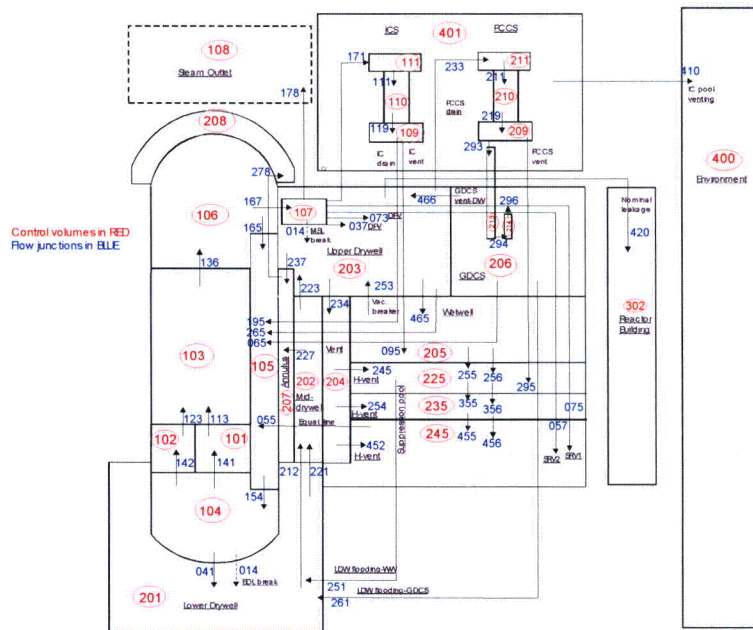


Enclosure 2

MFN 08-770

**Transmittal of Non-Proprietary Version of the Initial
Research Report No. VTT-R-04413-06, "*Estimation and
Modeling of Effective Fission Product Decontamination
Factor for ESBWR Containment, June 2006*"**

Non-Proprietary Version



Estimation and Modeling of Effective Fission Product Decontamination Factor for ESBWR Containment

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Confidentiality GE Proprietary Report

Report's title Estimation and Modeling of Effective Fission Product Decontamination Factor for ESBWR Containmentment	
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Keywords ESBWR, Severe accidents, Source term	Report identification code VTT-R-04413-06
<p>Summary</p> <p>Previous ESBWR MELCOR input file "ESBWWR_BDL6_NRC.txt" supplied by GE has been upgraded for fission product behavior analyses for version MELCOR 1.8.6YH. The key modifications are the updating of COR input to be compatible with the new models, checking and upgrading of most of the RCS and containment volume, flow junction and heat structure input, building up of RN package input for radionuclide calculations.</p> <p>A preliminary Bottom Drain Line Break scenario with successful depressurization of RCS and reflooding at 4100 s was performed with unverified MELCOR 1.8.6 input. The fission product release from the core was relatively low, e.g. for noble gases about 62 %, for Cs 57 % and CsI 62 % of the whole core inventory. The modeled single-hole leakage for containment nominal leakage resulted in release fractions of noble gases, CsOH and CsI to the reactor building to be $1.43 \cdot 10^{-3}$ %, $5.04 \cdot 10^{-4}$ % and $4.58 \cdot 10^{-4}$ % of the initial core inventory, respectively.</p> <p>When approximating the decontamination factor of CsI aerosol in the PCCS by dividing the airborne mass in the Drywell by the airborne mass in the GDCCS one obtains a PCCS decontamination factor varying between 4.4 and 853. The minimum is reached at time 4 h into the accident.</p> <p>The CsI decontamination factor for the whole containment can be defined as the ratio of total CsI released from the core divided by the total airborne mass of CsI in the containment. The value for containment decontamination factor ranges from 2 to 4976 on the basis of draft MELCOR calculation. The minimum is reached in the beginning of the accident (at 1 h).</p>	
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Preface

This report is proprietary report of General electric Nuclear under the GE Purchase Order No. 4431005566. The contact persons at GE were Mr. Wayne Marquino, Mr. Gilbert Hwang and Mr. Chris Pratt.

Espoo 29.6.2006

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1 Executive Summary

The purpose of this work is to investigate the capacity of Passive Containment Coolant System Condensers (PCCS) to remove airborne fission products from the containment atmosphere. A specific goal is to determine the decontamination factor of the PCCS units and validate the model against existing experiments. Further aim is to perform source term calculations with the integral MELCOR code in selected accident cases. For minimization of formation of volatile iodine compounds during the severe accidents a high pH in the containment pools is preferable. The estimation of pH in the containment with consideration of buffer injections is being performed with a dedicated analytical equilibrium chemistry tool.

The studied ESBWR plant has a rated power of 4590 MWt and the Reactor Coolant System (RCS) and Containment design is according to ESBWR Design Control Document Tier 1 and 2, rev 1. As to the containment passive safety systems, four double-module units of Isolations Condensers are capable of providing coolant injection to the RCS at high pressure and a total of 6 double-module PCCS provide long term pressure control of the containment. In addition to that an attractive feature of the PCCS is the potential for fission product retention to the heat exchanger tubes and to condensate flow.

The applied MELCOR version is 1.8.6 YH that was released in September 2005. The new features in MELCOR 1.8.6 comprise a more detailed lower head model addressing better the creep rupture failure of lower head. The core melt blockage and relocation model have been enhanced and a stratified molten pool model for lower head has been included. Also more output variables have been added for fission product transport and release results.

The first task is to update existing MELCOR input of ESBWR for the latest MELCOR version 1.8.6. For the first draft analysis the implementation a few key plant modifications will be implemented, including the venting of GDCS airspace to the Drywell. The MELCOR model will be updated to incorporate the current ESBWR design parameters for the Final Report.

Previous ESBWR MELCOR input file "ESBWWR_BDL6_NRC.txt" supplied by GE has been upgraded for fission product behavior analyses for version MELCOR 1.8.6YH. The key modifications are the updating of COR input to be compatible with the new models, checking and upgrading of most of the RCS and containment volume, flow junction and heat structure input, building up of RN package input for radionuclide calculations.

A preliminary Bottom Drain Line Break scenario with successful depressurization of RCS and reflooding at 4100 s was performed with unverified MELCOR 1.8.6 input. The fission product release from the core was relatively low, e.g. for noble gases about 62 %, for Cs 57 % and CsI 62 % of the whole core inventory. The modeled single-hole leakage for containment nominal leakage resulted in release fractions of noble gases, CsOH and CsI to the reactor building to be $1.43 \cdot 10^{-3}$ %, $5.04 \cdot 10^{-4}$ % and $4.58 \cdot 10^{-4}$ % of the initial core inventory, respectively.

When approximating the decontamination factor of CsI aerosol in the PCCS by dividing the airborne mass in the Drywell by the airborne mass in the GDCS one obtains a PCCS

decontamination factor varying between 4.4 and 853. The minimum is reached at time 4 h into the accident.

The CsI decontamination factor for the whole containment can be defined as the ratio of total CsI released from the core divided by the total airborne mass of CsI in the containment. The value for containment decontamination factor ranges from 2 to 4976 on the basis of draft MELCOR calculation. The minimum is reached in the beginning of the accident (at 1 h).

The second task is to quantification of the capacity of the PCCS to remove fission product aerosols and validation of model and estimates against existing VTT experimental work. The key phenomena to be investigated are diffusiophoresis and thermophoresis. The effect of different thermal hydraulic boundary conditions, i.e. water level in the PCCS pool, gas inlet temperature and the fraction of non-condensable gases in the flow to the tubes will be accounted for. The Draft Report contains the description of the key modeling principles. Currently, all models have been incorporated to a separate code model and validation effort has been started. The final result of task 2 is a correlation model for aerosol decontamination factor as a function of particle size.

The third task is to evaluate the pH in the containment water pools. The estimation will be performed with MELCOR and ChemSheet codes. The base model for ChemSheet has been built including the applied buffer solutions (sodium pentaborate and trisodium phosphate). The next step is to add the iodine pool model input to MELCOR input.

The fourth task is to perform the calculations for the Final Report with verified MELCOR model and by applying the validated decontamination factors for PCCS obtained from the task 2.

The fifth task is to find estimates for the fission product release rates from the reactor building to environment with MELCOR 1.8.6 code.

2 Introduction

The studied ESBWR plant has a rated power of 4590 MWt and the Reactor Coolant System (RCS) and Containment design is according to ESBWR Design Control Document Tier 1 and 2, rev 1. As to the containment passive safety systems, four double-module units of Isolations Condensers are capable of providing coolant injection to the RCS at high pressure and a total of 6 double-module Passive Containment Coolant System Condensers (PCCS) provide long term pressure control of the containment. In addition to that an attractive feature of the PCCS is the potential for fission product retention to the heat exchanger tubes and to condensate flow.

3 Goal

The purpose of this work is to investigate the capacity of PCCS condenser to remove airborne fission products from the containment atmosphere. A specific goal is to determine the decontamination factor of the PCCS units and validate the model against existing experiments. Further aim is to perform source term calculations with the integral MELCOR code in selected accident cases. For minimization of formation of volatile iodine compounds during the severe accidents a high pH in the containment pools is preferable. The estimation of pH in the containment with consideration of buffer injections is being performed with a dedicated analytical equilibrium chemistry tool.

4 Description of ESBWR plant model for MELCOR

1.8.6

The applied MELCOR version is 1.8.6 YH that was released in September 2005. The new features in MELCOR 1.8.6 comprise a more detailed lower head model addressing better the creep rupture failure of lower head. The core melt blockage and relocation model have been enhanced and a stratified molten pool model for lower head has been included. Also more output variables have been added for fission product transport and release results.

4.1 Reactor Core

The reactor core nodalization is depicted in Figure 1. The core region is divided into 6 radial rings and 14 axial levels. The radial rings in the active core region have equal cross-section area. The ring 6 is for lower head modeling and the ring 6 cells above the elevation of the bottom of downcomer (=1.544 m) are dummy. The lower head model is a new feature in MELCOR version 1.8.6. Tables 1, 2 and 3 collect the applied parameters in the COR model. The full core decay heat curve is given as a Tabular function power vs. time and represents the situation of a full core at the end of cycle. The axial and radial power peaking factors in the current input were maintained the same as in the unverified input from 2001. The axial peaking factors will be updated for the calculations in the Final Report.

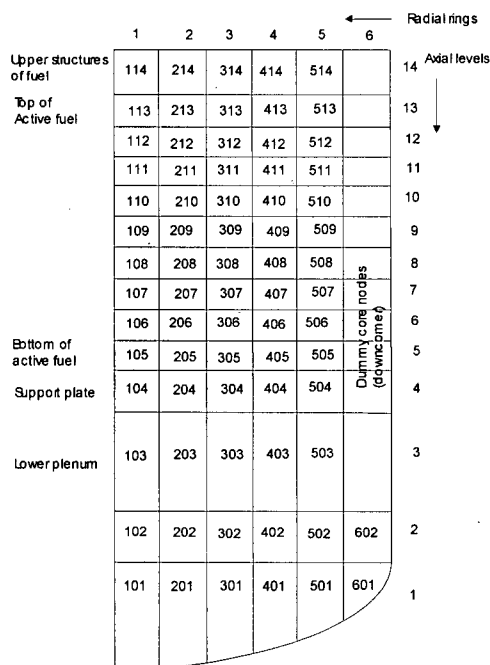


Figure 1. Schematic description of the COR model.

Table 1. Applied ESBWR core data in the MELCOR 1.8.6 code

Item	Data in the MELCOR 1.8.6 input	Data source
Outer radius of fuel pellet	[[unverified MELCOR input (2001)
Outer radius of cladding		unverified MELCOR input (2001)
Thickness of gap between the pellet and the cladding		unverified MELCOR input (2001)
Center-to-center spacing of fuel rods		unverified MELCOR input (2001)
Thickness of canister wall		unverified MELCOR input (2001)
Outer radius of core region		DRF 0000-0037-2687
Radius of curvature of inside of the lower head		DRF 0000-0037-2687
Inner radius of RPV cylinder		DRF 0000-0037-2687
Thickness of cylindrical vessel wall		DRF 0000-0037-2687
Thickness of lower head		DRF 0000-0037-2687
Elevation of baffle plate		DRF 0000-0037-2687
Elevation of (top of) lower core support plate		DRF 0000-0037-2687
Elevation at top of active fuel		DRF 0000-0037-2687
Elevation at top of core region		DRF 0000-0037-2687
Total mass of UO ₂		unverified, scaled with ratio of active core heights: 3.0483/2.1664=1.40708 2.1664 m is used in 2001 input
Total mass of Zircaloy (cladding)		
Total mass of Zircaloy (canisters)		
Total mass of stainless steel in active core		
Total mass of B ₄ C		
Mass of core support plate		unverified MELCOR 2001 input
Mass of control rod guide tubes		unverified MELCOR 2001 input
Support plate thickness]]	DRF 0000-0037-2687

Table 2. Core radial data.

Core ring	Outer radius of ring (m)	Data source	Power peaking factor	Data source
1	[[calculated*	[[unverified 2001 input
2		calculated*		unverified 2001 input
3		calculated*		unverified 2001 input
4		calculated*		unverified 2001 input
5		DRF 0000-0037-2687		unverified 2001 input
6]]	DRF 0000-0037-2687]]	

* The assumption that $A1=A2=A3=A4=A5$

Table 3. Axial core input data.

Axial level	Elevation at the bottom of cell (m)	height of cell (m)	Channel flow area per ring (m ²)	Bypass flow area per ring (m ²)	Axial power peaking factor	Data source
1	[[scaled from unverified 2001 input
2						scaled from unverified 2001 input
3						scaled from unverified 2001 input
4						scaled from unverified 2001 input
5						scaled from unverified 2001 input
6						scaled from unverified 2001 input
7						scaled from unverified 2001 input
8						scaled from unverified 2001 input
9						scaled from unverified 2001 input
10						scaled from unverified 2001 input
11						scaled from unverified 2001 input
12						scaled from unverified 2001 input
13						scaled from unverified 2001 input
14]]	scaled from unverified 2001 input

4.2 Reactor Coolant System volumes and flow paths

The reactor coolant system and containment nodalization of ESBWR for MELCOR 1.8.6 input are depicted in Fig. 2. The total volume of reactor pressure vessel nodes in the MELCOR 1.8.6 input is 942.126 m³. The total volume of RPV in (Figure 5.1-1 in [1]) is 959 m³. Tables 4, 5 and 6 gather the key input data for RCS nodalization and flow paths. The operation logic of valves connected to different flow paths is discussed in Chapter 4.6 of this report.

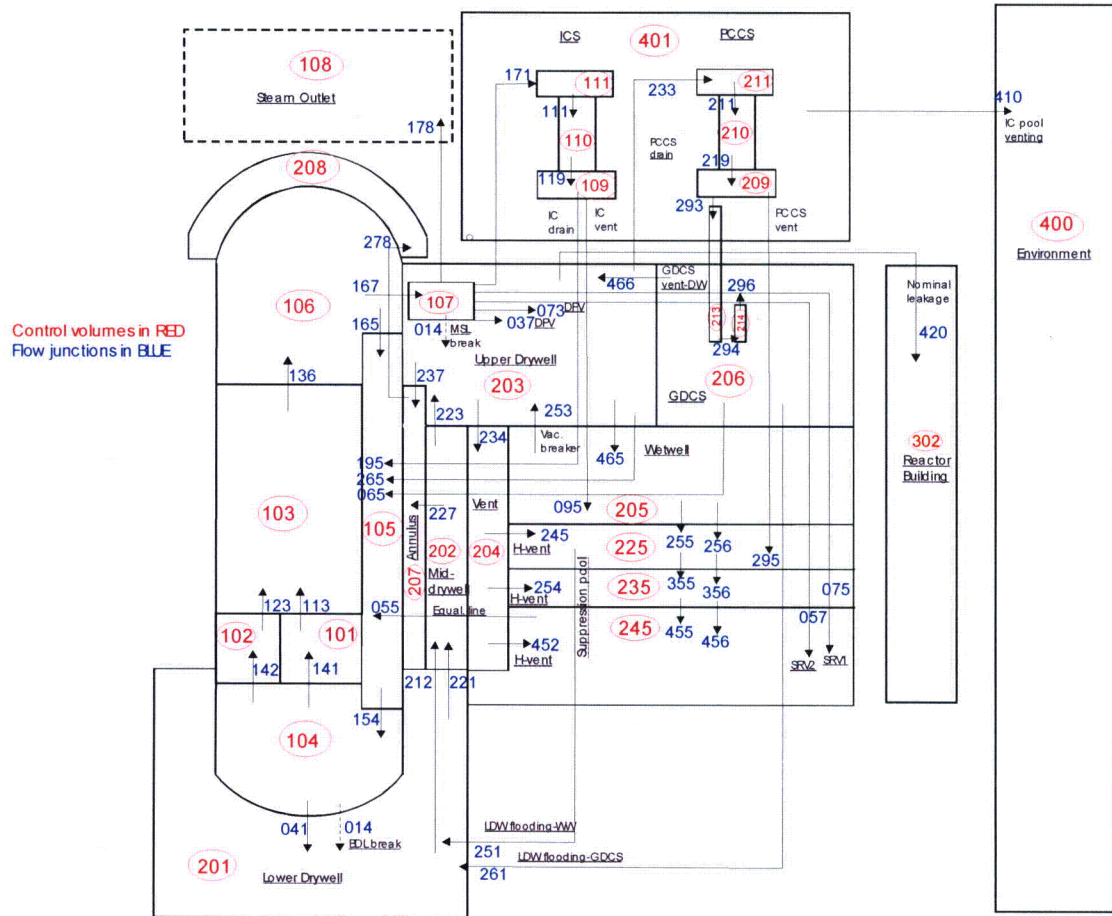


Figure 2. MELCOR 1.8.6 control volume and flow junction scheme of ESBWR model.

Table 4. Control volumes of reactor coolant system.

Control volume name	Control volume node	Elevation vs. volume of node		Volume of pool (m ³)	Initial temperature		Initial pressure (MPa)	Data source
		elev. (m)	vol. (m ³)		T _{atm} (K)	T _{pool} (K)		
Core	101	7.896 7.4533 4.405	59.46681 42.9312 0.0	30.0	sat.	sat.	7.21	DRF 0000-0037-2687 & ESBER DCD Tier 2, Ch. 6 rev1
Bypass	102	7.896 7.4533 4.405	54.138 39.08414 0.0	54.138	-	551.82	7.2042	DRF 0000-0037-2687 & ESBER DCD Tier 2, Ch. 6 rev1
Chimney	103	16.51 7.896	255.6355 0.0	66.79	sat.	sat.	7.1896	DRF 0000-0037-2687 & ESBER DCD Tier 2, Ch. 6 rev1
Lower plenum	104	4.405 4.0105 2.365 0.0	136.0938 123.6317 71.65127 0.0	136.09	-	550.9	7.2397	DRF 0000-0037-2687 & ESBER DCD Tier 2, Ch. 6 rev1
Downcomer	105	22.276 19.540 16.365 7.896 2.365	147.0625 135.2081 115.1544 39.2945 0.0	131.2605	sat.	551.0	7.1447	DRF 0000-0037-2687 & ESBER DCD Tier 2, Ch. 6 rev1
Upper plenum	106	27.56 25.24 19.5278 16.51	289.7294 226.2726 54.8177 0.0	26.862	sat.	sat.	7.17	
Main steam line	107	23.58 22.08	27.25 0.0	-	sat.	-	7.0881	
Steam outlet [*]	108	30.0 20.0	1·10 ⁸ 0.0	-	sat.	-	2.0	

^{*} steam outlet is an arbitrarily large volume representing turbine bypass

Table 5. Isolation condenser system (ICS) control volumes.

Control vol. name	Control vol. number	Elevation vs. volume table		Volume of pool (m ³)	Initial temperature		Initial pressure (MPa)	Data source
		Elev. (m)	Vol. (m ³)		T _{atm} (K)	T _{pool} (K)		
IC steam box	111	29.95 29.185	4.01 0.0	4.01	sat.	sat.	7.088	MFN 05-122 & MFN 06-003
IC tubes	110	29.185 27.385	2.173 0.0	2.0	sat.	sat.	7.088	MFN 05-122 & MFN 06-003
IC water box	109	27.385 26.755	4.077 0.0	4.075	sat.	sat.	7.088	MFN 05-122 & MFN 06-003

Table 6. Flow paths between RCS volumes

Flow path no	From volume	To volume	from elevation (m)	To elevation (m)	Flow area (m ²)	length (m)	fraction open	Data source
RPV flow paths								
113	core	chimney	7.896	7.896	S0: 9.48 S1: 15.858	0.914 1.356	1.0	
123	bypass	chimney	7.896	7.896	8.503	1.649	1.0	
136	chimney	upper plenum	16.51	16.51	S0: 32.94 S1: 49.253 S2: 7.761 S3: 11.533 S4: 38.114	8.008 1.156 3.381 0.779 5.141	1.0	
165	upper plenum	downcomer	21.91	21.91	S0: 20.388 S1: 33.977	2.845 2.470	1.0	
154	downcomer	lower plenum	2.365	2.365	S0: 6.647 S1: 6.647 S2: 8.191 S3: 7.522	5.118 2.890 1.815 4.272	1.0	
141	lower plenum	core	4.405	4.405	S0: 0.317 S1: 11.835	0.094 1.142	1.0	
142	lower plenum	bypass	4.405	4.405	S0: 26.83 S1: 0.166 S2: 8.503	2.145 1.327 1.649	1.0	
167	upper plenum	main steam line	22.83	22.83	S0: 0.3932 S1: 1.283	2.129 5.128	1.0	
178	main steam line	steam outlet	22.83	22.83	0.4276	7.543	valve (CF178)	
ICS flow paths								
195	IC water box	downcomer	26.755	13.025	0.1004	32.5	valve (CF195)	MFN 05-122
171	upper plenum	IC steam box	21.91	29.95	0.3936	31.5	1.0	MFN 05-122
111	IC steam box	IC tubes	29.29	29.185	1.207	0.8	1.0	MFN 05-122
119	IC tubes	IC water box	27.385	27.385	1.207	0.8	1.0	MFN 05-122
ECCS injection flow paths								
065	GDCS pool	downcomer	17.8	8.453	0.0912	10.57	valve (CF265)	unverified 2001 input
055	Suppression pool bottom	downcomer	5.0	8.453	0.0912	2.89	valve (CF070)	unverified 2001 input
RPV pressure control flow paths								
075	main steam line	suppression pool bottom	22.83	6.494	0.0673	14.795	valve (CF075)	unverified 2001 input
057	main steam line	suppression pool bottom	22.83	6.494	0.0673	14.795	valve (CF057)	unverified 2001 input
073	upper plenum	upper drywell	21.91	22.83	0.1224	0.2	valve (CF273)	unverified 2001 input
037	upper plenum	upper drywell	21.91	22.83	0.1224	0.2	valve (CF237)	unverified 2001 input
095	IC water box	wetwell	27.355	9.533	0.00278	27.3	valve (CF095)	MFN 05-122
014	lower plenum	lower drywell	0.0	-0.212	$2.165 \cdot 10^{-3}$	0.3	valve (CF142)	unverified 2001 input
041	lower plenum	lower drywell	0.0	-0.212	1.0	0.212	valve (CF141)	unverified 2001 input

4.3 Containment

The total gas space volume of the containment in the MELCOR 1.8.6 model is 12 342 m³ and water pool volume 6288 m³. The detailed description of the containment control volumes is given in Tables 7 and 8.

Table 7. Containment control volumes.

