Chapter 8 On Design Tools

8.1 Introduction

8.1.1 Chapter Overview

This chapter makes some comments on modelling in general and takes a quick look at a number of thermalhydraulic codes used by the Canadian nuclear industry.

8.1.2 Learning Outcomes

Objective 8.1	The student should be able to appraise which types of codes to use for a given thermalhydraulic problem.					
Condition	Open book examination.					
Standard	75%.					
Related concept(s)	Modelling approximations. Industrial computer codes.					
Classification	Knowledge	Comprehension	Application	Analysis	Synthesis	Evaluation
Weight	a	a				a

Objective 8.2	The student should be able to identify the possible sources of errors for a given thermalhydraulic model applied to a given problem and to appraise the situation to determine which of the sources of errors are the major ones..					
Condition	Open book examination or workshop investigation.					
Standard	75%.					
Related concept(s)	Modelling approximations. Industrial computer codes.					
Classification	Knowledge	Comprehension	Application	Analysis	Synthesis	Evaluation
Weight	a	a				a

8.1.3 Chapter layout

A short overview of sources of modelling errors is given as a reminder that models are just models, not reality.

> Models must always be be subjected to verification and validation to increase the confidence in their predictions.

A number of industrial strength codes are reviewed.

8.2 The Model's Tenuous Link to Reality

All process system endeavours, problems solutions, etc., can be conveniently classified by considering the fundamental relationships governing the phenomena (see chapter 2).

The fundamental relationships are:

1) Conservation laws: mass, energy, momentum;

2) Constitutive laws: state equations,

3) Empirical correlations.

This basic step of establishing mathematical statements to reflect reality is, in itself an approximation.

All component equations (fluid, pipes, heat exchangers, valves, pumps) are derivable from these fundamental relationships, even stress, water hammer, etc.

The state of the art is such that empirical relations are heavily relied on to compensate for the lack of understanding of the fundamental terms in the basic equations.

For example, stress tensors are invariably reduced or ignored, or replaced by friction factors.

Multiphase flow equations are invariably combined into mixture equations.

This is the second level of approximation.

Next, the solutions to the various approximate forms are usually not directly achievable.

This means discrete approximations (the third level of approximation) are made to continuous systems

and

unguaranteed numerical solution techniques (guaranteed only for linear systems) are used (the fourth level of approximation) to arrive at a solution, one which is thus, four-fold removed from reality.

Small wonder that our component modelling is lacking.

Not surprising, then, the more simplified component models used in systems analysis is even more lacking.

On that cheerful note, we look design tools.

8.3 Documentation, Verification and Validation

8.3.1 Documentation

The more mundane issue of full documentation is as important as it is neglected.

The code and the associated input data sets must be completely documented.

This includes:

a) derivation of equations, including assumptions;
b) description of coding;
c) description of input data, complete with sources, accuracy, and limitations;
d) description of correlations, complete with sources, accuracy, and limitations;
e) standard procedures for running the code, maintaining a standard data set, etc.;
f) description of verification and validation.

8.3.2 Verification

The issue of verification can be divided into:

a) programming checkout;
b) code-code comparison.

The basic thrust is to verify that the code is a faithful representation of the model.

The model may contain many approximations and even some errors, however, it must be established that that model is correctly coded.

8.3.3 Validation

The assessment of how well the model compares to reality is called validation.

It typically entails:

a) code-analytical solution comparison;
b) code-experiment comparison;
c) code-plant comparison.

Verification and validation has received considerable attention in the past and is discussed to some degree in the precursor to this course.

8.4 Design Tools

8.4.1 SOPHT

SOPHT models the plant hydraulics as a collection of modules for the system volumes, connected by links which model pressure drops (see figures 3.11 and 3.12).

The mass, energy and momentum equations are set up through the system in matrix form.

This set of equations is reduced to a smaller set of flow equations and, with the boundary conditions, are solved with the help of the Jacobian matrix.

The major components, such as, pumps, steam generators, reactor, turbine, "figure of 8" loops, pressure and inventory control, etc., are all modelled.

All of the details of the layout are supplied via input data, making circuit modifications straight forward.

The choice of boundary conditions and empirical correlation options are also supplied via input data.

The plant control model is essentially that of the plant. It is hard programmed in modular form, but parametric information is supplied by input data.

