Good Practice Guidelines

for

Practising Engineers

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.

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.

Contents

Preface 3
Scope 4
Copying 5
Legal & Professional Implications 5
Feedback & Comment 5

Summary of Key Messages 6

Guidelines For Engineers Using Software 7
Define Your Problem 9
Select the Program 10
The Input Data 13
Solving the Equations 15
Checking the Results 17
Keeping Records 18
Seeking Help 19

Appendices:

Errors & Their Potential Consequences 20
Thermophysical Properties, Models and Databases 24
Checking the Results 30
Uncertainty, Sensitivity and Design Margins 35
Legal & Professional Aspects 37

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.

Dr Rob Best, South Bank University
Chairman, Computer-Aided Process Engineering Subject Group

Scope

The principal feature of the computer tools 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.
- specific issues associated with dynamic behaviour or batch processes. Many of the basic issues are similar and it is believed that readers addressing such processes will find much useful guidance: feedback would be most welcome for inclusion in future editions.

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:

CAPE Subject Group Officer
IChemE
165-189 Railway Terrace
Rugby
Warwickshire, CV21 3HQ

or:

The document editor: Tony Perris (Tony.Perris@btinternet.com or t.perris@ucl.ac.uk)

Summary of Key Messages

- 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. **This means you!**

- 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.

- The purpose of these Guidelines is to suggest some **simple precautions** which should be taken to help protect the integrity of proposed engineering solutions and thus to adequately discharge professional responsibilities, for example:

    - what matters is the quality of the engineering decision: focus on "fitness for purpose" of both the computer-based system and the data which is fed into it

    - assume that everything is "guilty until proven innocent": you must check and ensure that the computer-based model is appropriate to your needs and that the data (including any data from databanks, etc) is correctly specified and adequately covers the expected ranges (for example, of temperatures, pressures and compositions)

    - you must check and ensure that the program has worked successfully and that the results are adequate for your purpose: you must satisfy yourself that you fully understand any weaknesses and that you apply them sensibly and with good engineering judgement

    - sensitivity analysis is a key weapon in identifying where the critical problems lie and in assessing their likely impact on your design decisions

- Do not hesitate to **seek help and guidance** from your more experienced colleagues, from your support services or even from the suppliers of the systems concerned (and seek it early, not when things have already gone wrong)

Guidelines
for
Engineers Using Software

The increasing availability of powerful Computer-Aided Process Engineering (CAPE) tools brings enormous benefits to process engineers in their day-to-day work - it is almost inconceivable that today's generation of tightly-integrated continuous plants or flexible batch processes could be designed or operated without such aids. However, their use requires careful attention to detail, or serious mistakes can be made: any significant mismatch between the problem, the CAPE tool and the input data may lead to expensive (or even dangerous) mistakes.

The guidelines and suggestions which follow are based upon two underlying principles:

- **You, the engineer,** are ultimately responsible for all decisions you make, whether or not those decisions are based on information generated by a computer program.

  The computer is an aid to decision-making not a substitute for judgement.

- **You, the engineer,** must establish whether the computer-generated information is "fit for your purpose". You must **always** challenge the results of a computer model and check in every way possible that the solution which it proposes is suitable for your needs. You must assume that all data, models and results are *"guilty until proven innocent"!*

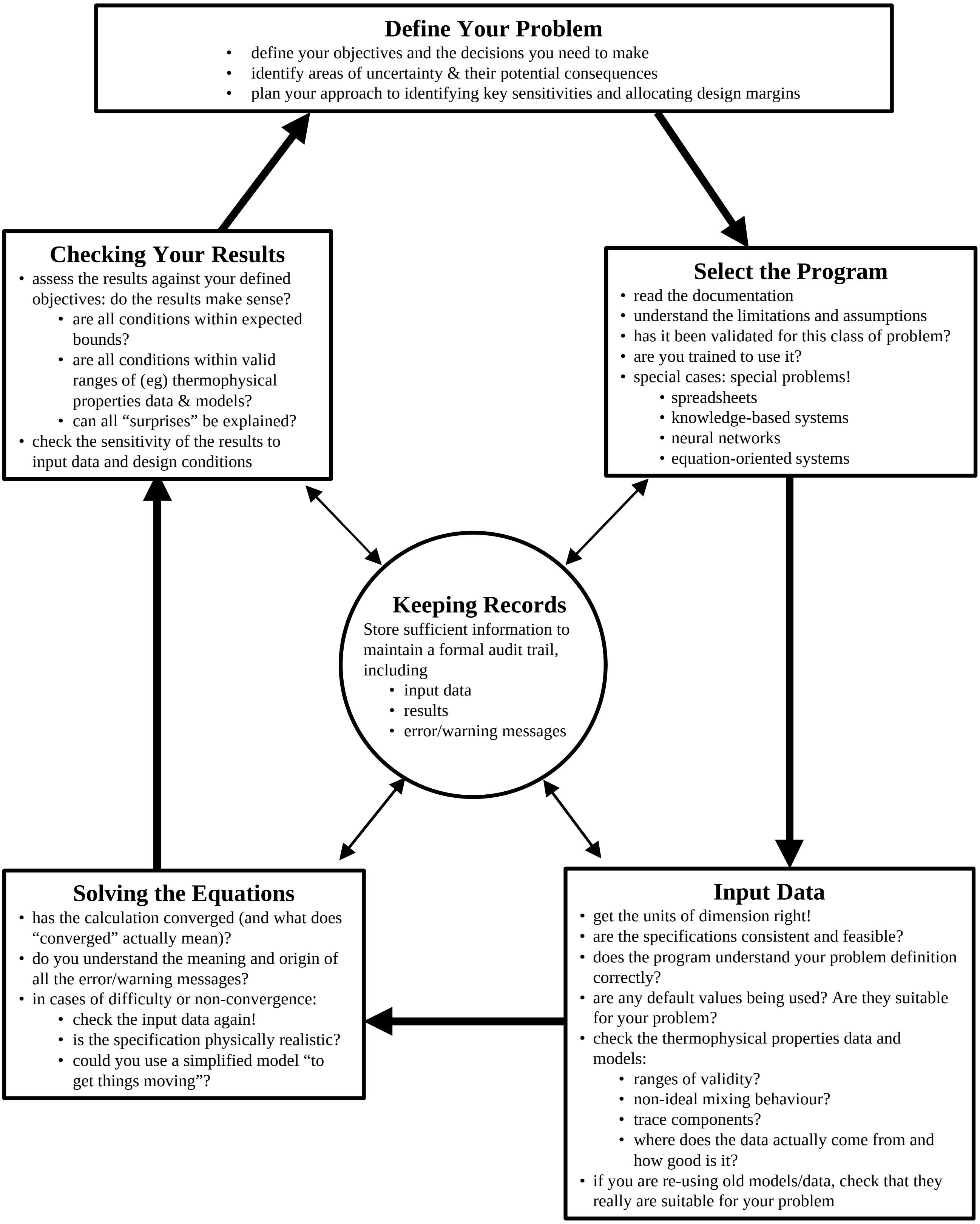
  You must fully understand your legal and professional responsibilities

As a starting point, you should:

- assume that all data, models and results are fallible
- explore the problem areas and eliminate potential sources of errors and inadequacies at the outset
- ensure that you understand where the residual problems are and how serious they may be, in terms of their effects on the final engineering decision which is being made.

Examples of the many areas in which problems can arise are given in Appendix A1.