Control vol. name	Control vol. number	Elevation vs. volume table		Volume of pool (m ³)	Initial temperature (K)		Initial pressure (MPa)	Data source
		elev. (m)	Vol. (m ³)		atm.	pool		
Lower drywell	201	7.443 -8.8	1190 0.0	-	330	-	0.1013	ESBWR DCD Tier 2, Ch. 6, rev 1
Central drywell	202	17.5 7.443	713.56 0.0	-	330	-	0.1013	ESBWR DCD Tier 2, Ch. 6, rev 1
Upper drywell	203	24.6 17.5	4589.44 0.0	-	330	-	0.1013	ESBWR DCD Tier 2, Ch. 6, rev 1
Vents	204	17.5 10.1 4.65	174.76 74.12 0.0	74.12	316	330.	0.1013	ESBWR DCD Tier 2, Ch. 6, rev 1
Wetwell	205	16.9 10.1 9.4	5991.3 559.3 0.0	559.3	300.	300.	0.1013	ESBWR DCD Tier 2, Ch. 6, rev 1
Suppression pool upper	225	9.4 8.1	1038.7 0.0	1038.7	-	300	0.1130	ESBWR DCD Tier 2, Ch. 6, rev 1
Suppression pool middle	235	8.1 6.7	1118.0 0.0	1118.	-	300.	0.1238	ESBWR DCD Tier 2, Ch. 6, rev 1
Suppression pool bottom	245	6.7 4.65	1637.95 0.0	1637.95	-	300.	0.1374	ESBWR DCD Tier 2, Ch. 6, rev 1
GDCS	206	24.6 24.1 17.5	1999.4 1859.0 0.0	1859.0	300.	300.	0.1013	ESBWR DCD Tier 2, Ch. 6, rev 1
Annulus	207	21.85 7.443	349.46 0.0	-	340.	-	0.1013	ESBWR DCD Tier 2, Ch. 6, rev 1
Head	208	35.35 29.35 21.85	277.0 68.254 0.0	-	330.	-	0.1013	ESBWR DCD Tier 2, Ch. 6, rev 1

Table 8. Passive Containment Cooling System (PCCS) control volumes.

Control vol. name	Control vol. number	Elevation vs. volume table		Volume of pool (m ³)	Initial temperature		Initial pressure (MPa)	Data source
		Elev. (m)	Vol. (m ³)		T _{atm} (K)	T _{pool} (K)		
PCC steam box	211	30.22 28.90	12.96 0.0	-	300	-	0.1013	MFN 05-122 & MFN 06-003
PCC tubes	210	28.90 27.563	12.94 0.0	-	300.	-	0.1013	MFN 05-122 & MFN 06-003
PCC water box	209	27.563 26.243	12.96 0.0	-	300.	-	0.1013	MFN 05-122 & MFN 06-003
PCC Drain 1	213	26.243 21.538	0.49884 0.0	0.26506	300.	300.	0.1013	MFN 05-122 & email communication with GE
PCC Drain 2	214	24.038 21.538	0.26506 0.0	0.26506	-	300.	0.1013	MFN 05-122 & email communication with GE

Table 9. Containment flow paths.

Flow path no	From volume	To volume	from elevation (m)	To elevation (m)	Flow area (m ²)	length (m)	fraction open	Data source
212	lower drywell	mid drywell	-8.256	7.443	0.01634	14.2	1.0	unverified 2001 MELCOR input
221	lower drywell	mid drywell	6.4	7.443	7.89	1.0	1.0	unverified 2001 MELCOR input
223	mid drywell	upper drywell	17.5	17.5	42.0	8.4	1.0	unverified 2001 MELCOR input
227	mid drywell	annulus	9.379	9.379	6.92	0.15	1.0	unverified 2001 MELCOR input
234	upper drywell	vent	17.5	17.5	9.05	9.56	1.0	unverified 2001 MELCOR input
237	upper drywell	annulus	21.85	21.85	8.04	0.15	1.0	unverified 2001 MELCOR input
465	upper drywell	wetwell	21.05	15.0	0.0001	6.05	1.0	DCD Tier 2, Chapter 6
466	GDCS	upper drywell	24.45	24.45	17.63	1.0	1.0	MFN 05-122
245	vent	suppression pool-upper	8.493	8.493	3.85	1.21	1.0	DCD Tier 2, Chapter 6
254	vent	suppression pool-middle	7.123	7.123	3.85	1.68	valve (CF358)	DCD Tier 2, Chapter 6
452	vent	suppression pool-bottom	5.753	5.753	3.85	2.14	valve (CF458)	DCD Tier 2, Chapter 6
255	wetwell	suppression pool-upper	9.91	9.4	600.0	1.6	1.0	unverified 2001 MELCOR input
256	wetwell	suppression pool-upper	9.71	9.2	600.	1.6	valve (CF259)	unverified 2001 MELCOR input
355	suppression pool-upper	suppression pool-middle	8.75	8.1	600.	1.6	1.0	unverified 2001 MELCOR input
356	suppression pool-upper	suppression pool-middle	8.55	7.9	600.	1.6	valve (CF365)	unverified 2001 MELCOR input
455	suppression pool-middle	suppression pool-bottom	7.4	6.7	600.	1.6	1.0	unverified 2001 MELCOR input
456	suppression pool-middle	suppression pool-bottom	7.2	6.5	600.	1.6	valve (CF465)	unverified 2001 MELCOR input
251	suppression pool upper	lower drywell	8.45	-6.565	0.01634	13.56	valve (CF253)	unverified 2001 MELCOR input
253	wetwell	upper drywell	16.9	17.5	1.13	1.61	valve (CF255)	unverified 2001 MELCOR input
261	GDCS	lower drywell	17.8	-6.565	0.01634	23.68	valve (CF263)	unverified 2001 MELCOR input
278	annulus	upper head	21.85	21.85	1·10 ⁻⁴	0.1	1.0	
PCC flow paths								
293 [*]	PCC water box	PCC Drain 1	26.243	26.243	0.10603	1.0	1.0	MFN 05-122 & MFN 06-003
294 ^{**}	PCC Drain 1	PCC Drain 2	21.538	21.538	0.10603	1.0	1.0	MFN 05-122 & MFN 06-003
296 ^{***}	PCC Drain 2	GDST tank	24.038	24.038	0.10603	11.0	1.0	MFN 05-122 & MFN 06-003
295 ^{****}	PCC water box	wetwell	26.965	9.350	0.3040	24.5	1.0	MFN 05-122 & MFN 06-003 & comm. with GE
233	upper drywell	PCC steam box	24.6	30.22	0.4241	8.15	1.0	MFN 05-122 & MFN 06-003
211	PCC steam box	PCC tubes	28.9	28.9	6.81	0.8	1.0	MFN 05-122 & MFN 06-003
219	PCC tubes	PCC water box	27.563	27.563	6.81	0.8	1.0	MFN 05-122 & MFN 06-003

^{*} modeled as vertical pool-first, forward flow only junction

^{**} modeled as horizontal pool-first, forward flow only junction

^{***} modeled as vertical pool-first, forward flow only junction

^{****} modeled as vertical atmosphere-first, forward flow only junction

4.4 Reactor building and environment volumes

The current MELCOR model has one control volume representing the whole reactor building. It is defined to be an artificially large volume to provide constant down stream thermal hydraulic conditions. Refueling pool volume is presented as a separate control volume. The water pool housing ICS and PCCS condensers is modeled as single large pool. The environment is modeled as a large control volume for purposes of being a heat sink to containment outer walls and a receiving volume for possible source term.

Table 10. Reactor building and environment control volumes.

Control vol. name	Control vol. number	Elevation vs. volume table		Volume of pool (m ³)	Initial temperature		Initial pressure (MPa)	Data source
		Elev. (m)	Vol. (m ³)		T _{atm} (K)	T _{pool} (K)		
Refuel floor	301	45.695 33.505 33.205 26.6	15540. 758.24 725.3 0.0	725.3	300	300	0.1013	unverified 2001 MELCOR input
Reactor building	302	50.0 -10.3	1·10 ⁸ 0.0	-	300.	-	0.1013	unverified 2001 MELCOR input
Environment	400	50.0 -20.0	1·10 ⁸ 0.0	-	300.	-	0.1013	unverified 2001 MELCOR input
IC pool	401	33.7 28.65 26.0	6100. 3180. 0.0	4900.	300.	300.	0.1013	unverified 2001 MELCOR input

Table 11. Reactor building and environment flow paths.

Flow path no	From volume	To volume	from elevation (m)	To elevation (m)	Flow area (m ²)	length (m)	fraction open	Data source
410	ICS pool	environment	33.7	40.0	1.131	30.0	1.0	unverified 2001 MELCOR input
420	upper drywell	reactor building	24.0	24.0	1.949·10 ⁻⁶	1.0	1.0	area calculated from Bernoulli's equation (0.5 % of contmnt volume per day at 310 kPa)

4.5 Heat structures

The heat structures act as heat sinks according to their material characteristics and as deposition surfaces for fission product aerosols according to their geometric alignment.

Table 12. Reactor coolant system and containment heat structures.

Heat structure number	name	bottom elevation (m)	top elevation (m)	area (m ²)	thickness (m)	material	type/orientation	
10002	shroud level 2	4.0105	4.405	7.86	0.05	SS	vertical cylinder	scaled from unverified 2001 MELCOR input
10003	shroud level 3	4.405	4.7437	6.74825	0.05	SS	vertical cylinder	same as above
10004	shroud level 4	4.7437	5.0824	6.74825	0.05	SS	vertical cylinder	same as above
10005	shroud level 5	5.0824	5.4211	6.74825	0.05	SS	vertical cylinder	same as above
10005	shroud level 6	5.4211	5.7598	6.74825	0.05	SS	vertical cylinder	same as above
10007	shroud level 7	5.7598	6.0985	6.74825	0.05	SS	vertical cylinder	same as above
10008	shroud level 8	6.0985	6.4372	6.74825	0.05	SS	vertical cylinder	same as above
10009	shroud level 9	6.4372	6.7759	6.74825	0.05	SS	vertical cylinder	same as above
10010	shroud level 10	6.7759	7.1146	6.74825	0.05	SS	vertical cylinder	same as above
10011	shroud level 11	7.1146	7.4533	6.74825	0.05	SS	vertical cylinder	same as above
10012	shroud level 12	7.4533	7.896	8.8203	0.05	SS	vertical cylinder	same as above
10305	chimney shroud	7.896	16.51	171.625	0.05	SS	vertical cylinder	same as above
11003	top guide ring 1	7.896	8.076	6.285	0.18	SS	horizontal slab	same as above
12003	top guide ring 2	7.896	8.076	6.285	0.18	SS	horizontal slab	same as above
13003	top guide ring 3	7.896	8.076	6.285	0.18	SS	horizontal slab	same as above
14003	top guide ring 4	7.896	8.076	6.285	0.18	SS	horizontal slab	same as above
15003	top guide ring 5	7.896	8.076	6.285	0.18	SS	horizontal slab	same as above
RCS to containment heat structures								
10001	shroud level 1	2.365	4.0105	32.785	0.05	SS	vertical cylinder	same as above
15207	vessel	7.443	20.259	285.865	0.154	SS	vertical cylinder	same as above
16208	vessel head	22.84	23.84	79.452	0.154	SS	upper hemisphere	same as above

ICS heat structures								
11041	IC tubes	27.385	29.185	0.28727 x 810	0.0023	SS	vertical cylinder manifold (810 tubes)	MFN 06-003
Containment heat structures								
25160	GDCS floor	16.9	18.5	234.2	1.6	concrete	horizontal slab	unverified 2001 input
25130	Upper drywell floor	16.9	18.5	484.25	1.6	concrete	horizontal slab	unverified 2001 input
26130	GDCS wall	17.5	23.55	338.32	0.2	concrete	vertical cylinder	unverified 2001 input
22170	Lower biological shield	7.443	17.5	302.68	0.016	SS	vertical cylinder	unverified 2001 input
23170	central biological shield	17.5	21.85	130.92	0.016	SS	vertical cylinder	unverified 2001 input
25220	vent wall 1	10.443	16.9	267.77	1.6	concrete	vertical cylinder	unverified 2001 input
25221	vent wall 2	9.4	10.4	41.47	1.6	concrete	vertical cylinder	unverified 2001 input
26210	GDCS ceiling	24.6	26.6	50.64	2.0	concrete	horizontal slab	unverified 2001 input
23210	Upper drywell ceiling	24.6	26.6	781.4	2.0	concrete	horizontal slab	unverified 2001 input
28220	Drywell head	26.6	32.76	226.195	0.16	SS	upper hemisphere	unverified 2001 input
25310	SP-RB wall	9.4	20.4	103.67	2.0	concrete	vertical cylinder	unverified 2001 input
25311	WW-RB wall	10.44	16.9	669.72	2.0	concrete	vertical cylinder	unverified 2001 input
25313	WW floor	2.65	10.75	633.63	2.35	concrete	horizontal slab	unverified 2001 input
33401	LDW- HCU wall	-8.8	2.6	637.49	2.0	concrete	vertical cylinder	unverified 2001 input
25320	LDW floor	-8.8	-6.8	116.9	2.0	concrete	horizontal slab	added (ESBWR DCD Tier 2)
25321	MID-DW floor	7.443	9.443	70.9	1.0	concrete	horizontal slab	added (ESBWR DCD Tier 2)
25323	Shield ann. floor	7.443	8.043	24.2	0.6	concrete	horizontal slab	added (ESBWR DCD Tier 2)
PCCS heat structures								
21041	PCC tubes top	28.2315	28.90	0.10669 (x3360)	0.00165	SS	vertical cylinder manifold (3360 tubes)	MFN 06-003 & MFN05-122
21042	PCC tubes bottom	27.563	28.2315	0.10669 (x3360)	0.00165	SS	vertical cylinder manifold (3360 tubes)	MFN 06-003 & MFN05-122

4.6 Engineered Safety Features

4.6.1 Isolation condenser system (ICS)

ICS drain line is modeled with valve operation. ICS drain line opens fully when Main Steam Line Valve has closed (in 4.2 s following a scram signal). In the Draft MELCOR calculation of this report, no ICS were assumed to operate at any time. ICS vent line is modeled to remain closed in the Draft MELCOR calculation.

4.6.2 Passive Containment Cooling System (PCCS)

PCCS Drain Line has a loop seal at the pipe end in the GDCS pool. The Drain Line is modeled with two vertical control volumes connected with a horizontal flow junction at the bottom of the volumes. The flow junctions from the PCCS water box to the Drain Line, the horizontal junction between the Drain Line volumes and the junction from the second Drain Line volume to the GDCS pool are defined to be pool-first junctions in MELCOR. A pool-first junction allows water to flow first and only after no pool exists in the upstream volume, gas flow is allowed.

The PCCS Vent line is modeled as respective atmosphere-first flow junction between the PCCS water box and the Suppression Pool.

4.6.3 GDCS injection to RPV Downcomer

Coolant injection from the GDCS pool is modeled to start at a user-specified time. In the Draft calculation the start of reflooding was set to 4100 s. The GDCS line opening fraction can be varied, in the Draft MELCOR calculation it was defined to be 100 % of full area.

4.6.4 Equalization line injection from Suppression pool to RPV downcomer

The opening of Equalization Line is modeled to occur after a user-specified time delay has the beginning of the core oxidation and the boiled-up water level in the downcomer of the Reactor Pressure Vessel (RPV) has fallen below level L1 (10.5775 m from the bottom of RPV). In the Draft Bottom Drain Line Break scenario, the time delay from start of core oxidation was set to 5800 s, which is 1700 s after the start of GDCS injection.

4.6.5 Safety Relief Valves (SRV#1 and SRV #2)

Two separate Safety Relief Valve Lines (SRV) are modeled. The SRV #1 and SRV #2 open when the pressure in the Upper Plenum of the RPV exceeds 8.723 MPa and closes when Upper Plenum Pressure decreases below 8.045 MPa. If the water level in the downcomer is below level L1, SRV#1 opens fully in 10 s and SRV#2 in 55 s, respectively. The flow areas of both SRVs are equal.

4.6.6 Depressurization Valves (DPV#1 and DPV#2)

Two separate RPV Depressurization Lines are models. The DPV#1 opens fully with a 100-s delay from the level L1 signal. DPV#2 opens respectively with 145-s delay from the level L1 signal. The flow areas of the two valves are equal.

4.6.7 Lower Drywell Flooding from Wetwell and GDCS Pool

The Lower Drywell flooding from the Wetwell and GDCS Pool start, when the gas temperature in the Lower Drywell exceeds 533 K.

4.6.8 Vacuum Breakers

The Vacuum Breakers open fully when the Wetwell pressure exceeds the Drywell pressure by 3445 Pa. In addition to Vacuum Breakers the Wetwell airspace is connected to the Drywell airspace via a small leakage flow path ($A=1 \cdot 10^{-4} \text{ m}^2$).

4.7 Decay heat

The operating power of the reactor is defined in the input to be $4.59 \cdot 10^9 \text{ W}$, which is 102 % of the rated power. The decay heat is defined as a Tabular Function of power vs. time through input (Table 13). MELCOR interpolates the values of power between the given time points. The reactor shutdown time is currently determined to be at time 0.

Table 13. Decay heat vs. time used in MELCOR input for ESBWR.

Time from scram (s)	Decay heat (W)
0.0	$4.5900 \cdot 10^9$
0.1	$4.5097 \cdot 10^9$
0.6	$2.6806 \cdot 10^9$
1.0	$1.5298 \cdot 10^9$
6.0	$2.6314 \cdot 10^8$
10.0	$2.2592 \cdot 10^8$
60.0	$1.5946 \cdot 10^8$
100.0	$2.4367 \cdot 10^8$
600.0	$1.0148 \cdot 10^8$
1000.0	$8.9872 \cdot 10^7$
2000.0	$7.3624 \cdot 10^7$
4000.0	$5.8981 \cdot 10^7$
6000.0	$5.2051 \cdot 10^7$
8000.0	$4.7920 \cdot 10^7$
10000.0	$4.5083 \cdot 10^7$
20000.0	$3.9635 \cdot 10^7$
40000.0	$3.3530 \cdot 10^7$
60000.0	$3.0252 \cdot 10^7$
86400.0	$2.7416 \cdot 10^7$
100000.0	$2.6314 \cdot 10^7$
150000.0	$2.3340 \cdot 10^7$
172800.0	$2.2326 \cdot 10^7$

All default fission product classes in the MELCOR 1.8.6 are used in the ESBWR model. The total masses of fission products in each class is defined to be the default values of MELCOR. The initial masses of the fission product classes will be updated according to ORIGEN calculations for ESBWR specific core for the final calculations.

Iodine and Cesium are assumed to form CsI following the release from the fuel. The excess Cs is assumed to be as CsOH. Table 14 shows the distribution different radionuclide elements into default radionuclide classes used for fission product transport and deposition models.

Table 14. Applied default classification of fission product elements and Initial fission product class masses.

Fission product class	Representative class element	Initial mass (kg)	Elements in the class
1	Xe	583.2	He, Ne, Ar, Kr, Xe, Rn, H, N
2	Cs	337.5	Li, Na, K, Rb, Cs, Fr, Cu
3	Ba	26.1	Be, Mg, Ca, Sr, Ba, Ra, Es, Fm
4	I	26.325	F, Cl, Br, I, At
5	Te	51.3	O, S, Se, Te, Po
6	Ru	386.1	Ru, Rh, Pd, Re, Os, Ir, Pt, Au, Ni
7	Mo	441.0	V, Cr, Fe, Co, Mn, Nb, Mo, Tc, Ta, W
8	Ce	747.0	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
9	La	718.2	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf
10	U	166500.0	U
11	Cd	1.76895	Cd, Hg, Zn, As, Sb, Pb, Tl, Bi
12	Sn	10.8	Ga, Ge, In, Sn, Ag
13	B	0	B, Si, P
14	H ₂ O	0	H ₂ O
15	concrete	0	--
16	CsI	0	CsI

4.8 Fission product release and transport

The release of fission products from the fuel is calculated with CORSOR-M model with multiplication with surface-to-volume ratio. The default number (10) of aerosol size sections are used in the calculation. The hygroscopicity model is activated. The input needed to activate Iodine pool model and pH calculation was not yet done for the Draft MELCOR calculation.

Fission products were assumed to be initially evenly distributed in the fuel in the core rings. The fission product release in the gap in the beginning of the calculation was 5% for noble gases (class 1), Cs (class 2) and I (class 4). For the other classes the initial gap release was 0. The initial gap inventory is according to the specification for BWR core inventory gap release in [2]. The fission product release to the reactor coolant system begins, when the specified failure temperature (1173 K) is reached in the cladding. Once the failure temperature is reached at any axial level of a core radial ring, the whole airborne inventory in that radial ring is released.

All heat structures act as deposition surfaces according to their defined orientation. The PCCS tube walls were modeled as cylindrical heat structures and a floor heat structure was defined for PCC water box. PCC steam box and the tube volume have no horizontal heat slabs. An aerosol settling area equal to the total cross section area of the tube bundle is defined for aerosol settling by gravitation from steam box volume to tube volume and from tube volume to water box, respectively.

The fission product pool scrubbing model (SPARC) is activated in the SRV and DPV lines, in the IC Drain Line and the Vent Line, Horizontal Vent Lines, Lower Drywell flooding lines and PCC Drain Line flow junction to the GDCS pool and PCC Vent lines.

5 Model for fission Product Removal in Passive Containment Cooling System Modules

5.1 The description of the modeling principles

5.1.1 Heat and mass transfer

The heat and mass fluxes of the system were estimated using a simple plug flow balance model with appropriate Nusselt (Nu) and Sherwood (Sh) numbers, [3]. If assumed that the latent heat associated with steam condensation is not conducted to the gas the following applies for the gas temperature T [K]:

$$\frac{dT}{dx} = -\frac{Pq^T}{\dot{m}_w c_{pw} + \dot{m}_n c_{pn}} \quad (1)$$

Analogously, for the water film temperature T_l [K]:

$$\frac{dT_l}{dx} = -\frac{P[-q^{Ts} + q^T + Lq^m + c_{pw}(T - T_l)]}{\dot{m}_l c_{pl}} \quad (2)$$

Here L is the latent heat [J/kg], which is calculated at T_l . It was assumed that the water film temperature profile is linear. T_l is the average liquid temperature [K] and T the average gas temperature [K]. P is the perimeter of the heat exchanger tube [m], c_{pn} the nitrogen gas heat capacity [J/kg K], c_{pw} the water vapor heat capacity [J/kg K] and c_{pl} the liquid water heat capacity [J/kg K], respectively. The mass fluxes for the water vapor, nitrogen gas and liquid water are \dot{m}_w , \dot{m}_n and \dot{m}_l [kg/s], respectively. The heat fluxes q^T and q^{Ts} [W/m²] are calculated from:

$$q^T = Nu \cdot k_g \frac{T - T_{ls}}{d_h} \quad (3)$$

and

$$q^{T_s} = k_l \frac{T_{ls} - T_s}{\delta}, \quad (4)$$

where k_g and k_l are the thermal conductivities of the gas-vapor mixture and liquid water [W/m K], respectively. d_h is the hydraulic diameter of the heat exchanger tube [m], T_{ls} the temperature at the liquid film surface [K] and T_s the temperature at the tube surface [K]. The assumption of the linear temperature profile across the liquid film satisfies:

$$T_l = \frac{T_{ls} + T_s}{2} \quad (5)$$

The liquid film thickness δ [m] can be approximated by [3]:

$$\delta = \left(\frac{3\mu\dot{m}_l}{\rho_l^2 g d_h} \right)^{1/3}, \quad (6)$$

where μ_l is the liquid viscosity [N/s m²], ρ_l the liquid density [kg/m³] and g the gravitational acceleration [m/s²], respectively.

