# SCDAPSIM REACTOR SYSTEMS ANALYZER FOR DESIGN AND BEYOND DESIGN BASIS ACCIDENT CONDITIONS

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### ABSTRACT

SCDAPSIM is being developed as part of an international SCDAP Development and Training Program. SCDAPSIM is designed to provide a detailed, mechanistic prediction of the response of a reactor system during design basis and beyond design basis accident conditions. SCDAPSIM is the result of merging models from SCDAP/RELAP5 with "state-of-the-art" containment and source term models. The objectives of this paper are to (a) describe the goals of the SCDAP Development and Training Program, (b) briefly outline the overall capabilities of SCDAPSIM, (c) describe the advantages of the SCDAPSIM modeling approaches, and (d) discuss the application of SCDAPSIM to the CANDU reactor design.

### Introduction

SCDAPSIM<sup>1,2</sup>, an enhanced version of the SCDAP/RELAP5 code<sup>a</sup>, is being developed as part of an international SCDAP Development and Training Program (SDTP). SCDAPSIM is designed to provide a detailed, mechanistic prediction of the response of a reactor system during design basis and beyond design basis accident conditions. As described in this paper, SCDAPSIM will offer a number of advantages relative to the current versions of RELAP5<sup>3</sup> and SCDAP/RELAP5<sup>4,5,6</sup> for design basis and beyond design basis accident analysis, including design-specific modeling options for CANDU reactors. In addition, SCDAPSIM will offer several advantages relative to the more simplistic severe accident codes such as MAAP<sup>7</sup> and MELCOR<sup>8</sup> for severe accident management and training. However, the development of SCDAPSIM also offers difficult technical challenges to insure that the code can be used as a practical analysis and training tool.

a. The SCDAP/RELAP5 code is being developed at the Idaho National Engineering Laboratory (INEL) under the sponsorship of the United States Nuclear Regulatory Commission (USNRC).

The objectives of this paper are to (a) describe the goals of SDTP, (b) briefly outline the overall capabilities of SCDAPSIM, (c) describe the advantages of the SCDAPSIM modeling approaches, and (d) discuss the application of SCDAPSIM to the CANDU reactor design.

#### SDTP Goals

The primary goal of SDTP is to provide access to "state-of-the art" severe accident analysis tools, expertise, and other training materials for those organizations that cannot afford or do not want to develop those capabilities on their own. Although SDTP does not provide access to proprietary data and models developed through international research or reactor-vendor-supported programs, SCDAPSIM and other reactor accident analysis tools available through SDTP embody the important lessons learned from these research programs. In addition, a large number of the organizations participating in SDTP also have been involved in these international research programs since their inception.

Although the specific goals of participating in SDTP will vary by individual organization, the application of SCDAPSIM and other reactor system analysis software to support the development of more robust accident management guidelines and procedures, to support Probabilistic Safety Assessment activities, and to support the training of technical and operational staff members will be the most visible aspect of the program.

The SCDAPSIM portion of SDTP consists of four primary activities. First, expanded modeling capabilities are being added to SCDAP/RELAP5 including (a) design-specific modeling options for the CANDU, RBMK, and VVER reactor designs and (b) containment modeling options for core-concrete interactions, hydrogen combustion, and other containment-specific processes. Second, SCDAP/RELAP will be rewritten to incorporate more advanced numerical techniques and parallel/vector-computer-specific algorithms to significantly reduce computer run times. These changes are anticipated to allow "real time" accident simulations on workstations and super computers. Third, enhanced graphical user interfaces are being developed to reduce the cost of plant model development and the analysis of complex transients. These three SCDAPSIM development activities will be supplemented by the fourth activity, the establishment of an international network of accident analysis experts, and associated training workshops and seminars, to promote the exchange of information between research, regulatory, and industry groups.

#### SCDAPSIM Modeling Approaches

SCDAPSIM is designed to provide a detailed, mechanistic prediction of the response of a reactor system during design basis and beyond design basis accident conditions. As indicated in Figure 1, SCDAPSIM maintains the detailed SCDAP/RELAP5 modeling approach for the response of the reactor coolant system. In addition, it will have modeling options to treat processes like diffusiophoresis that are unique to the containment.