(... continued)



Define Your Problem

- define your objectives and the decisions you need to make
- identify areas of uncertainty & their potential consequences
- plan your approach to identifying key sensitivities and allocating design margins

Select the Program

- read the documentation
- understand the limitations and assumptions
- has it been validated for this class of problem?
- are you trained to use it?
- special cases: special problems!
    - spreadsheets
    - knowledge-based systems
    - neural networks
    - equation-oriented systems

Input Data

- get the units of dimension right!
- are the specifications consistent and feasible?
- does the program understand your problem definition correctly?
- are any default values being used? Are they suitable for your problem?
- check the thermophysical properties data and models:
    - ranges of validity?
    - non-ideal mixing behaviour?
    - trace components?
    - where does the data actually come from and how good is it?
- if you are re-using old models/data, check that they really are suitable for your problem

Solving the Equations

- has the calculation converged (and what does “converged” actually mean)?
- do you understand the meaning and origin of all the error/warning messages?
- in cases of difficulty or non-convergence:
    - check the input data again!
    - is the specification physically realistic?
    - could you use a simplified model “to get things moving”?

Checking Your Results

- assess the results against your defined objectives: do the results make sense?
    - are all conditions within expected bounds?
    - are all conditions within valid ranges of (eg) thermophysical properties data & models?
    - can all “surprises” be explained?
- check the sensitivity of the results to input data and design conditions

Keeping Records

Store sufficient information to maintain a formal audit trail, including

- input data
- results
- error/warning messages

Seeking Help

If in any doubt whatsoever, seek guidance from:

- your more experienced colleagues
- your company’s support services
- the software suppliers

Define Your Problem

Define Your Objectives & Decisions

What matters is the quality of the final engineering decision that you make, not the accuracy of the information which leads you to take it.

It is, therefore, CRITICAL that you have a clear, agreed, definition of your purpose:

- establish your objectives clearly so that appropriate methods can be chosen
- ensure that you fully understand the problem which you are trying to solve. Some particular examples, which are often overlooked:
  - trace components: even minor traces of some components can have a marked effect on the behaviour of the system (and you will need to identify them for safety & environmental studies)
  - transient conditions: do not forget potential transient conditions and any requirements for flexible operation
  - are you working within proper engineering limits?
- form a clear view of the decisions which you need to make and, therefore, what level of modelling will be fit for your purpose (you can easily waste a lot of time and effort on inappropriate sophistication but when detail is required then it must be included). For example:
  - what are the potential consequences of an error (eg. a performance problem, economic viability or safety/environmental issues)?
  - is this a scoping study or a final design? (See, however, notes on "Screening Studies" in Appendix A1.)

(A more detailed review of the issues which must be considered is given in Appendix A1.)

Uncertainty, Sensitivity & Design Margins

All information is subject to uncertainty. Some areas will be more critical than others: your primary weapon for assessing uncertainty and fitness for purpose is Sensitivity Analysis and this technique should be used to explore and bound the areas of uncertainty.

Plan your approach to identifying key sensitivities and allocating design margins:

- **what if ...? studies** can be used to discover important cause & effect relationships
- **bounding the problem:** assess the performance of your proposed design not just at the most probable value of the key variables but at potential maximum and minimum values too (and do not forget potential transient conditions). ***These bounds should reflect your true level of confidence in the data.***
- remember to consider **combinations of effects**, not just single uncertainties: some may act as “triggers” for more serious problems.
- carefully explore **worst case scenarios** and the potential **consequences** which may result (see above)
- **design margins** must directly reflect your level of confidence and the potential consequences if you are wrong

(See Appendix A4 for a more detailed review and examples.)

Select the Program

If your company has an "approved standard program" for your class of problem, USE IT!

If, however, there is no approved standard, then the following checks are important. You should perform them thoroughly and should document them carefully, both as a part of your own record-keeping and as potential guidance to other users - depending on the outcome, this may *become* the Company standard and the way in which it was validated and approved will become a key part of the Company's procedures and practices.

Documentation

As a principle, never use any program which is not documented to at least a reasonable standard - you do not really know what risks you are taking and the quality of documentation may be a good indication of the quality of the program

- read the manuals or documentation carefully and ensure that you fully understand the limitations of the system being used - is it fit for your purpose?
- ensure that the correct models, physical property methods etc., are being used and that they are being used in an appropriate manner (for example, within their specified ranges).
- the documentation should also give information on the solution methods used, their source, applicability, accuracy, range of validity etc. You must satisfy yourself regarding:
    - the suitability of the method of solution
    - the probable reliability/accuracy of the results

If the documentation is deficient (which is frequently the case), then you should request the program suppliers to supply further information, if necessary under a confidentiality agreement

Limitations & Assumptions

- are there any program limits which you should stay within (such as flow regimes, ranges of correlations, etc.)?
- are the underlying assumptions fully explained and acceptable for your purpose?
- sometimes, you may need to use approximate models (for example, to generate “ballpark” information quickly) but you need to know just how approximate such models are in the context of your particular problem

(... continued)

Validation

- has the selected program been validated for use on this class of problem? (For example, you should not use a program designed for simulating oil and gas mixtures to simulate an acids process.)
- take care to ensure that the correct (i.e. validated) version of the software is being used
- extra care is required if using:
  - a program written especially for a particular project (as opposed to a properly designed, tested and documented general-purpose design tool)
  - a spreadsheeting program (see later)
  - especially, any program of uncertain origin (such as might be acquired via shareware, networks, etc.).

You should assume that any such program has not been tested or validated and is, therefore, particularly prone to error

Are you trained to use the program?

Are you appropriately trained in the use of the program? “Learning on the job” is as potentially dangerous with computer tools as with anything else and should be done only with great care, planning and checking.

Some Special Cases

Some types of program require special consideration in use, for example:

- **Spreadsheets:** spreadsheet programs can be very useful tools. However, their formulae are usually not visible and are difficult to check, so you must only use them with very great care as errors can readily arise:

  - wherever possible, make sure that you are using a true Company Standard spreadsheet (ie. one which has been developed, tested and validated for applications like yours) - be especially wary of unofficial "improved" versions.
  - When using a spreadsheet developed by someone else, you must take special care to check that the spreadsheet is correct and is suitable for your problem, including model equations, range checking, component list, units of measure, use of properties and so on.
  - There may also be audit trail implications (see Keeping Records, below): it may be necessary to store a copy of the spreadsheet itself with the results.

- **Knowledge-Based Systems (KBS):** KBSs can be thought of as tools for enhancing the initial screening process, and as such they do not, in principle, influence or participate in the final decision. However, as the user, you should exercise caution and not assume that the KBS knows everything. Such systems do not remove the responsibility from you, the engineer, to validate all decisions - you should use them only in “advisory mode” and treat their output only as suggestions.

  - the knowledge base is merely a different form of data supplied to the KBS - it should be checked very thoroughly as to its source, range, validation, internal consistency checks, etc
  - as with any other system or data, extrapolation should be treated with extreme care
  - you should interrogate the system to elicit the reasoning used and to verify the recommendations reached. If such an interrogation facility is not available, then you must exercise great care in checking results.

- **Neural Networks:** by their nature, Neural Networks tend to be very problem-specific and may not transfer readily to different problems.

  - the training data should be available and be checked very thoroughly, in the same manner as the knowledge base for a KBS (see above)
  - extrapolating beyond the region in which they have been trained is especially error-prone and you must exercise particular care (as a principle, you should never extrapolate - go back and retrain the NN on additional data)

- **Equation-Oriented Systems:** good programming and model-building skills are required for using the in-built modelling languages in some specialised engineering modelling tools, such as equation-oriented simulators. You should refer to the recommendations in the section on Model-Building, Programming and End-User Support, especially if you suspect that the resulting model may ever be used by other personnel.

The Input Data

You must carefully ensure that your input data (including any defaults, etc.) properly define the problem which you want to solve - if you define a different problem, then...! Like everything else, your input data must be fit for your purpose. For example:

Units of Dimension

Do all the units of dimension correspond to those required by the program?

- if the program claims to use "SI" or "British" units, does it conform rigidly to the definitions? (For example, is pressure expected in bar or Pa and in gauge or absolute and time in h or s?)
- be especially careful of the implied factors of 10 "hidden" within the prefixes m, M, k, etc.
- check any units conversions very carefully

Specifications

Are all your specifications consistent and physically feasible? For example:

- is the specified combination of temperature and pressure compatible with the expected phase?
- is the column product specification compatible with the thermophysical properties data?

