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A critical assessment of available software for forecasting the impact of accidents in chemical process industry

by

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Abstract

Chemical process industries which use hazardous chemicals and/or processes are prone to accidents involving fire, explosion, or toxic release ─ which occur singly or in combination. Forecasting the likelihood of such accidents, and assessing their likely consequences, forms the basis of all accident prevention and mitigation strategies. This paper has attempted a critical assessment of the software that is available presently, priced or unpriced, for assessing consequences of process industry accidents. Besides developing a gist of the state-of-the-art, this survey also aims at identifying the strengths and the weaknesses of the available tools so that priorities for further work can be set accordingly.

Keywords: Chemical process industries, accident forecasting, software, explosion, fires, toxic release

1. Introduction

The Bhopal gas tragedy of 1984, the Vishakhapatnam IPL refinery accident of 1997, the Bruncefield catastrophe of 2005, the Jaipur fires of 2009, and the BP offshore rig disaster of 2010 are examples of major accidents that keep occurring in process industry throughout the world (Khan and Abbasi 1997a, b, c; 1998 a, b, c, d; 1999a, b; 2001a, b, c, d; 2002; Abbasi *et al.*, 2010; 2013). Each of these accidents not only cause losses worth billions of dollars but badly harm the environment of large areas (Abbasi and Abbasi 2005; 2007 a, b, c; 2008; Tauseef *et al.*, 2010; 2011 a, b; Vasanth *et al.*, 2013).Many accidents trigger other accidents, enhancing the damage

(Abdulhamidzadeh *et al.*, 2010; 2011). The after-effects of Bhopal gas tragedy continue to be felt even today, and will perhaps go on forever.

The best way to 'counter' an accident is to avoid it. And avoiding any accident is possible only if we can learn of its likelihood and prevent it from occurring. Ideally an industry should go for zero accident probability. It is like aiming a road travel which is 100% safe. By taking simple precautions such as driving slowly and keeping to correct side we can reduce the probability of an accident to less than 1%. In other words reducing the likelihood of suffering an accident during road travel to less than 1 in 100 travels. But even this is a huge risk because a single accident can ruin our entire life. To further reduce the probability we can go for stronger vehicles with special safety features. This will reduce the probability of an accident but will greatly increase the cost of travel. If we aim at zero probability of accident in our tavels, it would be so costly as to be impossible to achieve.

In the like manner, even as every industry would like to be 100% safe from accidents, such level of safety is impossible to achieve. As one approaches the 100% safety goal, the cost of achieving such safety increases exponentially. What is possible is to reduce the probability of accidents and try to achieve the lowest probability within affordable cost.

This paper presents a critical assessment of the major software tools that have been developed with which occurrence of likely accidents and their likely impacts can be forecast. The knowledge is then used to allocate resources for accident prevention in proportion to the probability and severity of the likely accidents.

2. Consequence assessment software

The computer languages, C++, Visual Basic, and FORTRAN which can be used with the Microsoft Windows, Macintosh, Linux or Unix operating systems, have been employed in the past to develop consequence assessment software. These software packages are available at a fee as well as free as shown in Table 1. Attempt has been made to bring in all major packages in Table 1 and the list can be considered as representative of the most commonly used consequence assessment software. Each software employs earlier established empirical or analytical models to estimate the extent of, and the distance to which, damage to property or loss of life can occur as a consequence of an accident.

3. The capacity, strengths and limitations of the available software

3.1 ALOHA (Areal Locations of Hazardous Atmospheres)

Itis a stand alone software developed by the U.S. Environmental Protection Agency and the National Oceanic and Atmospheric Administration, in 1982 (taining.fema.gov). Its primary purpose is to simulate airborne releases of hazardous chemicals. It allows modelling for BLEVE (boiling liquid expanding vapour explosions), VCE (vapour cloud explosions), jet fires, and pool fires.

The distinguishing features of ALOHA are that it contains an extensive chemical library, which is expandable by the user. It uses weather data that can be entered by the user or directly from a meteorological station. It has easy-to-use graphic interface and display and it includes mapping program called MARPLOT which enables customized overlays showing area facilities and vulnerable populations.

Strengths of ALOHA can be catalogued as follows (response.restoration.noaa.gov):

- It is easy to use.
- It's user interface is designed to minimize operator error.
- The navigation through the model input screens is designed to be intuitive and quick.
- The user input data is checked for consistency and reasonableness.
- The results are presented graphically.
- It runs quickly on small computers that are easily transportable and affordable for most users.

Limitations of ALOHA (Documents.mx; www.homeland.ca.gov):

- ALOHA's results can be unreliable in situations of very low wind speeds, very stable atmospheric conditions, wind shifts,terrain steering effects, and concentration patchiness.
- ALOHA doesn't account for the effects associated with fires or chemical reactions, particulates, solutions/mixtures and buildings.

