Transient Analysis Needs for Generation IV Reactor Concepts

L. J. Siefken and E. A. Harvego
Idaho National Engineering and Environmental Laboratory

Abstract

The importance of nuclear energy as a vital and strategic resource in the U. S. and world's energy supply mix has led to an initiative, termed Generation IV by the U.S. Department of Energy (DOE), to develop and demonstrate new and improved reactor technologies. These new Generation IV reactor concepts are expected to substantially improve the economics, safety, proliferation resistance and waste characteristics of current generation reactors. Although a number of light water reactor concepts have been proposed as Generation IV candidates, the majority of proposed designs have fundamentally different characteristics than the current generation of commercial LWRs operating in the U.S. and other countries. This paper presents the results of a review of these new reactor technologies and defines the transient analyses required to support the evaluation and ultimate development of the Generation IV concepts. The ultimate objective of this work is to identify and develop new analysis tools and capabilities needed by INEEL to support DOE's Generation IV initiative.

1. Introduction

At this stage in the development of Generation IV reactors, licensing analysis requirements for these reactors have not been completely defined by the United States Nuclear Regulatory Commission (USNRC). However, just as calculations are required of the transient behavior of the current generation of reactors following a broad range of initiating events (USNRC 1981), so similar requirements are expected for Generation IV reactors. For the current generation of reactors, the initiating events required for consideration include; (1) break in coolant system piping, (2) anticipated transient without scram, (3) ejection of reactor control rods, (4) inadvertent opening of a valve, (5) break in shaft of coolant pump, (6) startup of an inactive coolant loop, and (7) loss of off-site power (Greene et al 2001). In general, these initiating events are any event that adversely perturbs the reactor during its normal state of power production. While these general categories of initiating events and the resulting transient responses may not be appropriate for all of the different Generation IV reactor concepts, they do provide a basis for assessing the vulnerability of the different designs to recognized potential accident initiating events, and provide a starting point for the evaluation of other potential initiating events that may be unique to a particular design concept.

The following sections provide a discussion of some of the Generation IV reactor concepts evaluated in this study, their analysis needs, and the transient analysis capabilities required to address these needs. Section 2 of this paper provides a brief description of representative designs in four general categories of Generation IV reactors. Section 3 presents a more detailed description of the designs of reactors in each category, their requirements for transient analyses, and the extensions in modeling capability required. Section 4 then summarizes the extensions required to RELAP5-3D and SCDAP/3D for the transient analyses of Generation IV reactors, and presents an arrangement for completing these extensions. Section 5 describes the integration of other computer codes and models with RELAP5-3D and SCDAP/3D to achieve the capability for efficient front to back analysis of Generation IV reactors. Section 6 describes ways in which user efficiency can be improved. The conclusions are presented in Section 7.

2. Range of Designs Proposed for Generation IV Reactors

Generation IV reactor designs can be grouped into four general categories. These four general categories are (1) gas-cooled reactors, (2) liquid-metal-cooled reactors, (3) molten salt reactors, and (4) light water reactors. After reviewing a number of reactor designs in each of these categories, it was concluded that representative designs in each of these general categories demonstrated characteristics that were common to most of the designs in a particular category. This observation led to the decision to focus the evaluation of transient analysis needs on one or two representative designs in each of the four general reactor categories. This approach allowed for an in-depth evaluation of representative designs in each category, while at the same time making the task of defining general analysis requirements more manageable.

In the category of gas-cooled reactor concepts, a pebble bed reactor (Brey 2000, Brey 2001, Yamashita 1990, Gittus 1999, McNeill 2001), and a graphite-block reactor (McCardell et al 1990, DOE 1994, Kunitomi et al 1998) core design were selected for more detailed evaluation. These designs are candidates for Generation IV reactors because they offer a very efficient conversion of nuclear power to electrical power as well as inherent safety features. Both reactor designs use direct Brayton cycle gas turbines for electric power generation and have an energy conversion efficiency of 40% to 45%. The Brayton cycle was selected for both concepts over the traditional Rankine cycle because the higher potential cycle efficiency is thought to more likely meet the "Competitive Busbar Cost" goal for Generation IV reactors. The graphite moderator material and gas (helium) coolant for the two selected reference designs are a common feature for all the designs in this category, and are the most important features in determining analysis requirements for reactors in this category.

In the category of liquid-metal-cooled reactors, both lead-bismuth (Pb-Bi) (MacDonald et al 2000, Sekimoto and Su'ud 1994, Spencer et al 2000, Weaver et al 2001), and sodium-cooled (Boardman 2000) reactors were chosen for more detailed evaluation. As will be discussed later, the need to evaluate the two liquid-metal coolants was necessary because of the vastly different properties and behavior of these coolants under normal and transient operating conditions. Since these two basic designs may have several different fuel composition and coolant configurations, evaluations were also made of the affect of these design parameters on reactor transient response and operating limits.

Although a number of molten salt reactors have been proposed as potential Generation IV concepts (Robertson 1971, Gat and Dodds 1997, Mitachi et al 1999), the viability of these reactor designs remains to be shown. However, these designs are being proposed because they offer the possibility for extremely safe production of electricity as well as having proliferation resistant attributes. For these reasons, and because of some very unique analysis requirements, a representative molten salt reactor concept was selected for more detailed evaluation. The common characteristic of these concepts is the use of a molten salt as the primary working fluid, with a fuel (Th-U) mixed into the fluoride salt working fluid. Although there are potential variations in the salt working fluid and fuel, issues associated with freezing and thawing of the fuel/working fluid, flow blockages, and reactivity events are common concerns for this group.

A number of light water reactor designs have been proposed as Generation IV candidates. Among these designs are (1) Supercritical Pressure Fast Reactor (SPWR) (Oka et al 1995, Jevremovic et al 1996, Kitoh et al 1998, Mukohara et al 1999, MacDonald et al 2001), (2) International New Generation Reactor (IRIS) (Carelli et al 2000, Carellli et al 2001), (3) Simplified Boiling Water Reactor (SBWR) (Upton et al 1993, Ishii 1999, Rao and Gonzalez

2000, Brettschuh 2001), (4) Multi-Application Small Light Water Reactor (MASLWR)(Modro et al 2000), and (5) Advanced Pressurized Water Reactor (AP1000) (Westinghouse 2000, Winters 2000). Although many of the transient analysis capabilities developed for the analysis of current generation light water reactors (LWRs) can be utilized in the analysis of these various Generation IV LWR concepts, LWRs operated above the critical pressure of water present some unique challenges to our current analysis capabilities, as will be discussed later in this paper.

The basic features or characteristics of several representative Generation IV reactor designs in each of the four general categories are described in Table 1. The abbreviations used in this table are defined in Table 2.

Table 1. Features of various proposed Generation IV reactors

Feature of reactor	**Proposed Generation IV Reactor**							
	Light water			Gas cooled		Liquid metal		Salt
	SBWR AP1000 MASLWR	IRIS	SPWR	PB-HTGR	BT-HTGR	HMFR	S-PRISM	MSR
Composition of primary coolant	H_2O	H_2O	H_2O, p>25 MPa	He	He	Pb-Bi	Na	Th-U
Composition of fuel	UO_2	UO_2 or MOX	MOX	UO_2	UO_2	Pu-Zr, UN	MOX	Sa
Configuration of fuel and surrounding material	Rod/f	Rod/f	Rod/f	Ball/C	Rod/C	Rod/f	Rod/f	liq
Neutron spectrum	mod	mod or hard	hard	mod	mod	hard	hard	mod and hard
Location of primary coolant loop	In-ves except AP1000	In-ves	Ex-ves	Ex-ves	Ex-ves	In-ves	In-ves	Ex-ves
Driving force for primary coolant	NC except AP1000	pump & NC	pump	tur-cmp	tur-cmp	pump or NC	pump	pump
thermal cycle	In-Dir except SBWR	In-Dir	Dir	Dir	Dir	In-Dir	In-Dir	In-Dir
Thermal efficiency (%)	~30	~30	45	40	40	39	40	44
Passive transfer of shutdown decay heat to large pool of water, air, or earth?	Yes	Yes	No	Yes	Yes	Yes	Yes	No
Active emergency cooling system?	Yes	Yes	Yes	No	No	No	No	No
Minimum size of reactor (MWe)	600, 1000, 20	100	1500	100	100	100	760	1000

Table 2. Definition of abbreviations used in Table 1.