SCDAPSIM is the result of merging models from SCDAP/RELAP5<sup>4,5</sup> with "state-

Analysis systems	SCDAP/ RELAP5 MOD3.1	<u>SCDAPSIM</u>
Fast-running (1D/2D) Simulation		
- Reactor core thermal-hydraulics		X
- Core and vessel damage progression		<u>X</u>
- Containment response		
- Fission product transport and deposition		X
Detailed analyses (1D/2D/3D)		
-System thermal-hydraulics		
- RCS	X	X
- Containment	P*	<u>X</u>
- Fuel/control/structure behavior	X	X
- Debris formation, heating, and melting behavior	X	X
- Molten pool formation, heating, and relocation	X	X
- Lower head heating and failure	X	X
- RCS piping failure	X	X
- High pressure melt ejection		<u>X</u>
- Core-concrete interactions		X
-Hydrogen combustion		x
- Fission product release and transport		
- RCS		X
- Containment	:	X
- Pool scrubbing		X
- Material properties	x	X

\* Explicit coupling between SCDAP/RELAP5 and CONTAIN using PVM

Figure 1 - Comparison of SCDAPSIM and SCDAP/RELAP5 Capabilities with Containment and Source Term Options.

of-the-art" containment and source term models. The RELAP5-based portion of the code calculates the overall Reactor Coolant System (RCS) response including the transport of fluid through the system, control system behavior, reactor kinetics, and heat conduction in lower temperature vessel structures and RCS piping and structures. The thermal-hydraulic models utilize a multi-dimensional, two-fluid, non-equilibrium approach. Hydrogen, fission products, and other non-condensible gases are also included. The SCDAP-based portion of the code calculates the heatup and damage progression in the core and surrounding structures. This portion of the code describes the (a) heating, deformation, oxidation, and melting of fuel rods, control rods/blades, and other structures and (b) formation, heating, and melting of debris. The heating, melting, oxidation, and changes in core and vessel structures are described using representative 2D component models. Physical processes predicted include (a) heat conduction within the structures, (b) fuel rod ballooning and rupture, (c) oxidation, (d) material interactions between the fuel, cladding, and structural and control materials, (e) fission product release, (f) spalling of protective oxide films, (g) relocation and freezing of molten films, rivulets, and droplets, and (h) fragmentation and collapse of the structures during reflood. The SCDAP-based portion of the code also describes the behavior of debris beds, molten pools, and associated structures. Physical processes predicted include heat conduction with the debris and embedded or adjacent structures, molten pool formation and growth, natural circulation heat transfer between the molten pool and boundary, molten pool crust thinning and failure, relocation of the molten material, and the failure of the structures due to thermal and creep rupture mechanisms. Physical processes described by the source term models include evaporation and condensation, chemisorption, agglomeration, and deposition. The containment modeling options are still in the design phase but are anticipated to use modeling approaches for hydrogen combustion, core-concrete interactions, and other containment-specific processes similar to those adopted for the CONTAIN<sup>9</sup> and MELCOR<sup>8</sup> codes. The RELAP5 portion of SCDAPSIM will be extended to treat both the RCS and containment.

SCDAPSIM is capable of modeling a wide range of system configurations from single pipes to different experimental facilities to full-scale reactor systems. The configurations can be modeled using an arbitrary number of fluid control volumes and connecting junctions, heat structures, core components, and system components. Flow areas, volumes, and flow resistances can vary with time through either user-control or models that describe the changes in geometry associated with damage in the core. System structures can be modeled with one-dimensional heat structures, two-dimensional representative core components, or debris bed models. The one-dimensional models are typically used for system piping and other structures that remain below their melting points. The two-dimensional core component models include representative U02-Zircaloy fuel rods, research reactor U-AI fuel plates and annuli, Ag-In-Cd and B<sub>4</sub>C control rods and/or blades, electrically heated fuel rod simulators, and general structures. The heating and melting of debris beds are described by a combination of two-dimensional and lumped parameter models. The two-dimensional debris models are used primarily to describe the regions of system where the debris is in contact with important structures such as piping, reactor tanks or vessels. The lumped parameter approach to typically used within the core region.

