CHAPTER 13B

DEVELOPMENT AND APPLICATION OF THERMALHYDRAULIC COMPUTER CODES

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ABSTRACT

The development of a thermalhydraulic computer code is shown to be an evolutionary process guided by continuous validation. Common foundations of thermalhydraulic code development are discussed. Codes are grouped as system codes or component codes. Examples of each are cited and features of codes are compared. Areas requiring further development are mentioned.

13.1 INTRODUCTION

As a nuclear reactor system relies entirely on fluid circuits for energy transport, mathematical modelling of thermalhydraulic phenomena plays an important role in reactor design and development, and methods of improving the accuracy and efficiency of thermalhydraulic computations are sought continually. It is rarely feasible to conduct detailed thermalhydraulic measurements inside operating reactors, so the engineering analyst must often rely on computational tools, which have been validated against simpler out reactor experiments, to assist him in design and development studies. The development of a validated computer code is thus an evolutionary process.

Before discussing individual computer codes, it is necessary to first examine the necessary ingredients in any thermalhydraulic analysis or code development.

13.2 THE FOUNDATIONS OF THERMALHYDRAULIC CODE DEVELOPMENT

13.2.1 The Geometric Framework

The first step in any thermalhydraulic analysis is the selection of the geometric framework on which the computation will be based. The choice is often dictated by the hardware, the decision required is what simplification of the geometry will best serve the purpose of the analysis.

A simplified fluid circuit diagram of a CANDU reactor is shown in Figure 1. Throughout most of the piping network, the fluid behaviour may be adequately described by one-dimensional (cross-sectional averaged) models. However, in the reactor fuel channel, flow must distribute itself amongst the intricate flow passages of the fuel bundle. In the secondary side of the steam generator, and in the calandria, the flow distribution is also complex. One-dimensional analysis is adequate to simulate bulk energy transfer, in an overall, or system sense, but multi-dimensional analysis is necessary to model detailed local distribution of flows and temperatures in any of these geometrically complex components.

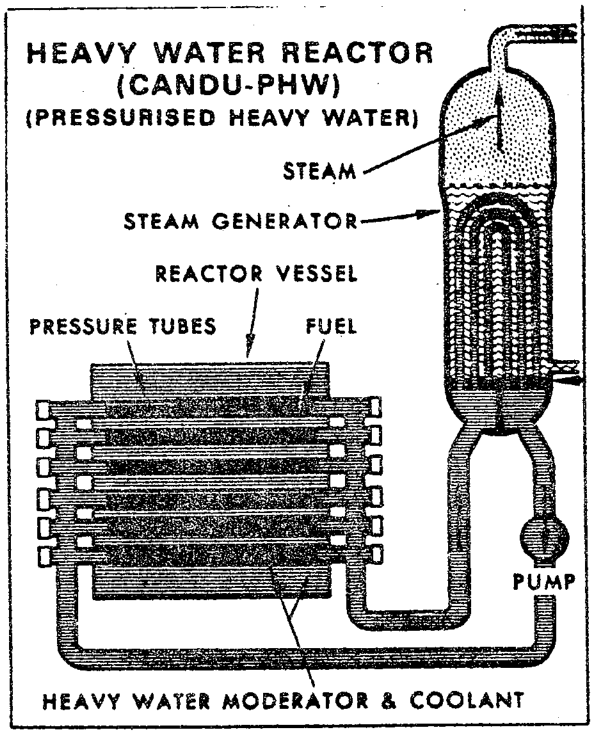

Figure 1. Simplified View of CANDU Reactor

The use of a one dimensional model of a pipe circuit is frequently dictated by practicality, but fortunately it can often provide a reasonable representation, particularly for transient studies involving high flows.

13.2.2 <u>The Flow Model</u>

The second step in an analysis is to decide on a flow model. Most reactor components are not always restricted to single phase flow. Again the most complicated available model of flow need normally not be used; simplifying assumptions are frequently valid and may reduce the complexity of the equations to be solved.

Single-phase flow is normally modelled adequately by solving the conservation equations of mass, momentum, and energy. The exact form of the equations will depend first on whether the fluid should be considered incompressible or compressible and secondly whether the fluid should be considered inviscid or viscous. These decisions affect both the form of the equations and the behavioural modes of the solution.