Abbreviation	Definition
Ball/C	400,000 fuel particles with diameter of 0.5 mm, each coated with graphite, contained in 60 mm ball with graphite matrix, and outer surface of ball in contact with coolant
Cmp/C	Rod-shaped compact of fuel particles with diameter of 0.47, each fuel particle coated with layer of ZrC or other material, and compact embedded in graphite block, and flow channels for coolant inside block.
Dir	Direct power cycle, electricity generating turbine driven by primary fluid, no steam generator
ex-ves	Part of primary coolant loop, such as steam generators or pumps, are outside of reactor vessel
In-Dir	Indirect power cycle, electricity generating turbine driven by fluid other than primary fluid, steam generator used
In-ves	Entire primary coolant loop is inside reactor vessel
liq	liquid
mod	Moderated (thermal) neutron flux
MOX	Mixture of UO_2 and PuO_2
NC	100% of driving force for primary coolant is supplied by buoyancy force (natural circulation)
p	Pressure (MPa)
Rod/f	Fuel with cladding in configuration of rod and outer surface of rod in contact with fluid
Sa	Fuel salt composed of LiF-BeF_2-ThF_4-UF_4

3. Transient Analysis Requirements for Various Categories of Generation IV Reactors

The licensing of any proposed new nuclear reactor concept will require the evaluation of the behavior of the reactor over a broad range of potentially adverse events. Although the specific analysis requirements may vary, as a minimum, new designs will be required to demonstrate acceptable response characteristics for a broad range of potential initiating events similar to those considered in the licensing of current generation light water reactors. For current generation reactors, the initiating events required for consideration include: (1) breaks in the primary coolant system piping, (2) anticipated transients without scram, (3) ejection of reactor control rods, (4) inadvertent opening of a valve, (5) break of a reactor coolant pump shaft, (6) startup of an inactive coolant loop, and (7) loss of off-site power.

The following sections of this paper describe some of the features of reactors within the four general categories of Generation IV reactors, potential transients events relating to the safety of these concepts, and the analysis capabilities needed to address these events.

3.1 Gas-Cooled Reactors

Two basic HTGR core designs were considered in this study. The first type, namely the pebble-bed core, has the fuel configured as a deep bed of porous pebbles through which the helium coolant is forced (Yamashita 1990, Gittus 1999, Brey 2001, McNeill 2001). The second type of core design, namely the block-type or prismatic-type, has the fuel configured as rods inside blocks of graphite (McCardell et al 1990, DOE 1994, Kunitomi et al 1998). Representative designs for the pebble-bed and graphite-block core designs are shown in Figures 1 and 2, respectively. For the pebble bed HTGR, the fuel pebbles are spherical in shape and have a diameter of about 60 mm. Each fuel pebble is composed of many small particles of uranium dioxide coated with carbon and silicon carbide. The coating on the fuel particles retains fission products. The fuel particles are placed in a matrix of graphite. Fuel pebbles can be continuously fed into the top of the operating reactor and then move downward due to gravity. The block-type HTGR has similar coated fuel particles in a matrix and configured as rods instead of as pebbles. The rods of fuel particles are places in graphite blocks.

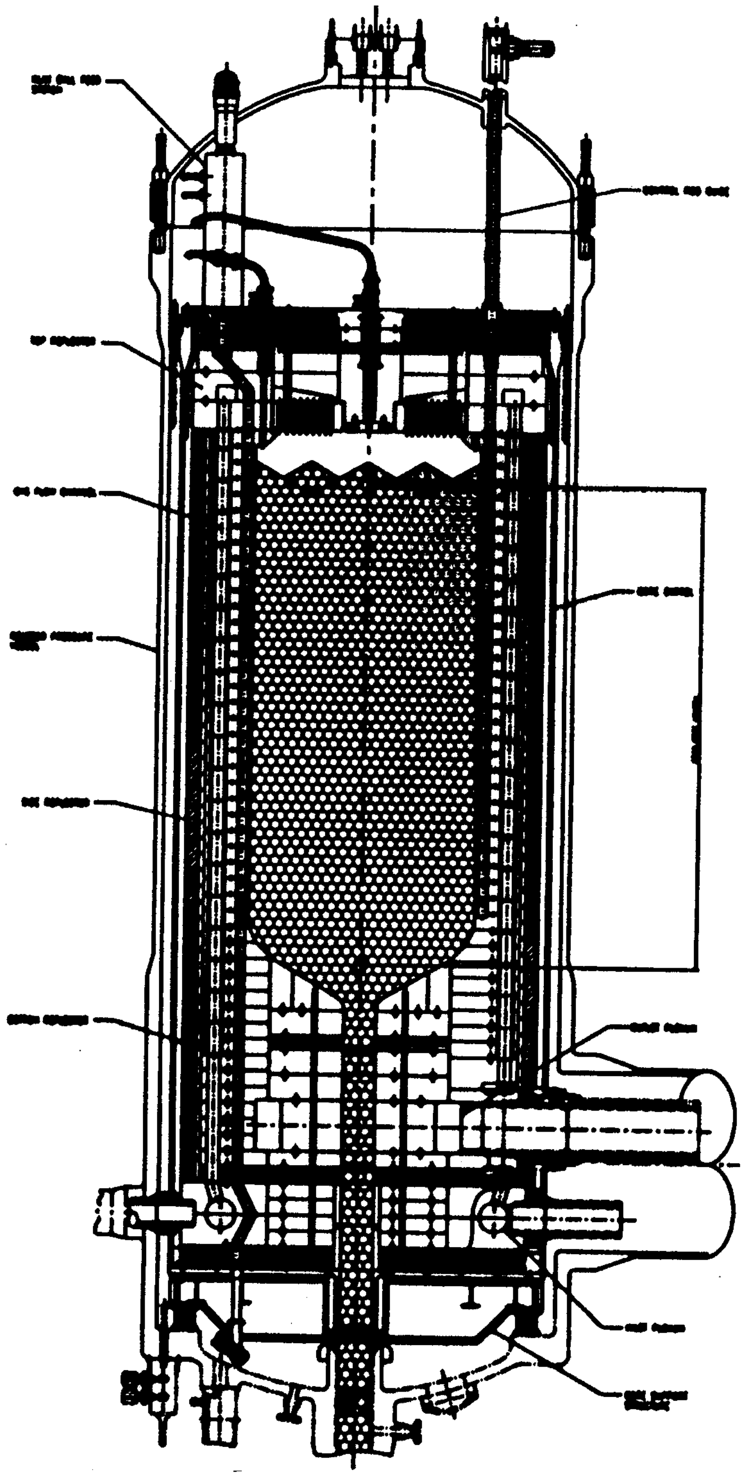

Figure 1. Reactor vessel for Pebble Bed High Temperature Gas Reactor

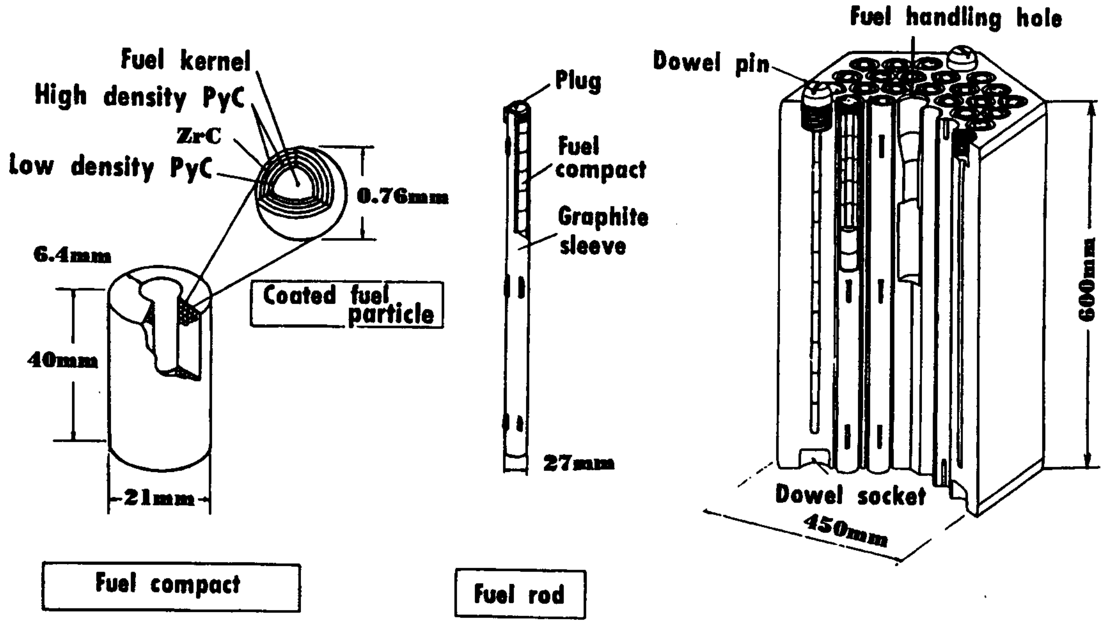

Figure 2. Configuration of reactor core for block-type High Temperature Gas Reactor.