Besides the energy balance equations, the mass balances are also formulated for solving a solution of the system simultaneously. For the nitrogen \dot{m}_n , water vapor \dot{m}_w and liquid water \dot{m}_l mass fluxes [kg/s] we obtain:

$$\frac{d\dot{m}_n}{dx} = 0, \quad (7)$$

$$\frac{d\dot{m}_w}{dx} = -Pq_w^m, \quad (8)$$

$$\frac{d\dot{m}_l}{dx} = Pq_w^m. \quad (9)$$

The water vapor condensation mass flux q_w^m [kg/s m²] is calculated from:

$$q_w^m = Sh \cdot D \cdot \frac{\rho_w - \rho_{ws}}{d_h}, \quad (10)$$

where D is the diffusion coefficient of water vapor in nitrogen [m²/s], ρ_w the mass concentration of water vapor in the gas [kg/m³] and ρ_{ws} the equilibrium vapor mass concentration at the film surface temperature T_{ls} [kg/m³]. The mass concentration and mass flux are related to the following:

$$\dot{m}_w = \rho_w UA, \quad (11)$$

where U is the gas velocity [m/s] and A the cross-sectional flow area [m²].

For the laminar and turbulent flow regimes, different correlations for the Nusselt and Sherwood numbers [3] were chosen:

For the laminar flow regime,

$$Nu = 3.66, \quad (12)$$

$$Sh = 3.66. \quad (13)$$

For the turbulent flow regime, the Dittus-Boelter correlations for were used:

$$Nu = 0.023 \cdot Re^{0.8} \cdot Pr^{0.3}, \quad (14)$$

$$Sh = 0.023 \cdot Re^{0.8} \cdot Sc^{0.3}, \quad (15)$$

where Pr , Re and Sc are the Prandtl, Reynolds and Schmidt number, respectively.

5.1.2 Particle deposition

In addition to steam condensation, the model includes the particle deposition onto the heat exchanger tube wall. The deposition mechanisms to be considered at the present study are: diffusiophoresis, thermophoresis, gravitational settling and the turbulent eddy impaction.

5.1.2.1 Diffusiophoresis

Diffusiophoresis is flow of aerosol particles down the concentration gradient of gas or vapor due to bombardment of particles by the gas or vapor molecules as they diffuse down the gradient. To maintain a constant total pressure near a condensing surface, the concentration gradient of vapor is balanced by an equal and opposite concentration gradient of non-condensable gas. The effect of gas molecules diffusing away from the surface on the transport of aerosol particles is however cancelled out by an aerodynamic flow of gas towards the surface (Stefan flow). Therefore the diffusiophoretic deposition velocity of particles onto the walls u_p^{DPH} [m/s] is directly proportional to the water vapor condensation rate q_w^m [kg/m²s] [4]:

$$u_p^{DPH} = \frac{x_w \sqrt{M_w}}{x_w \sqrt{M_w} + x_n \sqrt{M_n}} \frac{q_w^m}{\rho_w}, \quad (16)$$

where x_w and x_n are the mole fractions and M_w and M_n the molecular weights of water and nitrogen [g/mol], respectively and ρ_w is the mass concentrations of water [kg/m³] in the gas flow. Diffusiophoresis is approximately independent on particle size.

5.1.2.2 Thermophoresis

Thermophoresis is the result of the temperature gradients. On the hotter side, gas molecules colliding with particles carry on average a higher momentum than on the colder side, thus, causing a net transport in the direction of colder temperature. The thermophoretic deposition velocity is calculated using a generally accepted formula over a wide range of particle diameters [5]:

$$\mathbf{u}_p^{TPH} = -K \frac{\nu}{T} \nabla T, \quad (17)$$

where

$$K = 2C_s \frac{(\alpha + C_t Kn) Cn}{(1 + 3C_m Kn)(1 + 2\alpha + 2C_t Kn)}. \quad (18)$$

Here $C_s=1.147$, $C_t=2.20$, $C_m=1.146$, Cn is the Cunningham slip correction factor, ν the kinematic viscosity [m^2/s], T temperature [K], $\alpha = \lambda_g/\lambda_p$ is the ratio of gas to particle thermal conductivities, and Kn the Knudsen number. The Knudsen number $Kn = l_g/r_p$ is the ratio of the gas mean free path to the particle radius. In above equations, the thermophoretic velocity in the free molecular regime is interpolated with the corresponding expression in the continuum regime. Because thermophoresis is proportional to the temperature gradient, it is closely related to heat transfer. The actual value for the temperature gradient at the surface, which is required for calculating the thermophoretic deposition velocity \mathbf{u}_p^{TPH} , can be obtained using the heat transfer correlations for the Nusselt number Nu , which is the dimensionless temperature gradient at the surface. Consequently, we obtain the following simple equation:

$$\mathbf{u}_p^{TPH} = -K \nu Nu \frac{T - T_{is}}{Td_h} \quad (19)$$

5.1.2.3 Gravitational settling

Gravitational settling is caused by the effects of gravity on the particles. Settling affects particle transport in PCC only, if the tubes are not vertical. For spherical particles of density ρ_{den-p} [kg/m^3] and diameter d_p [m] in the range of 1-100 μm , the gravitational deposition velocity can be calculated from [6]:

$$\mathbf{u}_p^G = \frac{\rho_{den-p} d_p^2 \mathbf{g}}{18\mu} \cdot \mathbf{n}, \quad (20)$$

where \mathbf{g} is the gravitational acceleration [m/s^2] and \mathbf{n} the unit vector normal to the tube wall. For submicron particles gravitational deposition can be considered as negligible.

5.1.2.4 Turbulent impaction

Turbulent impaction is an important deposition mechanism for large particles, when the boundary layer between the surface and the host flow is turbulent. Inside the turbulent boundary layer turbulent eddies have a velocity component, which is normal to the main flow. Eddies may give enough momentum for particles to cross the laminar sub layer and finally to deposit on the wall.

At present there is no generally accepted mechanistic model available for turbulent deposition. Rough predictions can be made by using experimental correlations. The experimental deposition rate is usually given in such a way that the dimensionless deposition velocity u^+ is plotted as a function of the dimensionless stopping distance τ^+ . The dimensionless stopping distance τ^+ characterizes the ability of the particles to react to sudden changes of the fluid. In constant conditions it depends on particle size and other flow variables in the following way:

$$\tau^+ = \frac{1}{36} \frac{\rho_{den-p}}{\rho_{den-g}} \left(\frac{d_p}{d_h} \right)^2 \text{Re}^2 f(\text{Re}), \quad (21)$$

where f is the Fanning friction factor. The deposition velocity u^+ is the actual velocity, with which the particles deposit, normalized with “wall variables” [7]:

$$u^+ = \frac{u_p^{TUR}}{U \frac{f}{2}} \quad (22)$$

Submicron range particles ($\tau^+ < 0.2$) tend to follow the streamlines of fluid motion. This means that in the absence of thermophoresis Brownian motion is the mechanism mainly responsible for deposition. Therefore it is assumed that u^+ is independent of τ^+ and is a function of Schmidt number only:

$$u^+ = 0.086 Sc^{-0.7}. \quad (23)$$

($Sc = \nu/D$, where ν is the kinematic viscosity of the fluid [m^2/s] and D the Brownian diffusivity [m^2/s])

However, when τ^+ is greater than 0.2, the deposition velocity becomes independent of Sc . Particles in this range diffuse towards the wall due to radial velocity fluctuations (turbulent diffusion) and then deposit onto the wall by a free-flight mechanism through the viscous sub layer. This is caused by the inability of the particles to follow the turbulent eddies in the vicinity of the wall. This inability can be conveniently described by the concept of a stopping distance. In this range, the experimental deposition data can be roughly correlated using the following equation:

$$u^+ = 3.5 \cdot 10^{-4} \tau^{+2}. \quad (24)$$

Neither of the correlations above work properly, however, as the particle stopping distance increases beyond $\tau^+ > 30$. After this point the particles are too large to respond to the fluid

fluctuations, and the $u^+(\tau^+)$ curve levels off to an approximately constant value 0.17 (see [7] for details). This is also approximately the point, where gravitation starts to play an increasingly important role in particle depositions dynamics.

The reduction in the particle mass flux \dot{m}_p [kg/s], due to deposition can be obtained from:

$$\frac{d\dot{m}_p}{dx} = -\left\{P\rho_p(u_p^{DPH} + u_p^{TPH} + u_p^G + u_p^{TUR})\right\}, \quad (25)$$

where ρ_p is the particle mass concentration [kg/m³] in the gas flow.

5.2 Status of the program

The current version of the Fortran program, which will be applied in the study of deposition processes in PCC, is presented in appendix A. The program calculates heat transfer, condensation and deposition by diffusiophoresis in PCC tubes. Differential equations for temperature (Eqs. (1) and (2)) are integrated simultaneously with differential equations for mass fluxes (Eqs. (7) - (9)), and solved for obtaining the particle deposition rate along the tube wall. A simple Eulerian time marching scheme is to be used in this task.

Currently the models for all deposition processes including thermophoresis, turbulent eddy impaction and settling are added into the program. In the next stage the program will be validated by comparing the calculated results to the deposition velocities measured in VTT heat exchanger experiments. The first validation calculations are underway.

When the validation work is completed integral deposition and consequently the decontamination factor (DF) in PCC tubes is calculated using various sets of system parameters including inlet gas temperature, temperature of the pool, pressure, particle size distribution, steam partial pressure, submerged length of the tubes etc. Based on these results the most influential parameters will be determined. Lastly, DF will be presented as a correlation function of these parameters. Such correlation function is then to be included into MELCOR code for plant scale analysis.

6 Model to estimate pH in the containment sumps

The pH of the containment water pools will be estimated to assess the possibility of having highly volatile forms of fission product iodine in the containment. The estimates of the pool pH will be calculated with MELCOR model and with the ChemSheet model.

Iodine Pool model input will be added to the current MELCOR input for the final analyses. The effect of buffer injection (sodium pentaborate) to the RPV downcomer during reflooding and injection of trisodium phosphate into the Suppression Pool and RPV at 72 h from the accident beginning. The release of chlorine via radiolysis will be estimated with the MELCOR model. The time dependent pH in the containment pools will be calculated with both MELCOR and ChemSheet codes. ChemSheet analyses are used for verification of MELCOR results. The models of ChemSheet code are described in Appendix B.

7 Preliminary analysis of a source term from the containment in a selected test case

The following results are from a Bottom Drain Line Break run with an unverified and only partially updated ESBWR (4590 MWt) MELCOR 1.8.6 input.

The hypothetical accident scenario begins with a failure of reactor pressure vessel (RPV) bottom drain line ($A=2.165 \cdot 10^{-3} \text{ m}^2$). The reactor is scrammed at time 0 s. All Isolation Condenser Drain Lines are assumed to be blocked thus failing to provide any coolant injection to the RPV. GDCS pool injection is assumed to be unavailable until 4100 s from the accident beginning. This timing specification of reflooding was used in this run to allow high oxidation in the core but to prevent core support plate failure. During the reflooding the GDCS injection lines are fully open. Equalization line is opened late 26 910 s after the start of GDCS injection. All 6 PCCS units are operating through out the accident progression.

The following key event summary is for information of the overall time events in the scenario.

Table 15. Key event summary of the BDL Break scenario.

Event	Timing (s)
Reactor scram	0.0
MSIV closed	6.2
Level L1 signal	13.9
FP gap release, core ring 2	14.7
FP gap release, core ring 1	15.2
FP gap release, core ring 3	16.2
DPV valve # 1 open	114
DPV valve # 2 open	159
Level TAF (core uncovered)	301
FP gap release, core ring 4	711
FP gap release, core ring 5	753
Core fully uncovered	2125
GDCS injection line open	4100
Core fully recovered	9725
GDCS pool empty	25 880
Equalization line opened	31 010
In-vessel H ₂ production	532 kg

7.1 Reactor coolant system behavior

The reactor core is uncovered at 301 s (=5.0 min) from the beginning of accident due to of coolant through BDL break (Fig. 3). No core makeup is available till 4100 s (=68 min). The core is fully uncovered at 2125 s (=35 min). The core in uncovered for 33 min before start of reflooding. Core is fully recovered at about 9725 s (=2 h 42 min).

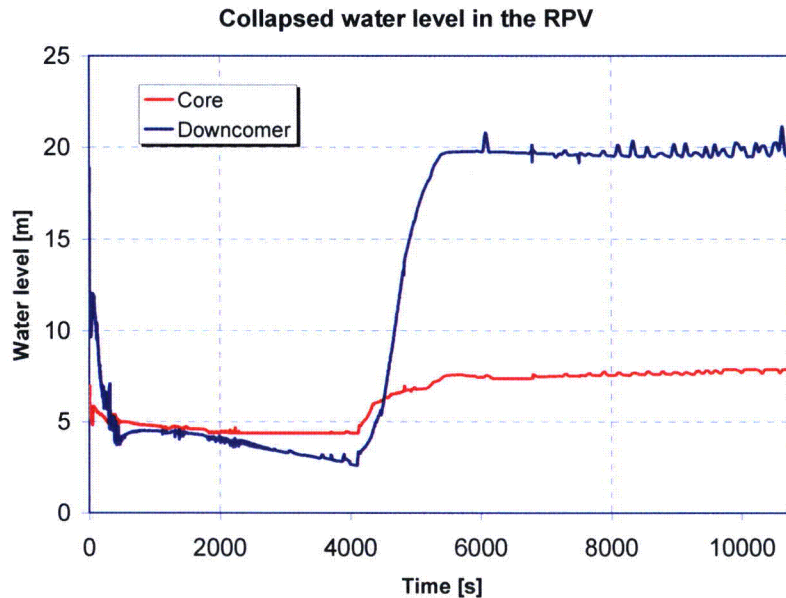


Figure 3. Collapsed and boiled-up water level in the core. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

The temperature of cladding and fuel in core ring 1 (Figs. 4 and 5) begin to increase after full uncovering of the core. The temperatures in the upper parts of the core reach Zr melting temperatures. Molten Zr, however, is set to be held up by ZrO_2 layer till the ZrO_2 temperature reaches 2400 K. Following the start of GDCS injection oxidation increases in the core and causes a rapid temperature escalation in the upper half of the core and causes relocation of molten Zr downwards. Material relocation is seen in Figs. 4 and 5 as rapid decrease of temperature to zero. As the surrounding Zr disappears in the uppermost node also the fuel pellets relocate downwards as particle debris.

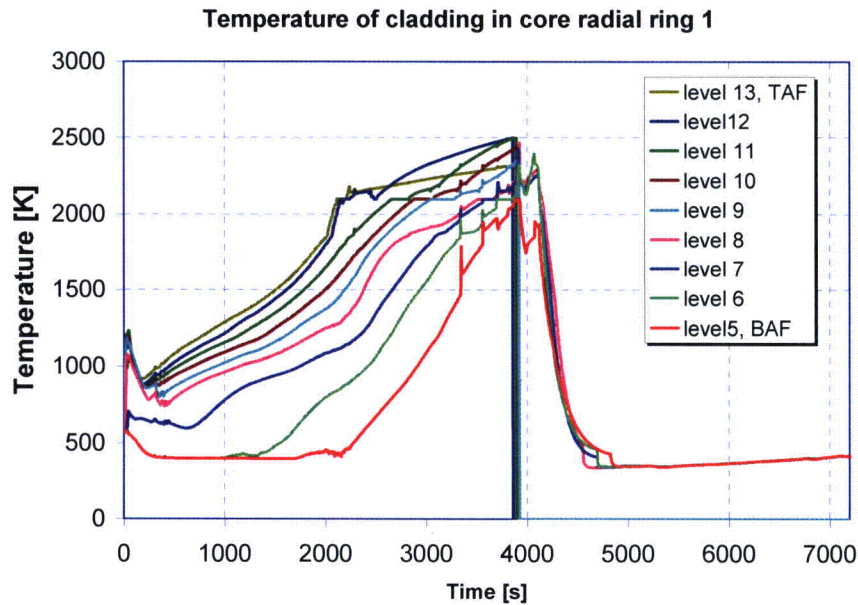


Figure 4. Cladding temperature in the core ring 1. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

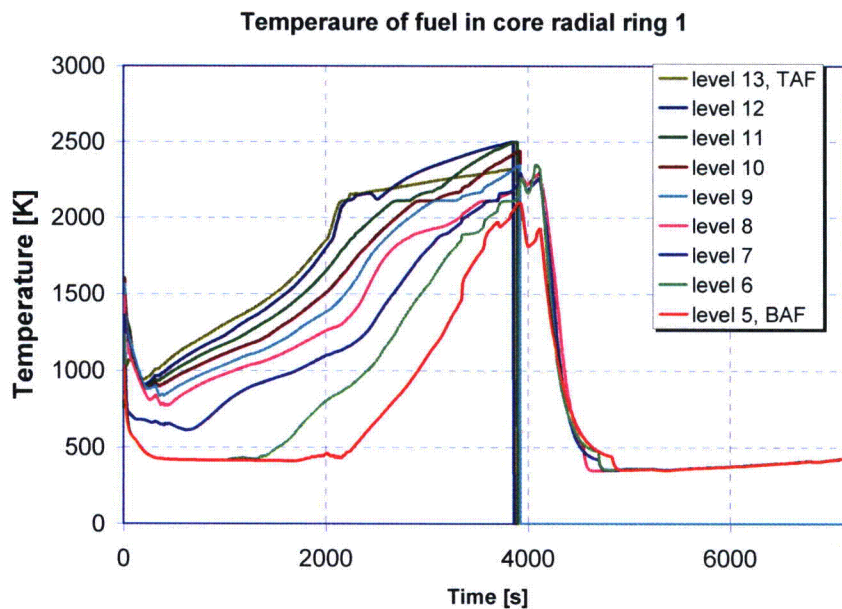


Figure 5. Fuel temperature in core ring 1. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

The total hydrogen mass generated in the core is 532 kg out of which 506 kg is produced from Zr oxidation (Fig 6). The total cladding mass is 50 572kg producing 2217.5 kg of hydrogen if completely oxidized. Thus the cladding oxidation fraction is 22.8 %.

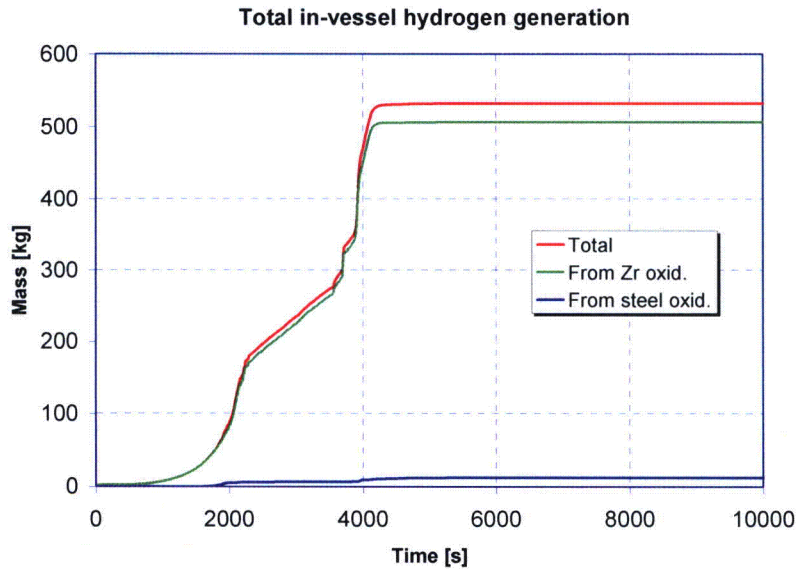


Figure 6. Cumulative hydrogen release from the core materials. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

The cumulative coolant injection to the RCS and break flow out of the RCS are presented in the Figs. 7 and 8, respectively. Reflooding is able to cool the core and prevent core support plate failure and pressure vessel failure. After about 9 h the water level in the Lower Drywell reaches the break elevation at the bottom of the RPV. This causes reverse (negative) flow through the Bottom Drain Line, which is seen as decreasing mass integral in Fig. 8.

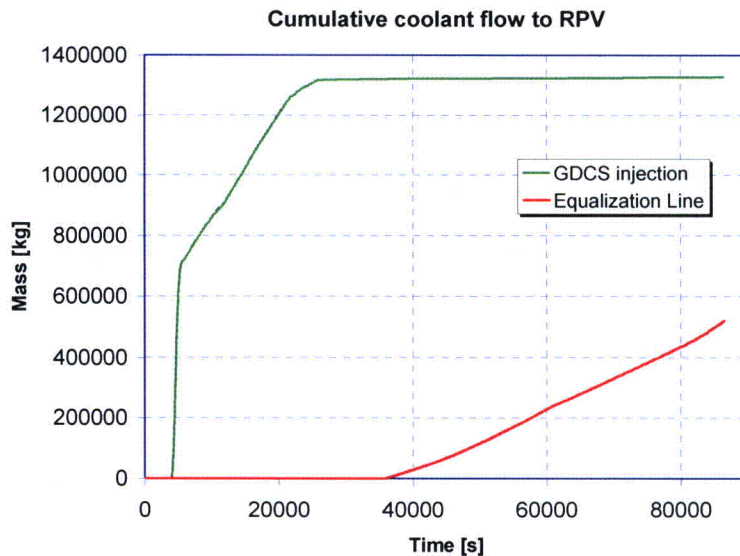


Figure 7. Cumulative coolant injection to the RPV from different water sources. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

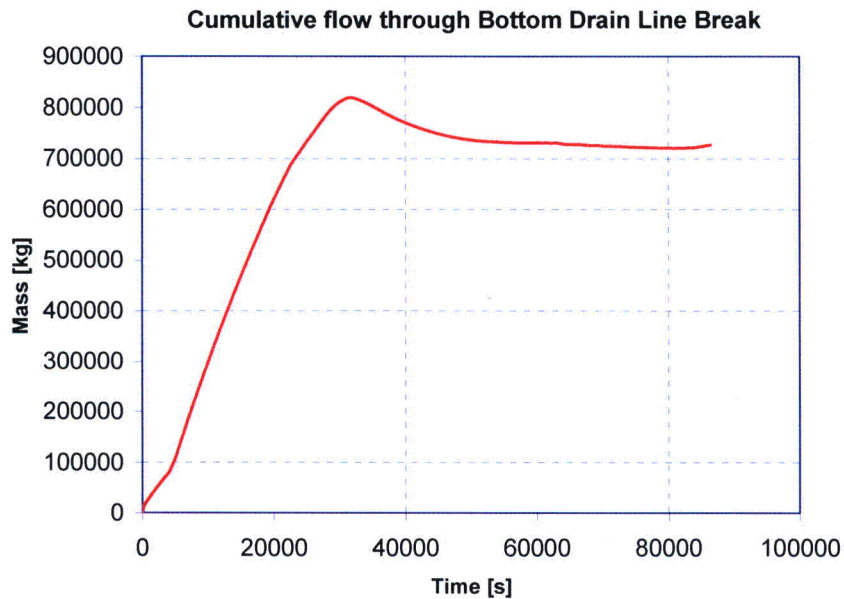


Figure 8. Cumulative coolant break flow. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

The pressure in the RCS is presented in Fig 9. The initial pressure in the RPV is 7.2 MPa. Following the opening of Depressurization Valves the pressure decreases to about 0.2 MPa. The initiation of reflooding increases steam production and RCS pressure to about 0.6 MPa.