3.2 EFFECTS

Developed by The Netherland Organisation TNO, EFFECTS allows the user to predict, calculate and present the physical effects of any accident scenario with toxic and flammable chemicals. It offers over 50 different calculation models for release, evaporation, fire, explosion, dispersion and damage.The key features of EFFECTS are:

- It has advanced chemical database containing toxic, flammable and thermodynamic properties of over 2000 chemicals. Also an integrated editor is available to detail definition of our own chemicals.
- Models can pass their calculation results as input to other models using a method called linking.
- In addition to the method of (manual) linking of models, EFFECTS offer combined models in a fully automatic process.
- GIS tool is incorporated within the software making it easy to overlay results over GIS drawings, Google earth screen captures.

The strengths of EFFECTS are:

- It is easy to use. The user interface is suitable for both experts and occasional users.
- The results are presented as series of graphs, special reports and contours on background maps, facilitating management steps.

3.3. ARCHIE (Automated Resource for Chemical Hazard Incident Evaluation; www.ofcm.noaa.gov; www.eng.utoledo.edu)

This software has been developed by U.S. Department of Transportation in association with Federal Emergency Management Association (FEMA) and USEPA. It is an emission and atmospheric dispersion estimation tool which can be used to assess the vapour dispersion, fire, and explosion impacts associated with episodic discharges of hazardous materials into the environment. The software can estimate the emissions and duration of liquid/gas releases from tank, pipelines and liquid pools, and the associated ambient concentrations downwind of these releases.

Strengths of ARCHIE:

- The model is very user friendly.
- Facilitates better understanding of the nature and sequence of events that may follow an accident and the resulting consequences.

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Limitations of ARCHIE

- It takes about 10-15 minutes to run the program including time required to respond to all the questions for a typical problem (www.eng.utolefo.edu).

3.4 BREEZE(Breeze Incident Analyst)

Developed by the U.S. Environmental Protection Agency and U.S. Military and Coast Guard, in 1987, it is a comprehensive tool incorporating toxic gas dispersion models, thermal radiation fire models and explosion models.

The features of BREEZE include a 3D Analyst for visualization of results, export to Google Earth etc. Further it has the ability to model multiple sources simultaneously. It is receptor/target locations can be user defined and drawn over a base map (AutoCAD DXF, ERSI Shapefile, or raster image) using a mouse for precise placement (www.chempute.com). There is a shortened model setup and execution time with intuitive ribbon bar interface and scenario templates. There is a built-in chemical database.

Strengths of BREEZE (www.chempute.com):

- Easy to use and quick to run.
- An intuitive interface guides the user through entering required and optional inputs associated with a potential chemical release (e.g. size and position of tank rupture, shape of storage tank, spill volume, and existence of an impoundment basin), and selecting the appropriate algorithms.
- Results are provided in both tabular and graphical formats including 2D contour, 3D volume, and time-series chart.
- Operator error is greatly minimized via a clear list of model run warnings.

3.5 CHARM (Complex Hazardous Air Release Model; (www.worldgeodata.com; cppwind.com)

This software enables calculations of air transport and dispersion, vapour cloud explosions, BLEVE, jet fire, and pool fire radiation. Two versions of the CHARM software are available: One assumes a single source in flat terrain and the second allows for multiple sources in complex terrain. The features of CHARM include nuclear radiation impacts which have been added in complex terrain version. Also, the complex terrain version uses 3D grid to perform simulation.

The strengths of CHARM are:

- Besides considering terrain effects it can be used inside and around buildings.
- Results are provided in 2D, 3D and table format.
- It can calculate the dynamics of particles.
- The model has the capability to set up nested grids automatically around a source to ensure a more detailed calculation in the volume where things are changing the quickest.

3.6 CANARY(www.questconsult.com)

Developed by Quest consultants, CANARY is a consequence assessment software that allows the user to assess the potential impacts following hazardous fluid release. It includes application-specific hazard models for vapour dispersion, fire radiation and vapour cloud explosions.

CANARY has auxiliary models to produce source term(s) required for consequence models such as multi-component thermodynamic calculation, liquid pool vaporization calculation and release rate calculation. CANARY allows the user to define the hazard endpoints (e.g. gas concentration, radiant flux, overpressure) that determine the extent of toxic or flammable gas clouds, radiation from several types of fire, or overpressure resulting from an explosion.

The strengths of CANARY are:

- It accepts wide range of user inputs.
- It is comprehensive; useful for any project that requires the calculation of process hazards.

3.7PHAST (Process Hazard Analysis Software Tool (www.dnv.com.ar)

PHAST is designed to contain models tailored for hazard analysis of scenarios like discharge and dispersion, jet fires, pool fires, fireballs and toxic hazards of a release including indoor toxic dose calculations. Its features includes the use of a geographical information system (GIS) for display of consequence results on maps and plot plans. It is able to undertake sensitivity studies to evaluate the need for mitigating measures such as changes in design, operation or response.

The strengths of PHAST are:

- Ease of use accomplished through predefined linking of discharge, dispersion, pool, flammable and toxic effect calculations.
- Quick and accurate results.

- Comprehensive reports and charts for easy, intuitive display of results.
- Considers releases from leaks, pipe ruptures, relief devices, vessel ruptures, venting.