The direct Brayton thermodynamic cycle was utilized by the HTGRs in this study. In this thermodynamic cycle, the helium heated by the reactor fuel flows out of the bottom of the reactor vessel, then drives a set of turbo-compressors before expanding into the turbine-generators. The expanded helium then passes through a regenerative heat exchanger and a water-cooled precooler before being repressurized in a set of turbo-compressors, regeneratively heated, and returned to the top of the reactor vessel. This thermodynamic cycle yields energy conversion efficiency in the range of 40% to 45%. The pressure of the helium in the reactor vessel is 7 MPa . The temperature of the helium entering the top of the core is 775 K and its temperature exiting the bottom of the reactor core is 1170 K.

Passive cooling systems have been designed for both the pebble bed and block-type HTGR. For the pebble-bed HTGR, decay heat is transferred by conduction, radiation and natural convection to the ground around the reactor building. The reactor building is designed to limit the ingress of air and the oxidation of graphite in the event of the rupture of a pipe (Gittus 1999). For the block-type HTGR, decay heat is transferred by conduction to the outer surfaces of the reactor core and then by radiation and natural convection to the reactor vessel (Kunitomi 1998). The reactor vessel is cooled by water surrounding it.

The evaluation of the safety of a HTGR requires the capability to calculate the transient behavior of the reactor following a broad range of initiating events. While the designs of HTGRs are radically different than those of LWRs, they are nevertheless vulnerable to accident initiating events similar to those occurring in a LWR. These initiating events include (1) pipe breaks, (2) loss of off-site power, (3) loss of generator load, and (4) ejection of control rods. Additional safety concerns for HTGRs include (1) ingress of water or air in the event of a pipe break, and (2) failure in gas turbomachinery.

A pipe break in an HTGR results in the possibility for ingress of water or air into the reactor core and thus the possibility of oxidation of graphite components in the reactor core (DOE 1994). The ingress of liquid water into the reactor core enhances neutron moderation and increases the reactivity of the core and the possibility of an excursion in reactor power. The ingress of air or steam into the reactor core causes oxidation and heat up of graphite and the hydrolysis of initially failed fuel particles. The oxidation of graphite releases fission products trapped in the graphite and reduces the strength of the graphite. The hydrolysis of failed fuel particles results in fission product release from these particles. For the direct Brayton-cycle designs, the sources for moisture ingress include the precooler, intercooler, and the shutdown cooling system heat exchangers. Thus, the transient analyses of HTGRs involves the calculation of the distance of penetration of water/air into the core.

An additional safety concern for HTGRs in the event of a pipe break is the damage to the reactor building caused by the hot gas escaping from the break. The rupture of a pipe connected to the reactor pressure vessel may cause formation of a high speed jet of hot gas that causes serious damage to the reactor building (van Heek 2001). The pressure and thermal loads imposed on the reactor building require the calculations of a multidimensional fluid behavior code. The high speed jet imposes both a pressure and thermal load on the reactor building.

An important safety concern for the direct Brayton-cycle HGTR is a possible failure of the gas turbomachinery (DOE 1994, Ball 2000b). The history of gas turbine operations indicates that parts from a gas turbine may break off and block flow through the turbine passages. The blockage of flow through the turbine could result in a large axial pressure drop that damages the core support structure and challenges the safety functions of heat removal and control of core heat generation. A blockage could also cause a reversal of flow through the core, which in turn may cause an ejection of control rods and challenge control of core heat generation (DOE 1994). Transient analyses of the behavior of a direct cycle HTGR following a turbine deblading event have been performed using the RELAP5/MOD3 code (DOE 1994).

While RELAP5-3D and SCDAP/3D codes have the capability to model a significant part of a HTGR after an accident initiating event (DOE 1994), nevertheless some features of the HTGR cannot be adequately represented by these codes. The features that cannot be adequately represented are (1) the reactor core, (2) passive transfer of decay heat from the reactor core to the environment beyond the reactor building, (3) configurations allowing for possible localized multidimensional fluid behavior, and (4) high temperature of coolant exiting the reactor core and thus the possibility for damage to the reactor building in the event of a pipe break. These unique features of a HTGR require new models to calculate the transient behavior of the reactor following accident initiating events. These new models result in the capability to calculate the temperature histories after accident initiating events of the reactor core, reactor vessel, and reactor building, which are fundamental measures of the safety of an HTGR following an adverse event such as a break in a pipe connected to the reactor vessel (DOE 1994, Gittus 1999, Kadak 2001, van Heek 2001).

The calculation of the transient behavior of the reactor core of a HTGR requires several extensions in modeling. For the pebble bed HTGR, extensions are required to model (1) conduction of heat through spherical fuel/graphite pebbles, (2) convective heat transfer and flow losses in bed of fuel pebbles, (3) oxidation of fuel pebbles, and (4) heat transfer by conduction, radiation, and natural convection through a bed of fuel pebbles to the outer surfaces of the reactor core. For the block-type HTGR, these extensions in modeling are similar, except that extensions are required for modeling the removal of decay heat by conduction through the graphite blocks to the outer surfaces of the reactor core.

The calculations of the transient thermal hydraulic behavior of a HTGR requires the capability to calculate multidimensional fluid behavior (Schultz 2001, van Heek 2001), and to calculate the ingress of air or water into the reactor vessel following a break in a pipe or other component. For accident initiating events with either forced flow or loss of forced flow, the possibility exists for local deficiencies in cooling that may result in hot spots in the reactor core. The identification of these local deficiencies in cooling and hot spots requires the application of a multidimensional Computational Fluid Dynamics (CFD) code. In an event resulting in complete loss of forced flow, a significant part of the removal of decay heat from the reactor core will occur by multidimensional natural circulation of the gas remaining in the reactor vessel. The modeling of this natural circulation of gas may also require the application of a CFD code. In the event of a pipe break, a jet of hot gas may impinge on the structure near the pipe break. The modeling of this jet of gas and the temperature and pressure loads it applies to the impinged structure may also require the application of a CFD code (van Heek 2001). These applications of a CFD code can be achieved by interfacing the RELAP5-3D or SCDAP/3D codes with CFDcodes such as FLUENT (Freitas 1995, Schultz 2001).

The calculation of the removal of decay heat from the reactor core of an HTGR may require multidimensional heat transfer modeling accounting for temperatures at many locations throughout the reactor system (Kadak 2001). The capability of the reactor core to endure high temperatures allows the design of a passive heat removal system involving the transfer of heat by conduction, radiation and natural convection from the inner parts of the reactor core to the inner surface of the reactor vessel, and then heat transfer by these same mechanisms from the reactor vessel to the environment beyond the reactor building. The modeling of this transfer in heat may require calculating temperatures at up to 50,000 different locations in the reactor and its surrounding environment (Kadak). The capability for modeling this heat transfer can be achieved by interfacing RELAP-3D and SCDAP/3D with a multidimensional heat transfer code such as HEATING7 (Kadak 2001).

3.2 Liquid-Metal Cooled Reactors

Liquid metal cooled fast reactors have been proposed as candidates for Generation IV reactors because they have a high thermal efficiency as well as having a fast neutron spectrum for burning actinides. The high boiling temperature of the liquid metal coolant permits high coolant temperatures, which in turn yields high overall plant efficiency (~40%) under very low system pressure. The high boiling temperature of the liquid metal coolant also has the advantage of counteracting the positive void reactivity coefficient of these reactors.

The majority of liquid metal reactors evaluated in this study used either sodium (Na) or a lead-bismuth eutectic (Pb-Bi) as the coolant. The design of the S-PRISM sodium cooled reactor (Boardman et al 2000) is shown in Figure 4 and the design of the STAR-LM Pb-Bi cooled reactor (Spencer et al 2000) is shown in Figure 5. The performance of sodium cooled reactors has been demonstrated by reactors such as the Integral Fast Reactor (Weaver et al 2001). The performance of Pb-Bi cooled reactors has been demonstrated by Russian submarine reactors and on-shore prototypes of these reactors (Weaver et al 2001).