The two-dimensional model utilizes a general finite element approach with an arbitrary user defined mesh to include any structures and thermal-hydraulic volumes within the RCS. However, the model is typically used to represent the lower plenum regions of the vessel and the accumulation of debris from the core and upper regions of the vessel. Other system components available to the user include pumps, valves, electric heaters, jet pumps, turbines, separators, and accumulators. Models to describe selected processes, such as reactor kinetics, control system response, and tracking non-condensible gases, can be invoked through user control.

## Advantages of SCDAPSIM

SCDAPSIM will offer a number of advantages over the "stand-alone" RELAP5 and SCDAP/RELAP5 codes for the analysis of design basis and beyond design basis accident conditions. First, SCDAPSIM will have options for integrated reactor coolant system and containment analysis. Although coupled RELAP5-CONTAIN and SCDAP/RELAP5-CONTAIN calculations have been demonstrated using the PVM (Parallel Virtual Memory) software, the coupling is machine-dependent, awkward to use, and requires duplicate input in many cases. Second, SCDAPSIM will include detailed fission product transport and deposition modeling options. Although SCDAP/RELAP5 originally offered such an option, that option was eliminated in the current versions of the code. Fission product calculations now require separate SCDAP/RELAP5 and VICTORIA<sup>10</sup> calculations. As a result, there is very little feedback between the system thermal-hydraulics, core damage progression, and fission product transport and deposition.

SCDAPSIM will retain two major advantages of SCDAP/RELAP5, the flexibility and the minimal use of user-controlled modeling parameters. The flexibility allows the code to analyze a wide range of facilities and also allows the user to employ exactly the same models to analyze reference experiments and perform full plant calculations. For example, the same representative fuel rod model and nodalization is typically used for the analysis of bundle heating and melting experiments as is used in a full plant calculation. Although the user may employ the fuel rod model to represent many more fuel rods in the actual reactor core than in the experiment, the only major difference between the experimental scale and plant scale is typically the number of thermal-hydraulic volumes used in the plant calculations. Minimizing the number of user-controlled modeling parameters reduces the variance of code calculations due to variations in user estimates. Instead, the important models in the code are mechanistic and defaults for the limited number of modeling parameters are established through code-to-data comparisons. These parameters do not need to be altered for the plant calculations.

SCDAPSIM also offers several advantages relative to the more simplistic severe accident codes for severe accident management and training. First, since the code has models that have been validated for both design basis and severe accident conditions, the same code and plant input models can analyze the accident from steady state operation, accident initiation and the successful termination of an accident (or the ultimate failure of the vessel and containment in unmitigated accidents). Second, mechanistic models can capture many more of the important process associated with accident conditions. Third, because of the mechanistic models and limited reliance on user parameters, the results from the code are much less subject to users' interpretations.

The ability to use one code for both design basis and beyond basis design accident conditions greatly simplifies the costs of multiple codes and training and maintenance activities associated with those codes. That has been one of the most significant benefits in the development of SCDAP/RELAP5. Although RELAP5 is normally used for design basis accident analysis and SCDAP/RELAP5 is used for severe accident analysis, there have been significant reductions in code development, maintenance, and validation costs associated with the two codes. First. SCDAP/RELAP5 and RELAP5 are maintained using a common RELAP5-based source code. The SCDAP portion of the source code is eliminated when RELAP5 is distributed in a "stand-alone" mode. Thus only one set of thermal-hydraulic models needs to be improved and validated. The ability to focus on severe accident model development and validation for the SCDAP/RELAP5 code has reduced the level of effort required by an estimated 40-50 man years over the 15 year life of the code, relative to that required if the RELAP5 and SCDAP/RELAP5 had been developed separately. Second, plant models developed for design basis or licensing calculations can be guickly extended for beyond basis analysis through the addition of SCDAPspecific input. While the development of a fully-guality-assured RELAP5 plant model can take between 1-2 man-years of effort, the extension of those models to severe accident transients can be a matter of a few days. Of course, since there are RELAP5 plant models available for nearly every plant design used in the world, the development of quality assured beyond design basis plant decks for SCDAP/RELAP5 has become a relatively minor part of an analysis effort. Third, the commonality of documentation has also resulted in significant cost savings. This has been particularly true in recent years as the code documentation has been moved into the "desk-top" publishing age where electronic copies of the manuals are maintained and distributed.