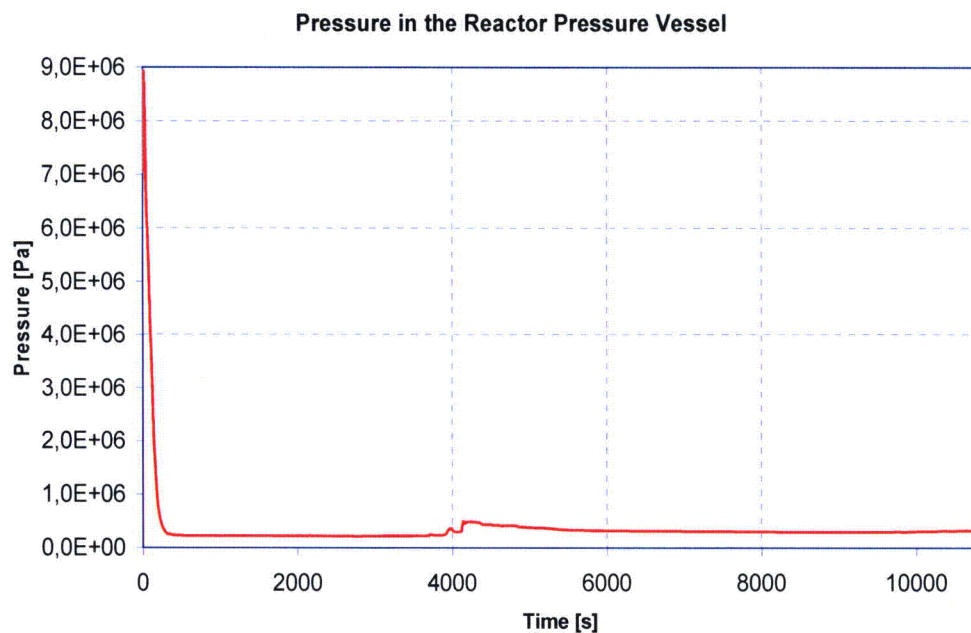


Figure 9. Pressure in the RPV. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

7.2 Containment behavior

The pressure in the containment increases due to blowdown through the DPV valves and the Bottom Drain Line Break to about 0.25 MPa (Fig. 10). The start of reflooding of over-heated core from GDCS pool at 4100 s (=68 min) increase the pressure in the containment rapidly peaking at 0.413 MPa at 4775 s (=80 min). The core becomes fully covered at 9725 s. The drywell pressure increases by continuous steam release from the RPV through Depressurization Valves (Fig. 11). Hydrogen is released from the RPV to the upper drywell and further vented via PCCS Vent Line and via horizontal vent at highest elevation to the Wetwell atmosphere. The partial pressure of non-condensables and steam increases in the Wetwell being about 0.4 MPa at the end of calculation (Fig. 12).

The gas temperature in the drywell peak at about 1800 K due to hot hydrogen and steam discharge from the RPV during reflooding (Fig. 13).

The water mass in GDCS is shown in Fig. 14. The inventory in the GDCS is depleted at 25 880 s (=7.2 h).

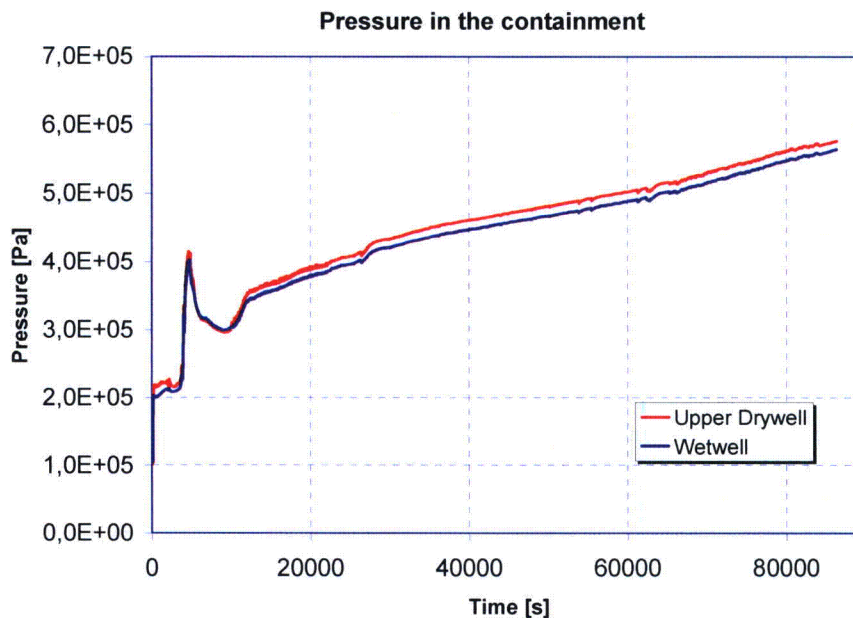


Figure 10. Pressure in the containment. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

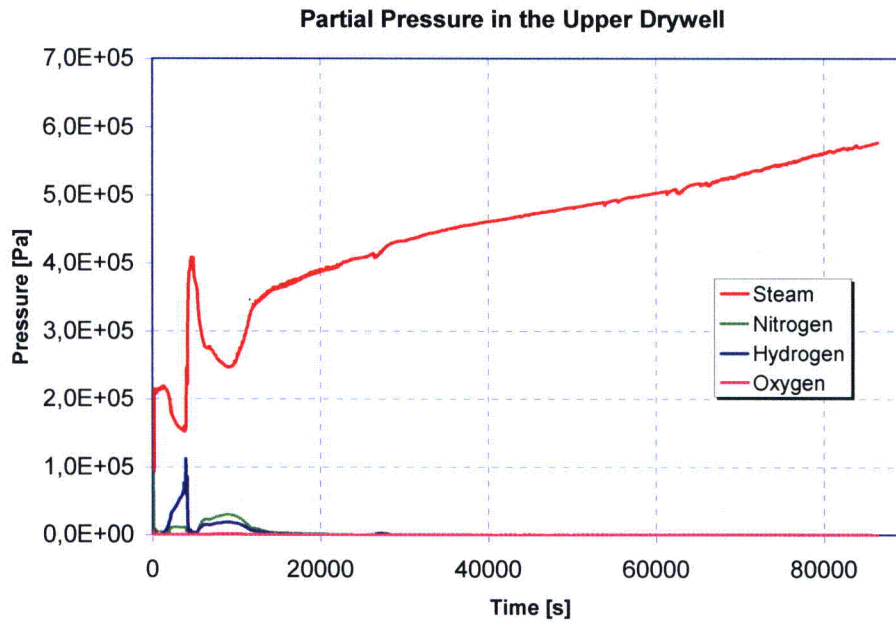


Figure 11. Partial pressures of steam, nitrogen and hydrogen in the upper drywell. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

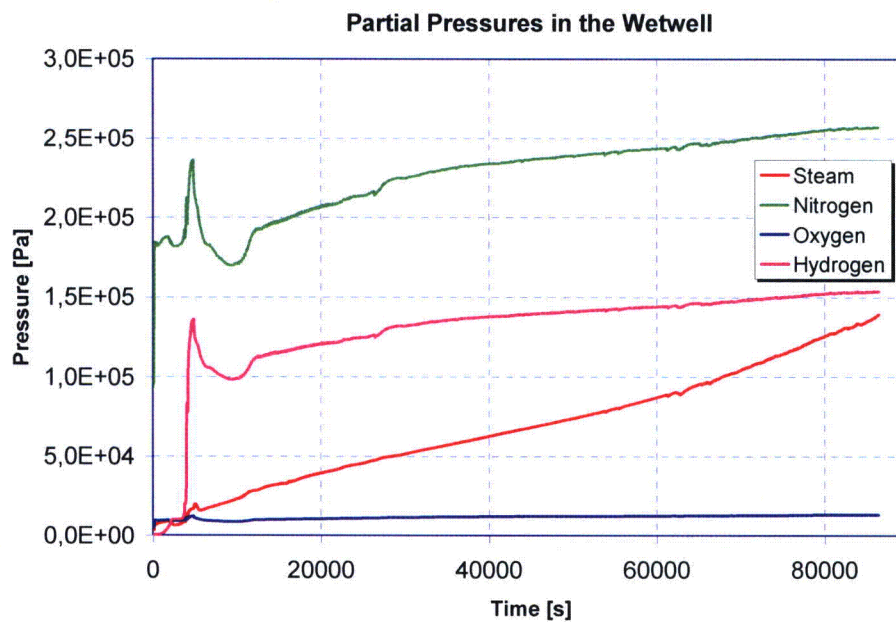


Figure 12. Partial pressures of steam, nitrogen and hydrogen in the wetwell. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

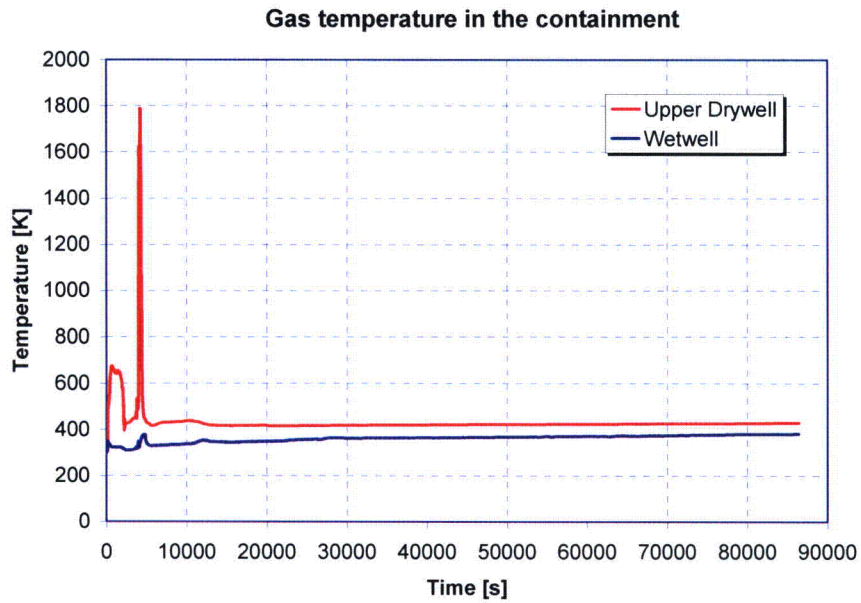


Figure 13. Atmosphere temperature in the containment. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

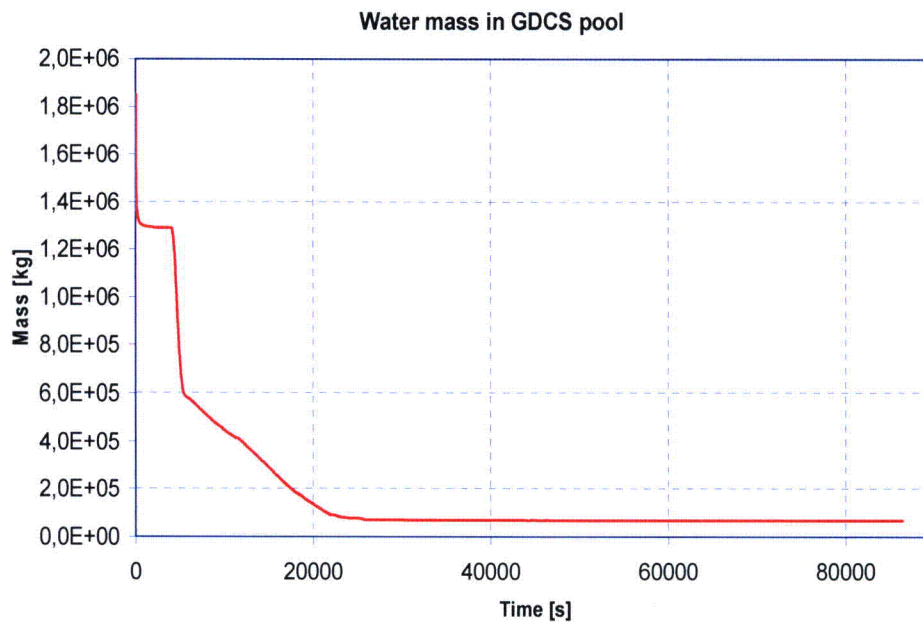


Figure 14. Water mass in the GDCS pool. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

Figure 15. illustrates the water pool temperatures in the GDCS pool. The temperature of GDCS pool increases due to condensate flow from the GDCS wall structure.

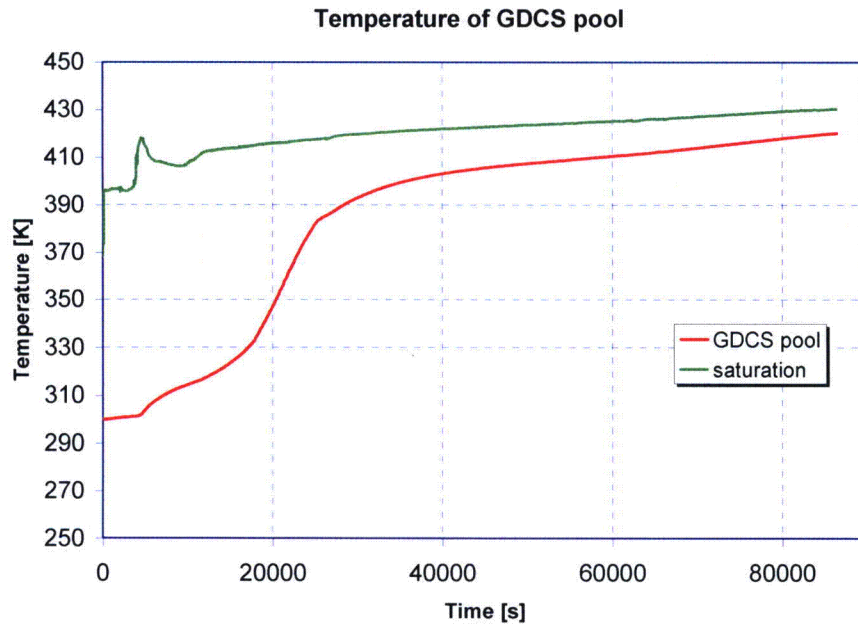


Figure 15. GDCS pool temperatures. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

The Suppression Pool temperature increases at the top of the pool but remains below saturation (Fig. 16). The temperature stratification in the suppression pool is modeled by dividing the pool volume into four vertically adjacent control volumes. The temperature difference between the top and the bottom of the pool is about 70 K at the end of calculation. However, this result should be considered as a rough estimate, since MELCOR code does not properly model fluid dynamics for mixing.

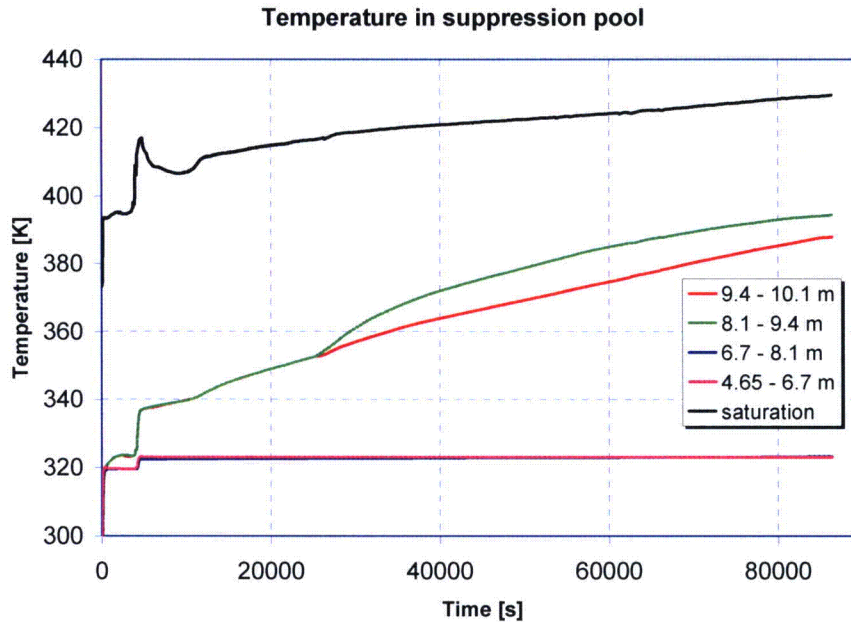


Figure 16. Suppression pool temperature. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

The nominal containment leakage is modeled as a single flow path from the upper drywell with the assumption the leakage rate is 0.5 % of the containment gas volume ($=12\,342 \text{ m}^3$) per day at 310 kPa (g). The respective average velocity is obtained from Bernoulli's equation

$$A \cdot v = \sqrt{\frac{2 \cdot \Delta p}{\rho}} = 0.005 \cdot 12342 / 86400 \text{ m}^3/\text{s},$$

where $\Delta p = 411.3 \text{ kPa}$, $\rho_{\text{steam}} = 6.12 \text{ kg/m}^3$. This yields $A = 1.949 \cdot 10^{-6} \text{ m}^2$.

The cumulative atmosphere flow rate through the containment leakage is presented in Fig. 17.

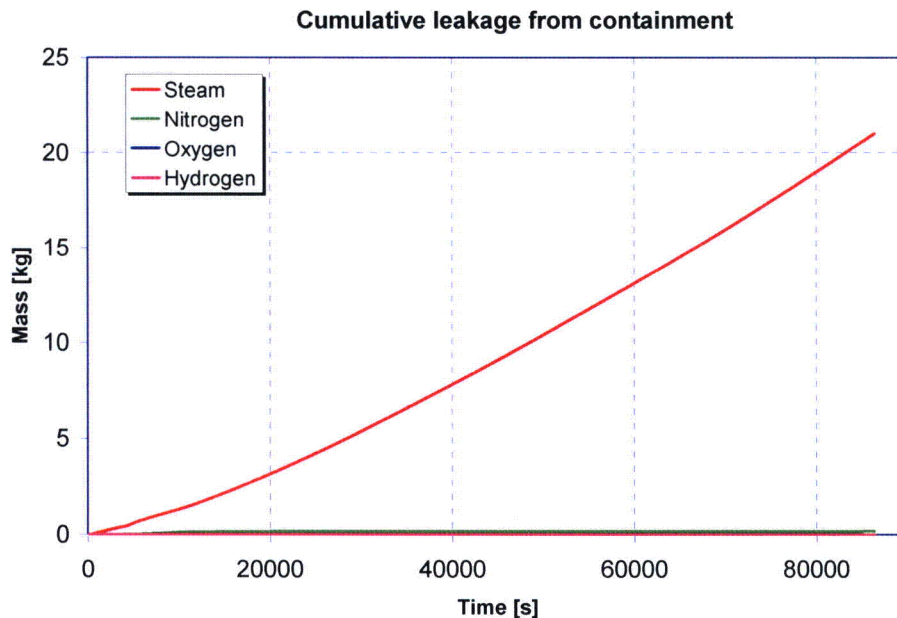


Figure 17. Cumulative containment (nominal) leakage from drywell. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

The cumulative water and non-condensable gas flow rates through the PCCS condensers are shown in Figs. 18, 19 and 20. The current model is not satisfactory in terms of describing the separation of condensate and gas flows between the Drain Line and the Vent Line. The current model setup of the Drain Line performs the loop seal function and directs the gas flow to the Vent Line, but also most of the condensate flows through the Vent Line to the Suppression Pool instead of GDCS Pool. The model will be upgraded for the calculations in the Final Report. However, the results are roughly representative in terms of airborne aerosol flow through the PCCS and it is possible that pool scrubbing in the Suppression Pool becomes more efficient when condensate at saturation temperature is directed to the GDCS pool. This may keep the Suppression Pool temperature lower.

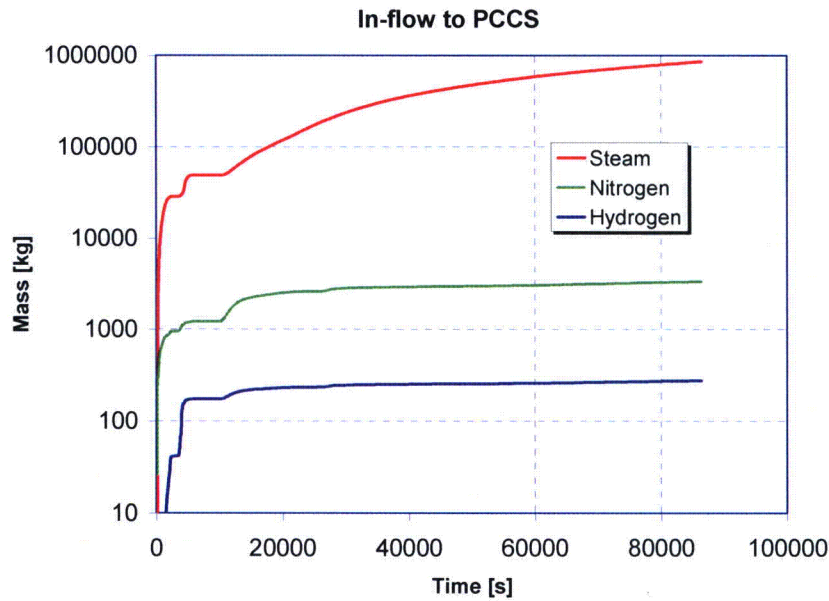


Figure 18. Cumulative mass inflow to PCCS units). Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

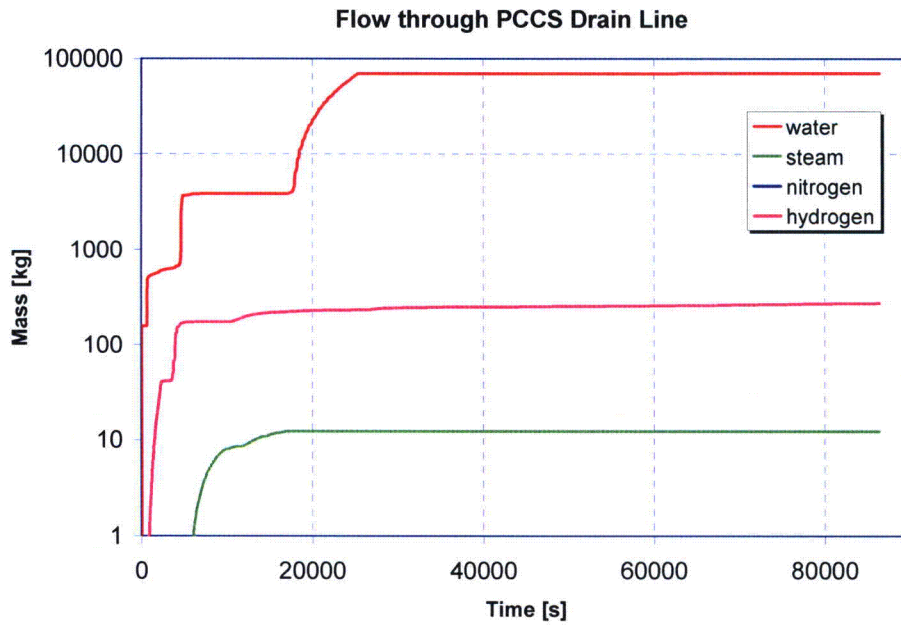


Figure 19. Cumulative mass flow through the PCCS Drain Lines. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

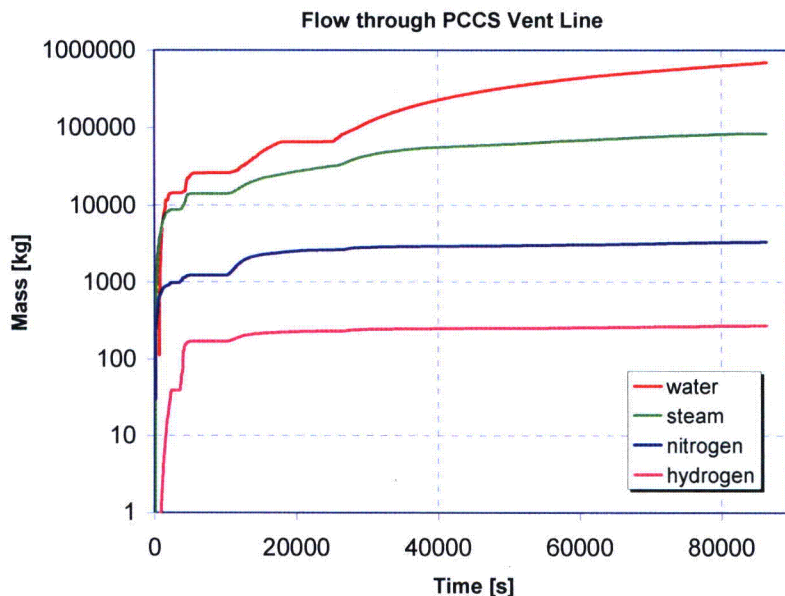


Figure 20. Cumulative mass flow through PCCS Vent Line . Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

7.3 Fission product behavior

The release fractions of fission products from the fuel were calculated using the CORSOR-M option in MELCOR. In general the release fractions remained lower than presented in [8] because of relatively early reflooding. Table 16 gathers the calculated release fractions at time steps 1500s, 1 h and 2 h. These are compared to the release fractions presented in NUREG-1465 [8].

