# DESIGN AND DEVELOPMENT OF AN INTEGRATED CHEMICAL ACCIDENT SYSTEM SOFTWARE FOR MONITORING RISK POTENTIAL OF HAZARD INSTALLATION

By

MOHANAD M-A. EL-HARBAWI

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirement for the Degree of Doctor of Philosophy

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**DEDICATED**

*TO*

*My parents, brothers and sisters for their real help*

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Doctor of Philosophy

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**Chairman: Associate Professor Sa'ari Mustapha, PhD**

**Faculty: Engineering**

Mathematical models are extremely useful tools to predict the impacts of chemical process accidents. The applications of these models require competency in mathematics and computer programming. Therefore the procedural and methodology for the calculation of consequences and risks from installations handling toxic or flammable materials have been computerized by using a software called the Simulation of Chemical Industrial Accidents (SCIA). The SCIA software was successfully developed using Visual Basic (VB) programming language with integration of GIS tools. The explosion, fire and toxic release models are implemented in an interactive VB environment.

The first step to evaluate the hazard consequence by using the SCIA software is to select whether the material is a toxic or flammable substance which is accidentally released into the environment, the specification of the position of the installations, and of all the damage states under analysis. For each and every plant damage state

the following tasks are performed. An outflow model calculates the rate of release of the hazardous substance. For a toxic material the software will precede the dispersion calculations, in order to estimate the concentration of the substance in the environment. In the case of a flammable substance a distinction is made on whether an immediate or a delayed ignition will occur. If the flammable substance along with the plant damage state results in an immediate ignition, an appropriate model is called to calculate the resulting thermal radiation. If delayed ignition is appropriate, the software will proceed to dispersion calculations to determine the explosive mass and its position in the resulting cloud. In the second step, the explosion, fire and toxic release models are used to calculate the overpressure, radiation and concentration effects around the site. Assessment of the dose follows the calculation of concentrations, thermal fluxes and overpressures as appropriate. The third step is to estimate the probability of fatality or injury that an individual will die or suffer as a result of its exposure to extreme phenomenon which is estimated in terms of dose-response models. All dose-response models employed in SCIA are based on a "probit" function for the substance and phenomenon. The results obtained from all three scenario models (explosion, fire and toxic release) were compared with results from previous software or data from real accidents, spreadsheets and manual calculations. However slight differences can be noticed with those results obtained from earlier studies. The final step is to present the hazard zones located in the vicinity of the accident area. This can be done by using GIS functionality to present the results as a circle around the point of release from the source.

The software is capable of handling multiple and alternative accident scenarios, complex terrain dispersion, uncertain quantification (including parameter and model

uncertainty) and is characterized by a user-friendly Graphic User Interface (GUI). Furthermore the software is linked to GIS for screening hazard displays. The development is done by customizing ArcGIS Engine using Visual Basic (VB). With ArcGIS Engine user can efficiently build and deploy custom desktop ArcGIS applications and use embedded GIS logic in non-GIS centric applications. Using the ArcGIS applications, users can create and manage maps used in custom applications which will save in development and effort.

The results from SCIA software were extensively validated and compared with other commercial softwares such as: FRED (developed by Shell Global company, 2004), BIS (developed by ThermDyne Technologies Ltd, 2003), EFFECT (developed by TNO, 1987) and MAXCRED (developed by Khan and Abbasi, 1998) and with established data. It was observed that the difference between results from the SCIA software in comparison to the others can be considered insignificant. Furthermore the SCIA software has been developed successfully to be utilized as a stand alone application, which allows users to run the software independently on a PC.

The SCIA software is useful due to various reasons; the cost of developing the software is cheap, the program size is small which enables users to run the application instantly, compatible to download for all windows operating systems, work as a stand alone application and finally contains a flexible database to add or delete records in the future. Furthermore the application includes an internal help option to provide and guide users with instructions to use the software. Therefore SCIA is considered as a user-friendly application.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

**REKABENTUK DAN PEMBANGUNAN SISTEM KEMALANGAN TERINTEGRASI BAGI PENGAWASAN POTENSI RISIKO KEMALANGAN PEPASANG BERBAHAYA**