For two phase flows, there are more degrees of freedom in the decision process.

The assumption of equilibrium produces the simplest model, in which the phases are taken to be homogeneously mixed, and to have equal velocity and equal temperature, hence the terminology EVET model. The two-phase mixture is treated as a single fictitious fluid having properties determined solely by the relative proportion by weight (quality) of vapour in the mixture. Thus the partial differential equations to be solved are the same as for single-phase flow: conservation of mass, momentum and energy of the mixture; algebraic relationships cater for the two-phase properties and the equation of state for the mixture. The homogeneous model is suitable for conditions in which departures from mechanical and thermal equilibrium are known to be minimal.

For cases in which gravitational or centrifugal forces are known to produce a tendency for phases to travel at different speeds, a two-velocity model is required, and an additional relationship is required for relative velocity. Early separated flow models used void correlations instead of the equation of state and a simple numeric slip factor to impose the higher velocity of the vapour phase in vertical flow. This was later quantified by relating relative velocity to the rise velocity of vapour bubbles in liquid and radial distribution of vapour under various conditions. This simple drift flux model, also referred to as DF-ET, unequal velocity equal temperature, uses an algebraic relationship for relative velocity, and hence still requires the solution of the same three partial differential equations of conservation, but an additional equation, usually based on gaseous phase continuity, is required for void distribution.

None of the above models permits the temperature of either phase to depart from saturation. In order to simulate non-equilibrium phenomena such as subcooled boiling, superheated liquid etc., a mechanism which permits these effects must be added. Again, early studies used algebraic relationships, but more rigorous models now use a separate energy equation, and equation of state for each phase and model heat transfer to and between phases. The EVUT model is, therefore, also a four equation model.

The "advanced drift flux" DF-UT model is a combination of both of the above, and, therefore, requires the solution of five conservation equations: a mixture momentum equation, two continuity equations and two energy equations.

Finally, the full six equation, two-fluid model or UVUT abandons the algebraic definition of relative velocity and instead computes phase velocities using two momentum equations containing models of wall to fluid and fluid to fluid stresses.

It is apparent that with each level of complexity of the two-phase model, additional partial differential equations are added, and hence more involved numerical schemes are required.

13.2.3 The Numerical Method

The choice of geometric framework dictates the dimensionality of the governing conservation equations, and the coordinate system on which they will be solved, the choice of the fluid model dictates the number of conservation equations which must be solved. The resulting partial differential equations must then be discretized with respect to the coordinate system by definite difference or finite element techniques discussed earlier and reduced through manipulation to a set of algebraic equations which can be solved numerically. The numerical method itself must be subjected to a verification process in which it is shown to be convergent and consistent. Usually convergence and consistency are not universally attained but are confined to a region in which the method is said to be numerically stable.

13.2.4 Constitutive Relationships

The three conservation equations for a fluid supply governing relationships between the primary flow variables: velocity, enthalpy, density and pressure. Since enthalpy, density and pressure are related through the equation of state, this latter relationship provides a fourth equation to complete the primary set. However, the conversion equations also contain auxiliary variables for which further algebraic relationships must be provided to ensure closure, in other words to balance the number of definitive equations with the number of variables appearing in them.

In single-phase flow, detailed expressions are required for friction and heat transfer and elements of the turbulence model. In two-phase flow, depending on the model, correlations are needed for void fraction, relative velocity, heat transfer and friction between hardware and each phase and between phases, and the question of flow regime affects all these.

Once a numerical scheme has been developed and exhibited convergence and consistence, the choice of the constitutive relationships determines the detailed results. These must obviously be chosen judiciously. A fairly satisfactory repertoire of relationships has been developed for the homogeneous model. Some doubt exists about the correct choice for the advanced models and further research is continuing.

13.2.5 Interacting Systems

Frequently it is insufficient to model the thermalhydraulic behaviour in isolation, the effects of interacting systems must also be incorporated. It is often necessary, for example, to model the temperature transients in contained or containing structures, the neutron kinetics in the reactor fuel, pump behaviour, and the secondary side of a heat exchanger or even structural changes. Each of these auxiliary systems has its own equation set and constitutive relationships which must be solved simultaneously and compatibly with the thermalhydraulic equations.

