Good Practice Guidelines

for

Education & Training

in the

Use of Computer Software in the Design of Process Plant

It is a professional engineer's legal and professional responsibility to exercise good engineering judgement in making design decisions and, therefore, to satisfy him/herself regarding the adequacy of the information upon which design decisions are based.

Much of this information is today generated by computer-based systems and so the quality of these systems and the skill and judgement with which they are applied to a design problem are a critical part of these responsibilities.

It is increasingly important, therefore, that all process engineering personnel should have at least a basic appreciation and understanding of such systems and techniques.

These Guidelines will continue to evolve and develop as our understanding of the issues and our experience of using existing and new tools and techniques develops. The Working Party therefore welcomes and encourages feedback from readers, both in general and on specific items (as noted in the text), regarding ways to make these Guidelines both better and more widely applicable.

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Preface

Computers are now indispensable in the design and operation of process plant. The great benefits provided by today's computers to undertake extensive calculations bring with them the need to recognise that they are also capable of delivering wrong answers to high degrees of precision if care is not exercised.

The detection of such errors becomes correspondingly more difficult as the extent of computerized activity grows and the complexity of programs increases. Nevertheless, Chemical Engineers are subject to the provisions of the law, such as the Health and Safety at Work Act 1974, and must pay due attention to the implications of the decisions they make, whether or not they are based on the results of computer calculations.

The CAPE Subject Group of the IChemE therefore decided that the time had come to bring this guide up to date. The Working Party which produced the revised guide has attempted to condense more than 150 manyears of their own collective experience of computing in process design along with that of the numerous other contributors.

We hope that it will receive the widest possible dissemination and, moreover, by making this experience available, that at least some of the disasters that might have occurred may be averted.

Readers should note that we do not regard this as in any way a final edition and we welcome and look forward to feedback for use in the next edition.

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Chairman, Computer-Aided Process Engineering Subject Group

Scope

These guidelines contain suggestions for those responsible for the training of engineers, managers and developers, either in academia or the providers of industry-based training.

The principal feature of the computer tools & techniques discussed in this document is that they are used in a decision support environment; computer tools can be used to provide information or even advice but, in all cases, a qualified engineer makes and is ultimately responsible for all design decisions.

These guidelines are primarily concerned with the use of computer tools by process engineers, such as for flowsheet simulation and equipment design.

They **do not address:**

- issues concerned with areas such as computer-aided draughting and the three-dimensional visualisation of plant and pipework layout, for which the reader is referred, for example, to the British Standards Institute, The Institution of Mechanical Engineers, etc.

- the use of embedded process control software, for which the reader is referred, for example, to "Safety Related Systems - Guidance for Engineers", The Hazards Forum, London, 1995, ISBN 0-9525-1030-8 or to a number of publications of the Institution of Electrical Engineers.

The working party believes that, although the guidelines are primarily concerned with the use of computer programs, many of the suggestions are just as valid when dealing with the results of hand calculations.

Readers should note that these guidelines are in no way intended to modify or replace engineers' responsibility under the appropriate legislation (see below): these guidelines must be treated as suggestions and in the spirit of "necessary but not necessarily sufficient". ***The working party accepts no liability whatsoever for the use which may be made of them.***

Note

This document is an extract from:

Good Practice Guidelines

The Use of Computers
by
Chemical Engineers

Guidelines for practising engineers, engineering management, software developers and teachers of chemical engineering in the use of computer software in the design of process plant

A copy of the complete document may be downloaded free of charge from either of:

http://CAPE.icheme.org
http://CAPENET.chemeng.ucl.ac.uk

Copying

The Working Party intends that these Guidelines should have the widest possible circulation amongst practising engineers and we hope that the style of presentation will allow sections to be copied for use in documents used in training and for display above the desks of engineers and managers; we ask only that the source is acknowledged, the copyright notice is not removed and that, unless by prior consultation, they are reproduced without alteration. Companies and/or HEIs are welcome to incorporate these guidelines into their own procedures, again, subject to acknowledgement, etc.

Note, however:

- The materials in these Guidelines are copyright and reproduction in any form for the purposes of commercial gain is expressly forbidden
- These Guidelines will be updated from time to time and it is the *sole responsibility* of anyone making a copy to ensure that their copy is kept up to date by reference to the most recent public version.

Legal & Professional Implications

Within the UK the work of the chemical engineer is subject to the provisions of various Acts of Parliament, including the Health and Safety at Work Act 1974.