Defaults

Does the program use any defaults (in either data or methods)? If so, are they clearly identified and are they right for your problem?

Thermophysical Properties Data

Thermophysical properties data are fundamental to all process engineering calculations. In addition to the typical problems which apply to all data, thermophysical properties data are subject to a range of special problems. These issues are described in Appendix A2 and are a frequent source of errors which can be difficult to trace. Some particular problem areas:

- identify as best you can what components (ie. chemical species) are in your system and over what ranges of composition, temperature and pressure properties will be required. Beware:

    - even minor traces, which can have a marked effect on system behaviour (you will need to identify them anyway for safety & environmental studies)
    - expected conditions which lie anywhere near the critical point of any of the components
    - other physical or chemical effects, such as ionic interactions, association/dissociation, etc

- where does the data really come from and how good is it?

    - what is its original source?
    - what is its range of validity (beware extrapolation, especially in composition)?
    - what is its documented accuracy over that range?

- use **Sensitivity Analysis** to identify where accuracy is important (see above and Appendix A4)

- what are the **potential consequences** of an error (for example, a performance problem, economic viability or safety/environmental issues)?

- some simple (but very important) checks:

    - make some simple property calculations and plot them on a graph
    - repeat these experiments with more complex properties, such as bubble and dew points, flash envelopes, etc.

A more detailed review of the issues which must be considered is given in Appendix A2.

Thermophysical properties is a very specialised area and you should not hesitate to seek expert help and/or to involve the suppliers of your CAPE and/or property systems.

Re-Using Models and/or Data

In principle, you may save significant time and errors by using models and/or data which have been used successfully on previous problems.

Despite this, you are **strongly recommended** to subject them to the same checking as all other models or data, however tempted you may be to assume that they are "proven" - the new problem will differ to some degree at least from the earlier one, so you need to check that both the models and the data are correct for your new problem.

Digest of Input Data

Does the program understand your problem definition correctly?

A program which has been designed with the user in mind will display a "digest" of the input data, including any default values which have been applied. ***This digest is a vital part of your Record Keeping*** (see later) and you should check it very carefully:

- is the program actually solving the same problem that you intended to define?
- has the program interpreted the input values as you intended/expected?

A particular problem arises, of course, in the case of an interactive session, where the problem definition may be altered many times before satisfactory results are obtained (see Record Keeping, below).

Solving the Equations

Most process engineering calculations involve the iterative solution of a large and complex set of differential and/or algebraic equations.

You obviously need to know, so far as is feasible, just how successfully these equations have been solved.

In general:

- always be suspicious and check everything very carefully
- you must always satisfy yourself that the results presented are fit for your purpose. In cases of doubt, seek help.

Has the calculation converged?

Take care to establish precisely what the program regards as “converged” (see Appendix A3)

- what is the physical or other significance of the convergence "measure"?
- make sure that the convergence criteria being used by the program are very “tight”, especially with "nested" calculations (see Appendix A3)
- carry out some sensitivity analyses (see Appendix A4): do the results vary with either the initial guess or the convergence specification? If so, tighten the convergence criterion and, if such variations persist, seek help.
- be especially wary in cases involving trace components (the traces may still be far from converged, even when the major components have done so, and such traces may be important for environmental or safety studies, fouling, etc) or highly-nonideal mixtures (which will often give asymptotic behaviour or other convergence problems, see below)

Error & Warning Messages

Read the error and warning messages carefully and make sure that you understand what they mean and how they might affect the validity of your results. Do not simply ignore any whose meaning is not instantly obvious - there is a problem somewhere and you need to find it.

Convergence Problems

Sometimes it will be obvious that there is a problem but sometimes it will not.

- If in any doubt whatsoever, prepare a plot of the nominal error versus the key variables - ***asymptotic behaviour usually means trouble!*** (see Appendix A3)
- If the calculation seems to be making no real progress, or has converged partly and then ceased to make further progress, check your input data very carefully:

    - is the problem that you have actually defined (which may not be the one you intended to define!) capable of solution?
    - is the specification in some way physically unrealisable? This can be a particular problem when attempting to impose a combination of design constraints.

(... continued)

- In cases of difficulty, you may be able to assist convergence by using simpler models to get an approximate answer, thus providing improved initial guesses for the more detailed calculations. You can make such simplifications in a number of ways:

  - use simplified thermophysical properties models
  - use a reduced component list
  - use fewer/simpler constraints
  - (in the case of a flowsheet) start with only a few unit operations

  It is, of course, vital to take care that you do not unwittingly use the results of these simplified calculations for making engineering decisions!

- If there is still a problem, can you force the program to select a different convergence variable (eg. a different "tear stream" in a flowsheet simulator)?
- Spreadsheet programs may give special problems, as discussed earlier

All of the above, of course, assume that the program output and/or documentation provides sufficient information on such matters for these checks to be carried out. If the information is deficient (which is frequently the case - most program suppliers tend to assume that their products work faultlessly!), then you should ask the suppliers to supply further information (if necessary, under a confidentiality agreement).

Checking the Results

It is vital to check the adequacy of results of computer runs, particularly where safety or environmental issues are involved.

- You must assess the correctness of the results and their fitness for your purpose. Compare the results, including sensitivity analyses and estimates of consequences, with your defined objectives (see Define Your Problem, above).

  Note, in particular, that the number of significant figures displayed for a value (i.e. its nominal precision) is not at all the same thing as its accuracy (typically, only the first 2-3 figures can be relied upon, often only 1-2).

- Does it all make sense?

  - are the results credible and self-consistent?
  - check overall and individual species mass balances and overall energy balance
  - do all temperatures, pressures and compositions lie in the expected bands and within the range of validity of the Thermophysical Properties data?
  - are there any “surprises”? If so, can they be explained?
  - do the flowsheet conditions imply any unusual behaviour within a unit operation (for example, temperature cross-overs in heat exchangers)?

  A more detailed review of the issues which must be considered is given in Appendix A3.

- **Sensitivity Analysis** should be used to test the dependency of the results on the data and the design conditions, see Appendix A4.

Keeping Records

For a number of legal and other reasons (such as ISO Standards 9000 & 14001), you must maintain a formal audit trail of the development of your design and the judgements and decisions which underpin it. Since computer based calculations now form an integral part of the design process, you must keep proper records of the calculations which form the basis of design decisions. Only in this way can you maintain such a formal audit trail.

The following are some suggestions for the information which needs to be kept. Full records of these items should be maintained for cross-checking, error identification and auditing. Usually, a company or project management team will develop a comprehensive and formal system for these records. The records themselves may be paper or electronic as appropriate and the records system should provide adequate back-up in case of accidental deletion.

Just filing computer print-out is not acceptable and does not adequately discharge your responsibilities.

Note especially, the need to keep proper records of errors or failures. Sometimes trivial-seeming errors can indicate serious problems but the cause may only become apparent through collating the occasional instances when they occur.

Your records should include **at least** the following:

- a clear statement of the problem to be solved, in engineering terms
- (where appropriate - for example, in the case of a flowsheet simulation) a clear statement of the modelling approach and any implied assumptions and limitations
- a clear reference to the version of the program being used and where its documentation is filed.

  For an interactive system, this may present special problems, as much of this documentation may take the form of “on-line help”. Since on-line help will change with program versions and releases, the audit trail is broken unless adequate written documentation is also filed. This may take the form of a printed listing of the help screens (which the supplier might be asked to provide) or a record of the interactive session which took place.

- the actual input data and a digest (produced by the program) of the program’s interpretation of it, including, especially, any defaults and measurement unit conversions.