Oleh

**MOHANAD M-A. A. EL-HARBAWI**

**September 2006**

**Pengerusi: Profesor Madya Sa'ari Mustapha, PhD**

**Fakulti: Kejuruteraan**

Model matematik adalah amat berguna dan mempunyai kelebihan sebagai alat untuk menduga kebarangkalian berlakunya kejadian sesuatu kemalangan semasa proses kimia. Aplikasi model tersebut memerlukan kemahiran atau kepakaran dalam bidang matematik serta penulisan perisian komputer. Oleh sebab itu, prosedur dan pengaturan cara mengira kejadian atau risiko berlakunya kemalangan di lokasi pengendalian bahan-bahan toksik atau mudah bakar dianalisakan dalam sistem perisian komputer "Simulation of Chemical Accidents (SCIA)". Program SCIA telah dikodkan dan memberi hasil yang memuaskan dengan menggunakan perisian Visual Basic (VB) berserta penggabungan kemudahan GIS. Model-model yang menganalisis kejadian letupan, kebakaran dan pembebasan bahan toksik sedang digunakan (dilaksanakan/ diamalkan) dalam suasana VB yang interakif.

Langkah pertama untuk mengenalpasti risiko berlakunya suatu kemalangan melibatkan bahan kimia dengan mengguna sistem program SCIA adalah dengan memilih samada bahan tersebut toksik atau mudah terbakar mahupun kedua-duanya yang secara tidak sengaja tersebar ke alam sekitar, spesifikasi atau lokasi tempat pemasangan sistem tersebut dan semua suasana kemusnahan yang dianalisakan. Untuk setiap satu kejadian kemalangan atau kemusnahan di kilang, kerja-kerja berikut dilakukan. Suatu model "outflow" akan mengira masa pembebasan bahan kimia berbahaya tersebut ke persekitaran. Untuk bahan toksik pula, system tersebut mula membuat perhitungan pembebasan bahan tersebut supaya dapat menilai kepekatan atau jumlah pembebasan bahan tersebut ke alam sekitar. Sekiranya bahan tersebut mudah terbakar, perbezaan dibuat untuk menentukan bahawa mula berlakunya nyalaan adalah secara spontan atau mengambil jangka masa lama. Sekiranya bahan mudah bakar berserta kemusnahan kilang tersebut mengakibatkan suatu kebakaran spontan, model bersesuaian akan digunakan untuk mengira jumlah radiasi secara pembebasan haba yang jangka diperolehi. Sekiranya nyalaan berlaku secara tidak spontan pula atau diperlambatkan, perisai tersebut akan mula menghitung pembebasan bahan tersebut untuk memberi jumlah berat dan lokasi terbentuknya awan. Sebagai langkah kedua, model-model berkaitan letupan, kebakaran dan pembebasan bahan toksik digunakan untuk menghitung kesan tekanan berlebihan, radiasi dan kepekatannya di sekitar lokasi tersebut. Penilaian berkaitan dos berikutan perhitungan kepekatan, fluks haba serta tekanan berlebihan yang sewajarnya dibuat. Langkah ketiga adalah untuk mengira kebarangkalian atau peratus kemungkinan terjadinya kemalangan yang mengakibatkan maut atau kecederaan di mana pesakit menerima tindakbalas dari kesan ekstrim berhubung model dos-respons. Kesemua model dos-respons yang digunakan dalam SCIA

berasaskan fungsi “probit” berkaitan bahan dan fenomena tersebut. Hasil yang diperolehi dari kesemua model scenerio (letupan, kebakaran dan pembebasan bahan toksik) berbanding hasil yang diperolehi dari program awal / lain atau data dari kejadian semasa, kertas kerja atau perhitungan secara manual. Walau bagaimanapun, perbezaan kecil dan tidak begitu ketara diperolehi hasil dari kajian awal. Langkah terahkir adalah untuk menyediakan dan mengenalpasti lokasi-lokasi yang melingkupi zon berlakunya kemalangan tersebut. Ini boleh dilakukan dengan menggunakan fungsi GIS untuk menyampaikan hasil kajian sebagai suatu kontur mengelilingi lokasi/ titik penyebaran bahan tersebut dari pusat atau punca asalnya.

