asked Questions (FAQs) →

Table of Contents

- RAST Overview
- CHEF Overview
- Case Studies
- Terms and Conditions
- Download and Install
- RAST Manual and CHEF Aid
- Frequently Asked Questions (FAQs)
- RAST Development History
- CHEF Guide

Models

Source models

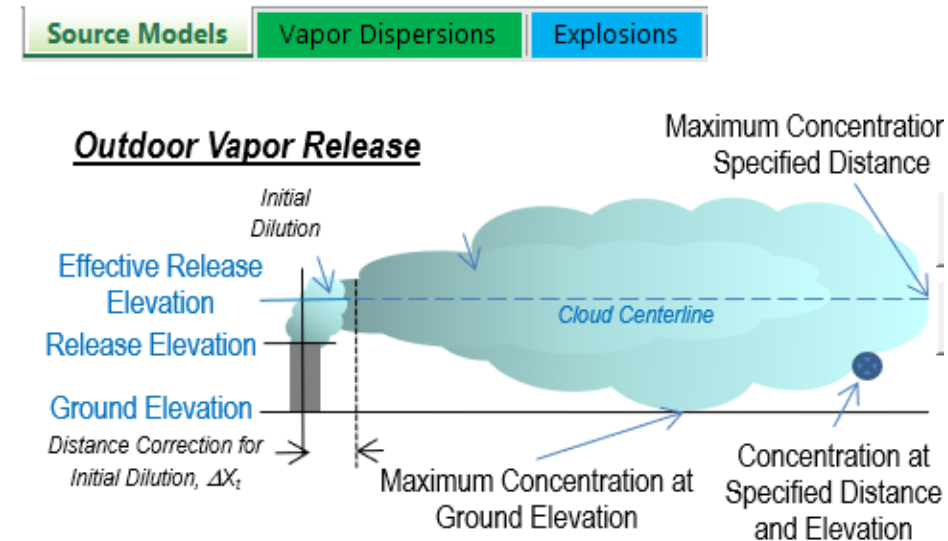
- Airborne quantity: hole size, flow rate, etc.

Dispersions

- Outdoor: 3D and 1,5F weather models
- Indoor: Volume, air exchange rate

Explosions

- VCE, headspace explosion: BST model (Baker–Strehlow–Tang)
- Physical explosion, condensed phase: simple TNT model



Dsm-firmenich Threshold Limits

➤ Flash (or Jet) Fire

*Exposure to flammable cloud of concentration > 0.5 * LEL*

➤ Building or Headspace Explosion

Indoor/inside average concentration exceeds LEL, else flashfire/fire ball

➤ (Physical) Explosion

Direct Blast Impact for humans: > 2.5 psi (200 mbar) overpressure

Building Impact: > 0.5 psi (30 mbar) overpressure

Vapor cloud explosion: Larger LOPC's in combination with (medium or high) congestion of the area.

➤ Toxic Vapor Release (Indoor, Outdoor)

- *On-site exposure to > ERPG-3 concentration (> 2 * ERPG-3 @ an occupied building).*

- *On-site exposure to a toxic vapor cloud > 5 * ERPG-3 concentration (direct ops personnel)*