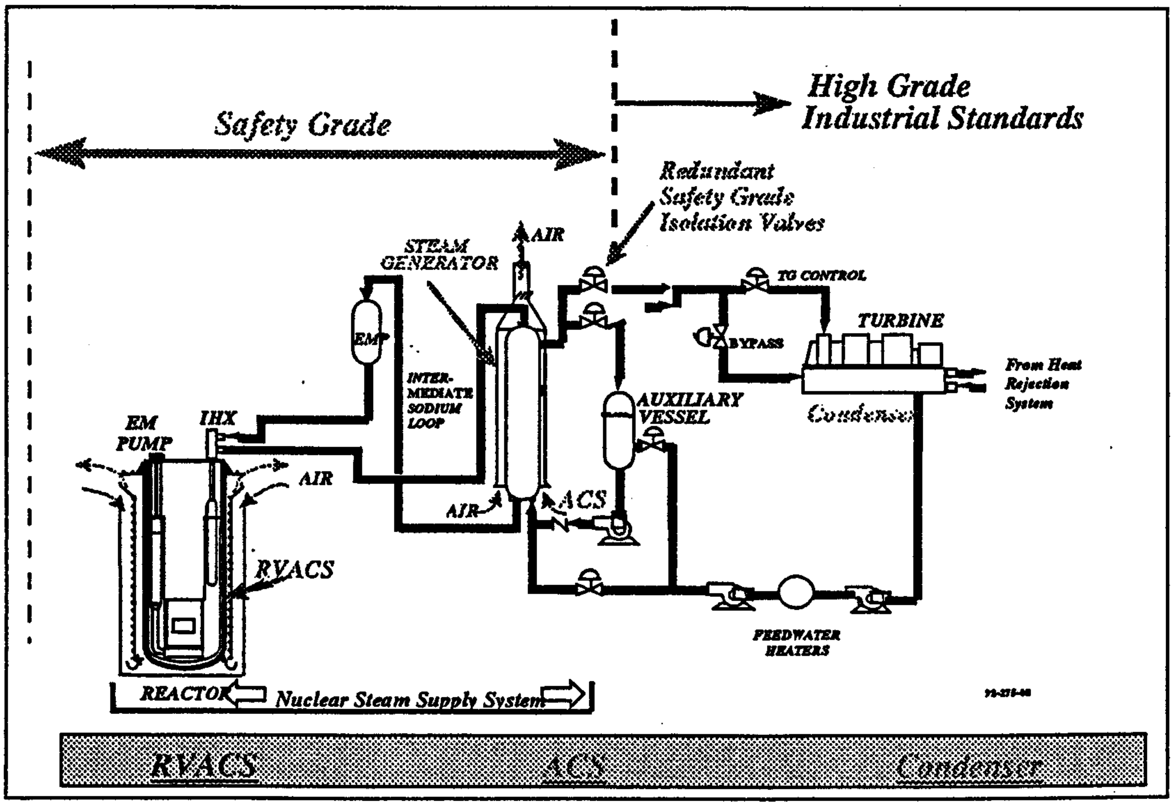

Figure 4. Schematic of S-PRISM sodium cooled reactor

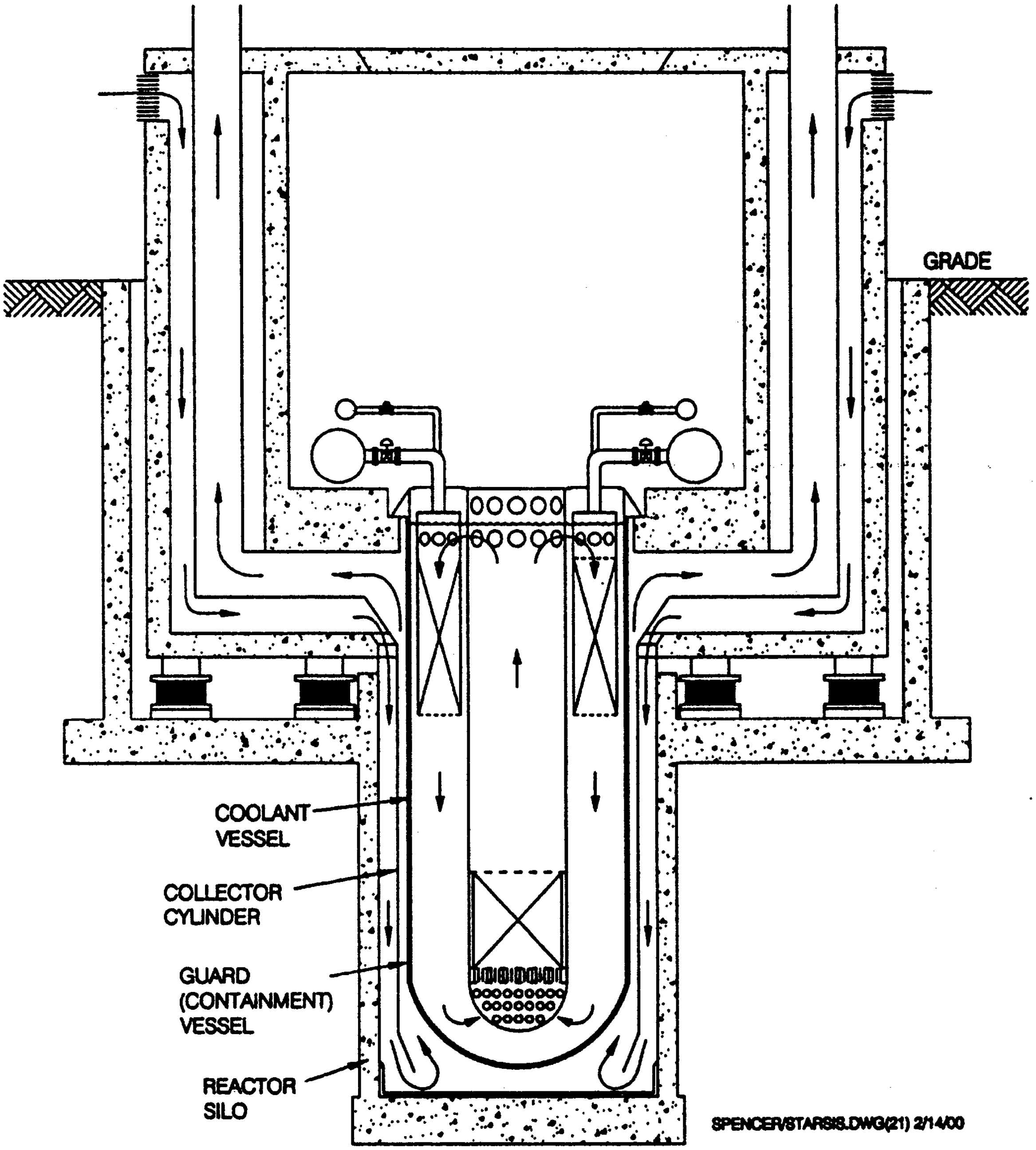

Figure 5. Cross section view of the STAR-LM Pb-Bi cooled reactor.

Sodium and Pb-Bi coolant have advantages and disadvantages. Sodium coolant has the advantages of (1) not being corrosive with structural materials, (2) having a relatively low materials cost, and (3) being based on well established technologies. Sodium coolant has the disadvantages of (1) reacting energetically with water, (2) having a low atomic number and as result a reduced neutron economy, (3) relatively low boiling temperature of 1165 K, (4) relatively low shielding against gamma-rays and energetic neutrons (5) producing a radiological hazard when irradiated (Jevremovic et al 1996), (6) solidification at a temperature significantly greater than room temperature (371 K), and (7) a relatively large volume change upon solidification. Pb-Bi coolant is superior to sodium coolant in some aspects and inferior in other aspects. Pb-Bi coolant has the advantages of (1) chemical inertness with air and water and thus compatible with a simplified containment structure, (2) high boiling temperature (1998 K) and potential for fuel rod cooling even during temperature excursions, (3) high atomic number and as a result a good neutron economy, (4) relatively high shielding against gamma-rays and energetic neutrons, and (5) a relatively small volume change upon solidification. Pb-Bi coolant has the disadvantages of (1) potentially corrosive to structural materials, (2) based on technology that is not well established, (3) solidification at a temperature significantly greater than room temperature (398 K), (4) producer of a radiological hazard (Po^{210}) when irradiated, and (5) relatively high material costs.

Both the S-PRISM and STAR-LM reactors have reactor cores consisting of an array of fuel rods. The fuel in the S-PRISM reactor may be composed of either oxidic or metallic fuel. A harder neutron spectrum and higher burnups can be achieved with metallic fuel than oxidic fuel. The fuel is clad with a ferritic alloy in order to minimize swelling associated with a high neutron fluence. The fuel in the STAR-LM reactor may be either metallic or nitride in composition. The fuel in the STAR-LM reactor is clad with stainless steel.

Both the S-PRISM and STAR-LM reactors have passive decay heat removal systems. These systems are designed to transport decay heat from the reactor core to the reactor vessel by natural circulation of the coolant in the reactor vessel and then transport the decay heat to the containment vessel and beyond by natural circulation of air and inert gases placed in the gap between the reactor and containment vessels.