  Note that this digest must correspond to the final results, as used for decision-making purposes. This may be a particular problem with an interactive session, when the input data may be modified many times in order to develop a satisfactory design. Unless the program has a capability to produce such a digest on-demand, it may be necessary to rerun the final conditions in order to obtain it. ***If the input and output are not properly consistent, then the audit trail is broken.***

- where a spreadsheet is being used, a copy of the listing of the cell contents of the entire spreadsheet
- the complete results, including error and warning messages, etc.
- the checks carried out
- the interpretation of the results, in design terms
- details of any circumstances which have led to unexplained errors or failures during normal usage.

Seeking Help

If in any doubt whatsoever, do not hesitate to seek help. Your more experienced colleagues may have some helpful suggestions and you should not hesitate to involve your internal computer support services or even the software suppliers themselves:

- they are the experts in the use of the packages
- they might have seen your problems before and already have a suitable “workaround”.

Appendix A1

Errors and Their Potential Consequences

All information is subject to uncertainty/error. A key question which faces any engineer is

"just how good is good enough and what are the potential consequences if it turns out to be wrong?".

Unfortunately, there are no simple universal rules to answer this question and each case must be considered individually, on its merits. The following are some examples of the kinds of errors which often arise and which you must guard against.

In the end, of course, you will have to "go with what you have" - it may simply not be feasible to get anything better. In this case, however, a thorough sensitivity analysis (see Appendix A4) and a "pre-flight drill" (such as that outlined in Appendix A2) will tell you where the problems are likely to be and what to watch out for - the less you know initially, the more important this procedure becomes.

Some Common Sources of Errors

As outlined in the various sections of these Guidelines, errors can arise from many sources, such as:

- inappropriate choice of software/model: the model does not apply to your problem
- simple errors in the input data: you must check it rigorously for mistakes
- problems with units of measurement: does your problem definition correspond exactly with the program's assumptions and have any conversions been carried out correctly?
- convergence problems
- ignoring error and warning messages
- applying models and/or data outside their range of validity:
    thermophysical property correlations & data
    knowledge bases
    neural network training data
- hidden spreadsheet formulae
- even minor trace components may have a disproportionate effect (eg. on fouling or on thermophysical properties - see Appendix A2)
- failure to consider transient conditions (for example, in flexible operations, in response to market dynamics)

All of these may cause problems and may lead you to take inappropriate design decisions and so you must be careful to exercise proper professional care to guard against them.

Fitness for Purpose

What matters is the quality of the final engineering decision, not the accuracy of the information which leads you to take it. If you can confidently make the right decision, then that information is "good enough", no matter what its absolute accuracy (i.e. it is fit for your purpose).

It is critical that you have a clear, agreed definition of your purpose, i.e. the decisions which you need to take. Otherwise, you have no means of assessing what is "fit".

Some areas will be more critical than others: your primary weapon for assessing uncertainty is Sensitivity Analysis (see Appendix A4) and this technique should be used to explore and bound the areas of uncertainty and thereby to establish the basic fitness of your information for your purpose. This will allow you to identify critical areas which must be subjected to more thorough analysis or where more time and money are needed, either to obtain more accurate information or to add an appropriate design margin.

Potential Consequences

There are several potential adverse outcomes if the quality of your information leads you to make an inappropriate decision. For example, in increasing order of severity:

- **A performance or capacity problem:** a key piece of equipment may be under-sized and so the plant capacity or product quality may not be completely achievable. Such problems can often be overcome, usually at the expense of extra energy, utilities or raw materials. (And, of course, the converse scenario: gross overdesign may have serious consequences for project economics!)
- **A non-viable process:** a far more serious situation can arise if the process configuration turns out to be wrong and the process simply doesn’t work. Typically, such problems can only be overcome by extensive redesign, involving delays, additional capital expenditure and possibly extensive reconstruction, depending on when the problem is discovered.
- **A dangerous or defective process:** which creates potential safety or environmental problems.

The same inadequacies in the same information may give rise to different "levels" of consequence.

The following examples are based on the often critical area of thermophysical properties (see Appendix A2) but the same general implications and logic (especially the need to differentiate between capacity and viability or safety/environmental problems) will apply to all potential areas of uncertainty.

A distillation system:

- Errors in relative volatility of a close-boiling mixture may have the effect of the column “inverting” (i.e. the products may come out of the “wrong” end of the column), with dramatic consequences for the viability of the process. Wide-boiling mixtures present fewer problems, but beware the effect of traces (see below). Note the potential impact on safety/environmental issues (for example, under relief conditions) and on the choice of materials of construction (for example, if a potentially corrosive mixture arises where it is not expected).
- Errors in heat capacity and latent heats will typically affect the sizes of the reboiler and condenser and thus capacity and/or utilities consumption.
- Errors in transport properties may seriously affect tray efficiencies, flooding, fouling, etc., and significantly affect capacity.
- Trace components (for example, arising from errors in reaction kinetics, fouling, etc.) can have a significant impact on all properties (see Appendix A2) and require careful consideration. For example, they may cause an unexpected azeotrope (or destroy an expected one), give rise to a 2-phase liquid region or have a disproportionate effect on critical points and properties (which might, for example, lead to excessive foaming or other problems).
- Failure to consider extreme or transient operating conditions (for example, flexible operations, in response to market opportunities) may give rise to operational, capacity or control problems, such as flooding or dumping.

(... continued)

An energy integration scheme:

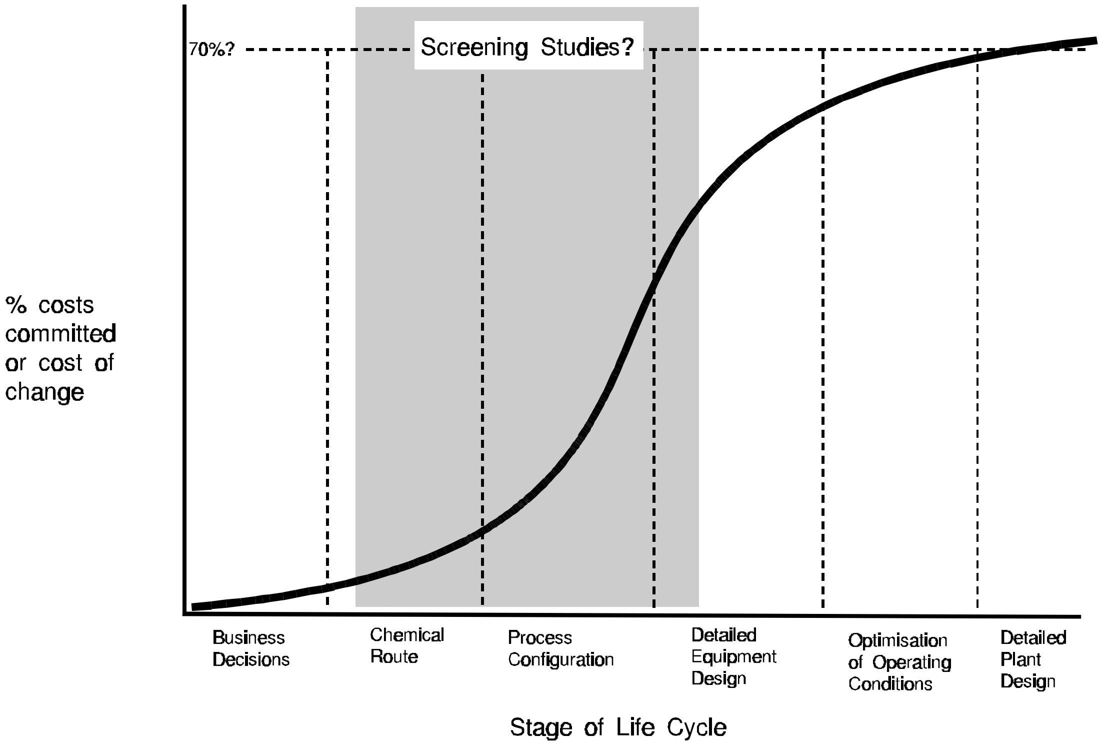
- Errors in heat capacity or latent heat may have a dramatic impact on the location of the “pinch point” and so may make the network non-viable. Less serious cases will lead to additional consumption of utilities.
- In the case of multi-phase mixtures, errors in equilibrium data can have serious effects on both temperature levels and latent heats, leading to changes in the “pinch point”.
- Errors in transport properties will affect pressure drops and pumping costs (which are essentially performance/capacity issues) but may also affect heat transfer coefficients and thus, potentially, the “pinch point”.
- The multiple operating regimes required for flexible operation may correspond to several different "pinch points". In selecting the optimal configuration, its inherent operability in **all** of the required operating regimes (and the transitions between them) must be established.