Affected number of people

People affected = Occupancy x vulnerability factor

explosion pressure @ human

200 mbar = 0 %

500 mbar = 100%

explosion pressure @ building

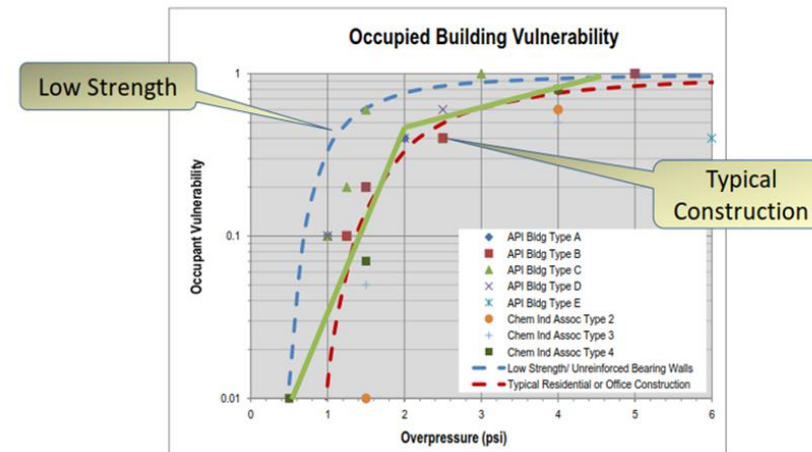
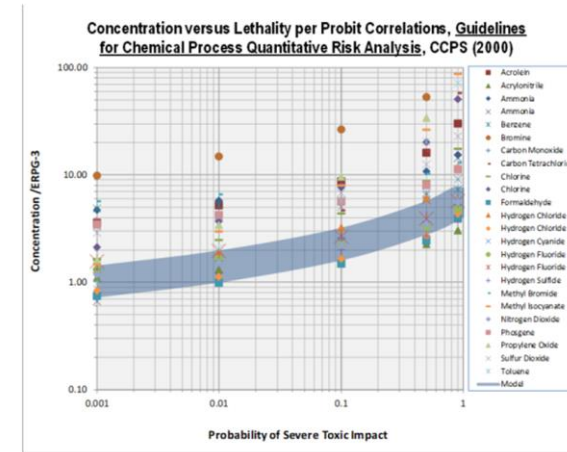
30 mbar = 0 %

300 mbar = 100%

toxic concentration

ERPG-3 = 0%

5 times ERPG-3 = 100%



CHEF Training

← CHEF effect distance calculation tool - CHEF effect distance calculation tool

DASHBOARD PATH PEOPLE SHARE

CHEF Introduction	
Introduction Editorial 5 min	5 PTS
CHEF Introduction Video Video 20 min	20 PTS
Self-study CHEF manual Editorial 60 min	60 PTS
Submit Questions Assignment 10 min	10 PTS
Knowledge Test Assignment 15 min	15 PTS
CHEF cases and submit results Assignment 30 min	30 PTS
Group session in TEAMS Teams activity 60 h	60 PTS

CHEF Toxicity

CHEF source models (airborne quantity)

CHEF dispersion modelling

CHEF explosions

Introduction

167 learners

- 98% (164) completed
- 2% (3) not started

164 learner views

Welcome to the CHEF web-based training.

Objective of this training is to enable you to use the CHEF tool for calculating effect distances for fire, explosion, and toxic scenarios. Estimated workload for this introduction is 2 hours, depending on your basic knowledge.

In this introduction module you will learn the basics of using the CHEF tool. It starts with an introduction video and self-study of part of the CHEF manual.

The CHEF tool and manual can be found via the [PS portal](#).

If you have questions about the content, you can submit your questions for an answer/discussion during the group session at the end of this module. This can be done in the "Submit questions" tab in the left menu. This module is all about starting to use CHEF, please keep in-depth questions about fire, explosion, and toxic scenarios for the upcoming modules.

After finishing all activities in this module (except the group session), you will receive an invitation to join a group session for discussion of your questions and the results of the CHEF cases.

Note: to download the CHEF tool, go to the PS portal OBRA section and open the tool in the Excel desktop app (not in SharePoint) and then save it to your computer. In this way you will keep all the macros. If you see the upper left 'clear inputs' button then you did it right.

NEXT >

Demo



Clear Inputs

VAPOR DISPERSION INPUT INFORMATION

Required inputs are Shaded "Yellow"

STEP 1 - Select Location, Type of Release, Concentration and Distance of Interest

Release Location (Assumed Outdoor if Blank)

Type of Release

Use Averaging Time Correction for Flammable Release If "Yes" dispersion concentration is approximately doubled

Input Units may be changed - Input Values in "blue" will be converted to appropriate equation units

Concentration of Interest Equation Input Equation Unit

Concentration of Interest for Hazard Analysis is typically 1/2 LFL, LFL, ER-2, ER-3 or LC50

Outdoor Downwind Distance of Interest, X m

Distance of Interest is typically to the property limit, to an unrestricted work area, or to an occupied building

Note that Concentration of Interest must be entered for estimation of instantaneous (or puff) releases

STEP 2 - Enter Chemical Properties (or Select Chemical Name from Pic List)

Chemical Name CAS No.