Since the code is capable of simulating steady states as well as transients with varying boundary conditions, the scope is wide. Some examples of typical cases may include:

1) 100% full power steady state;
2) Reactor trip;
3) Turbine trip;
4) Rapid cooldown of the steam generator;
5) Manoeuvring;

and 6) Loss of normal, interruptible power (Class IV).

We might look at these cases to investigate the transients seen by a piece of process equipment for design purposes or to answer safety related questions.

The 100% full power case is the usual starting point for many transients.

It is generated by supplying a rough estimate of the system parameters and a consistent set of boundary conditions.

Since one of the conditions is symmetry, the full representation of the hydraulic circuit can be simplified to the 1/4 cirucit representation of the hydraulic circuit shown in figure 3.11.

The main boundary conditions normally supplied are the reactor outlet header pressure, reactor power, primary system flow rate and steam drum pressure.

The Jacobian is used to update the trial solution until convergence is reached. Usually 10 iterations are sufficient to converge the flow solution to within an absolute discrepancy of $5x10^{-5}$ Kg/s (0.4 lb/hr).

Of course, the results give a detailed account of the pressure, temperature, density, enthalpy, quality and flow distributions. No information on the control system is needed for the steady state solution.

Information needed for the controllers during transients is supplied via additional input data.

The cost for such analyses is relatively cheap compared to the impact the results have upon the design.

Although the code has many attributes, it has a few limitations as well.

The reactor model used is the point kinetics approximation. For the CANDU type reactor this is inadequate for analysis involving non-uniform coolant voiding across the reactor face. For those cases, a 2 or 3-D reactor code must be used in conjunction with SOPHT in order to update the reactivity feedback due to the non-uniform voiding.

The turbine is modelled simply as a steam dump and the feedwater returning from the deaerator tank is assumed to be at constant temperature and pressure.

Another major limitation is the controller algorithms. Since they are hard programmed, altering the controllers from one plant to the next or from one design to another requires significantly more effort than say, altering the hydraulic circuitry.

More insidious limitations, by virtue of their nature are the many assumptions built into the many empirical formulae and models of the code. It is altogether too easy to make an erroneous judgment by not reviewing these assumptions and their relevance to your particular case study.

Obviously a code of this size and nature is not to be treated as a "black box".

In summary, SOPHT, used to simulate the heat transport system of nuclear plants, is viable for use as a design tool.

It is flexible, efficient, and for its comprehensiveness, cheap and easy to use.

It has being used in the design of the Darlington A GS, Pickering B GS, Bruce B GS., 950 MW design, and is used for support analysis on all CANDU stations although, in recent years, emphasis has moved to TUF (a two fluid version of SOPHT) and CATHENA [HAN95] (a two fluid version of FIREBIRD [LIN79]).

8.4.2 HYDNA

Historically, HYDNA [MER80] preceded SOPHT for HTS simulations.

HYDNA was used at AECL for design and safety purposes up to and including the standard 600's.

New designs use SOPHT or CATHENA for design and safety analysis.

The primary reasons for the switch away from HYDNA are twofold:

a) The code is not as flexible as required for design and analysis purposes.

b) The numerical procedure called for the separation of the momentum equation (for pressure distribution) from the mass and energy equations. This separation of equations leads to a restriction on the minimum time step allowed in the solution procedure. Now, as the degree of geometric detail is increased, the node size decreases requiring a smaller time step so that the properties don't change too quickly in the smaller node (Courant limit). But the minimum time step prevents sufficient nodalization to pick up the necessary detail in some cases (HT stability is a case in point). The code goes numerically unstable as the node size and time step are decreased.

However, HYDNA did serve as the work horse for many years and it gives valid results from most design and safety work.

It has compared well against experimental data for parallel channel stability [ELH80]. The basic equations and empirical correlations were employed in SOPHT and CATHENA but the above two limitations were removed.

8.4.3 NUCIRC

The computer program NUCIRC [CHE77] is a steady state thermalhydraulic analysis program designed to analyze the heat transport system for the complete range of operating conditions.

The program can select and optimize the feeder pipe sizes, evaluate critical power ratio, estimate the effects of single ended or double ended refuelling, and determine pressure, temperature and quality at any point in the feeders or fuel channel or heat transport system piping.