3.8KAMELEONFIREX(Springer Series in Reliability Engineering, 2014; www. firemodelsurvey.com)

Developed by ComputIT with the partners Statoil, ENI-group, ConocoPhillips, Gaz de France, Ruhrgas and Sandia National Laboratories. KAMELEON FIREEX is an advanced computational fluid dynamics (CFD) tool for three-dimensional, transient simulation of flares, gas dispersion, fire development and fire mitigation.

The features of this tool include efficient and user-friendly pre- and post-processor capabilities, including options for animation of simulation results and "moving cameras" through simulations. IT has CAD import capabilities where CAD geometries are converted automatically into solid constructions or surface/volume porosities used by the KFX calculation model. Its models can pass their calculation results as input to other models.

The strengths of KAMELEONFIREX are:

- It gives quick and accurate results.
- Operator error is greatly minimized *via* a clear list of model run warnings.

3.9 FLACS(Flame Acceleration Simulator (hse.gov.uk; www.homeland.ca.gov)

This is CFD tool developed by GEXCON. It is used extensively in explosion and atmospheric dispersion modelling. It has dedicated modules to simulate gas explosion, dust explosion and explosions involving chemical explosives like TNT. Its features include integrated explosion and dispersion modelling capabilities. It enables consequence modelling in Full-3D, with assessment of effects of mitigation and preventive measures. It includes a distributed porosity model for small sub-grid scale obstacles, a semi automated process for creating complex flow geometry and a simple Cartesian grid that enables simulations to be produced rapidly compared to other general-purpose CFD codes.

The strength of FLACS are: (hse.giv.uk; www.lavteam.org)

- It has various different options for viewing results in 2D, 3D, animations, and text file output..
- It provides better understanding of the phenomena and results.
- Atmospheric conditions at inlet boundaries can be specified which take into account upstream surface roughness and atmospheric stability.
- Wide applicability can do both dispersion & explosion with same setup.

The limitations of FLACS are (hse.gov.uk)

- Many of the validation studies reported for FLACS do not provide sufficient details to invoke confidence that the results are repeatable.
- Often the results are shown for only one grid and no grid-sensitivity tests are reported.
- FLACS uses a single-block Cartesian grid. This may lead to unreliable predictions of dense gas dispersion over sloping or undulating terrain due to the overly high dissipation of momentum from modelling a stepped surface. To simulate such flows, a body-fitted curvilinear or unstructured grid, or cut-cell approach, is needed. A single block Cartesian grid also introduces limitations in the approach that can be used to model gas jets. Since the code is not yet parallelised, grids cannot contain a very large number of cells.
- 4. FLACS lacks choice in its sub-models. Only one turbulence model is provided which, although well-established, has certain limitations, and the code lacks a Lagrangian model or an inhomogeneous Eulerian model for simulations of sprays or particles.

3.10 TRACE (www.ofcm.noaa.gov; www.ehsmanagementsoftware.com):

TRACE is an engineering analysis tool for dispersion modelling. It has provision for modeling accidental toxic releases including those caused by pipe/flange leaks, aqueous spills, hydrogen fluoride spills, fuming acid spills, stack emissions, or elevated dense gas emissions. It has updated its modelling capabilities for scenarios like vapour cloud explosion, solid explosives, pool fires and flares.

Its key features includes a comprehensive chemical database of over 600 pure component substances as well as liquid mixtures. sequential process that queries the user and leads to the right set of models to solve the problem.

3.11 WHAZAN (World Bank Hazard Analysis)

Developed by Technica International Ltd. in collaboration with the World Bank, WHAZEN is a consequence analysis package which calculates the consequences and hazard zones resulting from incidents involving toxic and flammable chemicals. It comprises models for toxic release dispersion, fires and explosion (Kiranoudis, 2002).

It contains an extensive chemical library, which is user expandable. It can run models individually or can link two or three models in a way such that outputs from one model can be used automatically as inputs for another model.

The strengths of WHAZEN are:

- Product is easy to use and quick to run
- User interface is designed to minimize operator error.

3.12 SCIA (Simulation of Chemical Industrial Accident; eprints.upti.edu.my; El-Harbawi et al., 2010):

Developed by Harbawi, et al., 2008, SCIA is designed for evaluating and analyzing all likely hazards from industrial accidents. It includes models for assessing fire, explosion and toxic release. These models can be used to examine radiation, overpressure and toxic dispersion hazards in various scenarios.

The features of SCIA include GIS for screening/scenario assessment. And it has incorporated MSDS.

The strength of SCIA are:

- Simulation estimates the consequences of possible accidents in a fast and reliable way.
- User-friendly and effective tool for evaluating the consequences of major chemical accidents, process decision making for land-use planning (eprints.utp.edu.my).
- The results can be saved using different formats, exported to Microsoft Excel and later plotted using Microsoft Excel or VB itself (El-Harbawi*et al.*, 2010).
- Operator error is greatly minimized via a clear list of model run warnings (www.chempute.com).