Despite all these pitfalls, process plants do usually work! The object of the above is not to induce a panic attack but to make it clear that careful thought is required to identify areas where uncertainties might have a dramatic effect on your proposed design (and to point out that it is not always the same areas which give rise to the more serious problems). You are then encouraged to use Sensitivity Analysis to try to define the limits of that uncertainty and to attempt to quantify its effects, so that you can be confident that your information really is “good enough” and that appropriate engineering decisions will be made or, alternatively, that you know what to watch out for at a later stage.

Screening Studies

It is always tempting to assume that screening studies require only approximate information. This may, however, be mistaken - you must **always** be able to justify your engineering decisions and recommendations, even in "screening mode". It is an essential part of the audit trail.

We are all painfully familiar with the increasing cost of change, which grows inexorably as design decisions are made and costs are committed (see diagram).



(It should be noted that this does **not** mean that later stages are unimportant - they may not be able to "turn a sow's ear into a silk purse" but it is quite simple to do the reverse by inappropriate or careless detailed design.)

Within process development and design, screening studies are usually designed to explore a number of alternative processes at the **structural** level, in order to select the most appropriate chemical route and process configuration and, perhaps, to guide research activities. The major design effort can then be focussed on optimising the equipment sizes and operating conditions for this optimal configuration and effort is not wasted in optimising processes which are already suboptimal (and, of course, operating conditions will be re-optimised during commissioning trials anyway).

All the major operating regimes and the principal transitions between them will be explored and the key issues will be not just steady-state operating efficiency but will include a range of other issues, such as flexibility, operability, control, safety, environmental impact, etc - it is now becoming more fully appreciated that a concurrent approach is required, even at the very earliest stages.

Many of the critical decisions will be taken and the inherent operating characteristics (and hence potential profitability) will be largely determined - our ability to influence these characteristics declines sharply beyond this point.

An appropriate **balance** must therefore be struck*:*

- it is vital to ensure **sufficient** accuracy, even at the earliest stages, to be confident that the key "structural" decisions are correctly made - if these are wrong, the eventual consequences may be very serious and they may be very difficult and expensive to change.
- demanding **excessive** accuracy can, of course, waste a lot of time and resources unnecessarily (for example in literature searches or laboratory or plant measurements).

Your key weapon in striking this balance is ***sensitivity analysis***:

- identify the critical inter-relationships and explore them thoroughly
- leave the less sensitive issues for later investigation

The critical decisions must be based upon good quality information, whereas the others may not require this degree of rigour at the screening stage.

Appendix A2

Thermophysical Properties, Models and Databanks

Models used for designing or operating a process plant are ultimately based on thermophysical property models & data (TPMD). The quality of such models and of the decisions which you make based upon their use is thus critically dependent on the adequacy of this TPMD. So far as is practically feasible, it is your professional and legal responsibility to satisfy yourself of its adequacy, to understand its weaknesses and to apply it sensibly, with good engineering judgement.

It is important to appreciate that TPMD (and, indeed any other basic data, such as reaction rates, fouling factors or plate efficiencies) undergo a significant number of transformations before they are finally used to provide the information upon which you base your engineering decision. Errors or inadequacies can be (and frequently are) introduced at any or several of these stages and, of course, some of the required information may be missing.

TPMD gives rise to a wide variety of special problems and uncertainties (see the examples in other Appendices) and probably causes more problems than all other areas put together. TPMD is a very specialised area and you should not hesitate to seek expert help from your colleagues and support teams or to involve the suppliers of your CAPE or TPMD systems.

To make matters worse, many TPMD systems are also “closed” and it may not be feasible to follow all the following Guidelines. Comprehensive information is seldom available regarding the underlying data and the models which are used to represent it. Moreover, the ability to modify parameters, for example to enable sensitivity analysis, is often not provided - the results must be taken on trust. Nonetheless, you should press your suppliers for access to the information and to the “controls” needed to carry out the appropriate sensitivity analyses or vary the convergence criteria. (You will almost certainly have to be very determined and you may [quite reasonably] have to enter some form of confidentiality agreement.)

These notes attempt to equip you with an awareness of where problems might be lurking, how best to flush them out and how to assess their importance. A five-step process is recommended:

- define your problem carefully
- choose an appropriate model
- assemble the available data
- fill in the gaps
- assess its adequacy for your needs

You may, in the end, have to “go with what you have” - it may simply not be feasible to get anything better. In this case, however, a thorough “pre-flight drill” (see below) will tell you where the problems are likely to be and what to watch out for - **the less you know, the more important this procedure becomes.**

(... continued)

Define your Problem

- Identify as best you can what materials (chemical species, psuedo-components, ...) are in your system and over what ranges of composition, temperature and pressure properties will be required.

- Even minor traces of some materials can have a marked effect on the thermophysical behaviour of the system (for example, enhanced or depressed volatility, dramatic changes in surface tension, etc.) and thus on the accuracy of your data and on the subsequent behaviour of your plant, so you really must find out what your mixtures contain - those “lights”, “heavies” and similarly lumped components could be important (and you’ll need to identify them for environmental studies anyway).

- Some important issues:

    - do the expected conditions lie well away from the critical point of all of the components? Take special care if any of the critical conditions lie within or near your expected range.
    - other effects, such as ionic interactions, association/dissociation, azeotropes, 2-phase liquids, reactions etc., can also occur and will lead to unforeseen complications and behaviour, though, in recent years, more sophisticated packages have become available to help predict and deal with them.

Choose an Appropriate Model

When used within a CAPE tool, TPMD are almost invariably represented by a model (i.e. a set of equations) of some kind, to which the TPMD will have been fitted. (In principle, a look-up table could be used but this is now rare.) Many CAPE tools will also be equipped with databanks of properties data - essentially correlation constants from the TPMD fitting calculations. The models can themselves be of many kinds and levels of sophistication and, even with the best of data, an inappropriate choice of model will cause severe errors.

The “pre-flight drill” below should expose most of the worst problems but their underlying cause (i.e. the adequacy of the data itself versus the adequacy of the model) may not be immediately apparent, so it is worth reviewing the choice of models directly, especially if extrapolation of any kind (e.g., in temperature, pressure or mixture/composition) is involved (which will almost invariably be the case).

This area is a major subject in its own right but some basic guidelines can be given:

- Many models assume that the vapour phase is a perfect gas: this is unlikely to be adequate at anything more than very moderate pressures, especially if conditions are anywhere near any of the critical points (and allowing for the potential impact of trace components)

- Equations of state are not a panacea: they work reasonably well for gases and the vapour phase but markedly less well for liquid phases (i.e. where the density is relatively high and where mixing effects become predominant, especially around the critical point). They also work best for homologous series of simple components (e.g., straight-chain paraffins) and considerably less well where strongly asymmetric components or components of widely different molecular structure (e.g., polar and non-polar compounds) are involved.

- Great care must be taken to ensure proper consistency between the models of each of the phases and, especially, density corrections based on mixing rules. Such a problem might be exposed by the “almost pure” tests in the pre-flight drill (see below), which might either fail completely, might predict a “false azeotrope” or might fail to predict an azeotrope which is known to exist. (See also remarks under "Fill in the Gaps", below.)