The program NUCIRC provides the following options:

1) For a given heat transport system geometry, the pressure, temperature and quality at any point in the heat transport system, feeders or fuel channels.
2) For a given flow, inlet temperature, channel power, outlet header pressure and fixed inlet and outlet feeder sizes and geometrical configuration, the program provides the header to header pressure drop.
3) For a given header to header pressure drop, inlet temperature, channel power, outlet header pressure, and fixed inlet and outlet feeder sizes and geometrical configuration, the program provides the channel flow.

4) For a given flow, header to header pressure drop, channel power, inlet temperature, outlet header pressure and fixed inlet and outlet geometrical configuration, the program sizes the feeders.
5) The provision to calculate CPR (critical power ratio) or CFR (critical flow ratio) in cases 2, 3 and 4, for 28 element or a 37 element fuel bundle has been provided.
6) For reactor at 100% power, assessment of the effect of cold water in-flows when the fuelling machine is connected to a channel, on the reactor fuel/fuel channel can also be done. The program can be used for single-ended, as well as double ended refuelling operations.
7) The temperature - pressure profiles for the fuel channels can be calculated.
8) The program has the capability to perform all the above mentioned analyses for heavy water or the light water as the primary coolant.

The following limitations apply:

1) The coolant conditions must be in the following range:

<u>Heavy Water</u>	
Temperature	(50 - 620)°F
Pressure	(1100 - 1760) psia
<u>Light Water</u>	
Temperature	(50 - 620)°F
Pressure	(700 - 1580) psia

2) The program can analyze a maximum of 25 fuel channels for ITYPE-4 option.

3) The program cannot analyze branches in the heat transport circuit I.e., it is unsuitable for Bruce Heat Transport circuit.

4) The program cannot model more than 1 (one) core pass at present and hence is unsuitable for cases such as operation with one heat transport pump tripped.

8.4.4 AESOP

AESOP [KAY79] contains the equations necessary to describe the design parameters and costs for a CANDU nuclear power station, cooled and moderated by heavy water.

The program can automatically optimize the values of up to 23 independent variables in order to minimize the Total Unit Energy Cost (TUEC) or to minimize the capital cost for a given maximum TUEC, subject to certain constraints.

The independent variables include reactor dimensions, steam cycle temperatures, heat transport temperatures and quality, and channel power or fuel rating.

Since all variables are changed simultaneously, second order iteration between the variables is accounted for.

With a given set of values for the chosen independent variables, the program calculates a detailed design of the plant, and then calculates the costs of the capital components, fuelling costs and operating and maintenance costs, to arrive at the TUEC.

A new set of values for the same set of independent variables is now chosen in an ordered way so as to reduce the TUEC (or capital cost), and the design and costing calculations are repeated to establish the new TUEC.

This process continues until no further reduction in cost can be achieved, that is the optimum has been found, or the computing time is exhausted, and the program prints out a very detailed description of the plant with the lowest TUEC or capital cost.

The values of any of the independent variables may now be perturbed in order to calculate the sensitivity of the design to these changes.

The calculation begins with the determination of the performance of the steam turbine cycle, which may be of the single or dual pressure type.

The turbine heat rate is multiplied by the demanded gross electrical power output to determine the thermal output of the reactor.

The gross power may be specified, or may be estimated from the demanded net power by using approximate values for station service load and heat losses.

These approximations are refined as the calculation proceeds.

Reactor physics calculations are based upon a one-group point model approach, but with bucklings determined for an inner flattened region and an outer region.

Axial flattening may also be included.

The mean discharge irradiations for the two regions are calculated by interpolation in the fuel tables, which contain the variation of nuclear properties with burnup rating and lattice pitch.

These tables may be set up externally using any lattice code, or may be set up at the start of an AESOP run using the built-in version of the code POWDERPUFFS-V.

Corrections are made later to the calculated discharge irradiations to allow for control flexibility and changes in parameters, such as moderator temperature and pressure tube thickness, from values assumed in setting up the fuel tables.

Options are available for using uranium or plutonium fuel, boosters or adjusters, and axial as well as radial reflectors. Also, either the maximum channel power or the fuel element power rating (proportional to the maximum bundle power) can be used as an independent variable.