13.2.6 Validation

As mentioned previously, validation against experimental evidence is essential to establish credibility. The validation process consists of comparing results from the computer code against as much experimental evidence as possible. If the code predicts experimental behaviour acceptably, it is considered to have been validated for those conditions. If it does not, then the reason for the discrepancy must be hypothesized, and the assumptions used must be revised until reasonable agreement is achieved. All computer codes proceed along such an evolutionary route, they have been adequately validated for only a limited number of scenarios, and therefore should be used only discriminatingly.

13.2.7 Robustness & Versatility

The property of robustness is a direct function of the extent of the validation that has been performed. A code should be sufficiently versatile that it can address a reasonable range of geometries without requiring extensive modification by the user, and sufficiently robust that it can perform adequately within this range or diagnose unacceptable conditions.

13.2.8 Documentation

As code development is an evolutionary process, documentation often lags out of phase. Frequently the document available to users describes the version of the code previous to that which the developers are currently using to get good results. There is no ready solution to this phase lag except to ensure that internal documentation of the code is maintained continually in such a form that new developments can be rapidly disseminated. The documentation at any stage is the users window on the code and must always be both precise and concise.

13.3 CLASSIFICATION OF THERMALHYDRAULIC CODES

As most thermalhydraulic codes have developed in an evolutionary manner in response to successive requirements for more precise particular analysis, each computer code is a unique product of its own history. However, it is useful to divide thermalhydraulic codes into two main groups, component codes, and system codes. The former are used to provide detailed analysis of a particular component, such as a fuel channel or a steam generator, whereas the latter are often used to analyse an entire system consisting of a number of interconnected components. Simple models of the individual components are used. System codes are addressed first as they have the most widespread use.

13.4 SYSTEM CODES

A well designed system code is a versatile tool which can be used to perform steady state and transient analysis of a one dimensional idealization of a thermalhydraulic circuit comprising a number of different components. The code should be able to perform open or closed loop analysis, and be sufficiently versatile that any reasonable fluid circuit and associated heat structures can be specified via input data. The minimum flexibility demanded is that the code can be used to simulate either an operating plant or a related experimental loop for validation.

13.4.1 Operation of a System Code

In the most general sense, the basic operation of a typical system code may be described as follows: given the status of the fluid circuit now, with boundary conditions, produce the status of the reactor at some future time. For example, if we have the status at time t_0, the code will produce the status at time t_1, (where the timestep is t_1-t_0). If we then repeat that process starting from the status at t_1 the code will produce the status at t_2, and so on. Thus the typical code can trace the evolution of a transient event, like a LOCA. If the reactor is operating steadily, or nearly steadily, its status is changing slowly if at all, and we would like to use large timesteps. However, during rapid transients - triggered by a changing boundary condition like a guillotine pipe break at a specified time - the reactor status can change very quickly and small timesteps are required. Automatic timestep control is a feature of most transient codes. Output from a system code is like a sequence of snapshots (status reports).

The information described as "reactor status" depends on the resolution desired when one is dealing with a system code. Clearly, any item of information which can change must be included - for example flow conditions throughout the circuit, piping network temperatures, fuel bundle temperatures and power, pump conditions, boiler conditions, break flow conditions, cold water injection flow conditions, and so on. However, the code user may select the number of flow condition stations in the circuit, for example, at the outset, thus defining ahead of time the resolution. Although some work is being done in automatically changing resolution during code operation, for most codes the user specifies it, and may have to respecify it, if the original estimate was inadequate. Just as there is an art to photography, there is an art to getting the most out of a system code.

We now turn our attention to what is inside the code: the rules for transforming the reactor status from time t_1 to t_2. As mentioned above, these rules end up being in the form of algebraic relationships whatever their sources. Some come directly - steam-water property routines, friction factors, heat transfer coefficients are, for example, often already in algebraic form. Some, however, come from the application of numerical methods to partial diffeential equations: for example the flow-boiling equations, and the conductive heat transfer equation, and these may be subject to timestep and spatial resolution criteria for accuracy and stability.