- Many TPMD models are polynomial: a polynomial will almost invariably extrapolate very badly! This is especially a problem with the transport properties, but even some of the more sophisticated equations of state contain a polynomial at their core.

- The TPMD model equations must, of course, be solved and this (typically iterative) calculation is by no means simple, especially anywhere near the critical point or when there are trace components involved. These calculations lie at the very heart of your equipment/flowsheet model and even the slightest lack of accuracy or reliability can cause serious problems with overall convergence and the validity of the results (see Appendix A3).

Assemble and Check the Available Data

- Draw together whatever data you can find and compare it with your requirements, as defined above. It is virtually certain that there will be significant areas where the coverage is inadequate.

- Ask yourself some questions:

  - where did the data originally come from? They may be measured (if you are lucky), estimated or gathered from the literature.
  - over what range (of temperature, pressure and, especially, composition) are they valid?
  - what is the documented accuracy of the data over those ranges?
  - how well does the fitted model represent the data?
  - what are the demonstrated extrapolation properties?
  - has any form of QA been applied?

- **Some remarks on TPMD Databanks**

  Many of the CAPE tools available today (especially the flowsheet simulators) are equipped with extensive physical properties databanks. Just because the TPMD comes from a recognised source, it does not mean that it is correct (see, for example: "Anomalous Results from Process Simulators", Sadeq et al, Chemical Engineering Education, Winter 1997)! Care must still be taken.

  - take care that the component names which you use to select your data from the databank **exactly** match those given in the documentation. The same component may appear several times (with very slightly different names or, worse still, numeric codes), corresponding to different possible applications (for example, one in an aqueous system and a separate one for organic mixtures). Selection errors are easily made and may not be easy to trace (the program will probably print out the "proper" name in all cases) and so great care must be exercised to avoid serious errors
  - do not assume that this data will be suitable for your particular problem just because it comes from a recognised source - subject it to the questions above, just the same

Involve the suppliers (of the CAPE tool and/or the TPMD) very early in this process, as soon as it becomes clear that you haven’t got all the data you require. Their advice and assistance can be invaluable.

(... continued)

Fill in the Gaps

It is very unlikely that there will be measured data for your particular range of mixtures under your particular range of conditions of temperature, pressure and composition. There are various ways of finding the missing information: some are more accurate but slower and more costly than others and you may need to carry out a number of sensitivity analyses (perhaps by several repetitions of the pre-flight drill, below, with different estimates of the missing information) to ascertain which of the missing data must be known accurately and which can be approximate without significantly affecting your engineering decisions. You should, however, never assume that trace components do not matter - they often have disproportionate effects on system behaviour and you must also be certain that your design properly "manages" them, for example, for environmental studies or to guard against build-up in recycles.

A variety of methods may be used to assemble missing data. ***Note that this is a highly specialist area and, in any but the simplest cases, you should seek expert assistance.***

- **Extrapolation: Temperature and Pressure**

  You will probably need to extrapolate the available information to conditions which may be far removed from the conditions under which the measurements were made. Extrapolation is a major source of problems, especially where the ubiquitous cubic equation is involved (or, indeed, any polynomial).

  One or two measurements are invaluable to check on the extrapolation properties of your data. It may be preferable to extrapolate the original data (e.g., by eye on a graph) and refit the equation, rather than using the original equation outside its fitted range.

- **Extrapolation: Mixtures**

  The additional mixture information you require will either have to be measured (potentially a lengthy and expensive process) or will have to be approximated using available data measured for pure components (and, maybe, for other mixtures) and then assembled to represent your mixture by using “mixing rules”. At best, this is an inexact science; at worst it is little better than alchemy and is very commonly the cause of all sorts of problems for anything other than the simplest of homologous series.

  A very common problem, which can cause severe distortions at "almost-pure" conditions but which is often not recognised, concerns the use of combined mixing data from different sources. Typically, a mixing model (ie. "mixing rules") is used to represent the deviation of the mixture's actual behaviour from the hypothetical behaviour of an ideal mixture of the same composition. The extent of this deviation thus depends on the model and data used to predict this "ideal" behaviour and so the coefficients of the mixing model will also depend on the pure component model and data used. Naturally, if this mixing model and data are then used in combination with a different pure component model or data, there will be an error, since the deviation is being "built upon a different base point". Often this escapes detection and may not be important but consequences can potentially be serious. It is important that you check carefully for such inconsistencies in both models and data when combining data from different sources.

- **Measured Plant Data**

  In principle, measured plant data are very valuable. They have the very real virtue that they apply to your conditions and your mixture. However, there are also problems - measured plant data often implicitly "lump together" a number of different effects, such as fouling, plate efficiencies, instrument inaccuracies/drift, non-steady states, etc. Measured plant data are very useful but must be treated with extreme caution - if the above factors can be allowed for, they are especially valuable for checking purposes - see below.

- **Estimation of Missing Data**

  Sometimes, there will be no basis of any kind for extrapolating information and so it will be necessary to estimate the data required “from first principles”. ***TPMD estimation is a highly specialist area and, in any but the simplest cases, you should seek expert assistance.***

- **Measurements**

  Depending on the results of your sensitivity analysis, you may decide that you need some measurements to be made - even a few not very accurate points can be very useful in establishing your level of confidence in the data, for example for checking extrapolation properties.

Assess the Adequacy for Your Needs: *“Pre-Flight Drill”*

Having assembled your data and filled in the holes, the time arrives to see if it all makes sense and if it is capable of providing the necessary support to you in making your engineering decisions. ***The basic principle is to start simple and then to gradually add necessary complexity to approximate the real situation.***

- First of all, you might use an abbreviated component list but you must also select some truly representative mixtures and operating conditions. Some should be fairly simple but some should be representative of the more complex aspects of the process and its behaviour - you must “look in all the corners”. For a variety of reasons given earlier, it is important not to ignore trace components.

- Begin by making some simple property calculations (for example, vapour pressures, specific and latent heats) and plotting them on a graph (a graph is much more immediately revealing than a table of numbers). If this can be done under conditions where at least some idea is available of the true property values, so much the better! Examine the results:

  - do they look reasonable - do they behave in the manner which you would expect?
  - how do the calculations behave at/near the extremes (e.g. an almost pure component)?
  - how well do they extrapolate?
  - are there any unexpected heats-of-mixing effects?

- Repeat these experiments with more complex properties, such as bubble and dew points, flash envelopes, etc. Check with whatever measured data are available and consult expert specialists wherever you are unsure and/or where sensitivity analysis indicates that accuracy is important.

(... continued)

Project Data Book

Once the above procedure has been completed and you are satisfied that you have chosen the most appropriate model for your purposes and assembled the best data which is available, it will be appropriate to prepare a Project Data Book (or its electronic equivalent):

- the above process then needs to be done once only and can be done properly with appropriate expert assistance

- if all design team members use the same model and data for all purposes, consistency is guaranteed

- it will form an important part of your audit trail

Appendix A3

Checking the Results

The following are some examples of checks which you should apply to your results. Such checking requires significant practical experience and you must be prepared to seek appropriate help from your more experienced colleagues whenever any doubts or uncertainties remain.

Note that these are suggestions and examples and should be used in the spirit of "necessary but not necessarily sufficient".

In assessing the validity of your results, you must check not only the results themselves but also the input data and the calculation which produced them.

It is important to appreciate that unexpected behaviour of your model may be due to two quite separate causes:

- the real behaviour of the process plant, as predicted by a correct model
- spurious effects which simply reflect errors in the model itself or in the data

In either case, this behaviour must be fully investigated and either corrected or explained, so that your engineering decisions can be properly justified for audit purposes.

Checks on the Input Data

Is your problem correctly specified?

- check the print-back of the input data for correctness (including units of measure, orders of magnitude and any units of measurement conversions)
- check where the software has supplied default values and what values were supplied: are these really suitable for **your** problem?