3.13HAZDIG (Hazardous Dispersion of Gases; Khan and Abbasi, 1999c)

As noted by Khan and Abbasi, (1999),HAZDIG (Figure 1) is "a tool for studying accidental release of hazardous chemicals and its consequences. HAZDIG is made-up of five main modules for data, release scenario generation, dispersion, characteristics estimation, and graphics. It incorporates the latest models for estimating atmospheric stability and dispersion".

The features of HAZDIG include "a database containing various proportionality constants and complex empirical data has been built into the system". It has a modular structure which enables swift processing of data and computation of result.

The strengths of HAZDIG are:

- The graphics module "enables presentation of the results in an easy-to-understand and visually appealing manner.
- The output of the software is formatted so that it can be directly used for reporting the results without the need of editing.
- Wider applicability: It incorporates larger number of models than existing packages dealing with accident simulation to handle larger varieties of situation with minimum data inputs.
- Greater sophistication: It incorporates more precise, accurate and recent models than handled by existing packages.
- User- friendliness".

3.14. MAXCRED (Maximum Credible Accident Analysis; Khan and Abbasi 1999a)

Also developed by Khan and Abbasi,(1999a), MAXCRED (Figure 2) "enables accident simulation and damage potential estimation". Different types of explosion and fire models such as confined vapour cloud explosion, unconfined vapour cloud explosion, BLEVE, pool fires, flash fires, and fire balls are included in this software (Figure 3).

A special feature of MAXCRED "is that it is able to handle dispersion of heavier-than-air, gases, as light-as-air and lighter-than-air gases". The software is able to verifies the plausibility of the proposed scenario.

The strengths of MAXCRED (Khan and Abbasi 1999a) are:

- It is capable of simulating second and higher order accidents.

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- "Wider applicability: It incorporates larger number of models than existing packages dealing with accident simulation to handle larger varieties of situation with minimum data inputs.
- Greater sophistication: It incorporates more precise, accurate and recent models than handled by existing packages.
- User- friendliness".

4. Models predominantly used in the package described above

Figures 4-8 provide glimpses of models predominatly used by different software described above.

Table 1: The available major software for process industry accident consequence assessment

Software acronym	*Source*	*Availability*
ALOHA	National Oceanic Atmospheric Administration & Environment Protection Agency, 1982	Free
EFFECTS	TNO, The Netherlands	"
ARCHIE	Department of Transportation, the Federal Emergency Management Agency, and the Environmental Protection Agency in 1989 (hazmat.dot.gov)	"
BREEZE	Trinity Consultants, 1987	Priced
CHARM	Mark Eltgroth,1981	"
CANARY	Quest Consultants, 1989	"
PHAST	DNV Technica, 1982	"
KAMELEON FIREX	StatoilHydro, Total, ENI-group, ConocoPhillips, Gaz de France, BP and Sandia National Laboratories (www.offshore-technology.com)	"
FRED	SHELL company	"
SAFETI	DNV Technica	"
FLACS	GEXCoN, 1996	"
TRACE	SAFER System, 1986	"
WHAZAN	DNV Technica, 1985	"
SCIA	Harbawi, et al., 2008	Not specified
TORAP	Abbasi and Khan in 1999	"

HAZDIG	Khan and Abbasi, 1999	"
MAXCREED	Khan and Abbasi, 1998	"

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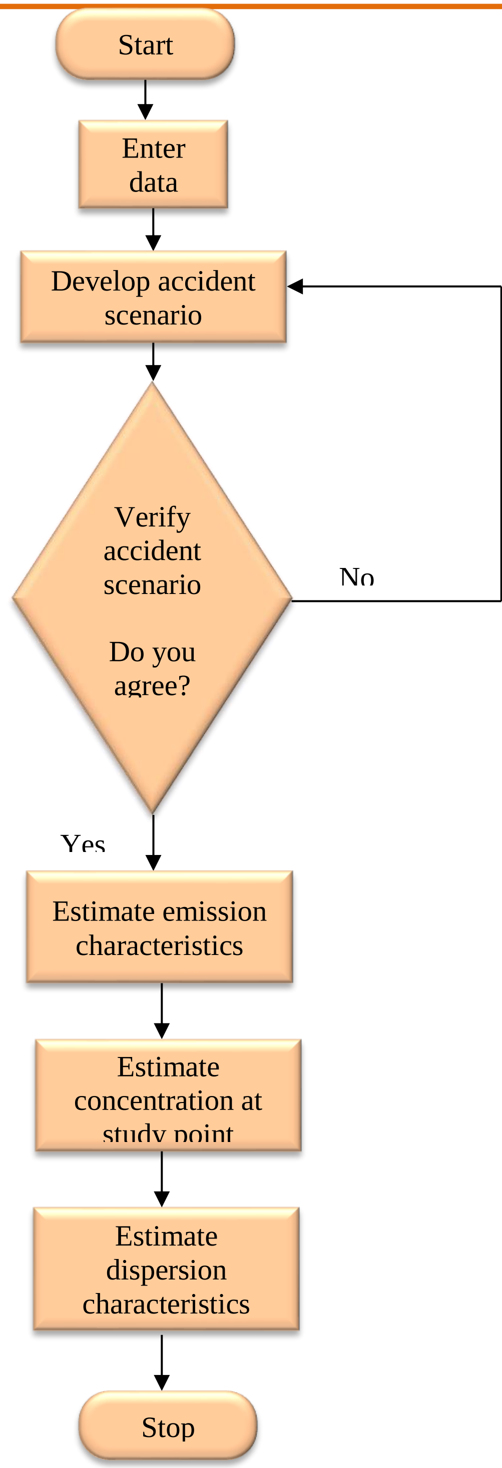