The use of a common code for design basis and beyond design basis also has benefits that are significant but more difficult to quantify. For example, one of the strongest criticisms of many risk assessment studies performed using the simplified risk codes is the inaccurate definition of thermal-hydraulic success criteria and the conditions associated with core uncovery. In many cases, the simplified codes are not adequate to predict the thermal-hydraulic response of the plant during accident initiating events or possible recovery actions. As a result, it has been necessary to perform separate detailed plant calculations using design basis thermal-hydraulic systems codes to initialize or to "tune" the more simplified codes. In addition, as noted below, many of the simplified codes neglect many of the important feedback mechanisms between the progression of damage in the core and system thermalhydraulic conditions. Thus, the simplified codes may predict the successful termination of an accident when, in fact, the accident would continue on through vessel failure and possibly containment failure. Of course, the reverse could also occur, where key processes not considered in the simplified codes could result in the successful termination of the accident.

The advantages of using mechanistic models has been demonstrated over many years of design basis and severe accident model validation activities. The SCDAP and

RELAP5 models have been validated over a wide range of conditions over the past 15-20 years. As a result, it has been demonstrated that the SCDAP and RELAP5 models. can reliably predict the critical features of design basis and severe accidents. Although the importance of different models varies, depending upon the system being analyzed, accident initiating and boundary conditions, and phases of the accident, four basic models stand out in the successful prediction of the response of a reactor system during an accident. The impact of two-fluid, non-equilibrium thermal-hydraulic models in successfully predicting the response of a system during design basis accidents is well established. However, these models are equally important to successfully predict the behavior of the system during severe accident conditions. Natural circulation in the vessel and reactor coolant system piping, flow diversions associated with changes in core geometry, and the reflooding of core and vessel are examples where the accuracy of the thermal-hydraulic models can have a major impact on the progression of the accident. The models that predict the melting and destruction of the fuel assemblies, the oxidation and fragmentation of Zircalov cladding, and the formation and growth of molten pools are other examples.

Changes in flow patterns in the vessel associated with the loss of core geometry is one of the most notable areas where mechanistic models have significant benefits. For example, the multidimensional two-fluid models in SCDAPSIM can predict the changes in flow patterns as portions of the core are damaged or hydrogen is produced. This is possible since the time-dependent changes in flow channel geometry are considered directly in the conservation and constitutive equations for the liquid and vapor fields. On the other extreme, the simplified codes either ignore the changes in geometry or use "hard-wired" flow patterns. The importance of changes in flow as the core geometry is lost has been amply demonstrated both experimentally and analytically. For example, in the LOFT LP-FP-2 experiment, which was conducted in the small scale LOFT pressurized water reactor, showed the changes in core heating, oxidation, and blockage formation as flow was diverted from the hotter, more damaged regions of the core to other colder regions<sup>11</sup>.

The initial heating and melting of the core is also strongly influenced by many processes that must be modeled mechanistically. Bundle heating and melting experiments conducted over the past 15 years have shown that the heating and melting of the core is a complex process, strongly influenced by interactions between different materials in the core and between the structures and steam<sup>12,13</sup>. These experiments have shown that the transition from the original fuel rod assembly geometry takes place over an extended temperature range varying from 1500 K to approximately 3000 K. The first regions to suffer extensive damage are at Inconel grid spacer locations and in control rod/blades due to the interactions between Inconel and Zircaloy and between stainless steel and Zircaloy. This occurs over a temperature range of between 1500 to 1700 K. The next regions to suffer extensive damage are the surfaces of the fuel rods as the Zircalov melts, dissolves a portion of the fuel, and then relocates either to lower grid spacer locations, other obstructions, or to a point where the rods were cooled by the water remaining in the assemblies. This starts at a temperature between 2050 to 2150 K and reaches a maximum at temperatures between 2400-2600 K. The final changes in geometry occur as temperatures near 2900 K are reached and the remaining fuel and oxidized material melt and start to

slump. In the experiments where the assemblies were reflooded, the upper regions of the assemblies above the quench front quickly heated up due to the rapid oxidation of any unoxidized Zircaloy, forming extensive blockages of metallic and ceramic materials<sup>12-14</sup>. In these experiments, peak bundle temperatures, maximum hydrogen production rates, and the formation of extensive blockages occurred during the reflood. Thus simplified parametric models requiring the user to define a single temperature where melting and slumping of the fuel occurs have little chance of predicting the actual progression of damage during a severe accident.

