

Ph.D. Thesis

**Quality Management Tools Of Chemical
And Bio Industrial Data Systems And
Procedures**

Gergely Viczián

M. Sc. in Electrical engineering and Economy

Ph.D. advisor:

Dr. Klara Kollár-Hunek

Consultant:

Dr. Maria Molnárné-Jobbágy

Budapest University of Technology and Economics
Chemical Information Department, 2003.

Introduction

The quality management of chemical and bio industrial data systems has extensive documentation, it is important to use adequately consistent and reliable data in the design and control of apparatus and procedures. Use of quality assurance methods in connection with databases is vital in cases when the data stored in the database is a result of measurements, and the application of the database happens in fields representing potential danger of life or risks of financial nature. A typical case for potential danger of life is in connection with the database of explosive substances. On the other hand an inadequately implemented market research study for instance can have great financial consequences.

The advancement of computer the graphics technology made it possible to use graphics not only for display statistical test values, but especially in industrial applications they are used for data adequacy test also. They present a quick feed back often with interactive control options from the data acquisition by measurements, through the comparison of the measured data systems, to process control and management.

As an informatics electrical engineer and economist, during the three years spent at the Chemical Information Department of Budapest University of Technology and Economics my ambition was to develop information technology tools – primarily software – which could be significant in the quality management and control of chemical and bio industrial data systems and procedures. My three most important innovations are:

- Accurate description of the explosion ranges of ternary gas systems, and quality managed document rendering from the corresponding data series based on online data.
- Visualization of explosion surfaces based on data sets of flammable substances for ternary systems measured on different temperatures or pressures.
- Implementation of Internet methods in the identification and analysis of customer requirements and satisfaction which is a key element of the process control and quality management ISO 900X:2000 standards.

Summary Of The Work Done

My PhD work included data visualization for quality assurance purposes. For this section of my research I had the opportunity to work with the database of flammable and explosive substances maintained by the BAM (Bundesanstalt für Materialforschung und prüfung – Federal Institute for Materials Research) institute located in Berlin, Germany. To get hands on experiences in the field I took part in laboratory measurements performed with prEN1839T tube method equipment. I made extensions to the visualization software TRIANGLE, which is in use for data acquisition and quality control purposes at the institute. In the next phase of the work I modified the Trigon software – a program we created for 3D surface visualization at our department at the Technical University of Budapest – to produce 3D explosion range surface diagrams based on the same data.

The original TRIANGLE program had been designed by BAM staff as an aid for data input in the CHEMSAFE[®] database. I enhanced this program within my PhD work with parts in connection with visualization and database quality assurance. I added the stoichiometric concentration calculation and visualization, which also serve as quality assurance checks in the program. There were many curve fitting problems in the original version of the TRIANGLE software, the identification and solution of these were also part of my PhD work.

In addition to the above enhancements in the TRIANGLE program there was demand for a handbook to be compiled based on CHEMSAFE[®] explosion range data. I added to the program a script based automation unit which would sequentially access several datasets and with the use of template files insert information from them in one editable and later printable document. This task involved further program modifications including the perfection of the triangular and Cartesian charts.

With the implementation of the automatic processing it also became possible to perform quality analysis on large number of datasets. Utilizing this new feature I implemented a testing technique for analyzing the quality of substituted missing turning points with respect to different extrapolation and curve fitting methods. I modified a real, complete data set, by eliminating one then two more points at the turning point of the curve. I examined the effects of the extrapolation on the characteristic values calculated for the explosion ranges, and compared the results for the different methods.

During the implementation of the curve fitting algorithms for the explosion range datasets came the idea to plot explosion surfaces when several sets of measurements were available for the same gas components at different starting temperatures or starting pressures. Tool for this was the Trigon program, which had been developed at the department of chemical engineering under my supervision. With some modifications this program could be made capable to visualize any ternary systems. During my PhD work, I adapted this program for the visualization of vapor liquid equilibrium data, after then for explosion limit surfaces of ternary gas systems. In case of the later I implemented a new interpolation method for the surface section near the turning line.