Since most parameters affecting the reactor thermal power are either fixed data or independent variables whose values are fixed in a case, the only dependent variables affecting the power output are the number of fuel sites and maximum channel power. (If the fuel element power rating is optionally chosen to be an independent variable, then the maximum channel power is proportional to the reactor length).

Either number of sites or maximum channel power is chosen to be an independent variable, and the other is calculated to produce the demanded power.

If the reactor design is fixed, both number of sites and maximum channel power are known.

In this case the power output is fixed in a case, depending upon rating and form factors, so that the input demanded power is merely a first approximation to evaluate the turbine heat rate.

An iteration scheme is used to determine consistent values of heat rate and thermal and electrical output.

The coolant temperatures at reactor inlet and outlet are independent variables, as is the coolant outlet quality, if any.

If the coolant is sub-cooled at the outlet, the reactor outlet pressure must be specified. The enthalpies of the coolant at inlet and outlet are found from property polynomials as functions of temperature, and thus the coolant flow in the maximum powered channel is derived.

This enables the pressure drops to be evaluated for the fuel channel (horizontal or vertical), end fittings and feeders, so that, based on the pressure at reactor outlet, the header pressures may be determined.

Knowing the temperatures and flows on both the primary and secondary sides of the main heat exchanger, the surface area is calculated, along with the pressure drops in the heat exchanger.

The overall pressure loss in the primary heat transport system is now known, so that the primary pump power calculated, and the heat loss from the primary piping may be calculated.

These values will in general be different from those assumed at the start, so that the reactor power requirement will change to maintain the required electrical output.

The program iterates through all the preceding calculations until the powers, or reactor dimensions, are correct.

Having established the major plant features, it now remains to calculate the critical power ratio (CPR), peak fuel surface temperatures, coolant tube thickness, heavy water inventories, and corrections to the discharge irradiation.

Finally, the capital cost of the plant is calculated using the costing equations from CANCAP 1973, including escalation and interest charges, and this is converted into the unit energy cost for capital.

To this are added the calculated unit energy costs for fuel, operation and maintenance, to provide the Total Unit Energy Cost (TUEC).

If any of the constraints specified in the data have been violated in this calculated plant, a penalty may be added to the TUEC in order to bias the optimization procedure away from such a combination of independent variables.

There are two methods built into the program to search for the optimum combination of the independent variables.

a) Random Search
In this method changes made to the values of the independent variables are of random magnitude and direction. However, a steepest gradient search is performed in order to weight the random choice in what appears to be a favourable direction. This method is, by its nature, not very efficient,

b) Simplex
The Simplex search requires as its starting point a set of (n+1) cases, where n is the number of independent variables being optimized. These cases are provided by an initial Random Search, which continues until there are (N+1) unpenalized cases. The values of TUEC from these cases are ordered in decreasing magnitude and are the vertices of an n sided polygon vertex (1) having the highest value of TUEC and vertex (n+1) the lowest.

One of four searching methods is used at each iteration to determine a new set of values of independent variables to replace the highest vertex. These are

Reflection,
Expansion,
Contraction and
Collapse.

With these new values, the design parameters and new TUEC (with penalty if necessary) are calculated. The new set of vertices is reordered as before, and iterations continue until the optimum is found.

If no suitable new vertex can be found by the Simplex algorithm, a Random Search is performed.

The overall optimization scheme in the program is as follows:

1) If Random Search only is requested, this method is used through the run.

2) If Simplex is requested, the Random Search stops when (n+1) unpenalized cases have been calculated.

3) Simplex is used for the next 40 seconds (CYBER 175) of the run.

4) Random search is used for the next 10 seconds, just in case Simplex has become stuck in a local minimum.

5) Simplex continues until the optimum is found, run time is exhausted, or a specified number of cases is tried.

At the end of the optimization, a univariate search may be employed to check whether the optimum has been reached. For each independent variable being opti-mized in turn, the program uses a simple Newton method to find the value of that variable which minimizes TUEC. This is really a fine tuning of the variables. A final case is calculated which employs the best values of the variables from the single searches.

When optimizing a small selection from the available independent variables it is often convenient to investigate the sensitivity of the design and TUEC to changes in the other variables, or to defined changes in the optimized variables.

This may be achieved by specifying a number of perturbation cases after the optimization. Multipliers may be specified for each of the independent variables, which are applied to the values in the optimized case, or the specified case if only a single case was run. The variables may be perturbed individually or in groups.