Data Table Value	Input Value	Equation Input
Lower Flammable Limit, LFL	1.1 vol %	
ERPG-3 Concentration	8600 ppm	
ERPG-2 Concentration	2900 ppm	
Vapor Molecular Weight, Mw	86.2	86.2
Normal Boiling Point, Tb	68.7	68.7

For reference in determining concentration of interest

STEP 3 - Enter Process Information

Process Inputs:

Equation Input	Equation Unit
Airborne Rate, Q <input type="text" value="18.4"/>	Kg/sec <input type="text" value="18.4"/>
Release Temperature, T <input type="text" value="20"/>	C <input type="text" value="20"/>
Total Release Quantity, Q* (Leave Blank if Unlimited) <input type="text" value="13200"/>	Kg <input type="text" value="13200"/>
Liquid or Two-Phase Release Velocity (Flashing Liquid) <input type="text" value=""/>	m/sec <input type="text" value=""/>
Initial Fraction Vapor, fi (Flashing Liquid Only) <input type="text" value=""/>	Fraction <input type="text" value=""/>
Vapor Pressure at Release Temp (Subcooled Liquid Only) <input type="text" value=""/>	kPa absolute <input type="text" value=""/>

STEP 4 - Enter Equipment and Plant Layout Information

Equipment and Plant Layout Inputs:

Input Value	Input Units	Equation Input	Equation Unit
Diameter of Hole or Discharge Piping, do <input type="text" value=""/>	m <input type="text" value=""/>		
Release Elevation, h (Blank assumed at Ground) <input type="text" value=""/>	m <input type="text" value=""/>		
Release Direction (Assumed Horizontal if Blank) <input type="text" value=""/>			
Enclosed Process Area Volume, Venc <input type="text" value=""/>	cu m <input type="text" value=""/>		
Enclosed Process Area Ventilation Rate <input type="text" value=""/>	Air Changes/Hr (Assumed 1 if Blank) <input type="text" value=""/>		

JET MIXING

Vapor Density at atmospheric pressure (equation 9-18), $\rho_v = 0.12 PMW / T$
 $= 0.12 (101.3) (86.2) / (293.15) = 3.574 \text{ Kg/m}^3$ (at initial temp)

Discharge Velocity (equation 9-5), $V_0 = 1.27 Q / (\rho_v d_0^2)$
 $= 1.27 (18.4) / ((3.574) (0)^2) = \text{m/sec}$

Concentration at Xi (Equation 10-2), $C_i = 1.18 C_0 u / (\rho_0 fi W)$ at $\rho_0 = 1.18 \text{ Kg/m}^3$
 $= 1.18 (1 \times 10^{-6}) (3) / ((3.574) (0)) = 1000000 \text{ ppm}$

Jet Mixing Transition Distance (equation 10-3), $X_i = 3.125 d_0 (W_0 / u) / (\rho_0 / \rho_{air})^{1/2}$
 $= 3.125 (0) (0) / (3) (3.574 / 1.18)^{1/2} = \text{m}$ at 3 m/sec wind

DISTANCE CORRECTION FOR INITIAL CONCENTRATION

Vapor from Liquid Evaporation, Equipment Rupture, or Low Vapor Velocity (equation 10-1) if $Q > (a/b) u Q^* X_b - b^2 \rightarrow$ Instantaneous Model (from equating Puff and Plume correlations)

$X_0 = 139115 [Q (F) / (u Mw C \text{ at } X=0)]^{0.59} - s h(z) X_i$ Continuous
 or $X_0 = 1934 [F Q^* / (Mw C_0)]^{0.5}$ Instantaneous