Checks on the Calculated Results

Does it all make engineering sense?

General Review

- are there any warning or error messages? (Make sure that any diagnostic "switches" are ON!)
- are the results credible and self-consistent? For example, are there any negative or otherwise unrealistic flowrates?
- have conflicting/competing design constraints created any problems? For example, are any of the conditions set to unexpected boundaries?
- check overall and individual species mass balances, **including trace components** (use proportional/percentage errors, rather than absolute values, so that large errors in small flows are not masked by the relatively small errors in larger flows)
- check atomic mass balances across reactors

- check the energy balance
- do all temperatures, pressures and compositions lie in the expected bands and within the range of validity of the data? Are all flows of the expected phase? Are there any “surprises”? If so, can they be explained? **Carry out any appropriate sensitivity analyses to establish critical areas of uncertainty, where better information is required to protect the integrity of your design**
- in the case of flowsheet simulations, these checks should be applied both to individual units and to the flowsheet as a whole

Equipment Items

- are equipment and piping sizes reasonable?
- are the predicted flow regimes in equipment/pipes within the expected ranges?
- are the heat transfer coefficients in exchangers reasonable?
- are there any implied crossovers within heat exchangers?
- do the light-end components appear at the top of a distillation column and the heavies at the bottom?

Warnings and Errors

- do not ignore warning and error messages: even if their meaning is not instantly obvious, there is a problem somewhere and it is your professional responsibility to find it and assess its likely impact on your engineering decisions
- has the printout or screen display truncated any of the results, labels, messages, ...?

Multiple Solutions

- is this solution the only solution and, if not, is it the correct solution?

  This can often be tested (but never fully confirmed) by repeating the calculations from (significantly) different initial guesses or with a different choice of convergence variable (see below).

Some “Classics”

- errors in units of dimension often occur (either on input or output) and a particularly frequent one, with potentially serious consequences, is mislabelling and/or misinterpretation of compositions - is that weight%, mole% or even volume% and on a wet or dry basis?
- thermophysical properties correlations and/or data are often used outside their range of validity. This may be unavoidable but when it occurs, careful use of sensitivity analysis becomes CRITICAL, to expose areas of risk.

Checks on the Calculations

Has it “converged” and what does that mean?

Convergence Variables and Measures

The solution of a chemical engineering model will almost always involve solving a set of simultaneous non-linear equations by an iterative (trial-and-error) method. The essence of this technique is to repeatedly guess values for one or more variables, in order to force some measure of the error to zero (or very nearly).

- a **convergence variable** (ie. what you guess) might typically be a physical quantity with an obvious significance, such as a temperature, pressure, flowrate, composition, etc. (In cases where there is no obvious physical significance, take great care to ensure that you understand what it **does** mean!) In the case of flowsheet simulators, the entire set of variables representing a whole stream (often referred to as a "tear stream") may be guessed.
- a **convergence measure** (ie. the measure of error) might typically also be a physical quantity, such as the error in mass or energy balance or the summation of component compositions or might be the difference between the estimated value of the convergence variable(s) and the new value(s) calculated from the model equations. (Again, take great care in cases where there is no obvious physical significance.)

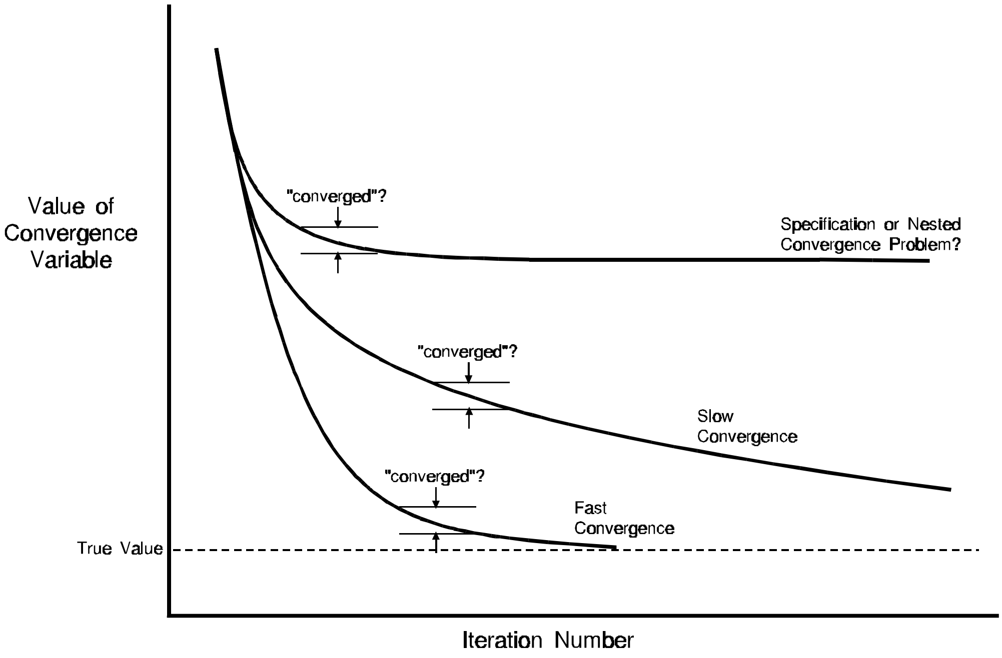
  Such a measure is only indirectly related to the “true” error (i.e. the discrepancy between the current estimate of the convergence variable and its “true” value, which, of course, we do not know) and under some circumstances that relationship can be very weak indeed. There are plenty of ways in which things can go wrong, for example:

  - large errors in small flowrates (ie. in the ubiquitous traces) can be masked by small errors in larger flows, thus hiding the build-up of traces in recycles, for example. ***(For this reason, it is good practice to make your checks in proportional/percentage, rather than absolute, terms).***
  - a mass balance may be extremely sensitive to a small variation in a key temperature or pressure (eg. phase separation of a narrow boiling mixture) and this may lead to non-convergent or even oscillatory behaviour.
  - it is easy to specify inconsistent or even conflicting design requirements and these may lead to non-convergence or to oscillatory behaviour.

Some care and experience is therefore required in selecting both convergence variables and measures in order to improve the convergence characteristics of the problem. Unfortunately, in many cases, the program may not allow you any realistic degree of control over the choice of such matters but, ***where it does, use it!***

Convergence Paths and Success Criteria

Convergence does not always proceed smoothly and may exhibit several sorts of behaviour, as illustrated in the figure below:



- **Fast Convergence:** a good well-behaved model - no problems! (But follow the General Advice, below.)
- **Slow Convergence:** progress is being made, so the model is apparently well-behaved but is badly scaled and/or ill-conditioned, resulting in slow progress. As you can see on the diagram, the "converged" solution is very far removed from the true value and a very large number of iterations will be required to force proper convergence.

  As an example, a quoted temperature error of “less than 0.25 K” sounds good but, if it is actually calculated as the difference between two successive estimates, one 20 K and the other 19.8 K different from the true answer, ...this is hardly “converged”! Trace components also often cause convergence problems (see below).

  In the case of slow convergence, it is essential to set a very tight convergence criterion or your results may be meaningless. A simple acceleration method, such as Wegstein, or a more powerful multi-dimensional technique, such as a variant of the Newton method, will be useful to improve the rate of progress.

- **Problem/No Convergence:** convergence appears to stop making progress and the calculation "wanders around" or even oscillates. Oscillation may be cured by "damping" but this type of behaviour often indicates that there may be no real solution at all (for example, there may be impossible or conflicting design constraints), that there are major interactions and/or non-linearities or that there is a lot of "noise" coming from inadequate convergence of calculations at lower levels (see "Nested Calculations" in Appendix A5). The behaviour of any non-standard models should also be examined very carefully.