The limitations of parametric models are also apparent when the user is trying to describe the reflooding of the core and the successful or unsuccessful termination of an accident. As noted above, bundle heating and melting experiments have clearly demonstrated that the reflooding of a hot damaged core following the start of a severe accident can lead to significant increases in the heating, melting, and oxidation of the core prior to the termination of the accident. The experiments indicate that the transition to accelerated heating typically occurs when the peak bundle temperature exceeds 1500 K. If reflood occurs when bundle temperatures range between 1500 to 2100 K, the accelerated heating of fuel rods results in limited melting of the fuel rod cladding and the associated flow restriction in portions of the bundle. In this case, the combination of oxidized cladding and rapid cooling can result in the fragmentation of a portion of the fuel and cladding material. If the peak bundle temperatures are above 2100 K when cooling water is added to the hot core region, the accelerated heating and oxidation can lead to increased melting and the formation of a non-coolable cohesive debris bed and molten pool. This is the situation that has occurred in the larger experiments. In addition, this is the process that is predicted to have occurred in early stages of the TMI-2 accident. If water is added after the core is extensively damaged, then the cooling of the core may not be adequate to terminate the accident. This was the case in the later stages of the TMI-2 accident, where reflooding of the core was unable to prevent the subsequent melting and relocation of a portion of the core material into the lower head.

The ability to minimize the influence of the code user is also a significant advantage of the mechanistic modeling approach. As noted earlier, elimination of "user-defined" modeling parameters also eliminates a significant source of uncertainty in analyzing plant transients. Although modeling parameter defaults can be defined through code-to-data comparisons or benchmarking using more detailed codes, the use of large numbers of modeling parameters make it very difficult to predict the overall conservatism or non-conservatism in a plant calculation. In addition, the modeling parameters may be strongly scale- and condition-dependent and require an extensive validation effort to quantify the influence of each parameter.

#### CANDU-Specific Features of SCDAPSIM

The CANDU-specific models for SCDAPSIM are still in the design phase. However, it is clear that the number of design-specific models will be relatively limited. The primary limitation of the code is associated with the horizontal geometry of the fuel assembly and primary cooling channels. Although the thermal-hydraulic constitutive models include correlations for horizontal flows, the assessment of these models against CANDU-specific experiments has been very limited. As a result, one of the highest priority activities will be to validate these constitutive models and add additional correlations where necessary. The second limitation is associated with the sagging and initial loss of geometry of the fuel. Although the code can use the representative fuel rod and other component models to describe the fuel assemblies, calandria, pressure tubes, and other vessel structures, the current fuel element deformation and melting models were developed for vertical geometries. Until these models are extended for horizontal geometries, a combination of the representative component models and debris bed/molten pool models will be used to analyze the plants.

## **Concluding Remarks**

SCDAPSIM is currently under development and testing for general release in early 1997. The initial test versions of the code are currently only available to the participants of the development program. However, a number of important milestones have already been reached. First, many of the specialized numerical techniques and parallel/vector constructs have been demonstrated. "Real time" and "faster-than-real time" have been demonstrated on a variety of workstations and super computers. Second, a generalized graphical user interface has been designed that allows the analyst or trainer to use the code on a variety of computers from personal computers, UNIX workstations, and centralized computer facilities. Third, a program of international training workshops and technical exchange meetings is being established to provide training on accident management, severe accidents, and other related areas necessary to qualify reactor systems analysts and trainers on the use of SCDAPSIM.