The evaluation of the safety of metal cooled reactors requires the capability to calculate the transient behavior of these reactors following a broad range of initiating events. These reactors are vulnerable to accident initiating events similar to those occurring in a LWR. These initiating events include (1) pipe breaks, (2) loss of off-site power, (3) loss of generator load, and (4) ejection of control rods. Additional safety concerns for metal cooled reactors include (1) freezing of the coolant in an event causing increased heat removal from the primary coolant, (2) ingress of water into the primary coolant after rupture of a steam generator tube and the possibility of an energetic reaction, and (3) formation of voids in the primary coolant and a resulting excursion in power due to the positive void reactivity coefficient of these reactors.

While RELAP5-3D and SCDAP/3D codes have the capability to model most of the phenomena occurring in a metal cooled reactor after an accident initiating event (MacDonald and Todreas 2000), nevertheless some features of these reactors and some phenomena occurring in these reactors cannot be adequately represented by these codes. The features and phenomena that cannot be adequately represented are (1) metallic fuel composed of Zr-Pu, U-PuN, or UN, and clad with stainless steel, (2) freezing of Pb-Bi coolant and representing the blockage to coolant flow caused by the freezing, (3) inter-component and interphase heat and momentum transfer in mixtures of metal coolant and water. To resolve these deficiencies in modeling, extensions required to the RELAP5-3D and SCDAP/3D codes include (1) material properties for the fuel, (2) structural properties of the cladding, (3) model for fission gas release in the fuel, (4) model for freezing of Pb-Bi coolant and the blockage caused by the freezing, and (4) model for inter-component and interphase heat transfer in a mixture of metallic coolant, liquid water and steam.

3.3 Molten Salt Reactors

Although relatively unproven, Molten Salt Reactors (MSRs) are candidates for Generation IV reactors because they offer the possibility for extremely safe production of electricity as well as having proliferation resistant attributes (Robertson 1971, Gat and Dodds 1997, Mitachi et al 1999). The primary working fluid in these reactors contains the fuel. The Th-U fuel is homogeneously mixed in the fluoride salt working fluid. Fission products can be continuously extracted from the working fluid so as to maintain a very low decay heat level and small radiological source term. Other advantages of the MSR include a high thermal efficiency (44%) (Robertson 1971) and the burning of actinides (Gat and Dodds 1997). A disadvantage of MSRs is that maintenance of its components may be difficult due to the radioactivity in the circulating molten salt (Gromov 1997).

The core of a molten salt reactor consists of vertical graphite moderating elements and the fuel salt moving through the moderating elements. The vertical cross section of a representative design of a molten salt reactor is shown in Figure 6. Heat in the fuel salt is transferred in a heat exchanger to coolant salt in the secondary coolant loop. The heat in the coolant salt is transferred in another exchanger to steam in the tertiary loop, which contains a turbine for producing electricity. Fission products are continuously extracted from the fuel salt. One design has a maximum of ten days inventory of fission products in the fuel salt, while another design has a maximum of one day inventory of fission products (Gat and Dodds 1997). The extraction of fission products greatly reduces the decay heat in the fuel salt and greatly reduces the source term of the MSR.

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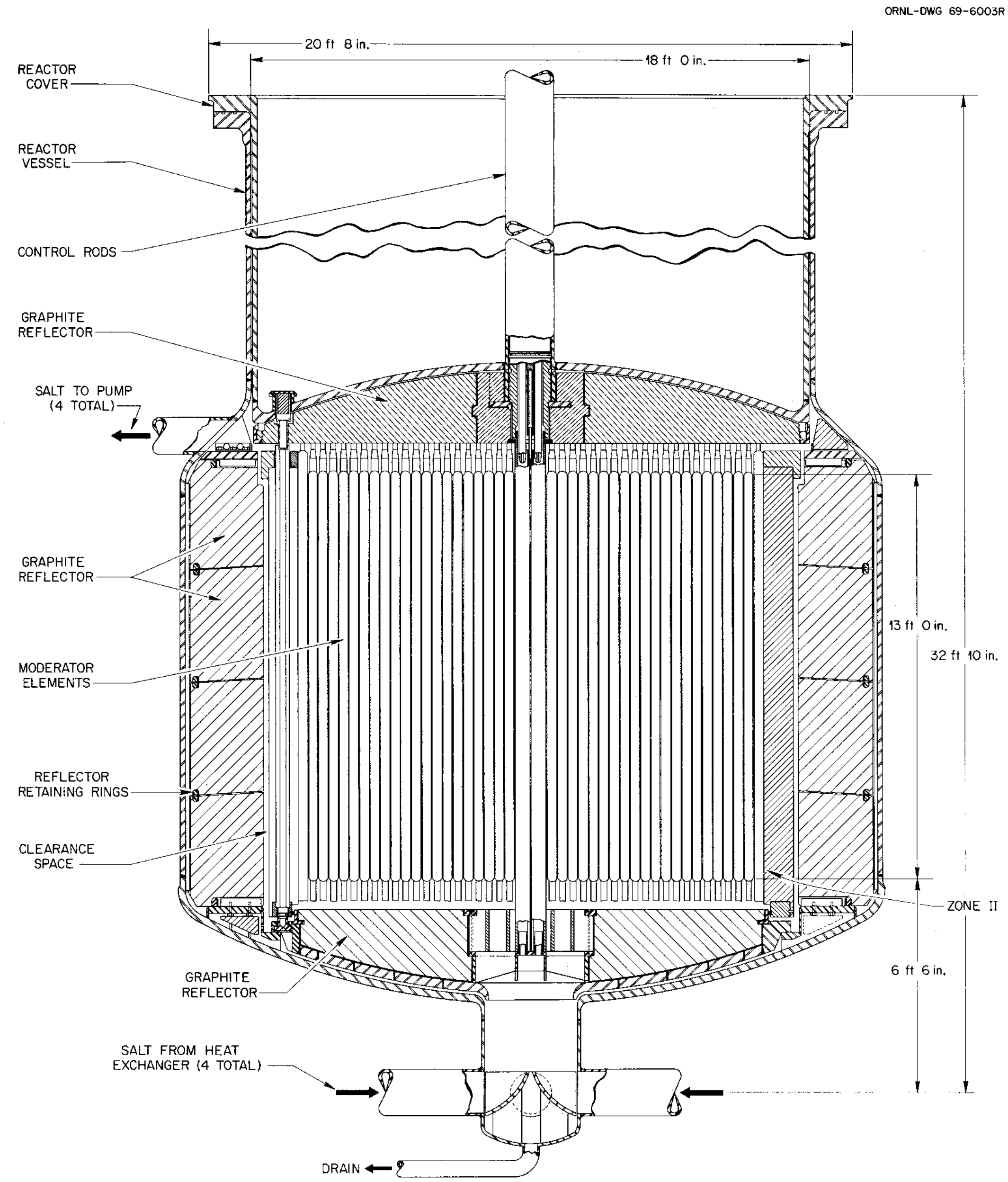

Figure 6. Cross section of reactor vessel of Molten Salt Reactor.

The fuel salt is generally composed of LiF-BeF_2-ThF_4-UF_4, with a composition of about 71.7 mole % LiF, 16 mole % BeF_2, 12 mole % ThF_4, and 0.3 mole % UF_4. The uranium is the isotope ^{235}U. During normal power production, the temperature of the fuel salt ranges from 839 K to 978 K, and its pressure is about 0.5 MPa. The liquidus temperature of fuel salt is 772 K and its boiling temperature is 1400 K at 0.1 MPa.

A drain tank for the fuel salt is connected to the bottom of the reactor vessel by a drain line having a freeze valve. This freeze valve can be an ordinary section of piping, exposed to a cooling stream of environmental gas to the extent that it creates a frozen plug of fuel salt. When the temperature of the fuel salt in the reactor vessel rises above a threshold temperature, the frozen plug melts and the fuel salt in the reactor vessel drains to a storage tank. At the discretion of the plant operator, the frozen plug can be thawed in a few minutes. The frozen plug would also thaw in the event of a major loss of electric power, or failure of the plug cooling system. This drain system is activated in case of a leak in the fuel salt loop. It also provides for safe storage of salt during maintenance operations.

Nearly all components containing fuel and coolant salt are constructed of Hastelloy-N, which is composed mostly of nickel, molybdenun, chromium, and iron. This alloy has the capability to resist the diffusion through it of the tritium in the fuel salt.