Figure 1: The HAZDIG algorithm

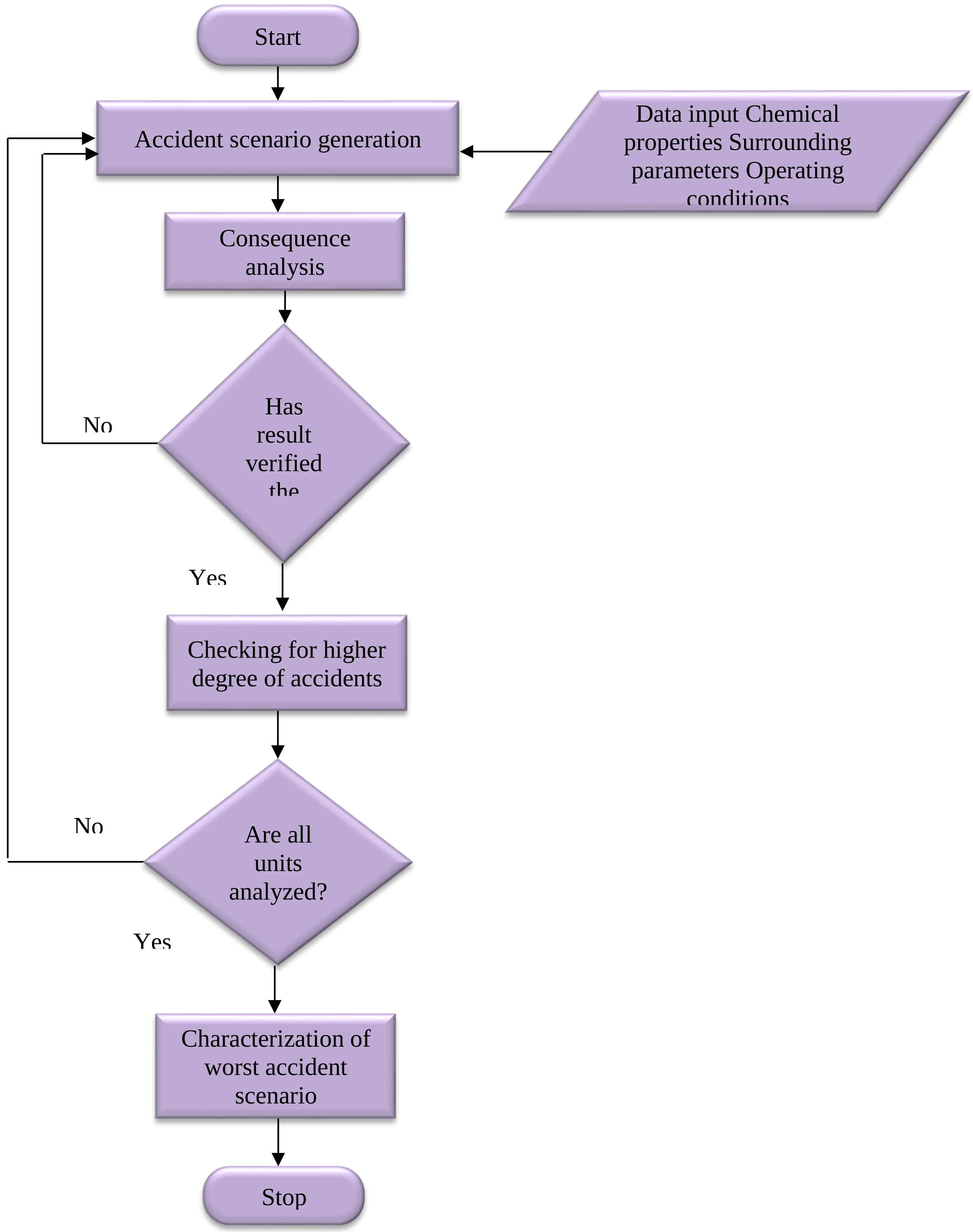
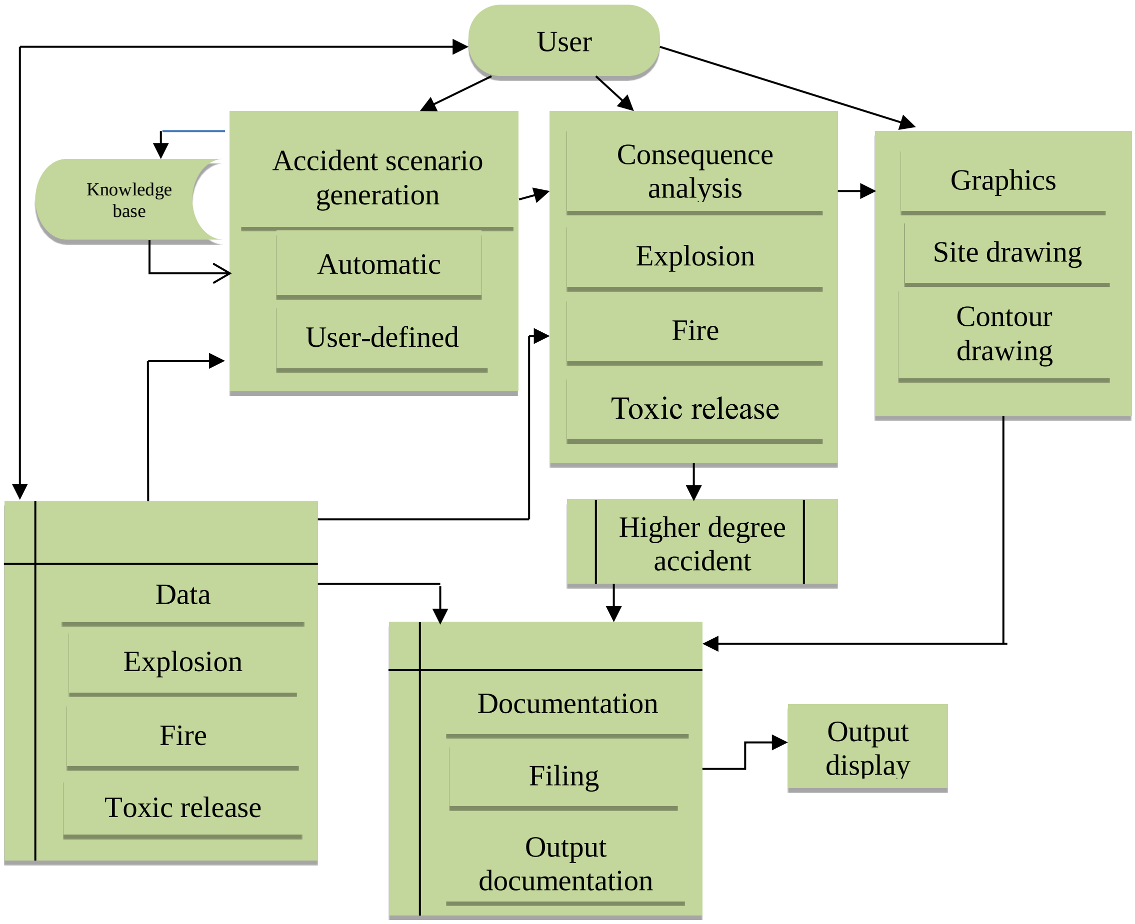