Some General Advice

- ***Start out with the simplest available method,*** such as resubstitution: it is far easier to see what is going on than if the program is making decisions of its own (such as differential acceleration of the different variables). Only use acceleration methods if they are really necessary and when you are confident that your model is basically well-behaved (see below).
- Usually, mass and energy balance errors will detect convergence problems but it is not guaranteed, and so ***it is good practice to do some sensitivity analysis*** - repeat the calculation with a different convergence criterion (say, 10-times tighter) and/or a different starting point and examine the effect this has on the results: if the results change, then there is a problem.
- ***ALWAYS specify a tight convergence criterion.*** As illustrated in the diagram, in the case of slow convergence your results may otherwise be meaningless and in the case of fast convergence it will take only a very few more iterations and so is effectively "free". Suitable values depend on the problem and can be found by appropriate sensitivity analysis but, as a starting point, a target convergence of the order of 0.01% should be set for flows (including traces) and, say, 0.01 K for temperatures. "Slack" values, such as 1% or 0.5 K should only be used with extreme care and subjected to rigorous checking.

Checking for Convergence & Fixing the Problems

- check the results, as described above, and ensure that the imbalances are consistent with the convergence criterion which you have set (eg. an error of 5% in the flow of a trace is not consistent with a convergence criterion of 0.01%).
- test the sensitivity of your results to the convergence criterion and the starting point (see above)

If this all seems to make good engineering sense, then you have some grounds for optimism! If, however, you are in **any doubt whatsoever**, then you must look more closely:

- has **every** component got an "exit route" from the flowsheet, or are they building up, either within individual units or in recycles? Growth of trace inerts within recycles is a "classic", just as it is on a real plant!
- review very carefully the behaviour of any non-standard models (see Appendix A5)
- examine the behaviour of the convergence: using a simple method such as resubstitution (see above), print out some key items of information (eg. the convergence measure and some of the critical flows, including important traces, and design parameters) at each iteration, plot them against the iteration number and compare with the convergence diagram above:

    - if it seems to be following the "fast track" - ie. it is taking significant steps in a broadly consistent direction (no less than a few percent, unless the convergence measure is very close to zero), then try

        - an improved starting point/initial guess
        - more iterations and/or an accelerator

    - if it is following the "slow track" - ie. it is taking small steps but in a broadly consistent direction, then

        - tighten the convergence criterion so that any "converged" results have at least *some* validity
        - try an accelerator to enable larger steps to be taken
        - try significantly different starting points
        - try to force a different choice of convergence variables and/or measures

    - if it is following the "problem track" - ie. if it seems confused and is either going nowhere, oscillating or stepping in apparently random directions, then:

        - check the design specifications, thermophysical properties, etc, again - does a solution actually exist?
        - look carefully at individual convergence variables: the overall convergence measure may appear to be "stuck" but individual variables may still be moving in broadly consistent directions (for example, if it is faced with a severely non-linear or interacting problem). Treat this as an extreme case of slow convergence and try a multi-dimensional acceleration method, such as Newton. You may even find it helpful to allow the global error to **rise** for a couple of iterations, while it "changes direction"
        - try a radically different starting point and/or try to force a different choice of convergence variables
        - try an accelerator: try a simple one first, such as Wegstein (which should also be capable of applying damping, which may help with any tendency towards oscillation), and then more powerful methods, such as Newton
        - review the nesting structure and the convergence criteria being set at each level (see Appendix A5), especially for any non-standard models: you may need to tighten some of the inner loops to increase overall stability

Help!

Do not hesitate to seek advice and assistance - this is a difficult area until you've built up a good base of real experience.

Appendix A4

Uncertainty, Sensitivity and Design Margins

It is important to appreciate that almost everything is uncertain - it is only the degree of uncertainty which varies. Your key weapon in identifying and quantifying the potential impact of that uncertainty is Sensitivity Analysis. This should be used to explore and bound the areas of uncertainty and to identify critical areas (i.e. where the potential consequences are most serious - see Appendix A1) which must be subjected to a more thorough analysis or where more time and money are needed, either to obtain more accurate information or to add an appropriate design margin.

The scale of the potential interactions (i.e. the sensitivity of everything with respect to everything else) is vast, so you cannot expect to study everything - the level of detail required and the number of calculations to study all possible combinations make it infeasible. You need to adopt a selective approach to render the problem tractable.

In the end, it is you, the responsible engineer, who must exercise your experience and judgement: not all questions can be answered completely - there are just too many of them. Your responsibility is to try to identify and quantify the critical areas and to allocate your design margins accordingly.

What if ...?

A practical approach is to use your intuition and experience (and advice from others) to guide you into areas where problems might lie and then to use the “what if ....?” approach:

- ***What if*** the reactor generates a bit more heavies and the heavies are not so heavy as we thought: where do they go and what impact might that have on fouling or corrosion or on safety or environmental issues?

- ***What if*** two liquid phases form, or an azeotrope?

- ***What if*** my estimate of volatility or latent heat turns out to be 20-30% out? Or a factor of two? Or ten?

You may discover some very informative cause and effect relationships!

To save time and resources, you might do initial explorations “at a high level” (i.e. using simplified models) to expose the critical sensitivities and then go into greater detail to identify those specific parameters which will cause problems and thus need to be known with greater certainty.

Bounding the Problem

It is unlikely that you will have sufficient information to know the probability distribution of your uncertainty. You should, however, be able to guess potential maximum and minimum values, to go with your estimate of the most probable value (MPV).

- You should then assess the performance of your proposed design at the MPV and at both bounds (the effects are very rarely symmetrical), not forgetting such issues as transient behaviour, requirements for flexible operation and the need to assess impact at the global (i.e. process-wide) level, not just on local conditions - the effects may cancel (if you are lucky) or they may be accentuated (if you are not).

- Your bounds should reflect your true level of confidence: do not just take an arbitrary 10% step. If you really have little idea of the true value, then vary it by a large amount (perhaps by a factor of five or even ten) to see if it really matters.

- Remember that you must consider combinations of effects, not just single uncertainties: some may act as "triggers" for more serious problems.

- Explore worst case scenarios but do it intelligently: what is the likelihood of them all occurring at once? A combined worst case could lead you to a very expensive design, even though the likelihood of its occurrence and the potential consequences might be extremely low.

Design Margins

The allocation of design margins is not, of course, an issue which is unique to the use of CAPE tools. However, CAPE tools and sensitivity analysis are critical to decisions on the optimum allocation of the design margins (and, thence, the additional capital and/or operating costs) and so it is appropriate to make some remarks within these Guidelines.

- design margins might be added for a variety of reasons/purposes, such as:

    fouling
    corrosion
    "for future expansion"
    "for control" (i.e. to allow for unknown dynamics)
    to allow for critical uncertainties

- it is almost certain that there will be a company guideline on such matters and/or that a project-specific policy will be included within the design brief.

- policy guidelines on design margins will also reflect prevailing commercial circumstances: whether it is more important to spend the time to get it "just right" (for example, in a static market, when significant overdesign would result in a serious cost-penalty) or whether it is more appropriate simply to add substantial overdesign because of the need for speedy market entry, in the expectation that any over-capacity will rapidly be absorbed by the rising market.

- it is very unlikely that it will ever be optimal to add a margin for all of the above factors independently: the indiscriminate addition of arbitrary design margins to everything not only fails to provide any guarantee of performance but can result in substantial overdesign and potentially serious extra costs, thus damaging project economics. A proper definition of your purpose (see Appendix A1) will provide guidance on a balanced approach.

- in some cases, the normal procedure of rounding up to the next standard size is sufficient to cover for a low/moderate level of uncertainty and no further action need be taken. You must be confident, however, that this really is the case.

- in the same manner as the bounds of your sensitivity analysis, design margins must directly reflect your level of confidence and the potential consequences if you are wrong (see Appendix A1).

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 (ie. to "safety critical standards").

- 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.

(... continued)

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 licensed 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."*