$= 139115 [(18.4) (1) / ((3) 86.2 (1000000))]^{0.59} = 8.7 \text{ m}$
 Alternate weather Initial Dilution Correction

$= 98535 [(18.4) (1) / ((1.5) 86.2 (1000000))]^{0.6} = \text{m}$

CORRECTION FOR RELEASE ELEVATION

Effective Release Elevation (equation 10-24): $H = h + 1.5 (u_0 / u) d_0 [s h(z) + 1.8 d_0 (1 - \rho_v / \rho_{air})^{1/2}]$

Sin $\theta =$ for assumed horizontal release $\rho_{air} = 1.18 \text{ Kg/m}^3$ at ambient conditions

$H =$ m for Vapor release

$H = 0 + 1.5 (0 / 3) (0) [0 + 1.8 (0) (1 - 3.574 / 1.18)] = \text{m}$
 limited to 0 elevation above ground at 3 m/sec wind

CONCENTRATION FOR RELEASE WITHIN ENCLOSED PROCESS AREA

Check Limit for Total Release Divided by Enclosed Volume (equation 10-30)
 $C_{limit} = 245 \times 10^7 (\text{Total AQ}) / (Mw (V_{enc})) = 5 \times 10^7 (13200) / (86.2 (0)) = \text{ppm}$

"Steady State" Concentration within Enclosed Process Area (equation 10-29)
 $C_{enclosed} = 8.8 \times 10^{10} (Q / Mw) / (VR V_{enc} + 880.20 Q / Mw) = \text{ppm}$
 $= 8.8 \times 10^{10} (18.4 / 86.2) / ((0) + 880.2 (18.4) / 86.2) = \text{ppm}$
 Limited to the Total Release divided by the Enclosed Volume

SIMPLE VAPOR DISPERSION

for 3 msec Wind Speed, Class D Atmospheric Stability, and Residential Surface Roughness

Outdoor Vapor Release

Maximum Concentration at Specified Distance

Maximum Concentration at Ground Elevation

Concentration at Specified Distance and Elevation

per Correlation Details with Concentration in ppmv

Plume or Continuous: $C_m = 5.5E+08 (Q / Mw) / (u X^2) 1.70$

Puff or Instantaneous: $C_m = 3.4E+08 (Q^* / Mw) / (X^2) 1.99$

per Correlation Details for 1.5 m/sec F Stability with Concentration in ppmv

Plume or Continuous: $C_m = 2.4E+08 (Q / Mw) / (u X^2) 1.88$

Puff or Instantaneous: $C_m = 8.5E+08 (Q^* / Mw) / (X^2) 2.17$

Test for Plume versus Puff Model at Dispersion Conditions: (equation 10-20)

if $Q > (a/b) u Q^* X_b - b^2 \rightarrow$ Instantaneous Model (from equating Puff and Plume correlations)

$18.4 \text{ kg/sec} < 0.00618 (3 \text{ msec}) 13200 \text{ kg} (121 \text{ m})^2 - 0.29 \text{ or } 61.14 \text{ kg/sec} \rightarrow$ Continuous

Alternate weather Puff versus Plume Model

$18.4 \text{ kg/sec} < 0.026875 (1.5 \text{ msec}) 13200 \text{ kg} (121 \text{ m})^2 - 0.49 \text{ or } 51.52 \text{ kg/sec} \rightarrow$ Continuous

Estimated Exposure Duration - Continuous Dispersion (Equations 10-21, 10-23)

$t = Q^* / Q$ for Continuous or $[-2 \ln(C/C_m)]^{1/2} [(2 \sigma_x / \text{Wind Speed}) \text{ min. for Instantaneous}]$

$t = 13200 \text{ Kg} / 18.4 \text{ Kg/sec} = 717.4 \text{ sec}$

Alternate weather Estimated Exposure Duration

$t = 13200 \text{ Kg} / 18.4 \text{ Kg/sec} = 717.4 \text{ sec}$

Maximum Downwind Distance to Concentration of Interest (equations 10-9, 10-13)