Figure 2: The algorithm of MAXCRED

Figure 3: The object-oriented architecture of MAXCRED



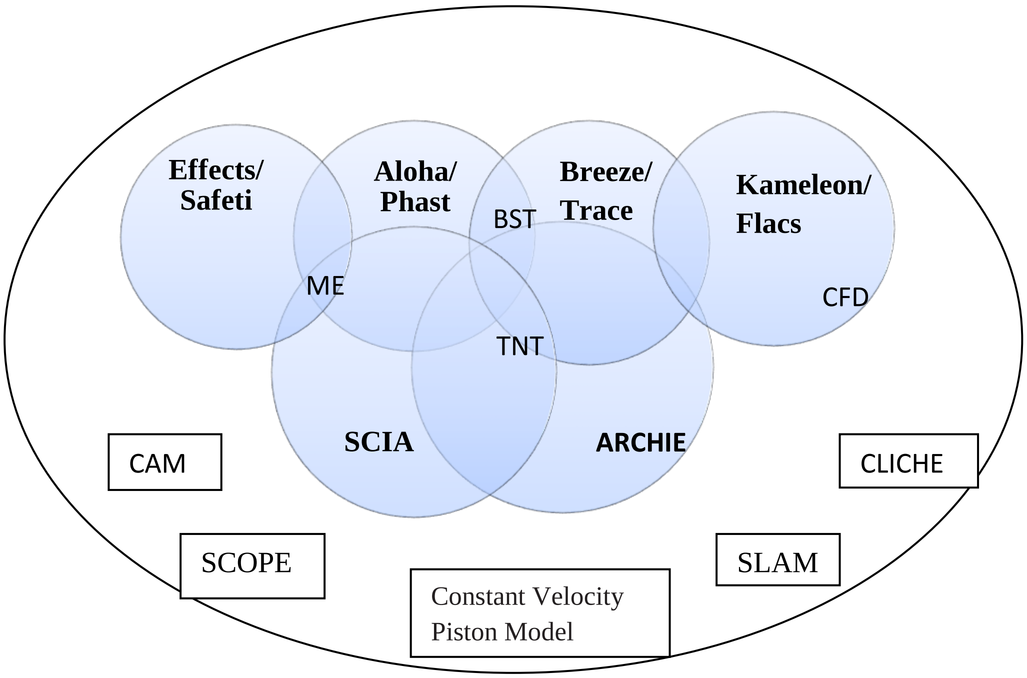


Figure 4: Models for vapour cloud explosion used in different software: ME: Multi Energy model; BST: Baker Strehlow model: TNT: TNT equivalence model