The evaluation of the safety of molten salt reactors requires the capability to calculate the transient behavior of these reactors following a broad range of initiating events. These reactors are vulnerable to accident initiating events similar to those occurring in a LWR. These initiating events include (1) pipe breaks, (2) loss of off-site power, (3) loss of generator load, and (4) ejection of control rods. Additional safety concerns for molten salt reactors include (1) coalescing of gases and volatile materials in the primary coolant into bubbles and then the collapse of these bubbles in the core region, resulting in a reactivity initiated accident due to the negative void reactivity coefficient of these reactors (Gat and Dodds 1997), (2) possibility of slug of cold fuel suddenly entering the core, resulting in a reactivity initiated accident due to the large negative temperature reactivity coefficient (Gat and Dodds 1997), (3) freezing of the primary coolant and blockage to coolant flow caused by the freezing, (4) heat transfer in the tertiary water coolant system operating at supercritical pressure, (5) properly timed melting during an accident of the frozen plug of fuel at the bottom of reactor vessel, and (6) containment of tritium, which is radioactive and produced at a relatively high production rate in the fuel salt due to the abundance of lithium (Robertson 1971).

While the RELAP5-3D and SCDAP/3D codes have the capability to model most of the phenomena occurring in a molten salt reactor after an accident initiating event, nevertheless some features of these reactors and some phenomena occurring in these reactors cannot be adequately represented by these codes. The features and phenomena that cannot be adequately represented are (1) primary coolant composed of LiF-BeF_2-ThF_4-UF_4 and secondary coolant composed of $NaBF_4$-NaF, (2) volumetric heating of the primary coolant due to the fissile isotopes in the coolant, (3) freezing of the primary coolant and blockage to flow caused by freezing, (4) heat transfer in water above the supercritical pressure, and (5) melting of the frozen plug of fuel salt at the bottom of reactor vessel after an initiating event causing heatup of the primary coolant. To resolve these deficiencies in modeling, the following extensions are required to the RELAP5-3D and SCDAP/3D codes (1) thermal and transport properties for the fuel and coolant salts, (2) model for volumetric heating of the primary coolant due to the fission and decay heat produced in the coolant, (3) model for the freezing of the primary coolant and the blockage caused by freezing, (4) heat transfer correlations for water above the supercritical pressure, and (5) model for the melting of the frozen plug of fuel salt at the bottom of the reactor vessel.

3.4 Light Water Reactors

While LWR candidates for Generation IV reactors have some common characteristics, such as a primary coolant composed of water and a reactor core with of UO_2 fuel in rod-like geometry, nevertheless other characteristics may vary significantly. Some of the differences in proposed Generation IV LWR designs are shown in Table 3. The acronyms identifying these reactors are defined in Table 4. Some of the LWR candidates have the primary coolant loop within the reactor vessel so as to eliminate the possibility of a loss of coolant accident and reduce the probability of other accident sequences. The use of natural convection (NC) as a driving force for the primary coolant is used in some of the designs to reduce reliance on pumps. A direct thermal cycle in which the coolant from the core outlet flows directly to the electricity producing turbines is used by some of the LWR designs, while other designs use a steam generator to heat the fluid that drives the turbines. Some of the LWR candidates for Generation IV reactors have a containment system that enhances passive cooling. Some of the candidates have a tight lattice reactor core so as to produce a hard neutron spectrum that burns actinides and extends the reactor core lifetime, and thus reduces radioactive waste and decreases operating cost. The cost of initial investment is less for a small LWR than a large LWR; as a result, some of the LWRs are designed as small in size as 100 MWe. One of the candidates operates with a primary coolant system pressure above water's critical pressure of 22.1 MPa so as to reduce cost by eliminating steam generators and increase thermal efficiency by operating at a higher coolant temperature at the outlet of the reactor core. Most of the candidates have active emergency cooling systems in addition to passive cooling systems.

Table 3. Some variations in designs proposed for LWR versions of Generations IV reactors.

Feature of reactor	Some proposed LWR versions of Generation IV reactors				
	IRIS	SBWR	AP1000	MASLWR	SPWR
Composition of primary coolant	H_2O	H_2O	H_2O	H_2O	H_2O
Pressure of primary coolant(MPa)	17.24	~7	15.5	7	25 ($>p_{crit}$)
Composition of reactor fuel	UO_2 or UO_2-PuO_2	UO_2	UO_2	UO_2	UO_2-PuO_2
Configuration of reactor fuel	rod-like	rod-like	rod-like	rod-like	rod-like
Location of primary coolant loop	in-vessel	ex-vessel	ex-vessel	in-vessel	ex-vessel
Driving force for primary coolant	Pumps + NC	NC	Pumps	NC	Pumps
Thermal cycle	in-direct	direct	in-direct	in-direct	direct
Thermal efficiency (%)	34	~30	~30	~30	45
Passive removal of shutdown decay heat?	yes	yes	yes	yes	no
Neutron spectrum	moderated or hard	moderated	moderated	moderated	hard
Lifetime of reactor fuel (years)	8	2	~2	?	~2
Minimum size of a reactor module (MWe)	100	~1000	1000	100	1500

Table 4. Reactor name corresponding with acronym in Table 3 and reference for reactor design.

Acronym	Name of reactor	Reference for design
IRIS	International Reactor Innovative and Secure	Carelli et al 2001
SBWR	Simplified Boiling Water Reactor	Rao and Gonzalez 2000, Brettschuh 2001
AP1000	Atomic Plant 1000	Schulz et al 2001
MASLWR	Multi-Application Small Light Water Reactor	Modro et al 2000
SPWR	Supercritical Pressure Water Reactor	Oka et al 1995, Suhwan et al 2001

The safety of LWR versions of Generation IV reactors has been enhanced by changes in the configuration of the primary coolant system. Those LWRs with primary coolant loops within the reactor vessel (IRIS and MASLWR) eliminate the potential for loss-of-coolant accidents caused by a break in the primary coolant system piping. These primary coolant systems, therefore, require less containment capacity, allowing for a smaller containment design. The spacing of components in the reactor core have been adjusted in some of the LWRs (IRIS, MASLWR, SBWR) so a significant part or all of the circulation of the primary coolant is driven by natural convection. These design changes prevent or reduce the probability of accidents initiated by events such as a locked pump rotor or loss of pump power. Natural circulation is enhanced by adjustments such as (1) increasing the spacing between fuel rods, (2) decreasing the height of reactor core, (3) decreasing fuel rod power so sufficient cooling and reduced flow losses can be achieved with a reduced core flow rate, (4) increasing the extent of boiling in the reactor core, (5) increasing the flow path between the downcomer and lower plenum, and (6) increasing the height of the reactor vessel to enhance the driving head for natural circulation. The possibilities for uncovery of the reactor core have been reduced in some of the LWRs by increasing the inventory of water in the reactor vessel above the fuel rods. In the Supercritical Pressure Water Reactor (SPWR), accidents initiated by a failure in the steam generator have been eliminated by removing this component from the reactor system.

The safety of candidate Generation IV LWRs have also been increased by changes to the configuration of the reactor containment. In general, the containment is designed so decay heat can be removed in a passive manner with simple heat exchangers. The containment may include large pools of water that condense steam to reduce the pressure load on the containment. In general, the containment is inerted with nitrogen to prevent hydrogen deflagration. In the case of the IRIS, the containment is pressurized to reduce the pressure differential that drives coolant out of a break and into the containment (Carelli et al 2001). In the case of one version of the SBWR, the containment has been designed with sufficient capacity to accommodate the hydrogen produced by oxidation of 100% of the reactor core (Brettschuh 2001).

The design of the SPWR is based on the behavior of water above the critical pressure (22.1 MPa). In one SPWR design, water at the supercritical pressure of 25 MPa circulates through the reactor vessel and power generating turbines (Oka et al 1995, Jevremovic et al 1996, Kitoh et al 1998, Mukohara et al 1999, MacDonald et al 2001a). For water above the critical pressure (22.1 MPa), the concept of boiling does not exist. This is because water above the critical pressure is a single-phase fluid with no discernible boundary between liquid and gas phases. As a result, convective heat transfer is not deteriorated by dryout such as occurs at subcritical pressure when the heat flux exceeds the critical heat flux. The specific heat exhibits a peak at the pseudo-critical temperature (~658 K). A plot of specific heat as a function of temperature is shown in Figure 7. The temperature of the coolant varies from about 580 K at the core inlet to about 750 K at the core outlet. The high temperature of the coolant at the core outlet results in a high thermal efficiency. Since convective heat transfer at supercritical pressure is proportional to specific heat to the 0.4 power, the heat transfer coefficient is large for temperatures around the pseudo-critical temperature (Oka 1995). The heat transfer and enthalpy change with respect to temperature in the range of the pseudo-critical temperature is so large that much heat is removed with low coolant flow. The density change with respect to temperature is also large around the pseudo-critical temperature. A plot of density as a function of temperature for a pressure of 25 MPa is also shown in Figure 7.