Continuous (equation 37): $X = a [Q (F) / (u Mw C_m)]^b - X_0$
 $= 139100 [(18.4) (1) / ((3) 86.2 (11000))]^{0.59} - 8.7 = 114 \text{ m}$

Instantaneous (equation 41): $X = a^* [(Q^* F) / (Mw C_m)]^{b^*} - X_0$
 $= 1930 [13200 (1) / (86.2 (11000))]^{0.5} - 8.7 = \text{m}$

Alternate weather Maximum Downwind Distance to Concentration of Interest

Continuous (equation 10-xx): $X = a [Q (F) / (u Mw C_m)]^b - X_0$
 $= 98500 [(18.4) (1) / ((3) 86.2 (11000))]^{0.6} - 0 = 121 \text{ m}$

Instantaneous (equation 10-xx): $X = a^* [(Q^* F) / (Mw C_m)]^{b^*} - X_0$
 $= 1400 [13200 (1) / (86.2 (11000))]^{0.45} - 0 = \text{m}$

Maximum Ground Level Concentration from Elevated Continuous Release per Neutrally Buoyant Plume Model (equation 10-27)

Beirut example

- ▶ August 4, 2020
- ▶ 2750 tons of stored ammonium nitrate in the harbor
- ▶ Ignited by an adjacent warehouse fire
- ▶ Biggest non-nuclear explosion of the 21st century
- ▶ 220 fatalities
- ▶ 6500 injured
- ▶ 250.000–300.000 people got homeless
- ▶ 3–5 Billion US\$ damage

Ammonium nitrate

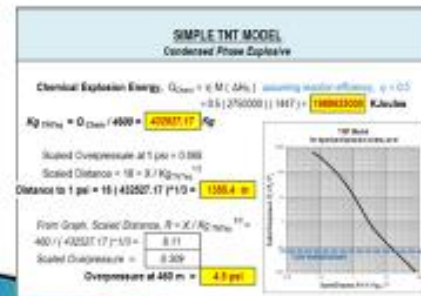
Thermal Decomposition of Ammonium Nitrate

Table 1. Properties of AN

Property	Property value
Molecular formula	NH ₄ NO ₃
Molecular weight	80
Heat of combustion	1,447.7 J/g
Heat of formation	4,594 J/g
Heat of explosion	1,447.7 J/g
Heat of fusion	76.7 J/g
Density	1.725 g/cm ³
Color	Colorless
Melting point	169.6°C
Specific volume	0.580 cm ³ /g
Solubility in water at 20°C	66 g/100 g
Oxygen content	60%
Available oxygen	20%
Estimated flame temperature	1500°C
Detonation velocity	1,250–4,650 m/s
Coefficient of thermal expansion at 20°C	$9.82 \times 10^{-4}/^{\circ}\text{C}$
Specific heat from 0 to 31°C	1.72 J/mol
Vapor pressure at 205°C	7.4 mmHg

Effect distance

- ▶ 30 mbar – appr 2600 meter
- ▶ 200 mbar – appr 800 meter
- ▶ 300 mbar – appr 460 meter
- ▶ 500 mbar – appr 340 meter



Clear Inputs

EXPLOSION INPUT INFORMATION

Required inputs are Shaded "Yellow"

STEP 1 - Select Type of Explosion and Distance of Interest

Type of Explosion: Condensed Phase Explosive

Input Units may be changed - Input Values in "blue" will be converted to appropriate equation units

	Input Value	Input Units	Equation Input	Equation Units
Distance of Interest, X	2600		2600	m

STEP 2 - Enter Equipment Burst Pressure and Volume for Physical Explosion Skip Step

Physical Explosion Inputs:

	Input Value	Input Units	Equation Input	Equation Units
Burst Pressure (gauge), $P_B - P_0$				kPa gauge
Equipment Volume, V_{EQUIP}				cu m
Burst Temperature, T_{BURST}				C
Fraction Liquid Level (if Superheated), F_L				
Flash Fract during Depressurization, F_F				

STEP 3 - Enter Quantity and Heat of Reaction for Condensed Phase Explosion

Condensed Phase Detonable Inputs:

	Input Value	Input Units	Equation Input	Equation Units
Mass of Material, M	2750000		2750000	Kg
Heat of Reaction per Mass, ΔH_R	1447	J/g	1447	Kjoule/Kg

STEP 4 - Enter Chemical Properties for Select Chemical Name from Pic-List Skip Step

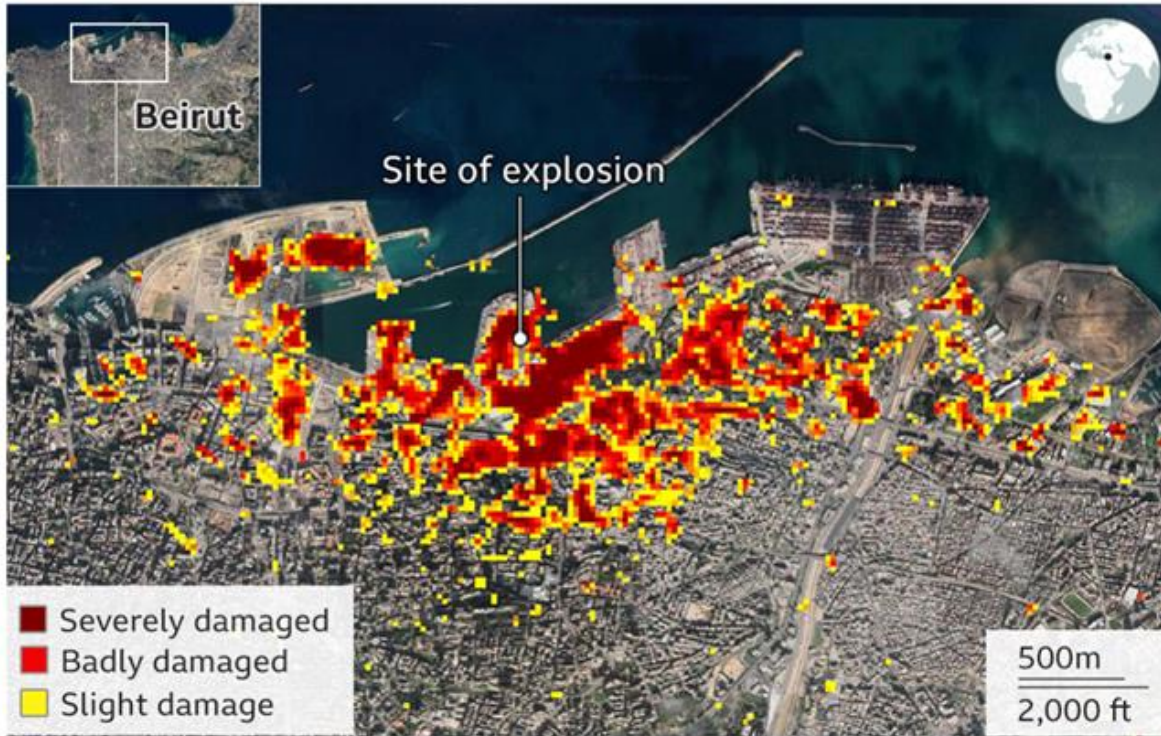
Chemical Name:

	Data Table Value	User Value	Equation Input	Equation Units
Vapor Molecular Weight, M_{VAP}				
Liquid Density, ρ_L (at Burst Temperature)				kg/m ³