The Trigon program can be controlled by three means: using a Turbo Vision user interface (character based windows/menu/mouse control), command line control, and control by external programs (such as web server side applications). The web-server controlled execution makes it possible for distant users to remotely use the program. Remote controlled programs offer several advantages, of which only some are utilized in this particular application, thus the significance of this development is mainly theoretical.

In every area of my PhD work I had to produce documentation that was adequate even for industrial applications. To meet an industrial sector's particular demands, I had to take into account the corresponding quality assurance and quality control standards in their complex arrangement and practice. The chemical and bio industrial databases can be created by not just experimental measurements, as part of my doctorate work I designed a generally applicable information processing method for market research as a tool for data acquisition in food industrial applications.

New Scientific Results

1. I have developed an algorithm for the interpolation of explosion range curve points by using vector spline functions. I implemented the corresponding functions and procedures in the TRIANGLE software developed at the BAM institute in Berlin, and tested it on several datasets with positive results.
2. I examined the effects of different curve fitting and approximating algorithms in case of missing turning points. I concluded that the substitution of missing turning points by extrapolation is not permissible.
3. I implemented the visualization of the line representing the stoichiometric concentration in the triangle diagram of the TRIANGLE software.
4. I enabled the Trigon software, which was developed under my supervision for the visualization of ternary vapor liquid equilibrium systems at the Chemical Information Department at the Budapest University of Technology and Economics, to be remotely controlled via Internet technologies. The Trigon software, also under my supervision, has been adapted for the visualization of the explosion surfaces for ternary gas systems. I solved the visualization problem around the turning point.
5. I created Internet based software solutions for the process control according to the ISO 900X:2000 quality control standard by implementing the most important input and output components, namely for the registration and analysis of customer requirements and satisfaction. These software solutions were successfully utilized in five areas of the bio and agro industry.
6. Also in view of the customer requirements and satisfaction I designed the automatic document rendering processes of the TRIANGLE software which make it possible to create and print quality assured handbooks that are adequate for industrial use. I implemented the necessary routines and built them into the program.

The Practical Use Of Results

Many of the results of my work are already in practical application. The enhanced version of the TRIANGLE program is in use for data acquisition at the Bundesanstalt für Materialforschung und Prüfung institute in Berlin. My quality assured publication system had been used to produce a handbook containing 200 datasets.

My automatic Internet based data acquisition solutions are used in real life agro and food industrial research by the Postharvest Department at the Szent István University.

The Trigon Remote program was available for experimental purposes at the Chemical Information Department's web site.

Acknowledgements

There were many people supporting my work through their advice and ideas. I express my thank for this first of all to my advisor Dr. Klara Kollar-Hunek, and my consultant Dr. Maria Molnar-Jobbagy, who suggested the elaboration of this subject and rendered me a great help with their advice. I'm also grateful to Beata Kapolna and Janos Heszberger for their great collaboration and work in data acquisition and programming. Many thanks to all colleagues at the Chemical Information Department, to the very kind and helpful people at the Chemical Safety Department at the Federal Institute for Materials Research and Testing (BAM) in Berlin, Germany, to Dr. Klara Csefalvay at the Department of Electromagnetic Theory, and to everyone at the Postharvest Department at the Szent István University.

Finally I thank for the financial support I got from Foundation "Varga Jozsef" of the Chemical Faculty of BME, and OTKA (T033005, T030241).