This Act has important consequences for the way we work, laying down a number of duties for employers and employees and making it a criminal offence to fail to discharge those duties. For an overview of the way in which the Act and other aspects of the law may impact upon the work of the chemical engineer, see Appendix A6.

Similar or equivalent legislation operates in other Countries and the implications are the same: you, the professional engineer, are responsible for all decisions which you make, whether or not a computer is involved.

Attention is also drawn to the Rules of Professional Conduct of the UK Institution of Chemical Engineers, an extract from which is included within Appendix A6.

Feedback & Comments

The Working Party welcomes and encourages feedback from readers, both in general and on specific items, regarding ways to make these Guidelines both better and more widely applicable.

Such feedback should be sent in the first instance to either:

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Guidelines
for
Education and Training

Individual requirements for skills and thus for education and training will, of course, depend on job function and on Company organisation. For this reason, no attempt will be made to set out specific recommendations regarding course content: each individual's needs must be driven by the requirements and responsibilities of their professional activities, as set out in earlier sections of these Guidelines. The following therefore focusses on fundamental topics which might be covered at a basic or advanced level, whether as part of undergraduate, post-graduate or post-experience training and whether this training takes place within a higher education institute or within a company.

The increasingly widespread use of computer-based systems in design activities, however, means that it is increasingly important that **all** process engineering personnel should have at least a basic appreciation and understanding of such systems and techniques. ***Further, computer applications for engineering are in a continuous state of development, with new concepts and techniques appearing on an increasingly frequent basis, and so even experienced engineers will, therefore, benefit from regular supplementary training, in order to keep up-to-date or to explore more specialised or detailed aspects.***

Basic Training

The basic training of process engineers should prepare them for work as users of engineering software as described in “Guidelines for Engineers Using Software”.

Engineers should be taught the use of models as an aid to the design and investigation of engineering systems and should have an awareness of the assumptions, approximations and limitations of such models and their potential consequences within the context of the particular question being addressed.

Basic training should therefore include familiarisation with the concepts and techniques of mathematical modelling and the use of computers and the potential problems associated with the use of modelling software, at least at a basic level. ***It is important that this familiarisation should precede attempts to develop software to implement such models.***

Students should also be acquainted with the legal and ethical framework within which they will operate as professional engineers and its implications for the use of computer tools.

To satisfy these requirements and thus to equip engineers to meet the professional standards set out in the Guidelines, the following areas (at least) should be addressed:

- Mathematical Modelling:

  basic approaches
  assumptions, approximations & limitations (and identifying their potential consequences)
  iterative calculations: convergence issues (and their potential consequences)

- The use of computers to solve mathematical models

  (a basic appreciation of) computer programming
  typical sources of problems

- (an introduction to) Numerical Methods:

    non-linear equations
    simultaneous algebraic equations
    ordinary differential equations
    differential-algebraic systems of equations
    partial differential equations

- Modelling of Fluid Flow:

    simple models
    (an introduction to) Computational Fluid Dynamics

- Thermophysical properties:

    measurement & estimation of data (especially mixtures)
    models & correlations (understanding their limitations and the potential consequences)
    simple methods of assessing adequacy

- Modelling of individual equipment items (eg. reactors, heat exchangers, distillation units)

- Modelling of flowsheets:

    steady-state: principles, applications, convergence
    (an introduction to) dynamics: operability, flexible operations, transients, safety, etc
    batch processes

- Uncertainty and Sensitivity Analysis

- The use (and potential misuse) of spreadsheets

- (an introduction to) the capabilities and limitations of knowledge-based systems and neural networks

More Advanced Training

The training of engineers who will be engaged in software development and/or support must equip them to satisfy all the requirements set out under “Guidelines for Model-Building & Programming". It should be emphasised that staff responsible for these activities will be markedly more effective in these roles if they are fully-conversant with the **end-use** of such software and so they must at least be familiar with the “Guidelines for Engineers Using Software” and preferably have direct experience of applying such software in project work.

In addition to the above Basic Training, the following areas (at least) should be addressed:

- More advanced coverage of all the above topics

- (basic principles of) Software Engineering

    Quality Management
    Requirements Specification

System Specification and Design
Programming Languages (both algorithmic and data-driven)
Structured Programming techniques
Testing and Validation
Configuration and Change Management
Data Management and Information Modelling

- Special requirements of Safety Critical Systems (such as process control systems)

Training for Engineering Managers

Most modern engineering software is very complex and the pace of development is such that many managers (especially senior managers) may have little recent direct experience in its use.