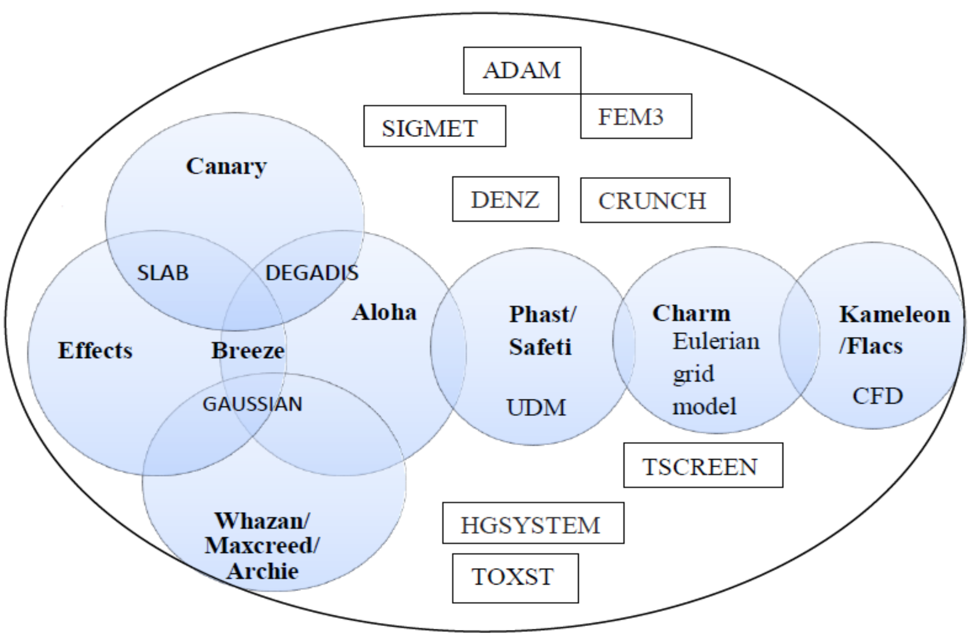


Figure 5: Models for Toxic Dispersion: DEGADIS: Dense Gas Dispersion UDM: Unified Dispersion

Model; ADAM: Air Force Dispersion Assessment Model; TOXST: Toxio Modelling System Short-Term; TSCREEN: Toxic Screening Mode.