8.4.5 RELAP4/MOD5

RELAP4 [REL76] is a computer program, written in FORTRAN IV, that was developed primarily to describe the thermalhydraulic transient behaviour of water-cooled nuclear reactors subjected to postulated accidents such as those resulting from loss of coolant, pump failure, or nuclear power excursions.

Fundamental assumptions inherent in the thermalhydraulic equations are that a two-phase fluid is homogeneous and that the phases are in thermal equilibrium.

Models are available in the code to modify these homogeneous assumptions.

The program is sufficiently general to be applied to experimental water reactor simulators and many other hydrodynamic experiments.

RELAP4 is a US code available through most of the major computing firms. It is used by process system designers to analyze feedwater break cases and other process piping failure cases.

The program requires numerical input data that completely describe the initial conditions and geometry of the system being analyzed.

The input data include physical characteristics such as fluid volume geometry, pump characteristics, power generation, heat exchanger properties, and material composition.

Starting with system initial flow, pressure, temperature, and power level boundary

conditions, transients can be initiated by the control action inputs to the program. These can describe breaks in fluid piping, valve actions, pump changes, and core power level variations.

The program computes (for each time advancement) fluid conditions such as flow, pressure, mass inventory, and quality.

Also computed are thermal conditions within the solid materials such as temperature profiles and power, and the fluid-solid interface conditions such as heat flux and surface temperature.

The degree of detail to which the system is described is specified by the program user.

This includes nodalization of fluid flow paths within the piping, vessels, and reactor core as well as heat transfer modelling within solids such as the fuel rods, piping, and vessel walls.

Both the reactor primary and secondary flow systems can be modeled.

The permitted system detail is limited by the maximum dimensions within RELAP4.

These dimensions can be adjusted to fit a particular computer.

From a practical viewpoint, the detail is most generally limited by computer time costs.

Computer running time increases rapidly with increasing detail of system modeling.

The definition of the thermalhydraulic system is also completely specified by the user.

A portion of a system, such as a single reactor channel, can be analyzed by supplying appropriate time-dependent boundary conditions.

The boundary conditions can be defined by the user if known, or they can be obtained from a previous RELAP4 analysis.

For example, analysis of a reactor blowdown transient may be performed using a RELAP4 integral system that describes the entire primary flow loop, and a simple nodalization of the total reactor core.

RELAP4/MOD5 was intended primarily as a blowdown code. It will calculate system phenomena from initial operating conditions at the time of pipe rupture through system decompression up to the beginning of core recovering with emergency core coolant.

The major parts of the RELAP4 program are the fluid equations, heat transfer and reactor kinetics. These are outlined as follows:

The fluid dynamics portion of RELAP4 solves the fluid mass, energy, and flow equations for the system being modeled. In order to provide a reasonable degree of versatility, a choice of the following five basic forms of the flow equation is provided:

1) Compressible single-stream flow with momentum flux,
2) Compressible two-stream flow with one-dimensional momentum mixing,
3) Incompressible single-stream flow without momentum flux,
4) Compressible integral momentum,
5) Incompressible mechanical energy balance.

The compressible two-stream flow equation has four sub-forms to represent different stream flow patterns.

A heat conductor model is used to transfer heat to or from the fluid in a volume.

The geometry and conditions of the heat conductor are specified by the user.

This model may be used to describe the thermal behaviour and effects of fuel rods, pipes, and plates.

The program contains correlations for calculating the critical heat flux (CHF), pre-CHF heat transfer, and post-CHF heat transfer. Several options are also available for describing heat exchangers.

Program options are available for describing the power internally generated in system components such as fuel rods or electric heaters. These options include user-supplied normalized power versus time curves and program solution of the space-dependent reactor kinetics equations with or without radioactive decay heat.

Although RELAP4 is a comprehensive program, it has approximations which must be recognized. The approximations include the use of:

1) Point reactor kinetics model,

2) Homogeneous fluid equations with the phases in thermodynamic equilibrium,

3) Air volumes to provide work without allowing the air to mix or flow (This assumption does not apply for the containment option).

4) One-dimensional fluid and heat conduction equations,

5) Steady state empirical correlations to estimate heat transfer coefficients, critical heat fluxes, two-phase friction factors, and critical mass fluxes.