As outlined in “Guidelines for Engineers Using Software”, the inappropriate use of software can have substantial safety and financial implications and it is therefore very important that staff with management responsibilities receive suitable update-training from time to time, in order to be properly equipped to discharge their responsibilities (see "Guidelines for Managers of Engineers Using Software").

Such training will normally be orientated towards developing an up-to-date appreciation of the capabilities of modern software systems but will also include material to raise their awareness of the potential limitations and consequences of such systems.

Managers requiring a more in-depth treatment would normally attend, for example, one of the courses for experienced engineers or even for development/support engineers (see above).

Appendix A6

Legal & Professional Aspects

It should be noted that there is, as yet, very little established precedent regarding the legal implications and liabilities associated with the use of software in engineering design activities. What follows, therefore, is necessarily a matter of opinion/judgement/interpretation on the part of the Working Party and input and suggestions from readers on potential enhancements to this Appendix would be welcomed.

1. Legal Aspects

The work of the chemical engineer in the UK is subject to the provisions of various Acts of Parliament, including the Health and Safety at Work Act 1974. This Act has important consequences for the way we work, laying down a number of duties for employers and employees and making it a criminal offence to fail to discharge those duties.

Some Points from the Act

- The duty is imposed on the individual, unless the individual can demonstrate that training or guidance from the employer is inadequate.

- If an employer's practice is faulty, or the individual is not adequately trained in good practice, then the employer would be held liable.

- If an individual is negligent, then it can result in criminal prosecution and/or being sued for damages through the civil court. Negligence implies a deliberate action done with knowledge, but ignorance would not be a defence if the individual was in a position of responsibility. A corporate body can equally be held to be criminally liable.

- Software which directly affects the operation of plant (eg. process control software or online optimiser) must be designed and constructed so as to be safe, adequately tested and supplied with adequate information to ensure that it is properly used.

- Penalties for breach of the Act are principally criminal (fines and custodial sentences).

- If an individual is injured following a breach of duty under the Act, liability will be deemed proven also.

Similar or equivalent legislation operates in other Countries and the implications are the same: you, the professional engineer, are responsible for all decisions which you make, whether or not a computer is involved.

Licensed Software

Note that software licences usually contain such broad-ranging exclusions and/or disclaimers as to be almost meaningless. It should also be noted, however, that the legal validity of such disclaimers is often unclear and may be subject to a judgement of what is and what is not considered to be "reasonable". Many licences almost certainly contain clauses which would be deemed "unreasonable exclusions" if challenged in court.

However, validation before use is often a critical issue, whether it is your own software or is licenced from a vendor. (Validation of your own developed software is covered in Appendix A5.) You would therefore be expected to take "reasonable steps" to validate the software for each of your intended applications, in order to establish "fitness for purpose" and the vendor would be expected to cooperate in a "reasonable" manner to facilitate this validation.

2. Professional Responsibilities

Most organisations will have established corporate standards and guidelines and, in general, it is your professional responsibility to take reasonable care to follow accepted good practice and your company's procedures. If you do not, you may be increasing your liability. It is therefore important to maintain records which show that you have: this is one reason for the emphasis placed on keeping records and the audit trail in the various chapters of these Guidelines.

The following is an extract from the UK IChemE's "Rules of Professional Conduct", Issue 2: October 1991:

> *"3. A member, when discharging his professional duties:*
>
> *(a) shall satisfy himself as to the extent of those duties, and, if in doubt, obtain such clarification or confirmation as is necessary to satisfy himself as to their extent before entering upon them, and shall not accept professional obligations which he believes he has not sufficient competence or authority to perform;*
>
> *(b) shall accept due responsibility for all work done by him or under his direct supervision, and shall take all reasonable steps to ensure that persons working under his authority are competent to carry out the tasks assigned to them, and that they accept personal responsibility for work done under the authority delegated to them;*
>
> *(c) shall, when called upon to give an opinion in his professional capacity and based on the facts disclosed to him, give an opinion that is objective and reliable to the best of his ability; and*
>
> *(d) shall, if his professional advice is not accepted, take all reasonable steps to ensure that the person over-ruling or neglecting his advice is aware of the possible danger which he believes may result from such over-ruling or neglect.*
>
> *4. A member shall take all reasonable care in his work to minimise the risk of death, injury, or ill-health to any person, or of damage to property. In his work, a member shall respect all laws and statutory regulations applicable to the design, operation and maintenance of chemical and processing plant. In addition, a member shall have due regard for the need to protect working and living environments, and the need to ensure efficient use of natural raw materials and resources."*