Table 19. Release fractions of fission products from the fuel.

Fission product class	Calculated release fractions from the fuel			Early in-vessel Release for BWRs in [8]
	1500 s	1 h	2 h	
Noble gases	$4.89 \cdot 10^{-2}$	0.33	0.62	0.95
Cs	$4.54 \cdot 10^{-2}$	0.30	0.57	0.25
Sr+Ba	$1.82 \cdot 10^{-10}$	$2.04 \cdot 10^{-4}$	$1.87 \cdot 10^{-3}$	0.02
I ₂	$5.19 \cdot 10^{-15}$	$4.07 \cdot 10^{-11}$	$9.51 \cdot 10^{-11}$	
Te	$7.068 \cdot 10^{-7}$	$4.20 \cdot 10^{-2}$	0.44	0.05
Ru	$4.58 \cdot 10^{-17}$	$1.18 \cdot 10^{-8}$	$1.05 \cdot 10^{-6}$	$2.5 \cdot 10^{-3}$
Mo	$3.60 \cdot 10^{-6}$	$5.11 \cdot 10^{-3}$	$1.51 \cdot 10^{-2}$	$2.5 \cdot 10^{-3}$
Ce	$9.75 \cdot 10^{-20}$	$9.92 \cdot 10^{-10}$	$5.04 \cdot 10^{-7}$	$5.0 \cdot 10^{-4}$
La	$8.98 \cdot 10^{-15}$	$8.61 \cdot 10^{-7}$	$4.80 \cdot 10^{-5}$	$2 \cdot 10^{-4}$
U	$8.99 \cdot 10^{-15}$	$8.71 \cdot 10^{-7}$	$4.80 \cdot 10^{-5}$	
Cd	$7.42 \cdot 10^{-8}$	$2.90 \cdot 10^{-3}$	$1.26 \cdot 10^{-2}$	
CsI	$4.23 \cdot 10^{-2}$	0.32	0.62	0.35

The calculated release fractions from the core are lower for noble gases but higher for cesium, iodine and tellurium and than presented in NUREG-1465.

Fig. 21 shows the history of the fission product release fractions of the classes with highest releases.

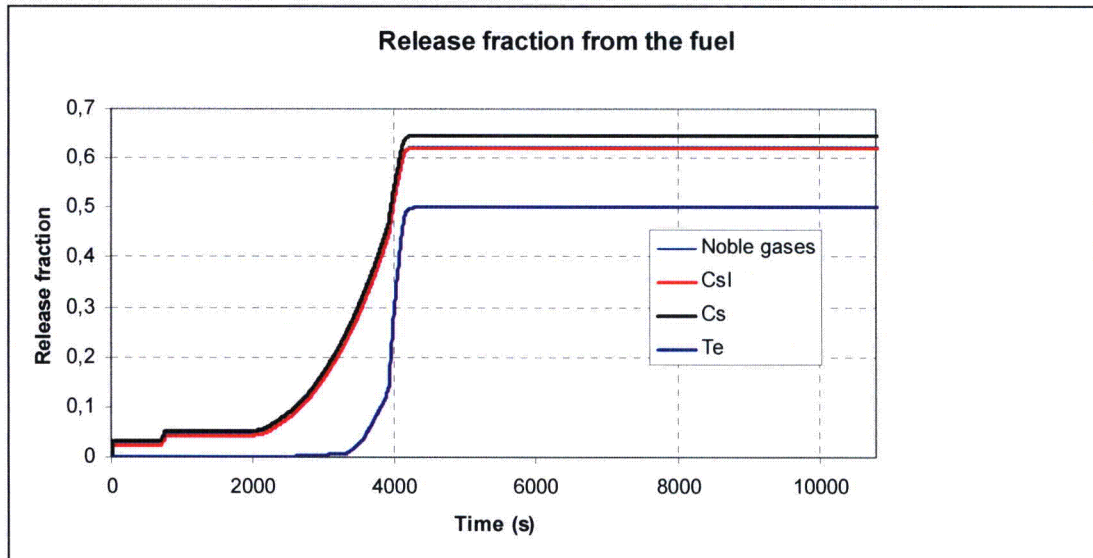


Figure 21. Release fractions of noble gases, Cs, CsI and Te from the fuel. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

The fission product release from the containment is low (Fig. 22). For noble gases, CsOH and CsI the release fractions of the initial whole core inventory to reactor building are $1.43 \cdot 10^{-5}$, $5.04 \cdot 10^{-6}$ and $4.58 \cdot 10^{-6}$, respectively.

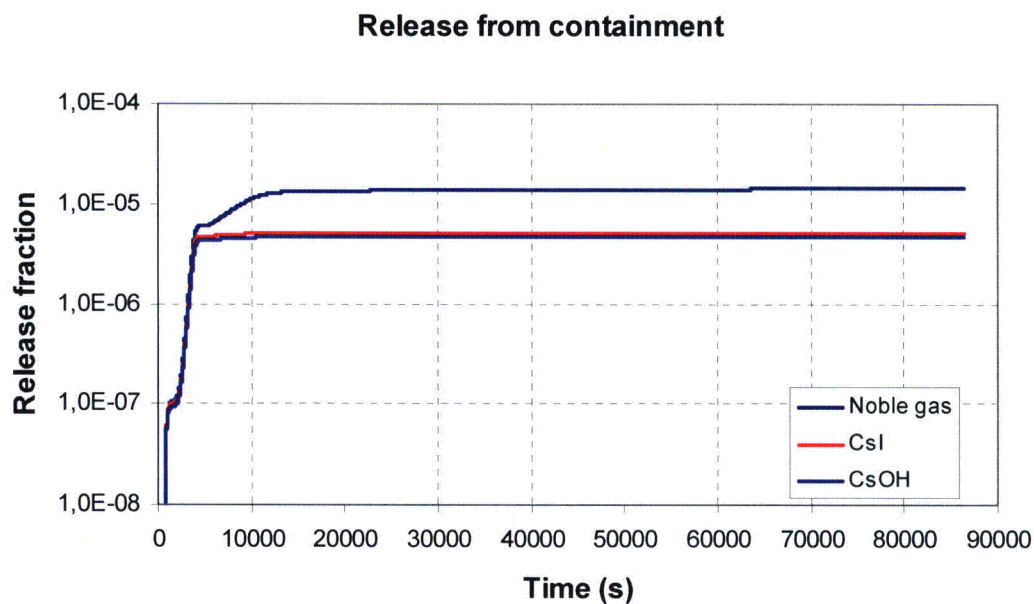


Figure 22. Fraction of initial core inventory of noble gases, CsI and Cs that is released from the containment through nominal leakage path. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

The total airborne CsI aerosol mass in the containment has a maximum value first in the upper drywell due to discharge of the DPV valves (Fig. 23). The airborne mass degrades rapidly after start of reflooding and scrubbing to suppression pool via horizontal vents. After recooling of the core the CsI aerosols are removed from the Drywell atmosphere by gravitational settling and condensation in the PCCS.

The total CsI aerosol concentration in the containment water pools is presented in Fig. 24. Suppression pool retains most of the CsI aerosols. The aerosol mass in the GDCS pool increases after start of the core heat up due to steam and aerosol flow from the upper drywell and rapid condensation on the walls. Concentration decreases along with the coolant injection to the downcomer.

The deposition of CsI aerosols on Upper Drywell structures is presented in Fig. 25. The decrease of deposited mass on the Drywell floor and the GDCS wall is due to steam condensation and wash-out with the water film.

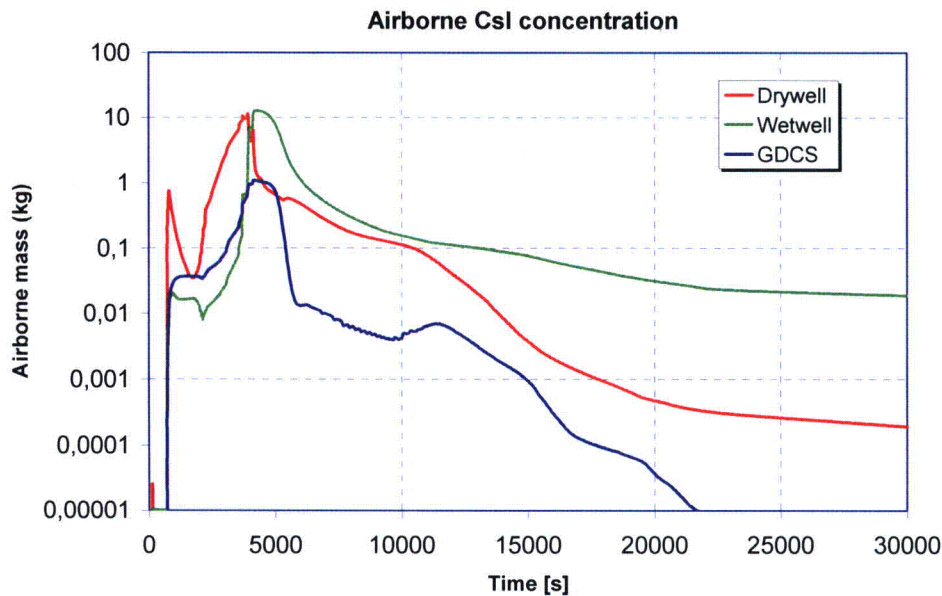


Figure 23. Total airborne CsI aerosol mass in the containment. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

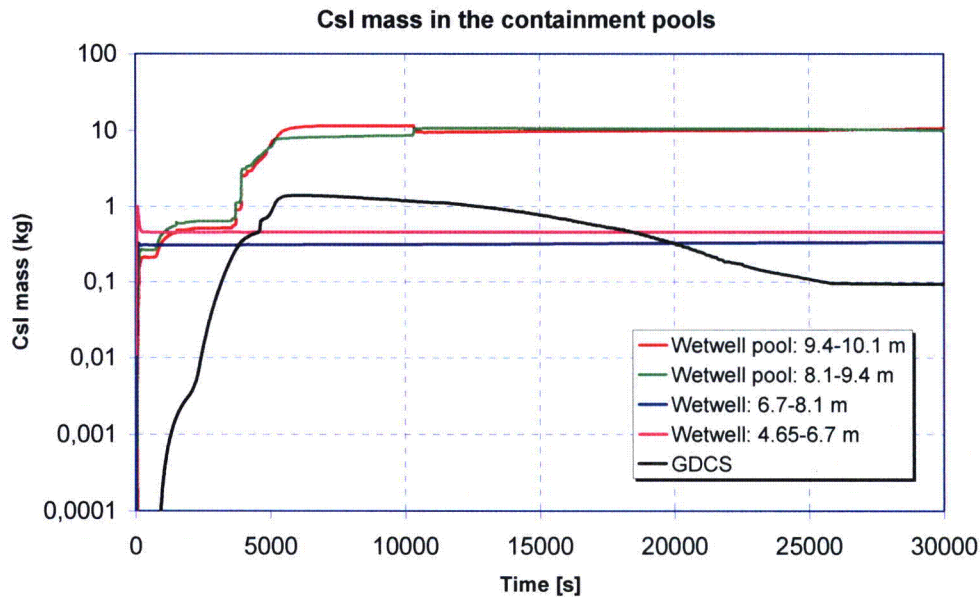


Figure 24. Total CsI aerosol mass in the Suppression Pool and the GDCS Pool. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

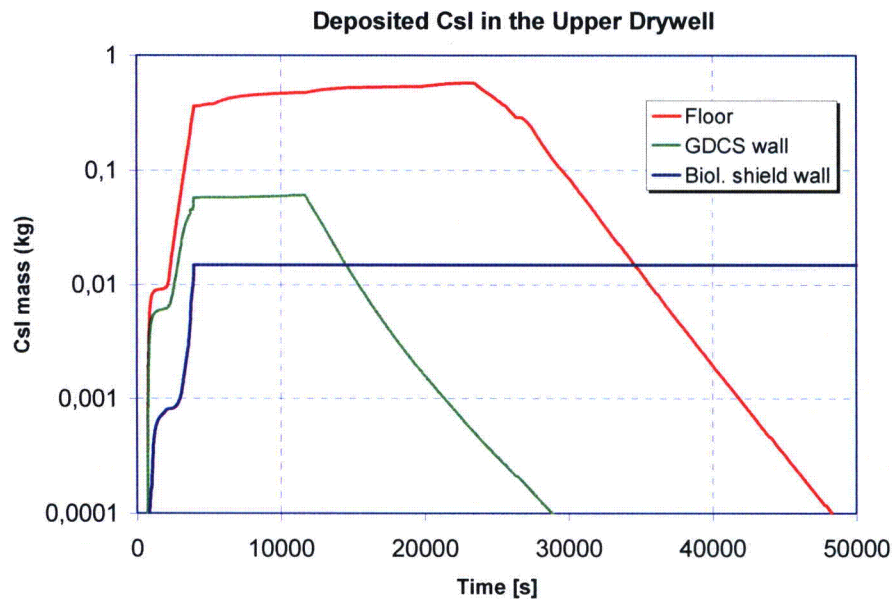


Figure 25. Total deposited CsI aerosol mass on Upper Drywell structures. Bottom Drain Line Break ($A=2.165 \cdot 10^{-3} \text{ m}^2$) case with reflooding by GDCS injection at 4100 s.

The airborne mass fractions of CsI in respect to the total release from the core for different containment compartments is presented in Fig. 26. When approximating the decontamination factor of CsI aerosol in the PCCS by dividing the airborne mass in the Drywell by the airborne mass in the GDCS one obtains a result shown in Fig. 27. The decontamination factor varies between 4.4 and 853. The minimum is reached at time 4 h into the accident.

Airborne fractions of CsI in respect to total release from the core

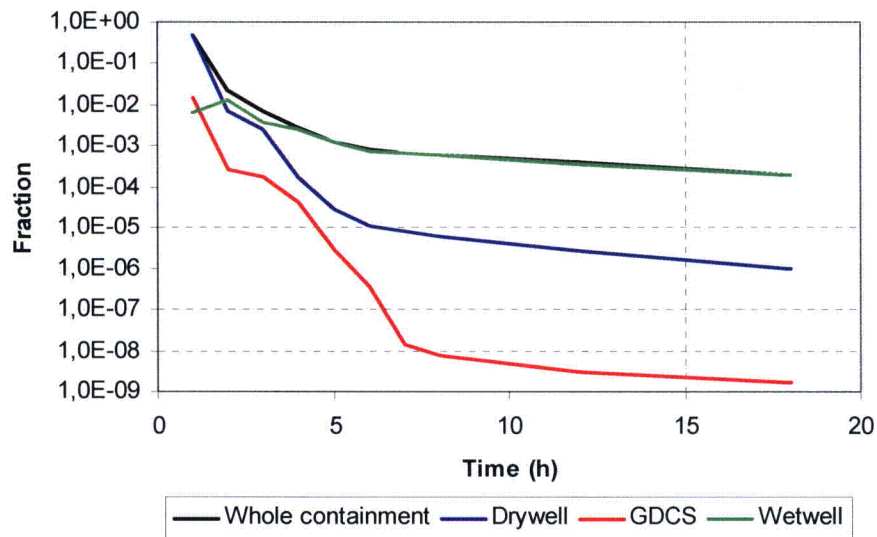


Figure 26. Mass fraction of airborne CsI in whole containment, Drywell compartments (upper+middle+lower), GDCS and Wetwell. Mass fraction is calculated from the release of CsI from the core.

Decontamination factor in the PCCS

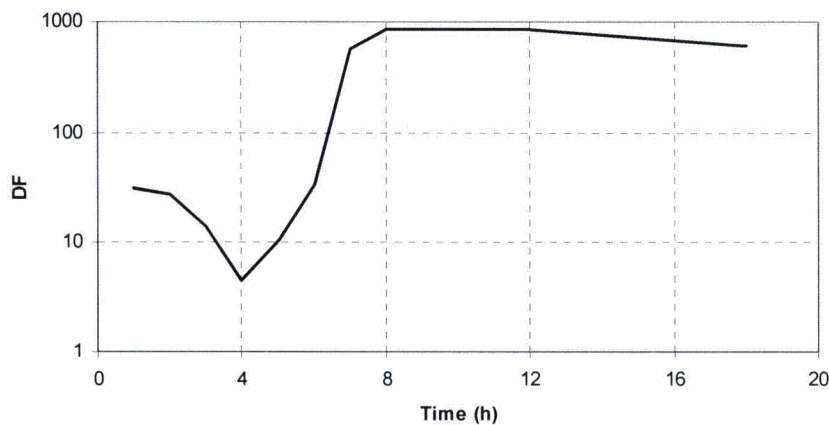


Figure 27. Estimate of decontamination factor in the PCCS calculated as airborne mass in the Drywell divided by airborne mass fraction in the GDCS.

The CsI decontamination factor for the whole containment can be defined as the ratio of total CsI released from the core divided by the total airborne mass of CsI in the containment. The value for containment decontamination factor ranges from 2 to 4976 on the basis of draft MELCOR calculation (Fig. 28).

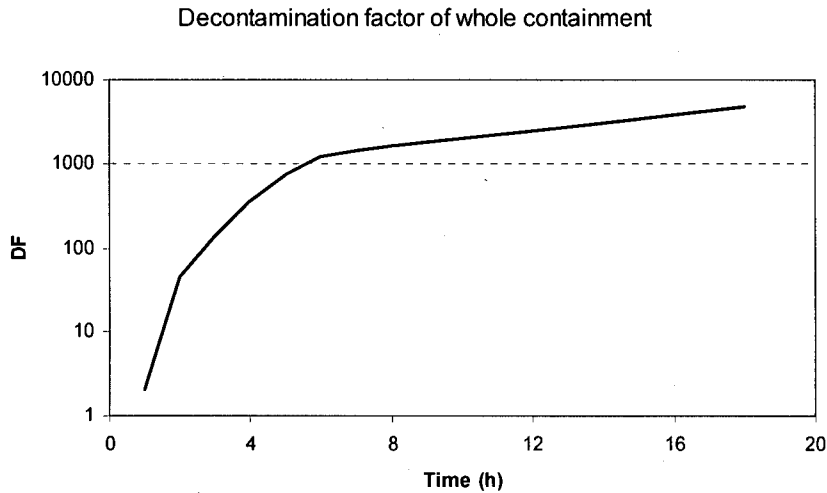


Figure 28. The decontamination factor of CsI aerosols for the containment calculated as total CsI mass released from the core divided by total airborne aerosol mass in the containment atmosphere.

The mass balance of CsI in the reactor coolant system and in the containment is reported in Table 20. The numbers in Table 20 are hand-calculated from the original CsI mass data in obtained from the Tabular Output for different printout intervals of the MELCOR run.

Table 20. Fractional distribution of CsI mass at different time steps (1, 2, 3, 4, 5, 6, 7, 8, 12 and 18 h). Fractions are determined as: Mass in a specified location/total mass released from the core.