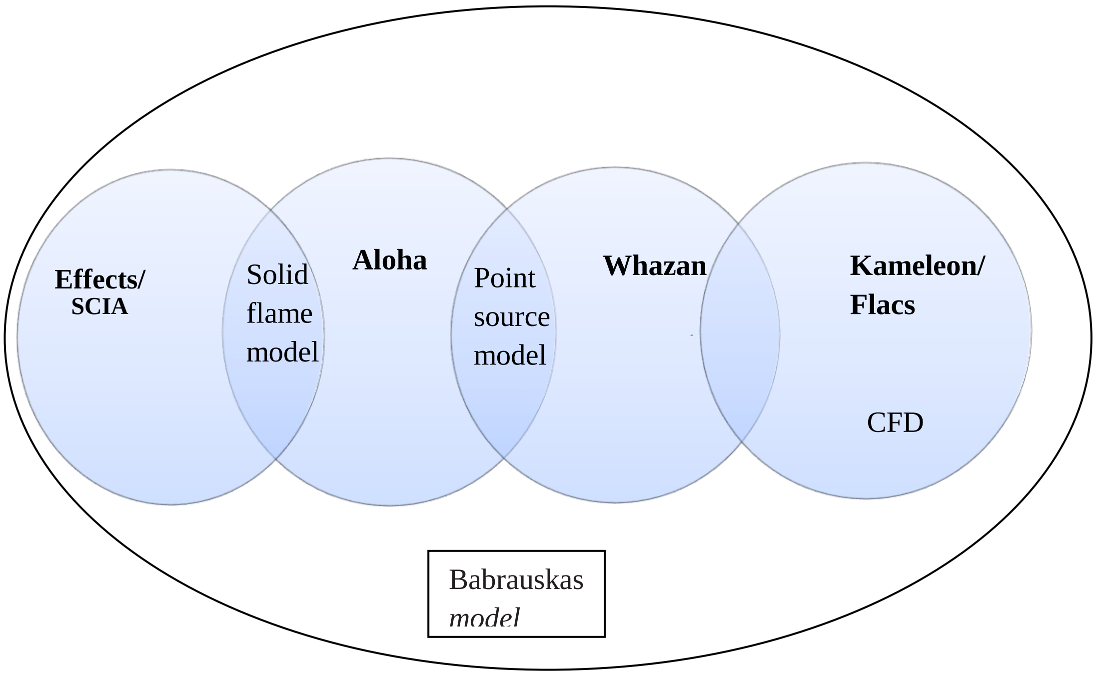


Figure 6: Models for pool fire used in different software

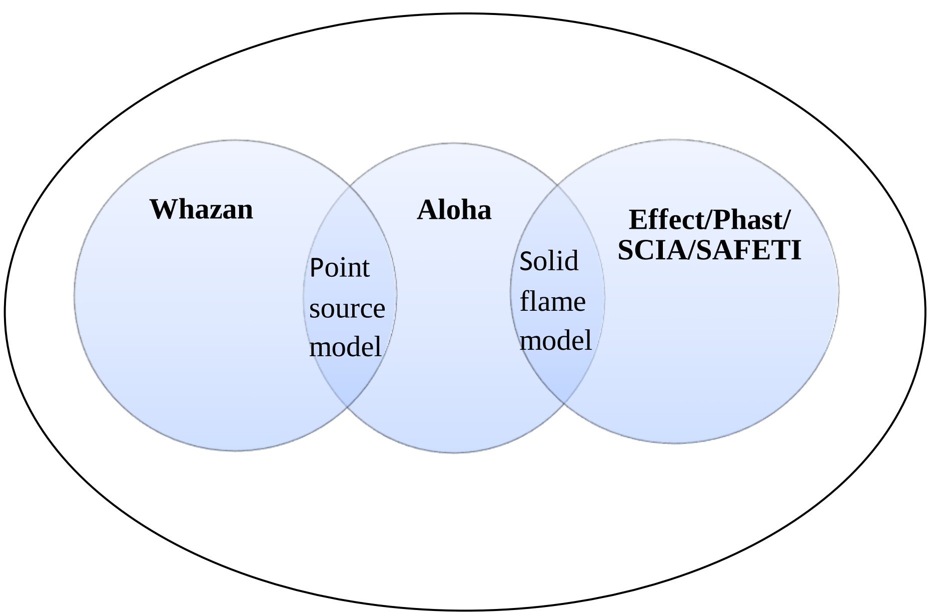


Figure 7: Models for Jet fire used in different software

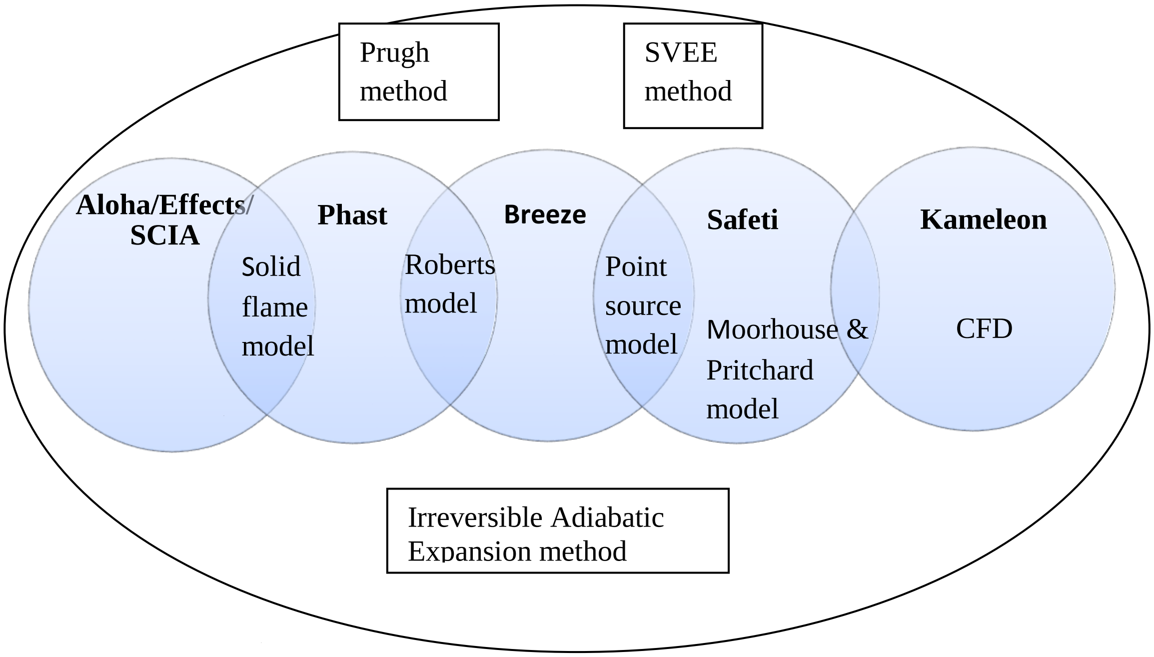


Figure 8: Models for BLEVE/Fireball used in different software

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