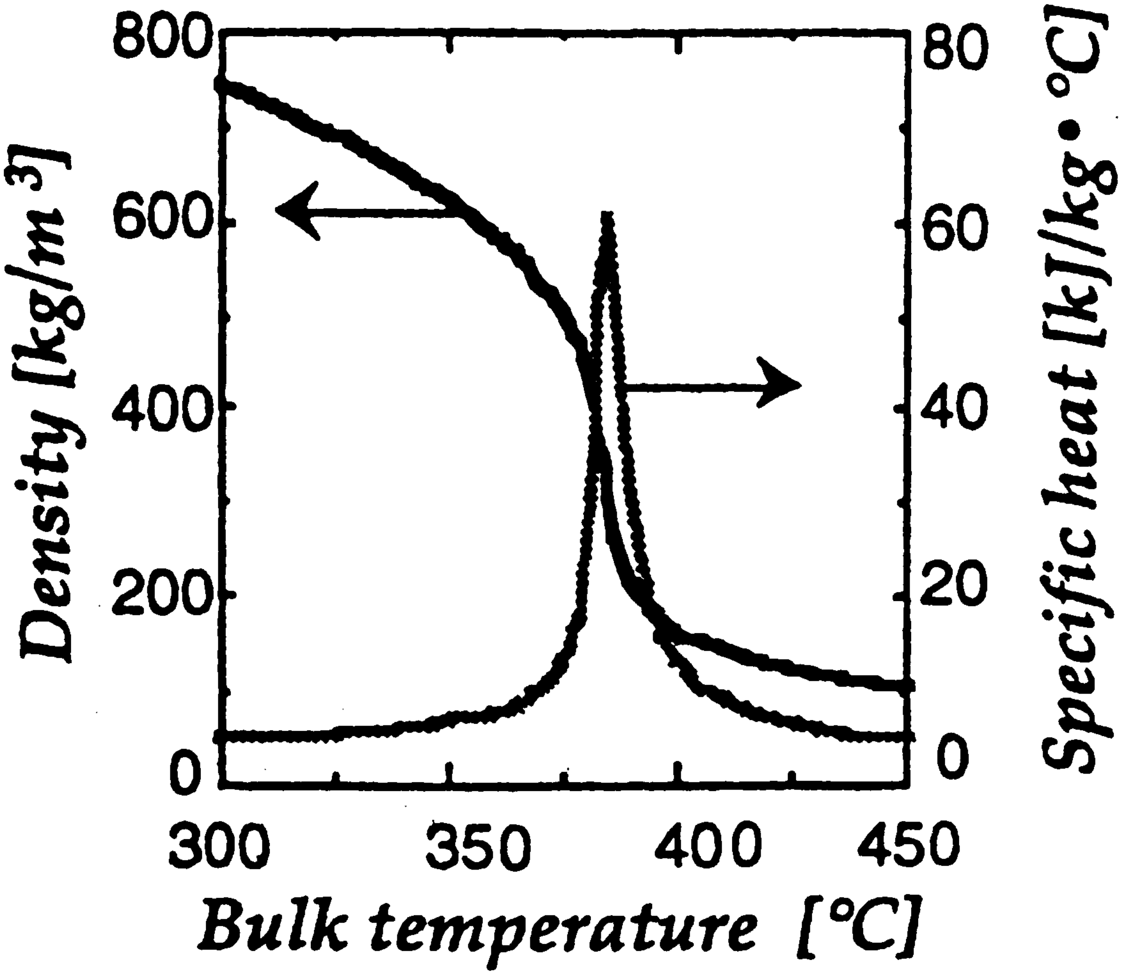

Figure 7. Density and specific heat as function of temperature for water at pressure of 25 MPa.

The evaluation of the safety of LWR versions of Generation IV reactors requires the capability to calculate the transient behavior of these reactors following a broad range of initiating events. These reactors may be vulnerable to accident initiating events similar to those occurring in Generation II LWRs. These initiating events include (1) pipe breaks, (2) loss of off-site power, (3) loss of generator load, and (4) ejection of control rods. An additional safety concern for Generation IV LWRs is the Minimum Departure fom Nucleate Boiling Ratio (MDNBR) for reactors relying mostly on buoyancy forces for circulation of the primary coolant, such as the IRIS and SBWR, or in reactors with a tight lattice reactor core so as to allow a hard neutron spectrum, such as in one version of the IRIS.

While RELAP5-3D and SCDAP/3D codes have the capability to model most of the phenomena occurring in Generation IV LWRs after an accident initiating event, nevertheless some features of these reactors and some phenomena occurring in these reactors cannot be adequately represented by these codes. The features and phenomena that cannot be adequately represented are (1) mixed oxide fuel in the supercritical pressure water reactor and IRIS reactors, and metallic fuel in the IRIS reactor, (2) Ni-based alloy cladding for fuel in the supercritical pressure water reactor, (3) pellet-cladding mechanical interaction in the supercritical pressure water reactor, (4) heat transfer in water above the supercritical pressure, and (5) potential localized cooling deficiencies in reactors with natural circulation of primary coolant or tight lattice of reactor core. To resolve these deficiencies in modeling, the following extensions are required to the RELAP5-3D and SCDAP/3D codes (1) material properties for mixed oxide fuel, metallic fuel, and Ni-based alloy fuel cladding, (2) model for pellet-cladding mechanical interaction, (3) heat transfer correlations for water above the supercritical pressure, and (4) interfacing with a code performing a sub-channel thermal hydraulic analysis.

4. Summary of New Capabilities Required for Transient Analyses of Generation IV Reactors

The transient analyses of Generation IV reactors require advancements in the current capabilities of RELAP5-3D and SCDAP/3D as described in the previous sections. This section summarizes these advancements. A series of relatively small development efforts applied to the RELAP5-3D and SCDAP/3D codes results in a gradual expansion in the range of designs of Generation IV reactors that can be analyzed. Table 5 shows one possible order for these development efforts and the reactor designs for which the development efforts are applicable. The order selected for model development starts with the Generation IV designs that are relatively small extensions of Generation II reactors. The focus of subsequent development effort follows the order of (1) IRIS, (2) Pebble Bed HTGR, (3) Block-type HTGR, (4) HMFR, (5) S-PRISM, (6) SPWR, and (7) MSR. The transient analyses of reactors such as the AP-1000 and SBWR can be performed without extensions to RELAP5-3D and SCDAP/3D.

Table 5. Extensions in modeling capability required for basic transient analysis of broad range of Generation IV reactors.

Extension in modeling capability	Reactor design requiring extension						
	IRIS	PB-HTGR	BT-HTGR	HMFR	S-PRISM	SPWR	MSR
Thermal and fission gas behavior in fuel composed of mixture of UO_2 and PuO_2	x					x	
Sub-channel thermal hydraulic analysis	x						
Transport of heat, flow losses, and oxidation in reactor core composed of graphite pebbles with coated fuel particles		x					
Transport of heat in reactor core composed of rods with coated fuel particles inserted in graphite blocks			x				
Multidimensional fluid behavior in reactor core or jet of gas resulting from pipe break		x	x				
Ingress of air/water into reactor vessel after break in pipe or other component		x	x				
Multi-dimensional heat transfer through complex shaped system		x					
Thermal, chemical, structural, and fission gas behavior in metallic fuel clad with stainless steel				x	x		
Freezing of coolant				x			x
Heat and momentum transfer in mixture of Pb-Bi and water or Na and water				x	x		
Convective heat transfer, $p>22.1$ MPa						x	x
Structural behavior of Ni-based fuel rod cladding						x	
Corrosion of surfaces contacted by supercritical pressure water						x	
Fuel-cladding mechanical interaction						x	
Thermal and transport properties of fuel and coolant salts, volumetric heat generation in fluid field, flow regime map							x
Melting during accident of frozen plug of fuel salt normally at bottom of vessel							x

The capability for the transient analyses of HTGRs is achieved by extensions primarily in the modeling of the reactor core and the capability for the transient analyses of metal-cooled reactors is achieved by extensions primarily in the modeling of thermal hydraulic behavior. The HTGRs have reactor core compositions and configurations radically different from those of Generation II reactors. As a result, extensions are required to model (1) conduction of heat through spherical fuel pebbles, (2) convective heat transfer from fuel pebbles, (3) oxidation of fuel pebbles, and (4) heat transfer by conduction, radiation, and natural convection through bed of fuel pebbles. The latter extension in modeling is required for the analysis of transients in which forced flow through the reactor core is lost. The metal cooled reactors have the possibility of the interaction of the metal coolant with water after an initiating event such as a rupture in a steam generator tube. As a result, extensions are required in the modeling of thermal hydraulic behavior. In particular, extensions are required to model the heat and momentum transfer occurring in a mixture of metal coolant and water. Since the coolant in Pb-Bi cooled reactors has a relatively high freezing temperature, extensions are also required to model the freezing of this coolant after initiating events causing an overcooling of the primary coolant.