<i>Time= 1</i>	Total	Airborne	In the pool	Deposited on structures
RPV	0.309	0.137	$3.5 \cdot 10^{-4}$	0.171
Drywell (upper+middle+lower)	0.513	0.469	0.025	0.019
Wetwell	0.126	$6.8 \cdot 10^{-3}$	0.120	$3.4 \cdot 10^{-3}$
GDCS	0.027	0.015	0.012	$1.6 \cdot 10^{-5}$
Annulus	$7.3 \cdot 10^{-3}$	$6.9 \cdot 10^{-3}$	$5.8 \cdot 10^{-5}$	$2.6 \cdot 10^{-4}$
PCCS	0.017	$3.2 \cdot 10^{-3}$	0.010	$4.2 \cdot 10^{-3}$
Reactor Building	$6.21 \cdot 10^{-6}$			
Total	0.999	0.638	0.167	0.198

<i>Time= 2 h</i>	Total	Airborne	In the pool	Deposited on structures
RPV	0.137	$4.6 \cdot 10^{-5}$	0.020	0.117
Drywell (upper+middle+lower)	0.131	$7.6 \cdot 10^{-3}$	0.047	0.076
Wetwell	0.677	0.014	0.659	$3.9 \cdot 10^{-3}$
GDCS	0.043	$2.8 \cdot 10^{-4}$	0.043	$8.3 \cdot 10^{-5}$
Annulus	$4.5 \cdot 10^{-3}$	$8.4 \cdot 10^{-4}$	$1.1 \cdot 10^{-3}$	$2.5 \cdot 10^{-3}$
PCCS	$7.8 \cdot 10^{-3}$	$1.3 \cdot 10^{-5}$	$7.8 \cdot 10^{-3}$	$2.7 \cdot 10^{-6}$
Reactor Building	$8.02 \cdot 10^{-6}$			
Total	1.000	0.0228	0.778	0.199

<i>Time= 3 h</i>	Total	Airborne	In the pool	Deposited on structures
RPV	0.141	$3.4 \cdot 10^{-6}$	0.025	0.117
Drywell (upper+middle+lower)	0.134	$2.7 \cdot 10^{-3}$	0.054	0.077
Wetwell	0.677	$4.0 \cdot 10^{-3}$	0.672	$1.8 \cdot 10^{-3}$
GDCS	0.036	$1.9 \cdot 10^{-4}$	0.036	$4.9 \cdot 10^{-5}$
Annulus	$4.6 \cdot 10^{-3}$	$2.8 \cdot 10^{-4}$	$1.4 \cdot 10^{-3}$	$2.9 \cdot 10^{-3}$
PCCS	$7.4 \cdot 10^{-3}$	$1.6 \cdot 10^{-5}$	$7.3 \cdot 10^{-3}$	$1.5 \cdot 10^{-5}$
Reactor Building	$8.3 \cdot 10^{-6}$			
Total	1.000	$7.19 \cdot 10^{-3}$	0.796	0.199

<i>Time= 4 h</i>	Total	Airborne	In the pool	Deposited on structures
RPV	0.146	$6.8 \cdot 10^{-7}$	0.029	0.116
Drywell (upper+middle+lower)	0.137	$1.9 \cdot 10^{-4}$	0.063	0.073
Wetwell	0.685	$2.6 \cdot 10^{-3}$	0.681	$1.4 \cdot 10^{-3}$
GDCS	0.026	$4.3 \cdot 10^{-5}$	0.026	$3.7 \cdot 10^{-5}$
Annulus	$4.4 \cdot 10^{-3}$	$8.3 \cdot 10^{-6}$	$1.6 \cdot 10^{-3}$	$2.9 \cdot 10^{-3}$
PCCS	$1.3 \cdot 10^{-3}$	$9.0 \cdot 10^{-7}$	$1.3 \cdot 10^{-3}$	$1.0 \cdot 10^{-6}$
Reactor Building	$8.4 \cdot 10^{-6}$			
Total	1.000	$2.84 \cdot 10^{-3}$	0.802	0.193

<i>Time= 5 h</i>	Total	Airborne	In the pool	Deposited on structures
RPV	0.151	$2.9 \cdot 10^{-7}$	0.038	0.116
Drywell (upper+middle+lower)	0.143	$2.9 \cdot 10^{-5}$	0.083	0.066
Wetwell	0.686	$1.3 \cdot 10^{-3}$	0.684	$6.6 \cdot 10^{-4}$
GDCS	0.016	$2.8 \cdot 10^{-6}$	$6.4 \cdot 10^{-3}$	$9.1 \cdot 10^{-6}$
Annulus	$4.4 \cdot 10^{-3}$	$1.1 \cdot 10^{-6}$	$1.7 \cdot 10^{-3}$	$2.8 \cdot 10^{-3}$
PCCS	$1.3 \cdot 10^{-5}$	$4.7 \cdot 10^{-8}$	$3.1 \cdot 10^{-7}$	$6.1 \cdot 10^{-12}$
Reactor Building	$8.4 \cdot 10^{-6}$			
Total	1.000	$1.33 \cdot 10^{-3}$	0.813	0.185

<i>Time= 6 h</i>	Total	Airborne	In the pool	Deposited on structures
RPV	0.154	$1.7 \cdot 10^{-7}$	0.038	0.116
Drywell (upper+middle+lower)	0.149	$1.1 \cdot 10^{-5}$	0.083	0.066
Wetwell	0.686	$7.9 \cdot 10^{-4}$	0.684	$6.6 \cdot 10^{-4}$
GDCS	$6.4 \cdot 10^{-3}$	$3.3 \cdot 10^{-7}$	$6.4 \cdot 10^{-3}$	$9.1 \cdot 10^{-6}$
Annulus	$4.4 \cdot 10^{-3}$	$8.1 \cdot 10^{-8}$	$1.6 \cdot 10^{-3}$	$2.8 \cdot 10^{-3}$
PCCS	$3.2 \cdot 10^{-7}$	$6.2 \cdot 10^{-9}$	$3.1 \cdot 10^{-7}$	$6.1 \cdot 10^{-9}$
Reactor Building	$8.4 \cdot 10^{-6}$			
Total	1.000	$8.02 \cdot 10^{-4}$	0.813	0.185

<i>Time= 7 h</i>	Total	Airborne	In the pool	Deposited on structures
RPV	0.152	$1.0 \cdot 10^{-7}$	0.036	0.116
Drywell (upper+middle+lower)	0.144	$8.0 \cdot 10^{-6}$	0.102	0.043
Wetwell	0.691	$6.6 \cdot 10^{-4}$	0.689	$5.6 \cdot 10^{-4}$
GDCS	$3.3 \cdot 10^{-3}$	$1.4 \cdot 10^{-8}$	$3.3 \cdot 10^{-3}$	$3.5 \cdot 10^{-6}$
Annulus	$8.5 \cdot 10^{-3}$	$1.1 \cdot 10^{-8}$	$5.8 \cdot 10^{-3}$	$2.8 \cdot 10^{-3}$
PCCS	$2.5 \cdot 10^{-8}$	$8.8 \cdot 10^{-11}$	$2.4 \cdot 10^{-8}$	$1.0 \cdot 10^{-10}$
Reactor Building	$8.4 \cdot 10^{-6}$			
Total	0.999	$6.68 \cdot 10^{-4}$	0.836	0.162

<i>Time= 8 h</i>	Total	Airborne	In the pool	Deposited on structures
RPV	0.148	$2.0 \cdot 10^{-8}$	0.032	0.116
Drywell (upper+middle+lower)	0.138	$6.4 \cdot 10^{-6}$	0.121	0.017
Wetwell	0.697	$6.0 \cdot 10^{-4}$	0.696	$4.5 \cdot 10^{-4}$
GDCS	$2.9 \cdot 10^{-3}$	$7.5 \cdot 10^{-9}$	$2.9 \cdot 10^{-3}$	$1.4 \cdot 10^{-6}$
Annulus	0.013	$6.4 \cdot 10^{-9}$	0.010	$2.8 \cdot 10^{-3}$
PCCS	$4.5 \cdot 10^{-9}$	$8.1 \cdot 10^{-12}$	$4.5 \cdot 10^{-9}$	$8.8 \cdot 10^{-12}$
Reactor Building	$8.4 \cdot 10^{-6}$			
Total	0.999	$6.06 \cdot 10^{-4}$	0.862	0.136

<i>Time= 12 h</i>	Total	Airborne	In the pool	Deposited on structures
RPV	0.167	$1.3 \cdot 10^{-8}$	0.052	0.115
Drywell (upper+middle+lower)	0.133	$2.7 \cdot 10^{-6}$	0.128	$5.4 \cdot 10^{-3}$
Wetwell	0.684	$3.9 \cdot 10^{-4}$	0.683	$1.3 \cdot 10^{-4}$
GDCS	$2.8 \cdot 10^{-3}$	$3.2 \cdot 10^{-9}$	$2.8 \cdot 10^{-3}$	$8.8 \cdot 10^{-7}$
Annulus	0.011	$1.1 \cdot 10^{-9}$	$8.6 \cdot 10^{-3}$	$2.8 \cdot 10^{-3}$
PCCS	$5.6 \cdot 10^{-10}$	$1.4 \cdot 10^{-12}$	$5.6 \cdot 10^{-10}$	$1.2 \cdot 10^{-12}$
Reactor Building	$8.4 \cdot 10^{-6}$			
Total	0.998	$3.93 \cdot 10^{-4}$	0.874	0.123

<i>Time= 18 h</i>	Total	Airborne	In the pool	Deposited on structures
RPV	0.228	$7.9 \cdot 10^{-9}$	0.114	0.114
Drywell (upper+middle+lower)	0.132	$9.6 \cdot 10^{-7}$	0.127	$5.3 \cdot 10^{-3}$
Wetwell	0.625	$2.0 \cdot 10^{-4}$	0.625	$1.6 \cdot 10^{-5}$
GDCS	$2.7 \cdot 10^{-3}$	$1.6 \cdot 10^{-9}$	$2.7 \cdot 10^{-3}$	$8.8 \cdot 10^{-7}$
Annulus	0.010	$2.3 \cdot 10^{-10}$	$7.5 \cdot 10^{-3}$	$2.8 \cdot 10^{-3}$
PCCS	$3.9 \cdot 10^{-10}$	$8.9 \cdot 10^{-13}$	$3.9 \cdot 10^{-10}$	$6.5 \cdot 10^{-13}$
Reactor Building	$8.4 \cdot 10^{-6}$			
Total	0.998	$1.91 \cdot 10^{-4}$	0.876	0.122

8 Work planned for Final Report

The more detailed deposition model validated against VTT experiments of aerosol retention to the PCCS tubes will define a Decontamination Factor of aerosols as a function of particle size and is underway. The model will be incorporated to MELCOR 1.8.6 input for ESBWR as a filter module in the flow path from PCC steam box to the PCC tubes and the PCC tubes will be deactivated from being deposition surfaces to the existing MELCOR deposition models.

The containment pool pH will be calculated with ChemSheet code using pool masses and flow rates between the pools obtained from the MELCOR calculations and considering the chemical (HCl and buffer solutions) additives to the system. The pH estimate gives input to the estimation of gaseous iodine in the containment.

As to the MELCOR 1.8.6 input, the following items still need to be done:

1. Update PCCS Drain Line and Vent Line models
2. Checking/upgrading if needed of the containment control volume elevations
3. Check fission product inventories based on separate ORIGEN calculation by GE to the scaled default ORIGEN inventories. Current results are applicable for dose calculations if used as fractions from the initial core inventory.
4. Modifications needed for high pressure scenario (switch for degraded/full operation of ICS)
5. Perform runs with more delayed start of reflooding in pursuit of higher releases of fission products from the core to meet better the definitions for Early In-Vessel Releases of Regulatory Guide 1.183.

The final MELCOR analyses will include also high pressure scenarios with failure of ADS and Loss of Preferred Power.

9 Validation of results

The separate aerosol retention model for PCCS will be validated against VTT experiments. The validation effort will be reported in the Final Report. ChemSheet code has been validated against specified titration experiments for buffer solutions. Sandia National Laboratories has performed an extensive validation effort for the previous MELCOR versions. Validation reports will be included as references in the Final Report of this assignment.

10 Summary

Previous ESBWR MELCOR input file "ESBWR_BDL6_NRC.txt" supplied by GE has been upgraded for fission product behavior analyses for version MELCOR 1.8.6YH. The key modifications are the updating of COR input to be compatible with the new models, checking and upgrading of most of the RCS and containment volume, flow junction and heat structure input, building up of RN package input for radionuclide calculations.

A preliminary Bottom Drain Line Break scenario with successful depressurization of RCS and reflooding at 4100 s was performed with unverified MELCOR 1.8.6 input. The fission product release from the core was relatively low, e.g. for noble gases about 62 %, for Cs 57 % and CsI 62 % of the whole core inventory. The modeled single-hole leakage for containment nominal leakage resulted in release fractions of noble gases, CsOH and CsI to the reactor building to be $1.43 \cdot 10^{-3}$ %, $5.04 \cdot 10^{-4}$ % and $4.58 \cdot 10^{-4}$ % of the initial core inventory, respectively.

When approximating the decontamination factor of CsI aerosol in the PCCS by dividing the airborne mass in the Drywell by the airborne mass in the GDCS one obtains a result shown in Fig. 27. The decontamination factor varies between 4.4 and 853. The minimum is reached at time 4 h into the accident.

The CsI decontamination factor for the whole containment can be defined as the ratio of total CsI released from the core divided by the total airborne mass of CsI in the containment. The value for containment decontamination factor ranges from 2 to 4976 on the basis of draft MELCOR calculation. The minimum is reached in the beginning of the accident (at 1 h).

11 References

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12 APPENDIX A: Listing of the separate FORTRAN code applied for the definition of decontamination factor of PCCS to be applied in MELCOR analyses

```

c -----
PROGRAM PROFILIT
c -----

REAL PI,KB,RG,GRAV
PARAMETER (PI=3.14159265,KB=1.380662E-23,RG=8.3145,GRAV=9.81)
REAL XSTART,XSTOP,X,DX,T0,T,TSSTART,TSSTOP,TS,DH,A,P,MN,MW,MDOTN
REAL
MDOTW,MDOT,PRES,RHO,U,RHOW,RHON,NW,NN,N0,PWS,RHOWS,KW,KN,K
REAL D,CPW,CPN,CP,NU,SH,QT,QM,QN,NDOTN,NDOTW,NDOT,LW,N,PW,STEF
REAL PNS,RHONS,FRW,FRWS,MUW,MUN,MU,NY,PR,SC,TW,M,KL,MUL,CPL
REAL
TL,TLS,QTS,MDOTL,MDOTW0,RHOL,DELTA,FRAC,MDOTP,RHOP,XW,XN,QP
INTEGER NCOUNT,NX

OPEN(UNIT=11,FILE="output",STATUS="UNKNOWN")

c-----initialization of variables
XSTART=0.                ! x-coordinate at start                [m]
XSTOP=0.8                ! x-coordinate at stop                [m]
X=XSTART                ! initial value for x                [m]
DX=0.00001              ! step size                          [m]
NX=10                   ! write-step                          [1]
NCOUNT=0                ! write step counter                 [1]
T0=203.+273.15         ! initial temperature                 [K]
T=T0                    ! initial temperature                 [K]
TSSTART=20.3+273.15    ! initial surface temperature         [K]
TS=TSSTART              ! initial surface temperature         [K]
TSSTOP=11.6+273.15    ! final surface temperature           [K]
TL=TSSTART              ! liquid water temperature            [K]
DH=0.022                ! hydraulic diameter of pipe          [m]
A=0.25*PI*DH**2        ! cross-area of pipe                 [m2]
P=PI*DH                 ! perimeter of pipe                   [m]
MN=0.028                ! molar mass of nitrogen gas          [kg/mol]
MW=0.018                ! molar mass of water vapour          [kg/mol]
MDOTN=5.23e-4          ! initial nitrogen mass flux          [kg/s]
MDOTP=100.              !
MDOTW=1.01e-3          ! initial water vapour mass flux      [kg/s]
MDOTW0=MDOTW           ! initial water vapour mass flux      [kg/s]
MDOTL=0.                ! initial liquid water mass flux      [kg/s]
MDOT=MDOTN+MDOTW      ! initial total mass flux             [kg/s]
    
```

NDOTN=MDOTN/MN	! initial mole flux of nitrogen	[mol/s]
NDOTW=MDOTW/MW	! initial mole flux of water	[mol/s]
NDOT=NDOTN+NDOTW	! initial total mole flux	[mol/s]
M=MDOT/NDOT	! initial effective molar mass	[kg/mol]
PRES=101300.	! total pressure	[Pa]
RHO=PRES*M/(RG*T)	! initial total density	[kg/m3]
U=MDOT/(RHO*A)	! initial velocity	[m/s]
RHOW=MDOTW/(U*A)	! initial density of water vapour	[kg/m3]
RHON=MDOTN/(U*A)	! initial density of nitrogen	[kg/m3]
RHOP=MDOTP/(U*A)		
RHOL=995.	! density of liquid water	[kg/m3]
RHO=RHOW+RHON	! total initial density	[kg/m3]
NW=RHOW/MW	! initial molar density of H2O	[mol/m3]
NN=RHON/MN	! initial molar density of N2	[mol/m3]
N0=NW+NN	! initial total molar density	[mol/m3]
N=N0	! initial total molar density	[mol/m3]
DELTA=0.	! initial liquid film thickness	[m]
FRAC=0.005	! allowed change in diff. eqs.	[1]

c-----initial output

```
WRITE(11,'(A9,A9,A9,A9,A9,A9,A12) 'x','t','tl','ts','mdot',
\      'mdotp','delta'
WRITE(11,'(F9.3,F9.3,F9.3,F9.3,F9.4,F9.4,F12.7)') 100.*X,
\      T-273.15,TL-273.15,TS-273.15,60000.*MDOTL,100.-MDOTP,DELTA
```

10 CONTINUE ! start of loop

NCOUNT=NCOUNT+1

c-----calculate surface temperature [K] and surface density [kg/m3]

```
TS=TSSTART+(TSSTOP-TSSTART)*(X-XSTART)/(XSTOP-XSTART)
TLS=2.*TL-TS
TWS=TS
PWS=7.7e+10*EXP(-5060./TLS) ! vapour pressure of water at surface [Pa]
PW=7.7e+10*EXP(-5060./T) ! vapour pressure of water [Pa]
PNS=PRES-PWS ! vapour pressure of nitrogen [Pa]
RHOWS=PWS*MW/(RG*TLS) ! mass concentration of H2O at surface [kg/m3]
RHONS=PNS*MN/(RG*TLS) ! mass concentration of N2 at surface [kg/m3]
```

c-----calculate transport data

```
KW=9.51e-5*T**0.941 ! thermal conductivity of water vapour [W/(m*K)]
KN=3.52e-4*T**0.757 ! thermal conductivity of nitrogen [W/(m*K)]
KL=-0.469+5.77e-3*TL-7.2e-6*TL*TL ! thermal conductivity of liquid water [W/(m*K)]
K=(KW*RHOW+KN*RHON)/RHO ! thermal conductivity of mixture [W/(m*K)]
MUN=2.94E-7*T**0.72 ! viscosity of nitrogen [N*s/m2]
MUW=8.64E-9*T**1.22 ! viscosity of water vapour [N*s/m2]
MUL=2.5E-5*EXP(561.5/(TL-141)) ! viscosity of liquid water [N*s/m2]
MU=(MUW*RHOW+MUN*RHON)/RHO ! viscosity of mixture [N*s/m2]
D=4.75e-10*T**1.95 ! diffusion coefficient of H2O in N2 [m2/s]
CPW=1900. ! heat capacity of water [J/(kg*K)]
CPN=1050. ! heat capacity of nitrogen [J/(kg*K)]
```

```

CPL=4185.                ! heat capacity of liquid water      [J/(kg*K)]
CP=(CPW*RHOW+CPN*RHON)/RHO    ! heat capacity of mixture [W/(m*K)]
NU=3.66                  ! Nusselt number          [1]
SH=3.66                  ! Sherwood number         [1]
LW=1000.*(2570+1.1*TL-5.17E-3*TL**2) ! Latent heat of condensation
                                [J/kg]
NY=MU/RHO                ! kinematic viscosity     [m2/s]
SC=NY/D                  ! Schmidt number          [1]
PR=CP*MU/K               ! Prandtl number          [1]
RE=U*DH/NY              ! Reynolds number         [1]
NU=MAX(3.66,0.023*RE**0.8*PR**0.3) ! Nusselt number          [1]
SH=MAX(3.66,0.023*RE**0.8*SC**0.3) ! Sherwood number         [1]

C-----calculate mass fractions
FRW=RHOW/(RHOW+RHON)    ! average mass fraction    [1]
FRWS=RHOWS/(RHOWS+RHONS) ! mass fraction at surface [1]
NW=RHOW/MW
NN=RHON/MN
XW=NW/(NW+NN)
XN=NN/(NW+NN)

c-----calculate wall fluxes
QT=MAX(0.,NU*K*(T-TLS)/DH) ! heat flux to liquid surface [J/(m2*s)]
STEF=1./(1.-0.5*(FRW+FRWS)) ! Stefan-flow correction term [1]
QM=MAX(0.,SH*STEF*D*RHO*(FRW-FRWS)/DH) ! wall mass flux
                                                [kg/(m2*s)]
QN=QM/MW                ! wall mole flux           [mol/(m2*s)]
QP=(XW*SQRT(MW))/(XW*SQRT(MW)+XN*SQRT(MN))
\ *(RHOP/RHOW)*QM

c-----calculate new average gas temperature
T=T+DX*(-P*QT)/(CPN*MDOTN+CPW*MDOTW)

c-----calculate new average liquid film temperature
IF (MDOTL .GT. 1.E-5*MDOTW0) THEN
    QTS=KL*(TLS-TS)/DELTA
c    explicit:
c    TL=TL+DX*P*(-QTS+QT+LW*QM+CPW*(T-TL))/(CPL*MDOTL)
ENDIF

c-----calculate new amounts of moles, molar fluxes and velocity
N=N0*T0/T
NDOTN=NDOTN
NDOTW=NDOTW-DX*P*QN
MDOTP=MDOTP-DX*P*QP
NDOT=NDOTN+NDOTW
U=NDOT/(N*A)
NN=NDOTN/(U*A)
NW=NDOTW/(U*A)
RHOP=MDOTP/(U*A)

c-----calculate new densities and mass fluxes
    
```

```

MDOTN=NDOTN*MN
MDOTW=NDOTW*MW
MDOTL=MDOTW0-MDOTW
MDOT=MDOTN+MDOTW
RHON=NN*MN
RHOW=NW*MW
RHO=RHON+RHOW

```

c-----calculate thickness of liquid film

```

DELTA=(3.*MUL*MDOTL/(RHOL*RHOL*GRAV*DH))**(1./3.)

```

c-----implicit liquid film temperature:

```

IF (MDOTL .GT. 1.E-5*MDOTW0) THEN
  TL=(TL+P*DX*(NU*K*(T+TS)/DH+2.*KL*TS/DELTA+LW*QM)/(CPL*MDOTL))/
  \ (1.+2.*P*DX*(NU*K/DH+KL/DELTA)/(CPL*MDOTL))
ENDIF

```

c-----output

```

X=X+DX
IF (NCOUNT .EQ. NX) THEN
  WRITE(11,'(F9.3,F9.3,F9.3,F9.3,F9.4,F9.4,F12.7)') 100.*X,
  \ T-273.15,TL-273.15,TS-273.15,60000.*MDOTL,100.-MDOTP,DELTA
  NCOUNT=0
ENDIF

```

```

IF (X .LT. XSTOP) GOTO 10 ! end of loop

```

```

WRITE(11,'(F9.3,F9.3,F9.3,F9.3,F9.4,F9.4,F12.7)') 100.*X,
\ T-273.15,TL-273.15,TS-273.15,60000.*MDOTL,100.-MDOTP,DELTA
WRITE(11,'(A9,A9,A9,A9,A9,A9,A12)') 'x','t','tl','ts','mdotl',
\ 'mdotp','delta'

```

```

STOP
END

```

13 Appendix B: ChemApp

13.1 Introduction

ChemApp is derived from the renowned ChemSage family of thermochemical calculation programs, which are widely used in universities, corporate and government laboratories. It offers new possibilities and perspectives for the use of thermochemical calculations across a wide spectrum of applications by providing an easily programmable interface to complex equilibrium calculation techniques.

ChemApp consists of a library of subroutines for data handling and phase equilibrium calculation purposes. It is available as an object code library for a variety of platforms and can be added as a module to virtually any existing or new software, major application areas are CFD (computational fluid dynamics) and process simulation programs.

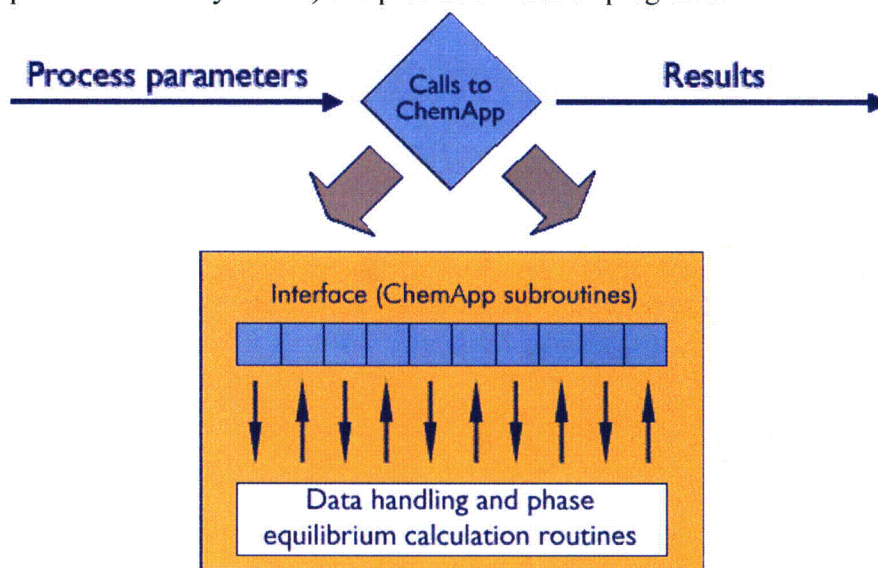


Figure 12-1. Schematic representation showing the integration of ChemApp into a process modeling or simulation program.

ChemApp provides the powerful calculation capabilities of ChemSage in the form of a programmer's library. It consists of a rich set of subroutines which provides all the necessary tools for the calculation of complex multicomponent, multiphase chemical equilibria and the determination of the associated energy balances.

ChemApp uses the 'engine' and data handling capabilities of the renowned ChemSage thermochemical application program. You find the same speed and reliability of convergence of calculations. You can use the same thermochemical data combined with the same comprehensive library of models for non ideal solution phases. ChemApp is modular, which makes it easy to integrate into third party applications and also facilitates the incorporation of future improvements and extensions.