8.4.6 BOILER

BOILER [KIN73] can be used to calculate the boiler heat transfer area, boiler size, boiler tube pressure drop, and the boiler heavy water holdup in order to satisfy a given set of input parameters.

The program also estimates some of the direct and indirect costs involved with the calculated boiler design.

The steam generator on which the program is based is similar to that found at Pickering Generating Station. That is, it is of the "light bulb" type having integral feedwater preheaters and individual steam drums.

Light water on the secondary side with heavy water on the primary side are the only fluid mediums which can be considered. The primary inlet flow, however, may be subcooled or have net quality up to 10% by weight.

The program is set up to consider a variety of tube outlet velocities, tube sizes and types, and primary side inlet conditions.

For a variety of reasons, the program has the following restrictions:

1) The primary inlet temperature must be below 620°F,
2) The primary outlet temperature must be above 300°F,
3) The primary inlet quality should be below 10% by weight.

8.4.7 THIRST

The THIRST[1] [CAR81a] computer code is the latest in a series of three-dimensional steady state computer codes developed at CRL for the detailed analysis of steam generator thermalhydraulics.

The original code, designated BOSS[2], arose from the DRIP[3] program of Spalding and Patankar, and was adapted for application to CANDU type steam generators.

Although the equations to be solved remain the same, extensive changes have been made to the program structure, the numerical computation sequence,the empirical relationships involved, the treatment of the U-bend, and the numerical and graphical presentation of results.

The code has therefore been renamed THIRST.

---

1 THIRST: Thermal-Hydraulics In Recirculating STeam Generators

2 BOSS: BOiler Secondary Side

3 DRIP: Distributed Resistance In Porous Media

In conjunction with these developments, the program has been used to successfully analyze the thermalhydraulic performance of a number of different steam generator designs, from CANDU to American PWR nuclear plants. The program has also been used for extensive design parameter surveys.

8.5 Notes on Steam Generator Modelling

8.5.1 Basic Equations and Modelling Intent

The mass, momentum and energy conservation equations that must be satisfied can be approached from a lumped (i.e., macroscopic or integral) or a distributed (i.e., microscopic or differential) view. The choice is guided by the intent and cost.

The macroscopic view is usually taken in systems modelling since it is cost effective and sufficiently accurate. This limits the analysis to a one dimensional approach with the inherent assumptions.

The microscopic approach is needed for detailed analysis of, say the flow penetration in a tube bundle. Such a code is available in THIRST, a CRL code. This type of code is not useful for the bulk of the overall design and analysis. Rather a macroscopic based code, such as SOPHT, is cost effective, flexible and proven.

Experience has shown that the specification and verification of input data for these codes tends to be a major portion of the whole task of analysis.

There exists two main intentions for modelling codes:

- design
- analysis.

The design code usually has the process output (in this case: steam and water flows, temperature, pressure, etc.) as input to the code and the design (in this case: heat transfer area, etc.) as output.

The analysis code, on the other hand, uses the design as the input and outputs the resultant process.

If the design algorithm is very simple, one can indeed arrive at a design in a straight forward, once-through manner.

Any serious design code, however, involves a number of non-linearities and convolutions so that it is not possible, in general, to specify an algorithm that directly generates a geometrical design given a process requirement.

Consequently, the normal route is to perform an analysis of a given design to determine the resulting process output and to iterate on the design until the desired process output is obtained.

The iterations can be automatically controlled to some degree, but the designer usually maintains a large degree of control over the feedback, especially if each iteration is expensive.

So we see that, irrespective of the modelling intent, the basic requirement is for an analysis code. Thus, this code will simulate transient steam generator performance. The output and level transients will be predicted based on the input values of geometry, primary flow conditions and secondary pressure and feedwater conditions.

8.5.2 Boundary Conditions

In addition to the analysis/design duality is the system/component condition duality.

For system work the reactor power, heat transport pressure, and drum pressure are usually given. The system seeks its own equilibrium with just enough primary to secondary side temperature difference to transfer the given heat load.

For component work, the power can be specified as in the system approach or the heat duty of a particular design can be assessed by supplying the temperatures.

Either approach is acceptable and the analysis/design code should be able to work either way. We must be aware of the difference, however, because reported design and performance information can be easily misinterpreted if the basis of the calculation is not made clear.