The quality of the model as well as the quality of its algebraic representation are both important to code performance. During any step, one model will be more dominant than the others in prescribing the change in reactor status. If that model is mathematically capable of describing the physics, and its numerics are of good quality, the change in reactor status will describe reality quite well, and within reasonable efficiency. However, if the models or the numerics are incompetent, either quality of prediction or efficiency (or both) will suffer. Experience suggests that sooner or later more developmental work will be required to improve the operation of any code.

13.4.2 Features of System Codes

It would be counter-productive to launch a discourse on each individual code, as we would have to discuss the particular features of each under each of the above headings of geometry, fluid model, numerical method, etc. Table 1 covers these features in summary fashion and readers can turn to the references to do homework on the details. This is not a comprehensive table by any means, but does contain codes used by, or being considered for future used by CANDU thermalhydraulic analysts.

13.4.3 Some Current Concerns

Physical Modelling

For most fast transients, particularly at high mass fluxes, the homogeneous model is considered to provide adequate simulation, hence the small break loss of coolant problem is considered to have been adequately analysed. Discrepancies arise when flows are lower, particularly in horizontal pipes where two phase flows tend to stratify. This causes considerable disparity of heat transfer in a fuel bundle and may cause CHF at powers well below those which a homogeneous flow model would predict, so a two fluid model must be invoked. Separation also introduces further dimensionality into the problem as the separation is normal to the axial coordinate. Currently this is handled in one dimensional codes by extracting the probability of separation from flow regime correlations and accordingly modifying heat transfer, but the practice is at best an artifact.

Departure from homogeneous conditions at low flows also occurs in vertical pipes, where local areas of counter current flow can be set up when the gravitational force on the liquid exceeds the combined forces of the vapour and the pressure gradients. Again a two fluid model is required even to begin to analyse this phenomenon.

In both the above cases, the modelling of the physics is difficult because of the lack of widely proven constitutive equations describing interphase phenomena. In the subject of quenching fronts, however, both the models and the numerics are currently inadequate. The manner in which a quenching front travels down a heated surface is yet to be adequately quantified, and the associated thermal gradients in the heater are quite severe. A standard fixed grid scheme merely diffuses the gradient, thus ignoring the steep front and its effects. Current practice is to attempt to refine the grid in the neighbourhood of the front and permit the refined grid to travel with the front. RELAPV uses a refined grid in the heat structures for this purpose. RAMA has refined the fluid grid. A combination of both refinements is required to improve precision. These concerns are addressed more fully in chapter 4.

13.5. COMPONENT CODES

Component Codes are generally more specialized than system codes. They provide a far more detailed analysis of flow and phase distribution in a particular component than the very simplified model of that component which is normally used in a system code. Although