13.2 Thermochemical data

The same comprehensive library of models for non-ideal solution phases available in ChemSage is also built into ChemApp. Thus, the wide range of existing thermochemical data

for ChemSage is available for ChemApp too. ChemApp also uses the same thermochemical data-file format as ChemSage.

Table 13-1. Solution models available in ChemApp

Model	Application area
Redlich-Kister-Muggianu Kaufman-Kohler Four-suffix Margules Kohler-Toop Hoch-Arpschhofen	for general use with substitutional or associated solution phases
Compound energy formalism Species chemical potential/bond energy formalism	solid alloys
Ionic two sublattice model	ionic liquids
Equivalent fraction sublattice model	molten salts
Gaye-Kapoor-Frohberg cell model	ionic oxidic mixtures
Blander-Pelton modified quasichemical model	ionic oxidic mixtures with non-oxidic solutes
Wagner	metallic dilute solutions
Pitzer	concentrated aqueous solutions
Virial equation	non-ideal gas phases

13.3 Programming steps

Only three stages of simple programming are necessary to proceed from initialisation of ChemApp to collection of results

1. Initialize the interface, read a thermodynamic data-file, and adjust the chemical system.
2. Set initial conditions for the equilibrium calculation.
3. Perform the calculation and collect results.

In the simplest cases, each programming step requires calling only one or two of the ChemApp interface routines. For more complicated applications, the number of routines called in each step increases; however, the demands on programming capabilities are never particularly difficult.

13.3.1 Initializing the interface and reading a thermodynamic data-file

This first step of each program entails initializing the interface, reading a thermodynamic data-file into the program, and changing default units, if necessary.

A further series of programming subroutines enable the chemical system to be adjusted to match the requirements of the calculation

- identification of phases, phase constituents, and system components
- delete or activate phases and/or constituents from a calculation

The latter group of routines provide a very useful set of tools, since they allow the suppression of otherwise stable phases in order to calculate metastable conditions. Also, by elimination of phases and/or constituents which are known not to be stable under the chosen conditions, considerable increase in computation speed can be gained.

13.3.2 Setting the initial conditions for the equilibrium calculations

ChemApp offers considerable flexibility for defining initial conditions for a chemical equilibrium calculation. Two different methods are available that will cover most cases experienced in practice.

- By defining the global conditions of the system.

Using this method, it is merely needed to set single conditions for pressure and temperature, and enter incoming species to define the composition of the system. For example, if the thermodynamic equilibrium for the system SiO₂-CaO is to be calculated, using a ChemSage - compatible data-file that contains the elements Ca, Si, and O, it is only required to define the temperature and pressure of the system, and the total amounts of SiO₂ and CaO present. Instead of temperature and pressure, other variables of state can be chosen too.

- By defining streams.

A stream is considered as a medium for transferring non-reacted matter to a reaction zone. It has constant temperature and pressure, and contains one or more phases of given composition. Hence, when using this method, the conditions for the three variables - composition, temperature and pressure - need to be defined for one or more input streams. For instance, one stream entering a reaction zone can consist of O₂(g), preheated to a temperature of 1500K, while the other consists of CO(g) at room temperature. This method must be used for calculation of the extensive properties of reactions; for example, those involving the heat balance or the adiabatic temperature of a combustion process. It is also convenient to use it for reactor calculations, where it is known what is entering the system and it is desired to calculate results at various stages during and at the end of the process.

13.3.3 Performing the calculation and collecting results

Only one subroutine needs to be called to execute phase equilibrium calculations defined by pressure, temperature, and input composition.

Like ChemSage, ChemApp is also able to perform extensive property target calculations (defined by an extensive property change) and phase target calculations (defined by the search for a particular phase). If, in the previous step, such a target calculation has been defined, the necessary additional information is supplied upon calling the equilibrium calculation routine. Results from a phase equilibrium calculation are retrieved by using only a single subroutine. For the following variables results can be obtained

- Total pressure, total volume, temperature
- Equilibrium amount of phases, phase constituents, and system components
- Chemical potential and activity
- Heat capacity, enthalpy, entropy, and Gibbs energy of the equilibrium state
- Mass or mole fraction of a system component or phase constituent

ChemApp can also calculate the thermodynamic properties, Cp, H, S, and G, of a phase and its constituents.

For full online documentation of ChemApp-interface see:

<http://gttserv.lth.rwth-aachen.de/~cg/Software/ChemApp/IndexFrame.htm>

14 Appendix C: ChemSheet

14.1 Introduction

ChemSheet combines the flexibility and practicality of spreadsheet applications with the thermodynamic and simulation capabilities of Gibbs Energy minimization. Its applications are appropriate for metallurgical, chemical and process industries as well as for geochemists and environmentalists. Also there is a special appeal to those in universities and chemical education.

ChemSheet allows rigorous chemical and thermodynamic calculations to be computed within the familiar environment of Microsoft Excel spreadsheet. Even though ChemSheet uses complex numerical procedures with extensive thermodynamic data linked with appropriate reaction kinetics, it produces the results on a simple Excel spreadsheet and thus makes the simulation accessible to the general user.

ChemSheet applies the ChemApp thermodynamic programming library, which handles repetitive complex equilibrium calculations for a diverse range of chemical and thermodynamic applications. ChemApp can be used to calculate both the composition and the thermodynamic properties of a multi-phase, multi-component system at given conditions.

With ChemApp, versatile one-dimensional phase-mapping and target calculations can also be done.

The applications range from analysis of laboratory and environmental data to practical process simulation and design. In ChemSheet each process chemistry model can be formatted to practical worksheet from which calculations are made.

14.2 Definition of Terms

A thermodynamic system consists of a number of phases, where some may have a composition expressed as amounts of a number of phase constituents, and others can have an invariant composition. Phases are divided into three groups:

1. The gaseous phase.
2. Condensed mixtures (liquid and solid state).
3. Condensed stoichiometric phases (liquid and solid state).

Phases and phase constituents always have thermochemical properties (activities, chemical potentials, enthalpies, volumes, etc.). Phase constituents have compositions expressed as amounts (i.e. stoichiometric coefficients) of a number of components. A component is a system-wide entity, which is stressed by calling it a system component. Usually components are elements, but it is also possible for them to be stoichiometric combinations of elements. For example, in an oxide system based on calcia and silica, CaO and SiO₂ may be used, as well as Ca, Si, and O

14.3 Nomenclature Used in ChemSheet

Names of components, constituents of a phase, phases and streams are case sensitive and can consist of a string of letters up to 24 characters in length. For example, 'CO' and 'Co' are two different phase constituents. Some names are reserved because they have some special meaning in ChemSheet:

14.4 Using ChemSheet

Several concepts are introduced which are important to know about when beginning to use ChemSheet. They include the description of the two ways initial conditions can be defined (global conditions and streams)

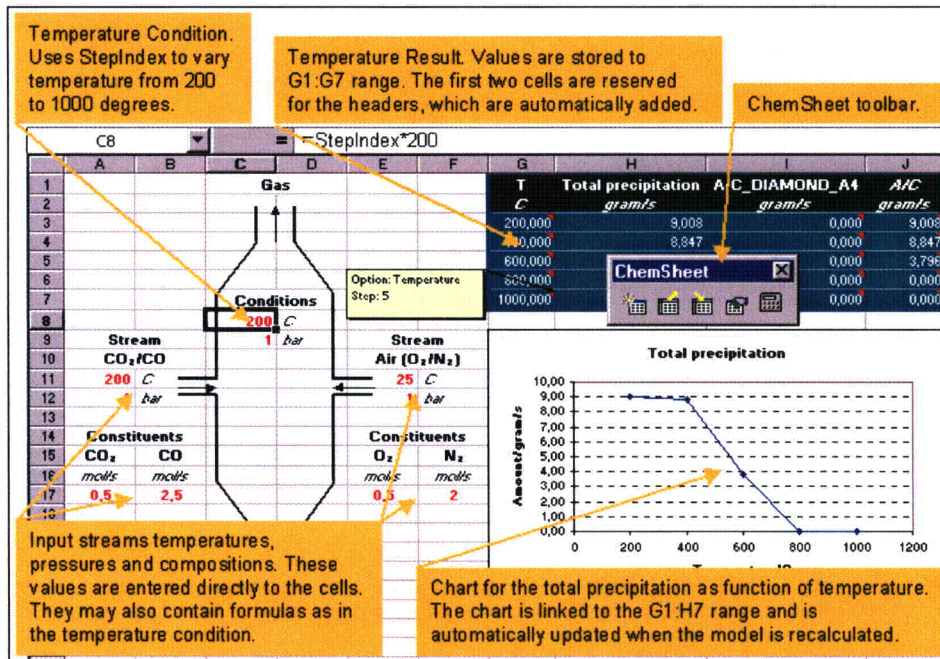


Figure 13-2. Example ChemSheet Application.

Here is a picture with some comments added of a more advanced ChemSheet application using Streams. It contains many features of Excel that can be used with ChemSheet. In this application all the necessary input values are entered to worksheet cells, so they can be quickly changed without opening the ChemSheet dialog box. The cells are linked to the ChemSheet model using cell references and the values of cells are evaluated for each calculation step. After changing one or more values in the linked cells the model needs only to be recalculated by clicking the Calculate ChemSheet Model command in ChemSheet toolbar and the result values and charts linked with them are automatically updated. ChemSheet dialog can be opened by clicking New ChemSheet Model or Edit ChemSheet Model commands in ChemSheet toolbar. In ChemSheet dialog you can define all the necessary input values for one or more equilibrium calculations and also the results you wish to retrieve and store to Excel worksheets.

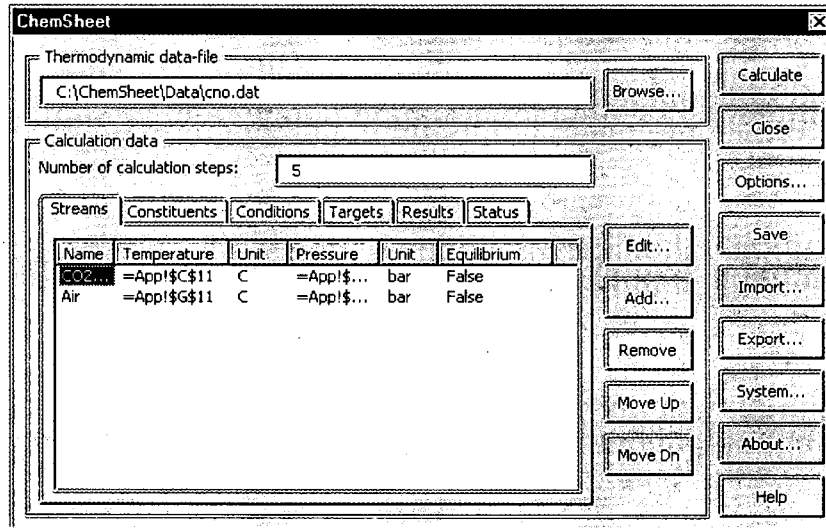


Figure 13-3. ChemSheet dialog.

14.5 Using Initial Conditions

ChemSheet offers you considerable flexibility for defining initial conditions for a chemical equilibrium calculation. Two different methods are available that will cover most cases experienced in practice:

1. Using Global Conditions of the System
2. Using Streams

Below is a schematic picture of an equilibrium calculation when using Global Conditions.

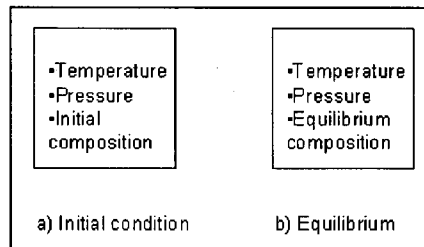


Figure 13-4. Global conditions.

You merely need to set single values for temperature and pressure, and enter amounts of incoming species to define the composition of the system at its initial stage. This input method is used if the amounts of the incoming species are merely given to define the overall composition of the system.

Below is a schematic picture of equilibrium calculation when using Streams.

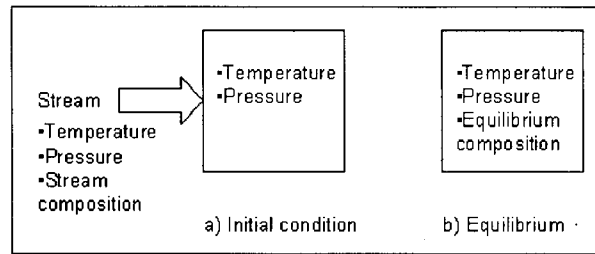


Figure 13-5. Streams.

You set three variables – temperature, pressure and composition – for one or more input streams and set single values for temperature and pressure of the system. This input method is used if the reaction between the input streams is to be calculated, especially in the respect to the change of the extensive properties: heat capacity, enthalpy, entropy, Gibbs energy, or volume.

You have also an option to make target calculations, if some of the variables used above are unknown but some other variables are known, e.g. the heat balance (enthalpy of the equilibrium condition minus enthalpy of the initial condition) or the presence of a phase at equilibrium.

14.6 Using Global Conditions of the System

Using this method, you merely need to set single values for pressure and temperature, and enter incoming species to define the initial composition of the system. For example, if you wish to calculate the thermodynamic equilibrium for the system SiO₂-CaO, using a thermodynamic data-file that among others contains the elements Ca, Si, and O, he would only need to define the temperature and pressure of the system, and the total amounts of SiO₂ and CaO present. You can also enter incoming amounts as components, i.e. total number of elements Ca, Si, O present. As a result of the calculation you will be given the amounts of the stable phases in the system, and if a phase is a mixture phase, also the equilibrium composition of the phase.

14.6.1 Selecting Global Conditions

1. Choose the Edit command in the ChemSheet menu or press the Edit ChemSheet model button in the ChemSheet toolbar. If you don't have the ChemSheet toolbar visible, select it with the Toolbars command in View menu. The ChemSheet dialog box appears.
2. Click the Options. The Options dialog box appears.
3. Click the Global conditions in Initial Conditions.

Note – Global Conditions is the default value when you start a new ChemSheet model. If you change the Initial condition all the Calculation data will be reset. So you should change the Initial condition first and only then start defining the Calculation data.

14.6.2 Adding a New Condition

The procedure to define conditions is the same regardless of the method you have chosen to define the initial conditions in the Options dialog box – only incoming species are defined

differently. When you are using Streams, the incoming species are defined as stream constituents. To add a new Condition:

1. Choose the New command in the ChemSheet menu or press the New ChemSheet Model button in the ChemSheet toolbar. If you don't have the ChemSheet toolbar visible, select it with the Toolbars command in View menu. The ChemSheet dialog box appears.
2. Click Conditions tab in the Calculation data.
3. Click Add to add a new Condition. The Condition dialog box appears.
4. Select the state variable and necessary options for it and give its value. If some controls are greyed, then their values are not needed for the selected set of options.
5. Click Ok.

If you add other conditions than temperature, pressure, or incoming amount, then you have to add a target variable.

14.7 Using Streams

A stream is a means for transferring non-reacted matter to a reaction zone. It has constant temperature and pressure, and contains one or more phases of fixed composition. When using this method, user sets the three variables – temperature, pressure and composition for each input stream and set single conditions for temperature and pressure of the system. For example, one stream entering a reaction zone may comprise O₂(g) pre-heated to a temperature of 1500 K, and the other may consist of CO(g) at room temperature. The Streams method must be used for calculation of the changes of extensive properties of reactions; for example, those involving the heat balance of a combustion process. It is also convenient to use it for reactor calculations, where you know what is entering the system and you wish to calculate results at various stages during and at the end of the process.

When setting the incoming amounts for a stream, only phases and phase constituents can be used for this purpose. If one wants to enter the incoming amounts for a stream in terms of the system components (i.e. usually the elements), but the phase constituents of that phase are not elements, one has to perform an intermediate calculation using another ChemSheet model that uses Global conditions.

Other conditions, especially temperature and pressure of the system, are defined just as when using Global Conditions.

14.7.1 Selecting Streams

1. Choose the Edit command in the ChemSheet menu or press the Edit ChemSheet model button in the ChemSheet toolbar. If you don't have the ChemSheet toolbar visible, select it with the Toolbars command in the View menu. The ChemSheet dialog box appears.
2. Click Options. The Options dialog box appears.
3. Click Streams in Initial Conditions.

Note – Global conditions is the default value when you start a new ChemSheet model. If you change the Initial Condition all the Calculation data will be reset. So you should change the Initial Condition first and only then start adding the Calculation data.

14.7.2 Adding a New Stream

To add a new Stream:

1. Choose the New command in the ChemSheet menu or press the New ChemSheet Model button in the ChemSheet toolbar. If you don't have the ChemSheet toolbar visible, select it with the Toolbars command in View menu. The ChemSheet dialog box appears.
2. Click Streams tab in Calculation data.
3. Click Add to add a new Stream. The Stream dialog box appears.
4. Give the stream name, the temperature and its unit and the pressure and its unit.
5. Click Ok.

14.7.3 Adding a New Stream Constituent

To add a new Constituent to a previously defined Stream:

1. Choose the New command in the ChemSheet menu or press the New ChemSheet Model button in the ChemSheet toolbar. If you don't have the ChemSheet toolbar visible, select it with the Toolbars command in View menu. The ChemSheet dialog box appears.
2. Click Constituents tab in Calculation data.
3. Click Add to add a new constituent. The Constituent dialog box appears.
4. Select the stream, the phase and the phase constituent and give its value.
5. Click Ok.

14.8 Getting Results

In ChemSheet getting results comprises two things: selection of the state variable and the range of worksheet cells used to store the values of that state variable for each calculation steps. The range can be a reference to a cell or range of cells or can refer to multiple areas. An area is a range of contiguous cells or a single cell. The values are stored to the areas from left to right and top to bottom. So the value for the first calculation step is stored to the first cell in the first area (upper left corner of the area) and the value for the last step is stored to last cell in the last area (lower right corner of the area).

Note – If you have selected Headers for a Result, then the first two cells in the first area are reserved to them.

Here is an example where three results have been defined:

Option	Phase	Output range	Unit
Amount	C_DIAMOND_A4	=Sheet1!\$K\$1:\$K\$7	gram/s
Amount	C	=Sheet1!\$L\$1:\$L\$7	gram/s
Temperature		=Sheet1!\$I\$1:\$I\$7	C

Figure 13-6. Results in ChemSheet dialog.

If the Headers and Comments options are selected then the results are stored as follows:

	I	J	K	L
1	T	Total precipitation	A/C_DIAMOND_A4	A/C
2	C	grams	grams	grams
3	200	Option: Temperature	0	9.008019045
4	400	Step: 1	0	8.846683183
5	600		0	3.795954012
6	800		0	0
7	1000		0	0

Figure 13-7. Results in worksheet.

The first cells in each range contain the ID of the Option (state variable) and the second cells contain the Unit of the state variable.

14.8.1 Adding a New Result

To add a new Result:

1. Choose the New command in the ChemSheet menu or press the New ChemSheet Model button in the ChemSheet toolbar. If you don't have the ChemSheet toolbar visible, select it with the Toolbars command in View menu. The ChemSheet Dialog box appears.
2. Click Results tab in Calculation data.
3. Click Add to add a new Result to the list. The Result dialog box appears.
4. Select the result variable and the necessary options for it and give the range where to store the values for each calculation step. If some controls are greyed, then their values are not needed for the selected set of options.
5. Click Ok.

14.9 Using Formulas

You can use formulas in any value field in ChemSheet. When you normally do any calculation you change some value between the successive calculation steps and see how that affects the new equilibrium.

The names *StepIndex*, *StepCount*, *MapIndex*, and *MapIndex2* are defined when you start a new ChemSheet model or open a workbook that contains a ChemSheet model. The value of *StepCount* is the same as the Number of Steps that is given in ChemSheet dialog box. The value of *StepIndex* varies from one to the number of steps so that you can always use it in your formulas to refer to the index number of the current calculation step. Their values are updated at the start of each calculation step before the results for that step are written. After

all the calculation has ended its value is restored as one. Here is an example where the equilibrium temperature is changed using the *StepIndex*:

Option	Value	Unit
Temperature	=StepIndex*200	C
Pressure	=Sheet1!\$E\$9	bar

Figure 3-8. Using formulas.

So initially its value is 200 C and then it increases by 200 at each successive calculation step. The value of the equilibrium pressure is defined as a cell reference. Its actual value is the same as the value of the cell E9 in worksheet Sheet1. The value of cell is evaluated in each calculation step so it too can contain a formula that uses *StepIndex*.

The previous formula is a very simple one. If you want to calculate at temperatures that are not incremented by a constant value you can enter the temperature values to a range in a worksheet and use the Index function. For example you can enter the following values to range A1:A5:

	A
1	201.354
2	405.464
3	600.462
4	798.098
5	979.231

Figure 13-9. Random temperatures.

and then set the formula for temperature as follows:

Option	Value	Unit
Temperature	=INDEX(A1:A5,StepIndex,1)	C
Pressure	=Sheet1!\$E\$9	bar

Figure 13-10. Using INDEX-worksheet function.

You can use any of the worksheet functions that are available. For the list of functions select the Functions command in Insert menu in Excel.

You can also use you own functions if you know how to program with Visual Basic

14.9.1 Using Units of State Variables

ChemSheet supports several units for each quantity. The quantities are:

- Pressure
- Volume
- Temperature
- Energy
- Amount
- Time

Time is only available when you have chosen to use Streams as Initial Conditions. Time is added to all the units when it is applicable: amount means amount of flow (e.g. mol/s),

enthalpy means enthalpy of flow (e.g. J/s), and so on. This way you can use different time scales when giving initial conditions (as it may be the case with the real world application that you are simulating) and need not to do the unit conversion yourself.

For all variables there are lists of example units. If the unit combination you want to use is not present in a list, just type it to the text box. The numerator and the denominator are divided with the slash character and other quantity units with the dash character. Blanks are ignored.

For example these are both the same unit for entropy flow:

$J/K\cdot s$

$J / s - K$

But this is not valid unit for entropy flow:

$J/K/s$

Note – If you use streams and are not interested in time scales, just give all the time units as seconds (or with any time unit as long as you make sure that you use the same time unit everywhere).

14.10 Available units for Quantities

Table13-2. Available units.

Quantity	ID	Unit	Comment
Pressure	P	bar	P/bar
		atm	$P/atm = P/bar/1.01325$
		Pa	$P/Pa = P/bar/0.00001$
		kPa	$P/kPa = P/bar/0.01$
		psi	$P/psi = P/bar/0.06894757$
		torr	$P/torr = P/bar/1.01325/760$
		Volume	V
cm ³	$V/cm^3 = V/dm^3/0.001$		
m ³	$V/m^3 = V/dm^3/1000$		
ft ³	$V/ft^3 = V/dm^3/28.316846592$		
in ³	$V/in^3 = V/dm^3/0.016387064$		
Temperature	K	K	T/K
		C	$T/C = (T/K - 273.15)$
		F	$T/F = 1.8 * (T/K - 273.15) + 32$

Energy	E	J	E/J
		cal	$E/\text{cal} = E/J/4.184$
		Btu	$E/\text{Btu} = E/J/1055.06$
		kWh	$E/\text{kWh} = E/J/3,600,000$
Amount	A	mol	M/mol
		gram	M/gram
		kg	$M/\text{kg} = M/\text{gram}/1,000$
		tonne	$M/\text{tonne} = M/\text{gram}/1,000,000$
		pound	$M/\text{pound} = M/\text{gram}/453.59237$
Time	t	s	t/s
		min	$t/\text{min} = t/s/1/60$
		h	$t/\text{h} = t/s/1/3600$
		d	$t/\text{d} = t/s/1/86400$

14.11 Thermodynamic Data

There are three different kinds of data-files that can be used with ChemSheet:

1. Ascii files (*.DAT)
2. Binary files (*.BIN)
3. Transparent files (*.CST)

Ascii files can be made with ChemSage and HSC programs and they can be freely edited by hand. When making data-files with HSC program you must convert the generated ChemSage 3.0 data-file to 4.0 format with ChemFile program that is included in ChemSheet package.