Program ini boleh mengendalikan beberapa kejadian/ situasi kemalangan berlainan, pembebasan bahan kompleks ke kawasan berbukit, melingkupi kawasan yang saiznya belum ditetapkan (termasuk perimeter dan jenis model belum ditentukan) dan berdasarkan GUI (Graphic User Interface) yang mudah digunakan atau difahami. Selain itu, program ini dikaitkan dengan GIS untuk membolehkan gambar zn bahagian berlakunya kemalangan dipaparkan. Usaha dan hasil pebentukan sistem ini dilakukan secara mengubahsuaikan Engine ArcGIS dengan menggunakan Visual Basic (VB). Dengan menggunakan Engine ArcGIS para pengguna boleh membina dan menggunakan sistem komputer persendirian dengan aplikasi ArcGIS yang diubahsuaikan bersesuaian keperluan pengguna yang mempunyai “embedded logik GIS” yang ada kelebihan untuk berfungsi sebagai aplikasi bukan GIS. Apabila mengguna aplikasi ArcGIS, para pengguna boleh mencipta atau mereka bentuk peta yang diperlukan dalam sistem/aplikasi yang diubahsuaikan menurut keperluan penggunanya supaya boleh menjimatkan masa pembentukannya, usaha berserta tenaga diperlukan.

Hasil dari perisaian SCIA telah dipastikan dan dibandingkan dengan perisaian komersial lain seperti; FRED (hasil ciptaan syarikat Shell global, 2004), BIS (ciptaan ThermDyne Teknologies Ltd, 2003), EFFCT (hasil rekaan TNO, 1987) dan MAXCREED (ciptaan Khan dan Abbasi, 1998) atau dengan data yang siap/ sah. Perbezaan SCIA berbanding dengan sistem perisai lain boleh dikatakan teramat kecil dan tidak ketara. Selain itu program SCIA yang siap dibina boleh dipergunakan sebagai aplikasi tunggal di komputer.

Sistem SCIA adalah amat berguna disebabkan kelebihan berikut; kos untuk mencipta serta membangunkan program murah atau berpatutan, saiz aplikasi kecil membolehkan pengguna terus melancar program tersebut tanpa masa download lama, bersesuaian atau kompatible digunakan dengan sistem operasi berlainan, berfungsi sebagai sistem "stand alone" dan mempunyai kemudahan database untuk menambah atau menyingkir (memusnahan) rekod pada masa akan datang (masa depan). Tambahan pula, aplikasi ini mempunyai suatu fungsi dalam menu untuk membantu pengguna dengan memberi panduan utuk menggunakan sistem itu. Oleh itu, SCIA boleh dikatakan program yang teramat mudah atau senang diamalkan atau digunakan.

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I certify that an Examination Committee has met on 20 September 2006 to conduct the final examination of Mohanad M-A. A. El-Harbawi on his Doctor of Philosophy thesis entitled "Design and Development of an Integrated Chemical Accident System for Monitoring Risk Potential of Hazard Installation" in accordance with Universiti Pertanian Malaysia (Higher Degree) Act 1980 and Universiti Pertanian Malaysia (Higher Degree) Regulations 1981. The Committee recommends that the candidate be awarded the relevant degree. Members of the Examination Committee are as follows:

**Jamarei Otheman, PhD.**
Associate Professor
Faculty of Engineering
Universiti Putra Malaysia
(Chairman)

**Luqman Chuah Abdullah, PhD.**
Associate Professor
Faculty of Engineering
Universiti Putra Malaysia
(Internal Examiner)

**Nor Mariah Adam, PhD.**
Associate Professor
Faculty of Engineering
Universiti Putra Malaysia
(Internal Examiner)

**Mohd Sobri Takriff, PhD.**
Associate Professor
Faculty of Engineering
Universiti Kebangsaan Malaysia
(External Examiner)

**HASANAH MOHD. GHAZALI, PhD**
Professor/Deputy Dean
School of Graduate Studies
Universiti Putra Malaysia

Date: 14 December 2006

This thesis submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy.
The members of the Supervisory Committee are as follows:

**Sa'ari Mustapha, PhD.**
Associate Professor
Faculty of Engineering
Universiti Putra Malaysia
(Chairman)

**Thomas S. Y. Choong**
Associate Professor
Faculty of Engineering
Universiti Putra Malaysia
(Member)

**Abdul Rashid Shariff**
Associate Professor
Faculty of Engineering
Universiti Putra Malaysia
(Member)

_____

**AINI IDERIS, PhD**
Professor/Dean
School of Graduate Studies
Universtit Putra Malaysia

Date: 14 December 2006

## DECLARATION

I hereby declare that the thesis is based on my original work except for quotation and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any degree at UPM or other institutions.

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**MOHANAD EL-HARBAWI**

Date: 14 December 2006

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