Table 1

TABLE 1

System Code Features

		HYDNA	FIREBIRD	SOPHT	RAMA	TRACP1	RELAP IV	RELAP5
A.	Numeric Solution							
1.	Explicit	-	-	-	-	-	-	-
2.	Semi Implicit	Momentum Integràl	Porshing	Porshing	Pseudo Character- istic	Ice	Ice	Ice
3.	Implicit	-	-	-	-	-	-	-
4.	Time Step Control	Yes	Yes	Yes	Yes	Yes	Yes	Yes
5.	Space Grid	Standard	Mode/Link	Mode/Link	Standard	Staggered	Staggered	Staggered
6.	Space Grid Control	No	No	No	Yes	No	No	No
7.	Type of Transient	Slow	Fast/Slow	Fast/Slow	Fast/Slow	Fast/Slow	Fast/Slow	Fast/Slow
B.	Flow Model							
1.	Conservation Eqns	3	3	3	3,(6)	6	3	5
2.	Slip Model	Opt	Opt	Opt	no	N/A	Yes	N/A
3.	Drift Flux	No	Opt	Opt	no	N/A	No	N/A
4.	Momentum Eqns	3	1	1	1,(2)	2	1	2
5.	Subcooled Boiling	Void & HT	HT Only	HT & Void	HT Only	HT Only	HT Only	HT Only
6.	Energy Eqns	1	1	1	1,(2)	2	1	1
7.	Flow Regime H.T.	Some	Yes	Yes	Yes	Yes	Yes	Yes
8.	Critical Flow Model	No	Yes	Yes	Yes	Yes	Yes	Yes
C.	Loop Components							
1.	Loop Topology	Limited	Specifiable	Specifiable	Specifiable	Specifiable	Specifiable	Specifiable
2.	Boundary Conditions	Specifiable	"	"	"	"	"	"
3.	Closed Circuits	Yes	Yes	Yes	Yes	Yes	Yes	Yes
4.	Branched Circuits	Yes	Yes	Yes	Yes	Yes	Yes	Yes
5.	Heat Structures	Some	Yes	Yes	Yes	Yes	Yes	Yes
6.	Secondary side	Yes	No	Boiler	Boiler	No	No	No
7.	Horizontal Fuel Channel		Strat Model	Strat Model	Strat Model	No	No	No
D.	Related Systems							
1.	Neutron Kinetics	Pt	No	Yes	(Some)	Pt	Pt	Pt
2.	Prompt/Del Groups	1/6	-	1/6	1/6	1/6	1/6	1/6
3.	Fuel Model	Yes	Yes	Yes	Yes	Yes	Yes	Yes
4.	Gap Model	Yes	Yes	Yes	Yes	Yes	Yes	Yes
5.	Pump Dynamics	Yes	Yes	Yes	Yes	Yes	Yes	Yes
6.	Heat Exchangers	Yes	Yes	Yes	Yes	Yes	Yes	Yes
7.	Control	Yes	No	Specific	Some	No	No	No
E.	References							
		1,2	3	4,5	6,7	8,9	10	11,12

the flow models and numerical methods used are applicable generally, a particular code cannot usually be readily converted to address a different type of component. Detailed description of flow and phase distribution usually requires multidimensional analysis.

Table 2 contains a summary of the features of component codes, again details can be gleaned from the references.

13.5.1 Current Concerns

Apart from the uncertainties of constitutive relationships in two fluid models, the main concerns in the development of component codes revolve around multidimensional analysis. Numerical methods in several dimensions are inevitably costly, particularly for transients, and the problem of adequately representing both internal and external geometrical boundaries is often difficult. Finally the problem of modelling turbulent effects is peculiar to multidimensional analysis. In single phase the turbulent model is applied through the friction factor, but in multidimensions correct velocity distributions can be obtained only through simulating turbulent effects. This is normally done in single phase by computing an effective viscosity due to turbulence, however this too is, at best, an artifact and in two phase no satisfactory rationale has yet been developed. These concerns are addressed further in Reference [4].

ACKNOWLEDGEMENTS

On request of the course program committee, this chapter was written to combine the contents of two chapters in the previous course of 1982, one by Dr. B.M. MacDonald, and one by myself. A few excerpts from both 1982 contributions therefore appear in this chapter almost verbatim.

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Table 2

TABLE 2

Component & Specialized Codes

Code	COBRA	ASSERT	SPORTS	MODCIR	MOTH	THIRST	TOFFEA
Type or Use	Subchannel (homog)	Subchannel (non equil)	Stability (transient)	Moderator	Moderator	Steam Gen.	General (2 Fluid)
Dimensions	3	3	1	3	2	3	2(3)
Flow Model							
single phase	yes	yes	yes	yes	yes	yes	yes
turbulence	corr	corr	N/A	k-e	k-e	no	k-e
two phase	yes	yes	yes	no	no	yes	yes
homogeneous	yes	opt	yes	no	no	yes	no
separated	yes	no	yes	no	no	no	no
drift flux	no	opt	no	no	no	no	no
two fluid	no	no	no	no	no	no	yes
thermal equilib	yes	opt	no	no	no	no	no
thermal disequilib	no	opt	no	no	no	no	no.
Geometry Boundaries	Subchannel between headers	Subchannel between headers	1D between headers	Cylinder	Cylinder	Cylinder	Cylinder
Internal Structures	rods	rods	N/A	Porous Medium	Porous Medium	Porous Medium	none
Steady State	yes	yes	yes	yes	yes	yes	yes
Transient	yes	yes	yes	yes	yes	no	no
Explicit	yes	no	no	yes	no	no	no
Implicit	yes	yes	yes	no	yes	no	no
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