5. Integration of Computer Codes for Complete Front to Back Transient Analysis

The integration of the RELAP5-3D and SCDAP/3D codes with other computer codes or subroutines is desirable in order to achieve the capability for the complete front to back transient analyses of Generation IV reactors. These other codes calculate phenomena that are not calculated by RELAP5-3D and SCDAP/3D but which may be important for evaluating the overall safety of Generation IV reactors. These phenomena include (1) multidimensional fluid behavior in a fluid field with a complex configuration, (2) sub-channel thermal hydraulic behavior in a tight lattice reactor core or a reactor core with mostly natural circulation of the coolant, (3) fission product transport and deposition, and (4) structural behavior of reactors during an earthquake. Computer codes or subroutines to calculate these phenomena can be integrated with RELAP5-3D and SCDAP/3D in three ways: (1) time-dependent interfacing of other computer codes with RELAP5-3D and SCDAP/3D, (2) time-independent interfacing of other computer codes with RELAP5-3D and SCDAP/3D, and (3) extraction of subroutines from other computer codes and implementing them into RELAP5-3D and SCDAP/3D.

The time-dependent interface of other computer codes with RELAP5-3D and SCDAP/3D is appropriate where the other codes are modeling phenomena affecting the phenomena calculated by RELAP5-3D and SCDAP/3D. Examples of such phenomena are multidimensional fluid behavior in part of the reactor system and sub-channel thermal hydraulic behavior in the reactor core. The time-dependent interface can be accomplished by a Message Passing Protocol (MPP). An applicable MPP is the PVM (Parallel Virtual Machine) message passing software (Geist 1993, Weaver et al 2001) developed to convey information calculated by one computer code to other computer codes requiring this information for boundary conditions. An executive program initiates a PVM daemon process on a group of computers, wherein each computer performs the calculations for one of the computer codes. The executive program integrates the execution of the various computer codes and coordinates the time step sizes used by the various computer codes. Data items are passed between the various computer codes as messages having unique message identifiers. The executive program is given input data defining the information to be sent and received by each computer code. Each item of input data consists of a pair wherein one part of the pair defines the computer code to send a certain calculation result and the other part of the pair defines the computer code to receive the calculation result. The item of input data also defines the name of the variable in the sending computer code containing a calculation result needed by another computer code. The item of input data also contains the corresponding name for this variable in the computer code receiving this calculation result. Each computer code can be executing on a different computer and the exchange of information occurs through a network.

In addition to coordinating the information sent and received by the various computer codes, the executive program also compiles calculation results for printing and plotting.

The time-independent interface of other computer codes with RELAP5-3D and SCDAP/3D is appropriate where these other codes model phenomena not affecting the phenomena calculated by RELAP5-3D and SCDAP/3D. Examples of such phenomena are the transport and deposition of fission products and the structural behavior of a reactor during an earthquake. A time-independent interface can be accomplished by one computer code writing a data set that is read by another computer code after the first computer code has completed its analysis.

An example of a time-independent interface is the use of RELAP5-3D and SCDAP/3D to calculate the thermal behavior of the reactor core and thermal hydraulic behavior of fluids in the reactor system and another code using these calculations to calculate the fission product transport and deposition in the reactor system. RELAP5-3D and SCDAP/3D can write a data set defining the transient distribution in fluid conditions and structure temperatures in the reactor system. The data set can also define the dimensions and configuration of the reactor system. A computer code such as VICTORIA (Bixler 1998) can then read this data set and calculate the transient distribution in fission products throughout the reactor system. This code can write a data set defining the fission product inventory at locations within the reactor system at which fission products can leak to the atmosphere. Another code such as RSAC (Wenzel 1993) or MACCS (Chanin et al 1998) can then read this data set and calculate the radiological consequences of the transient behavior of the reactor. The calculations of these radiological consequence codes include doses to the thyroid and whole body at various locations from the reactor. These calculated doses can be compared with acceptance limits established for Generation II reactors in order to make a preliminary evaluation of the safety of Generation IV reactors.

Another example of a time-independent interface is the use of RELAP5-3D and SCDAP/3D to calculate the temperature distribution in the pipes and vessels in a reactor system and the pressures of the fluids in the pipes and vessels and then passing this information to another code to calculate the structural behavior of the reactor during an earthquake. For this analysis, RELAP5-3D and SCDAP/3D can write a data set defining the transient temperatures in the structures throughout reactor system and the internal pressure of these structures. A structural analysis code such as ABAQUS (ABAQUS 1990) can then read this data set to obtain the temperature distribution in the reactor structures and the pressures at the boundaries of these structures. The structural analysis code can then calculate the transient structural behavior of the reactor during an earthquake and evaluate the damage to the reactor caused by the earthquake.

The extraction of subroutines from other codes and implementing them into RELAP5-3D and SCDAP/3D is an appropriate method of model integration in some cases. These cases include (1) the code from which the subroutine is being extracted for the most part calculates phenomena not required for a front of back analysis of Generation IV reactors or calculates phenomena already calculated by RELAP5-3D and SCDAP/3D, and thus the interface of the complete code with RELAP5-3D and SCDAP/3D is not appropriate, (2) the code from which the subroutine is being extracted requires almost the same definition of the reactor system as RELAP5-3D and SCDAP/3D, and thus the interface of that code with RELAP5-3D and SCDAP/3D results in a redundancy in defining the reactor system, and (3) the phenomena being calculated by a subroutine extracted from another code affects the phenomena being modeled by RELAP5-3D and SCDAP/3D.   An example of the subroutine extraction and implementation method of model integration is the extraction of subroutines for fission product transport and deposition from the VICTORIA code (Bixler 1998) and the implementation of these subroutines into RELAP5-3D and SCDAP/3D. This method of integration has the advantage of an instant distribution of calculation results, and thus in some cases may reduce the computer time required to perform a front to back analysis of Generation IV reactors.

6. Improvements in User Efficiency

The efficiency of performing the transient analyses of Generation IV reactors may be increased an order of magnitude by developing an analysis tool to build the input files required by RELAP5-3D or SCDAP/3D. These codes require the compilation of an enormous amount of data into a specific format in order for the reactor system to be adequately defined for calculating the transient behavior of the fluids in the reactor system. In general, an effort of one to two staff-years is required to build the detailed input file for performing the transient analysis of a reactor design for which previous analyses have not been performed. Since many different designs have been proposed for Generation IV reactors, many staff-years of effort may be required to perform transient analyses of the full range of proposed Generation IV reactors. The effort to compile this data can be reduced by an order of magnitude through coupling of a GUI with an analysis tool that transforms data describing the reactor system into the format required by the analysis tool for calculating reactor system fluid behavior.

The GUI for building an input file describing a reactor system can operate in two different ways. In the first way, the GUI receives figures describing the design of the reactor and transforms the figures into data describing the reactor system. In the second way, the GUI generates a template of the reactor system on a computer screen and transmits requests for data defining dimensions, extent of nodalization, and composition. The evolution of the reactor system is continuously displayed so corrections and extensions can be made to the computer generated representation of the reactor system.

7. Conclusions

Plans are being developed for extending RELAP5-3D and SCDAP/3D for the transient analyses of each major category of proposed Generation IV reactors. These codes already have the fundamental modeling capabilities for the transient analyses of Generation IV reactors. A series of relatively small development efforts to address the unique features of Generation IV reactors achieves the basic capability to perform the transient analyses of a broad range of proposed Generation IV reactors. These development efforts achieve the capability to model (1) transport of heat in reactor cores composed of fuel/graphite pebbles and fuel/graphite blocks, (2) thermal, chemical, and mechanical behavior of fuel rods composed of metallic fuel and clad with stainless steel or a Ni-based alloy, (3) freezing of coolant, (4) convective heat transfer in water at a pressure greater than the critical pressure, and (5) thermal and transport properties of fuel and coolant salts. The categories of reactors that can be analyzed with the completion of these development efforts include (1) advanced light water reactors and the supercritical pressure water reactor, (2) pebble bed and block-type high temperature gas reactors, (3) sodium cooled and Pb-Bi cooled reactors, and (4) molten salt reactors.

Plans are being developed for interfacing other codes and models with RELAP5-3D and SCDAP/3D so as to achieve a complete front to back capability of Generation IV reactors. These interfaces achieve the capability to integrate calculations of multidimensional fluid behavior in certain regions of the reactor system with the RELAP5-3D and SCDAP/3D calculations of system-wide fluid behavior. These interfaces also achieve the capability to efficiently calculate the radiological consequences of the transient behavior of Generation IV reactors. Until acceptance limits on various aspects of reactor behavior such as maximum fuel temperature have been established for each category of Generation IV reactor, the safety of these reactors can be assessed by comparing calculations of radiological consequences in these reactors with the acceptance limits on radiological consequences established for Generation II reactors.

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