List of Publications

Publications

1. Tóth, N., **Viczián, G.**, Viczián, Zs., Dióspatonyi, I.: Computer Network in Chemistry - Problems and results at the Chemical Engineering Faculty of the TU Budapest, Hung. Journal of Ind. Chem., Vol 27, p57-60, 1999
2. Dióspatonyi I., Horvai Gy., Tóth N, **Viczián G**, Schay D.: Computer network in education and research at the Chemical Engineering Faculty, TUB, Computers & Chemical Engineering, Vol 23. p116-119, 1999
3. Láng-Lázi M., Dióspatonyi I., **Viczián G.**, Heszberger J.: Thermodynamic consistency calculations on Internet, Hung. Journal of Ind. Chem., Vol. 27, p317-320, 1999
4. **Viczián G.**, Láng-Lázi M, Heszberger J, Dióspatonyi I., Kollár-Hunek K.: Graphic software for 3D consistency testing in thermodynamics, Hung. Journal of Ind. Chem., Vol 28, p311-318, 2000
5. **Viczián G.**, Molnárné-Jobbágy M., Heszberger J., Kollár-Hunek K.: Explosion areas of flammable substances and their numerical approximation, Hung. Journal of Ind. Chem., Vol 29, p143-148, 2001
6. Kollár G., Syposs Z., **Viczián G.**, Mészáros L., Kollár-Hunek K.: Quality management system as a tool of process control for food and agro industries, Hung. Journal of Ind. Chem., Vol 29, p135-138, 2001
7. Kollár G., **Viczián G.**, Syposs Z., Mészáros L., Hunek K.: Postharvest aspects in quality management system for fruit and vegetable production, Fruit, Nut and Vegetable Production Engineering, Inst. für Agrotechnik Bornim e.V. ISBN 3-00-008305-7, p351-355, 2001
8. Molnárné-Jobbágy, M., **Viczián, G.**: Software solution to produce the handbook "Explosion Range of Gas Mixtures – based on the CHEMSAFE[®] Database", Internary Report der Bundesanstalt für Materialforschung und –prüfung, Berlin, 2002
9. **Viczián G.**, Molnárné-Jobbágy M.: Gázelegyek robbanási területének és ezzel kapcsolatos jellemzők megjelenítésének informatikai problémái, Proc. of Műszaki Kémiai Napok '02, KE MÜKKI, ISBN 963-7172-95-5, p102-106, 2002
10. Kollár G., **Viczián G.**, Syposs Z., Mészáros L., Hunek K.: Aspekte der Nachernte Prozesse von Obst und Gemüse in Qualitätsmanagement Systemen, Obstbau, Ed.: Organ der Fachgruppe Obsbau im Bundesausschuss Obst und Gemüse, Bonn, Z-4055E, Vol. 27, 2002 (elfogadva)
11. Kápolna B., Szabó R., **Viczián G.**, Kollár G.: Internet based survey as I/O support in process approached QMS of food/agro industries, Hung. Journal of Ind. Chem., Vol 30, p229-234, 2002

12. **Viczián G.**, Molnárné-Jobbágy M., Kollár-Hunek K.: Gázelegyek robbanásáthatár-mérési adatainak minőségellenőrzése informatikai eszközökkel, Proc. of Nemzetközi Vegyészkonferencia, Kolozsvár, ISBN 973-85809-8-6, p350-354, 2002
13. Kápolna B., Szabó R., Kollár G., **Viczián G.**, Kollár-Hunek K.: Élelmiszer fogyasztói szokások Internet alapú vizsgálata, Proc. of Nemzetközi Vegyészkonferencia, Kolozsvár, ISBN ISBN 973-85809-8-6, p146-150, 2002
14. Molnárné-Jobbágy M., Bulin M., **Viczián G.**, Kollár-Hunek K.: TRIANGLE - ein Computer-Programm zur Darstellung und Auswertung der Explosionsbereiche von Dreistoffsystemen, Technische Überwachung Springer-VDI Verlag, Bd.44, Nr.1/2, S32-35, 2003