Binary files are stored in a way that doesn't permit the end user to extract or change thermochemical data from the data-file. This is mainly done in cases where the license agreement with the supplier of the data doesn't permit the distribution in plain text format. In these cases the distribution of the data-file in non-ASCII form is the only way to make it available to the users of our software. Due to the nature of FORTRAN standard for writing binary data to files, or rather, the lack thereof, binary data-files are usually not portable across platforms

Transparent files are more portable than binary files. Transparent data-files, like binary data-files, are stored in a way that doesn't permit the end user to extract or change thermochemical data from the data-file. This is mainly done in cases where the license agreement with the supplier of the data doesn't permit the distribution in plain text format. In these cases the

distribution of the data-file in non-ASCII form is the only way to make it available to the users of our software. Transparent files can be made with FactSage program.

A comprehensive list of readily available standard data-files that are adequate for many applications can be obtained from GTT-Technologies. Customized data-files can also be prepared to meet a user's specific requirements. ChemSage data-files are mostly in the form of an ASCII text-file and can easily be updated and refined, if necessary.

A significant feature of the ChemApp thermodynamic programming library used with ChemSheet is that it incorporates a comprehensive library of excess Gibbs energy models for various types of non-ideal solution phases. Additional 'customer-specified' models can be added upon request from GTT-Technologies.

14.12 Sodium pentaborate

These reference values are from Eagle-Picher (<http://www.eaglepicher.com/EaglePicherInternet>) report on enriched sodium pentaborate products for BWR operators: http://www.eaglepicher.com/NR/rdonlyres/1183A34B-F387-4D85-A79A-C4C5F1FB806C/0/w_c_03.pdf

Table 13-3. Physical properties of sodium pentaborate

Form	White Crystals
Enrichment	To 99% at 1% ¹⁰ Boron
Formula	Na ₂ O*5B ₂ O ₃ *10H ₂ O
Specific gravity	1.71 g/cm ³
Boron Content	17.21% at ¹⁰ Boron

Table 13-4. Solubility in water (natural isotopic composition)

Temperature/C	% anhydrous salt by composition
0	6.28
10	8.10
20	10.55
30	12.20
40	17.40
50	21.80
60	26.90
70	32.25
80	37.84
90	43.80
100	50.30

14.13 Sodium diborate (common name Borax)

Borax ($\text{Na}_2\text{O} \cdot 2\text{B}_2\text{O}_3 \cdot 10\text{H}_2\text{O}$) is the most common of sodium borate based buffer solutions. In this project it is used as a reference solution to validate the thermodynamic model as measured titration curves for it were found in the literature¹.

Table 13-5. 100 mL of 0.025 M Borax buffer solution titrated with 0.1 M HCl¹

HCl mL	pH
4.0	9.1
9.2	9.0
14.2	8.9
19.2	8.8
23.2	8.7
27.0	8.6
30.4	8.5
33.2	8.4
35.4	8.3
37.6	8.2
39.4	8.1
41.0	8.0

Table 13-6. 100 mL of 0.025 M Borax buffer solution titrated with 0.1 M NaOH¹

NaOH mL	pH
1.8	9.2
7.2	9.3
12.4	9.4
17.6	9.5
22.2	9.6
26.2	9.7
30.0	9.8
33.4	9.9
36.6	10.0
39.0	10.1
41.0	10.2
42.6	10.3

14.14 Thermodynamic System

The thermodynamic system used in pH calculation is shown below.

¹ Robinson, R. A., and Stokes, R. H., Electrolyte solutions, the measurement and interpretation of conductance, chemical potential, and diffusion in solutions of simple electrolytes, 2nd ed., rev. London, Butterworths, 1968

Table 13-7. Thermodynamic system.

Phase	Constituent	Components					
		B	Na	H	O	Cl	e
Gas	H ₂ O			2	1		
	HCl			1		1	
Water	H ₂ O			2	1		
	H ⁺			1			-1
	OH ⁻			1	1		1
	B(OH) ₃	1		3	3		
	B(OH) ₄ ⁻	1			2		1
	Cl ⁻					1	1
	Na ⁺		1				-1
	NaCl	NaCl		1			1
NaOH	NaOH		1	1	1		
Na ₂ O·2B ₂ O ₃ ·10H ₂ O	Na ₂ O·2B ₂ O ₃ ·10H ₂ O	4	2	20	17		
Na ₂ O·5B ₂ O ₃ ·10H ₂ O	Na ₂ O·5B ₂ O ₃ ·10H ₂ O	10	2	20	26		

Thermodynamic system consists of ideal gas phase (Gas), aqueous phase (Water) and for condensed salts, NaCl, NaOH, sodium diborate (Borax) and sodium pentaborate. Aqueous phase is modeled using Pitzer formalism.

14.15 Calculation Results

Initial calculations were made with ChemSheet software using the thermodynamic system in Table . At this stage no calculation is made with any real or estimated process values. These calculations are used to verify the thermodynamic system and its applicability to pH calculations with sodium pentaborate and HCl systems in general.

First two reference calculations were made where results were compared against measured pH values with 0.025 M Borax buffer solution (Figs. 3 and 4).

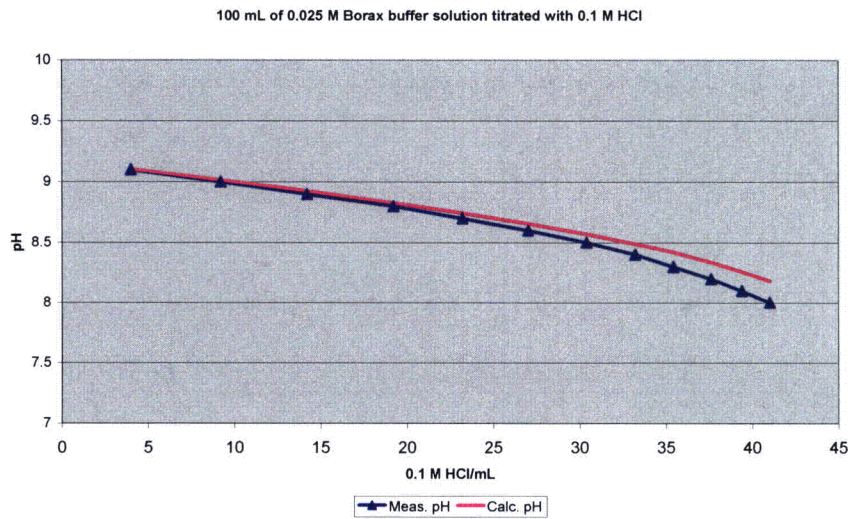


Figure 13-11. Comparison of calculated and measured pH in a case of Borax buffer solution titrated with 0.1 M HCl.

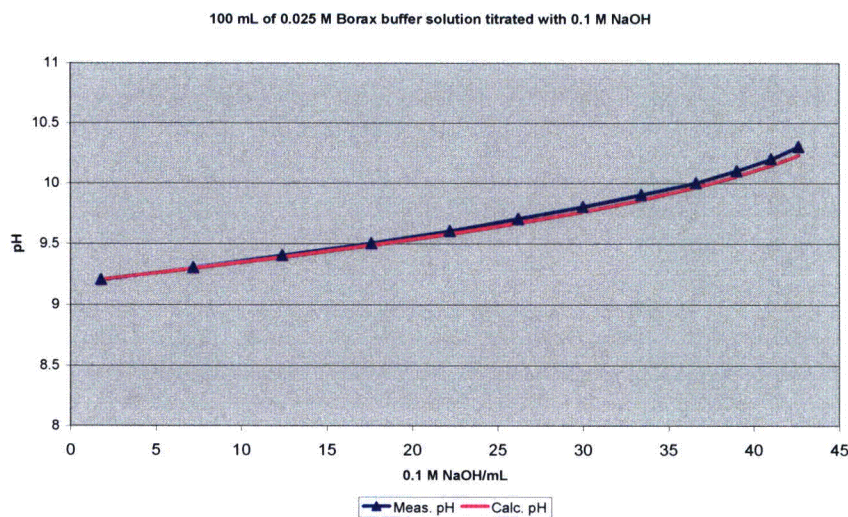


Figure 13-12. Comparison of calculated and measured pH in a case of Borax buffer solution titrated with 0.1 M NaOH.

With low acid and base concentrations calculated and measured values are almost equal but especially with higher acid (HCl) concentration there is a clear difference but the result is still adequate.

Next calculation was made with sodium pentaborate solution where natural boron concentration is 1600 ppm (according to standby liquid control system specifications).

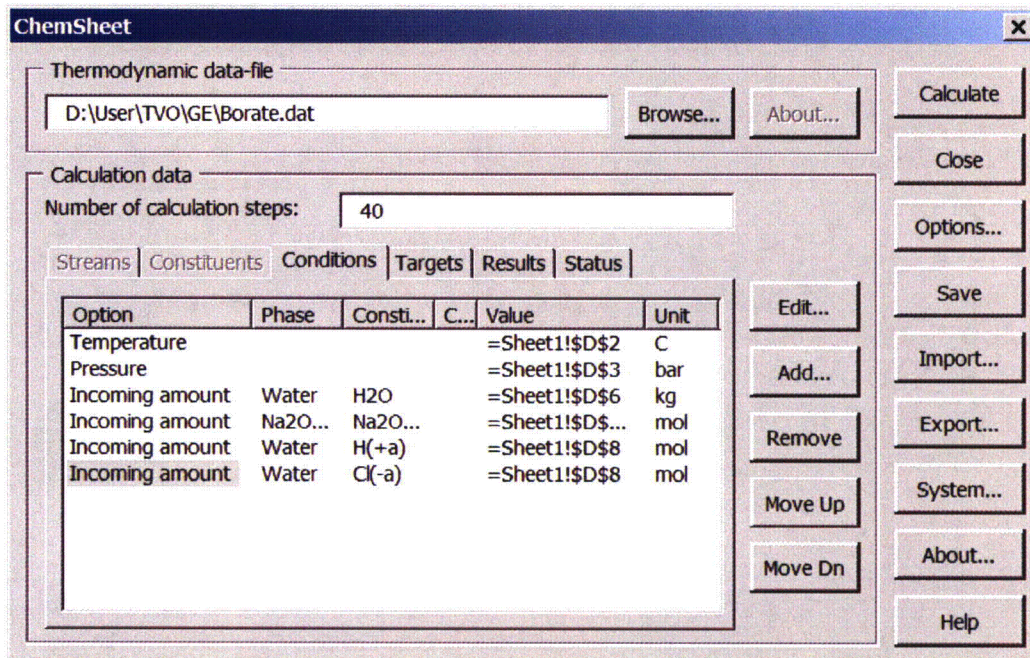


Figure 13-13. ChemSheet dialog showing the initial conditions of pH calculation. Actual values were given in Excel worksheet cells.

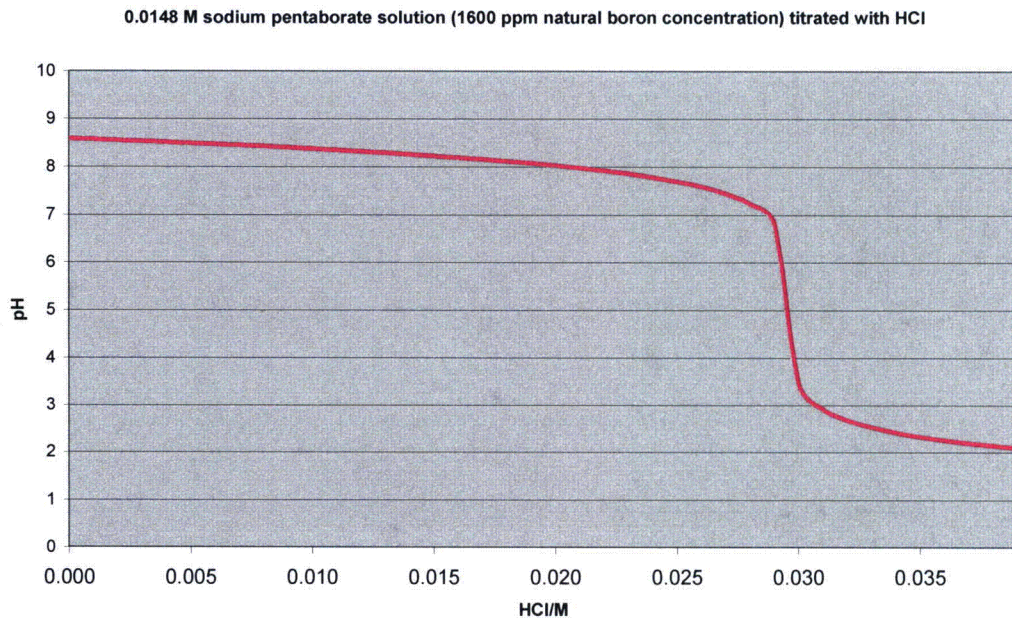


Figure 13-14. Calculation of pH in case of 0.0148 M sodium pentaborate titrated with HCl.

It can be seen that pH changes to acidic when HCl concentration is greater than 0.029 mol/kg_{H₂O}. This result is not verified yet (it is only based on calculation).

Similar titration curve was found for sodium diborate (Borax) at <http://www.borax.com/detergents/pheffect.html>.

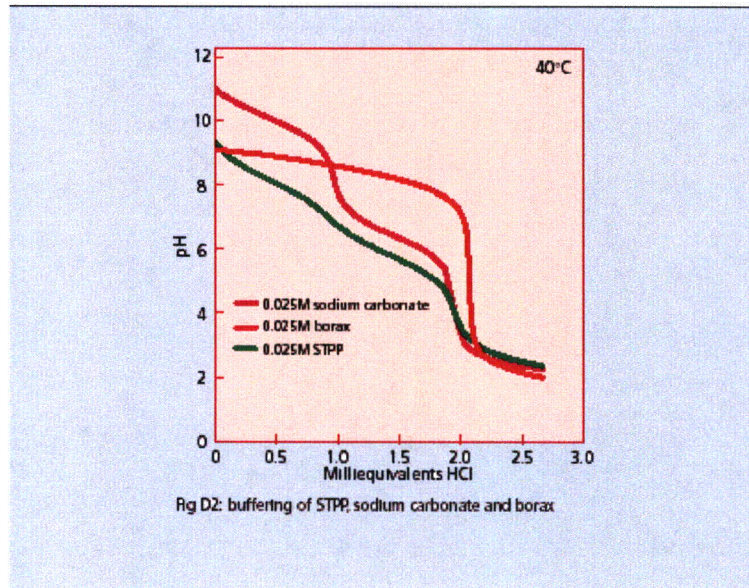


Figure 13-15. Titration curve for 0.025 M Borax buffer solution found at <http://www.borax.com/detergents/pheffect.html>.

The same titration curve was also calculated with ChemSheet.

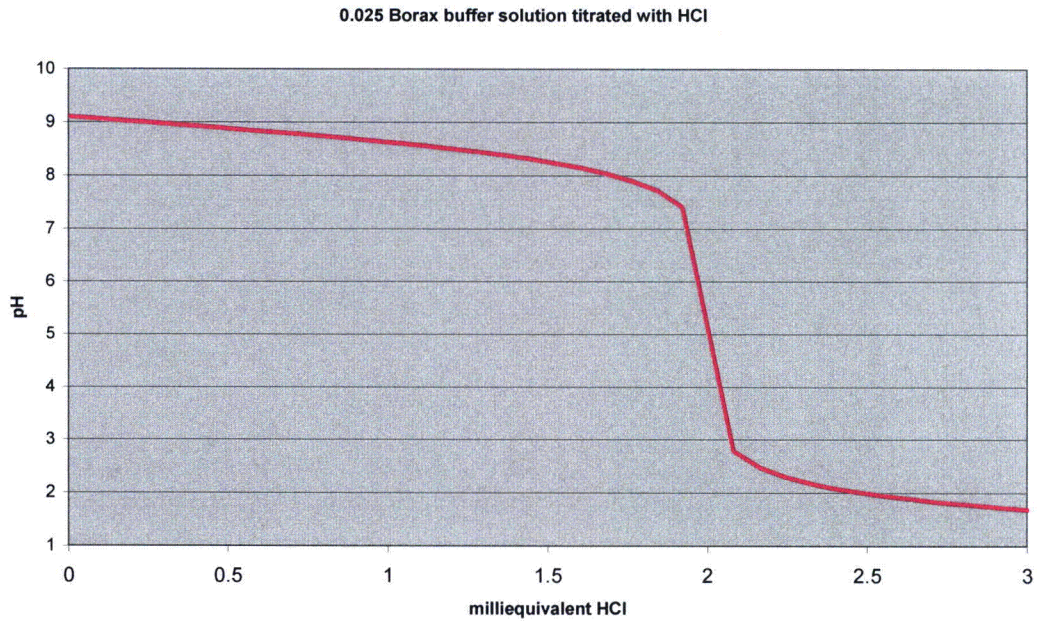


Figure 13-16. Titration curve at 40 C for 0.025 M Borax buffer solution calculated with ChemSheet.

It can be seen that the calculated titration curve is quite similar.

It can be concluded that the used thermodynamic data is applicable to pH calculations at temperature range between 25-50 degrees Celsius and at moderate pressure (1-5 atm). Probably it can be used at temperatures even close to boiling point of water (depending on the absolute pressure).

In the next stage a ChemSheet pH model will be made where process data is taken from MELCOR simulation.

Enclosure 3

MFN 08-770

Affidavit – David H. Hinds

GE-Hitachi Nuclear Energy Americas LLC

AFFIDAVIT

I, **David H. Hinds**, state as follows:

- (1) I am General Manager, New Units Engineering, GE-Hitachi Nuclear Energy Americas LLC ("GEH"), have been delegated the function of reviewing the information described in paragraph (2) which is sought to be withheld, and have been authorized to apply for its withholding.
- (2) The information to be discussed and sought to be withheld is delineated in the letter from Mr. Richard E. Kingston to U.S. Nuclear Regulatory Commission, entitled: "*Transmittal of Non-Proprietary Version of the Initial Research Report No. VTT-R-04413-06, Estimation and Modeling of Effective Fission Product Decontamination Factor for ESBWR Containment, June 2006*," dated October 8, 2008. The information to be withheld: "*Transmittal of Non-Proprietary Version of the Initial Research Report No. VTT-R-04413-06, "Estimation and Modeling of Effective Fission Product Decontamination Factor for ESBWR Containment, June 2006 – GEH Proprietary Information"*" contains proprietary information, and is identified by [[dotted underline inside double square brackets⁽³⁾]]. Figures and other large objects are identified with double square brackets before and after the object. In each case, the superscript notation ⁽³⁾ refers to Paragraph (3) of this affidavit, which provides the basis for the proprietary determination.
- (3) In making this application for withholding of proprietary information of which it is the owner or licensee, GEH relies upon the exemption from disclosure set forth in the Freedom of Information Act ("FOIA"), 5 USC Sec. 552(b)(4), and the Trade Secrets Act, 18 USC Sec. 1905, and NRC regulations 10 CFR 9.17(a)(4), and 2.390(a)(4) for "trade secrets" (Exemption 4). The material for which exemption from disclosure is here sought also qualify under the narrower definition of "trade secret", within the meanings assigned to those terms for purposes of FOIA Exemption 4 in, respectively, Critical Mass Energy Project v. Nuclear Regulatory Commission, 975F2d871 (DC Cir. 1992), and Public Citizen Health Research Group v. FDA, 704F2d1280 (DC Cir. 1983).
- (4) Some examples of categories of information which fit into the definition of proprietary information are:
 - a. Information that discloses a process, method, or apparatus, including supporting data and analyses, where prevention of its use by GEH's competitors without license from GEH constitutes a competitive economic advantage over other companies;

- b. Information which, if used by a competitor, would reduce his expenditure of resources or improve his competitive position in the design, manufacture, shipment, installation, assurance of quality, or licensing of a similar product;
- c. Information which reveals aspects of past, present, or future GEH customer-funded development plans and programs, resulting in potential products to GEH;
- d. Information which discloses patentable subject matter for which it may be desirable to obtain patent protection.

The information sought to be withheld is considered to be proprietary for the reasons set forth in paragraphs (4)a. and (4)b. above.

- (5) To address 10 CFR 2.390(b)(4), the information sought to be withheld is being submitted to NRC in confidence. The information is of a sort customarily held in confidence by GEH, and is in fact so held. The information sought to be withheld has, to the best of my knowledge and belief, consistently been held in confidence by GEH, no public disclosure has been made, and it is not available in public sources. All disclosures to third parties, including any required transmittals to NRC, have been made, or must be made, pursuant to regulatory provisions or proprietary agreements which provide for maintenance of the information in confidence. Its initial designation as proprietary information, and the subsequent steps taken to prevent its unauthorized disclosure, are as set forth in paragraphs (6) and (7) following.
- (6) Initial approval of proprietary treatment of a document is made by the manager of the originating component, the person most likely to be acquainted with the value and sensitivity of the information in relation to industry knowledge, or subject to the terms under which it was licensed to GEH. Access to such documents within GEH is limited on a "need to know" basis.
- (7) The procedure for approval of external release of such a document typically requires review by the staff manager, project manager, principal scientist, or other equivalent authority for technical content, competitive effect, and determination of the accuracy of the proprietary designation. Disclosures outside GEH are limited to regulatory bodies, customers, and potential customers, and their agents, suppliers, and licensees, and others with a legitimate need for the information, and then only in accordance with appropriate regulatory provisions or proprietary agreements.
- (8) The information identified in paragraph (2) above is classified as proprietary because it contains the ESBWR model for the containment fission product decontamination factor, developed by GEH. Development of this containment fission product decontamination factor model was achieved at a significant cost to GEH.

- (9) Public disclosure of the information sought to be withheld is likely to cause substantial harm to GEH's competitive position and foreclose or reduce the availability of profit-making opportunities. The information is part of GEH's comprehensive BWR safety and technology base, and its commercial value extends beyond the original development cost. The value of the technology base goes beyond the extensive physical database and analytical methodology and includes development of the expertise to determine and apply the appropriate evaluation process. In addition, the technology base includes the value derived from providing analyses done with NRC-approved methods.

The research, development, engineering, analytical and NRC review costs comprise a substantial investment of time and money by GEH.

The precise value of the expertise to devise an evaluation process and apply the correct analytical methodology is difficult to quantify, but it clearly is substantial.

GEH's competitive advantage will be lost if its competitors are able to use the results of the GEH experience to normalize or verify their own process or if they are able to claim an equivalent understanding by demonstrating that they can arrive at the same or similar conclusions.

The value of this information to GEH would be lost if the information were disclosed to the public. Making such information available to competitors without their having been required to undertake a similar expenditure of resources would unfairly provide competitors with a windfall, and deprive GEH of the opportunity to exercise its competitive advantage to seek an adequate return on its large investment in developing and obtaining these very valuable analytical tools.

I declare under penalty of perjury that the foregoing affidavit and the matters stated therein are true and correct to the best of my knowledge, information, and belief.

Executed on this 8th day of October 2008.



David H. Hinds
GE-Hitachi Nuclear Energy Americas LLC