Area assessment

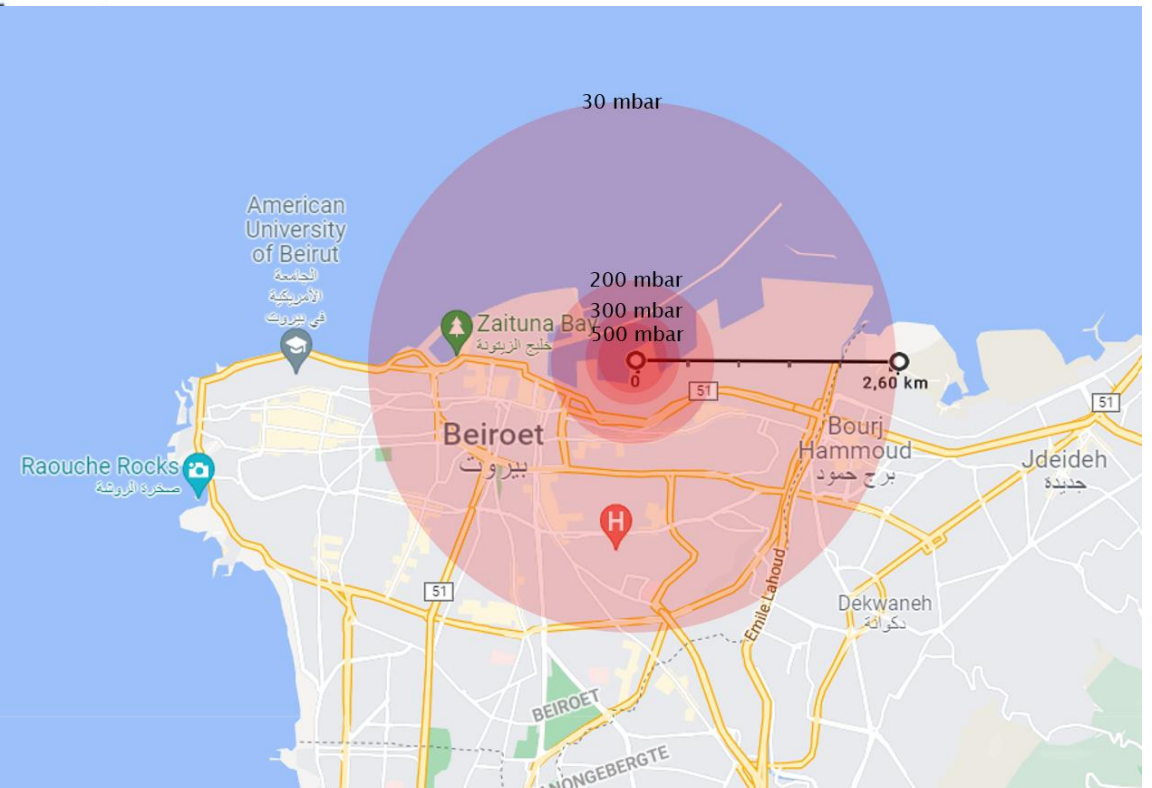
Beirut blast damage

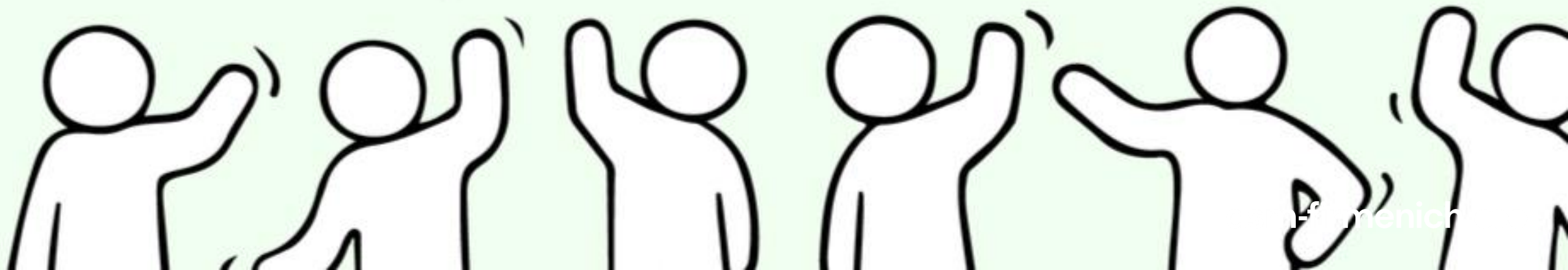
Damage assessment carried out 7 Aug



Source: ASA/JPL-Caltech/Earth Observatory of Singapore/ESA

BBC





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