The SCDAPSIM features will significantly improve the ability to perform detailed severe accident analysis and simulation. The detailed models developed as part of SCDAP/RELAP5 embody nearly two decades of severe accident research programs. Although SCDAP/RELAP5 is currently used by research and regulatory organizations in more than 20 countries around the world, the code has had limited impact on the operation and design of commercial nuclear power plants, because of the high cost of performing detailed calculations. However, the improved numerics and incorporation of more specialized parallelized coding being developed for SCDAPSIM will significantly reduce the running time of the code for typical applications. For example, initial testing of these techniques have demonstrated increases in code performance by a factor of 10 or more. As multiple-CPU workstations become more widely available, these changes will allow "real time" detailed plant calculations for a wider range of organizations. The enhanced graphical user interfaces will also significantly reduce the cost of detailed plant calculations. Addition of interactive graphical interfaces, and the ability to animate the response of the plant and important components have already been demonstrated to substantially reduce the cost of interpreting complex plant transients. The addition of preprocessors should provide comparable reductions in building detailed models of the plant. The incorporation of models for other reactor designs not only makes detailed calculations possible for a wider variety of plant designs, but also allows the incorporation of the lessons learned from non-LWR severe accident research programs.

# References

- C. M. Allison, "Development of a Mechanistic SCDAP/RELAP5-Based Nuclear Power Plant Analyzer for Simulator Applications", Paper presented at the 3rd Workshop on Supersimulators for Nuclear Power Plants, Tokyo, Japan, December 7, 1995.
- C. M. Allison, et al., "Impact of Recent Code Development Activities for SCDAP/RELAP5 and SCDAPSIM", Paper accepted for the International Topical Meeting on Probabilistic Safety Assessment, Park City, Utah, September 29-October 3, 1996.
- 3. <u>RELAP5/MOD3 Code Manual, Volumes I through IV</u>, NUREG/CR-5535, EGG-2596, DRAFT, June 1990.
- 4. <u>SCDAP/RELAP5/MOD3.1 Code Manual, Volumes 1-5</u>, NUREG/CR-6150, EGG-2720, Idaho National Engineering Laboratory, June 1995.
- C. Allison, et al., "SCDAP/RELAP5 Code Development and Assessment", Proceedings of the U.S. Nuclear Regulatory Commission Twenty-First Water Reactor Safety Information Meeting, NUREG/CP/0133, Vol. 2, April 1994.
- C. Allison, et al., "SCDAP/RELAP5 Code Development and Assessment", <u>Transactions of the Twenty-Third Water Reactor Safety Meeting</u>, NUREG/CP-0148, Bethesda, October 23-25, 1995.
- 7. M. G. Plys, et. al., "MAAP 4 Model and Validation Status", Second International Conference on Nuclear Engineering, San Francisco, March 21-24, 1993.
- 8. R. M. Summers, et al., <u>MELCOR 1.8.0: A Computer Code for Severe Nuclear</u> <u>Reactor Accident Source Term and Risk Assessment Analyses</u>, NUREG/CR-5531, SAND90-0364, Sandia National Laboratories, January, 1991.
- K. D. Bergeron et al., <u>User's Manual for CONTAIN 1.0, A Computer Code for</u> <u>Severe Nuclear Reactor Accident Containment Analysis</u>, NUREG/CR-4085, SAND84-1204, May 1985.
- 10. T. Heames et al., <u>VICTORIA: A Mechanistic Model of Radionuclide Behavior in</u> <u>the Reactor Coolant System Under Severe Accident Conditions</u>, NUREG/CR-5545, SAND90-0756, Rev. 1, December 1992
- Edited E. W. Coryell, <u>Summary of Important Results and SCDAP/RELAP5</u> <u>Analysis for OECD LOFT Experiment LP-FP-2</u>, NUREG/CR-6160, NEA-CSNI-R(94)3, EGG-2721, April 1994.
- S. Hagen, P. Hofmann, C. Allison, "Lessons on In-Vessel Severe Accidents from Experiments at KfK and the INEL", American Nuclear Society Transactions, 1993 Winter Meeting, San Francisco, November 14-18, 1993.
- C. M. Allison, et al., "Lessons Learned from Severe Accident Fuel Damage Tests", Paper accepted for the International Topical Meeting on Probabilistic Safety Assessment, Park City, Utah, September 29-October 3, 1996.
- S. Hagen, et al., "Influence of Reflood in the CORA Severe Fuel Damage Experiments", Heat Transfer and Fuel Behavior in Nuclear Reactor Accidents, 27th ASME/AIChE/ANS National Heat Transfer Conference, Minneapolis, July 29-31-1991, AIChE Symposium Series 283, Vol. 87, pp. 120-129.