Lectures And Posters In Foreign Conferences

1. Tóth, N., **Viczián, G.**, Viczián, Zs., Dióspatonyi, I.: Computer Network in Chemistry - Problems and results at the Chemical Engineering Faculty of the TU Budapest, 4th International Workshop on Chemical Engineering Mathematics, Bad Honnef, Germany, 1998
2. Dióspatonyi I., Horvai Gy., Tóth N, **Viczián G**, Schay D.: Computer network in education and research at the Chemical Engineering Faculty, Escape-9 Conference, Budapest, 1999
3. Láng-Lázi M., Dióspatonyi I., **Viczián G.:** Thermodynamic consistency calculations on Internet, 5th International Workshop on Chemical Engineering Mathematics, Bad Honnef, Germany, 1999
4. Kollár, G., Syposs Z., **Viczián, G.**, Mészáros L., Kollár-Hunek, K.: Quality Management System as a tool of process control for food and agro industries, 8th International Workshop on Chemical Engineering Mathematics, Bad Honnef, Germany, 2001
5. Molnárné-Jobbágy, M., **Viczián, G.**, Kollár-Hunek, K.: Explosion envelopes of flammable substances and their numerical approximation. 8th International Workshop on Chemical Engineering Mathematics, Bad Honnef, Germany, 2001
6. **Viczián, G.**, Molnárné-Jobbágy, M., Heszberger J., Kollár-Hunek, K.: 3D visualization of T or P dependence in explosion surfaces, 8th International Workshop on Chemical Engineering Mathematics, Bad Honnef, Germany, 2001
7. Kollár, G., **Viczián, G.**, Syposs Z., Mészáros L., Hunek, K.: Postharvest aspects in quality management system for fruit and vegetable production, 6th International Symposium on Fruit, Nut, and Vegetable Production Engineering, Potsdam, Germany, 2001
8. Kollár, G., **Viczián, G.**, Syposs Z., Kollár-Hunek, K., Kápolna B.: Information technology for Quality Management in process control of food and agro industries, Workshop on QM of special DS and Process Engineering in Chemistry and AGRO-Biotechnology, Berlin-Budapest, 2001

9. Molnárné-Jobbágy, M., **Viczián, G.**, Kollár-Hunek, K.: Explosion limits of flammable substances and their approximation – the Triangle program, Workshop on QM of special DS and Process Engineering in Chemistry and AGRO-Biotechnology, Berlin-Budapest, 2001
10. **Viczián, G.**, Molnárné-Jobbágy, M., Heszberger J., Kollár-Hunek, K.: Information technology of triangular surfaces in chemical database – the Trigon program, Workshop on QM of special DS and Process Engineering in Chemistry and AGRO-Biotechnology, Berlin-Budapest, 2001
11. Kápolna B., Kollár G., **Viczián G.**, Kollár-Hunek K.: I/O support in process approached QM systems of food/agro industries, 9th International Workshop on Chemical Engineering Mathematics, Bad Honnef, Germany, 2002
12. Szabó R., **Viczián G.**, Kollár-Hunek K.: Internet based survey of meat consumption patterns in Hungary, 9th International Workshop on Chemical Engineering Mathematics, Bad Honnef, Germany, 2002

Lectures And Posters In Hungarian Conferences

13. Dióspatonyi I., **Viczián G.**: Kémiai és fizikai információs rendszerek az Interneten, BME Ipari Nyílt Nap, Budapest, 1999
14. Láng-Lázi M., **Viczián G.**, Heszberger J.: Termodinamikai ellenőrzés és a matematikai vizualizációs programok, MKN 2000 (Veszprém), p106, 2000
15. **Viczián, G.**, Molnárné-Jobbágy, M., Kollár-Hunek, K.: Háromkomponensű rendszerek robbanáshatár-görbéjének numerikus közelítési problémái, MKN 2001 (Veszprém), p106, 2001
16. Molnárné-Jobbágy, M., Heszberger J., **Viczián, G.**, Kollár-Hunek, K.: A Trigon program kiterjesztése robbanáshatár-felületek megjelenítésére, MKN 2001 (Veszprém), p92, 2001
17. **Viczián G.**, Kollár G., Kápolna B., Kollár-Hunek K.: Folyamatszemplélet a minőségirányításban – az I/O rendszer Internetes támogatása, MKN 2002 (Veszprém), p162, 2002
18. **Viczián G.**, Molnárné-Jobbágy M., Kollár-Hunek K.: Informatikai és matematikai eszközök alkalmazása gázelegyek robbanáshatár-méréseinek minősítésében, MKN 2003 (Veszprém), elfogadva, 2003
19. Kápolna B., **Viczián G.**, Kollár G., Kollár-Hunek K.: Informatikai eszközök az agrár-élelmiszer ágazat minőségirányításában, MKN 2003 (Veszprém), elfogadva, 2003

