# ChemPool

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Summary

In severe accident scenario the water vaporized by the melting core flows through compartments where it condenses again. Hydrochloric acid can be formed from organic materials containing chlorine. Cesium hydroxide and cesium iodine are formed from released fission products. Controlling the pH in the containment is important as in acidic conditions radioactive iodine could be formed and released into atmosphere. Injected buffer solutions can be used to keep the pH neutral or alkaline in the pools. Currently MELCOR code is not able to consider aqueous species and how they affect the pH in the pools. ChemPool is a new program to be used with MELCOR to calculate the equilibrium composition and the pH values of the pools. After MELCOR simulation the results from MELCOR are exported to external datafile containing the temperatures, the pressures and the compositions of the pools at each time steps. The estimated formation rates of acids and dissolved salts from fission products are then coupled with these and the equilibrium compositions and the pH values of the pools are calculated with ChemPool. Internally ChemPool uses thermodynamic programming library, ChemApp®, for calculating the equilibrium composition of a thermodynamic system (gas, aqueous water and solids like fission products) by minimizing the Gibbs energy of the system. ChemPool is an easy to use tool for adding simulation of pH chemistry to a MELCOR simulation.

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# Contents

# 1 Introduction

Reactor core meltdown accidents in pressurized or boiling water reactors are caused by insufficient cooling of the core; first, the water in the core is heated, and evaporation of the coolant finally unveils the core either partly or totally. Within hours, the core is heated up by the decay heat, and then melts down. Finally, the hot molten core material will collect at the bottom of the rector pressure vessel, melt through the bottom, and gradually drop into the reactor cavity, which is part of the containment compartments. As core is exposed, fission products can directly enter the steam atmosphere of the primary system. Most fission products are transported through the primary system as aerosols until they reach the leak in the primary system and are discharged into the containment. This sequence of accident steps is possible only if the redundant emergency core cooling systems fail after the event initiating the accident. Typical hypothetical accident scenario begins with failure of reactor pressure vessel, RPV, bottom drain line after which all drain lines are blocked until reactor core becomes uncovered. After reactor core is uncovered and core has melted, RPV can be flooded with water from emergency water pool known as GDCS (see Figure 1).
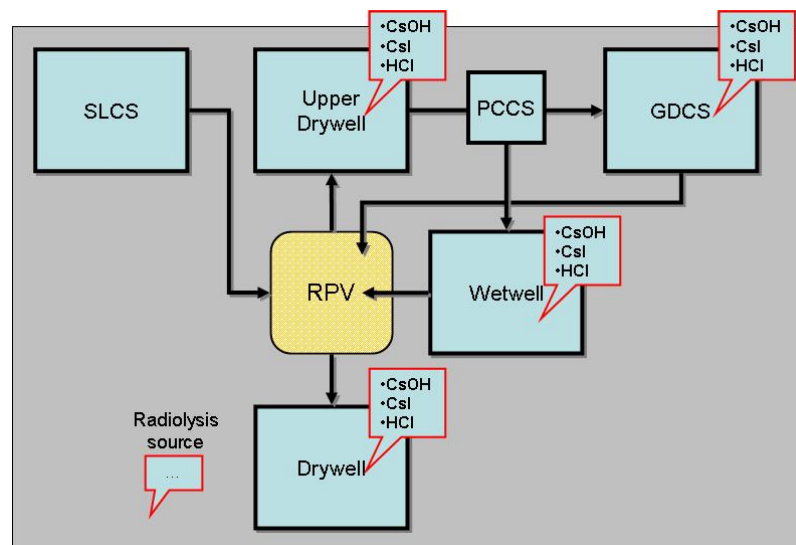


*Figure 1 Example accident scenario.*

MELCOR ("melting core") is a fully integrated, engineering-level computer code by Sandia National Laboratories whose primary purpose is to model the progression of accidents in light water reactor nuclear power plants. A broad spectrum of severe accident phenomena in both boiling and pressurized water reactors can be treated in MELCOR. Current uses of MELCOR include:

- Core uncovering (loss of coolant), fuel heat-up, cladding oxidation, fuel degradation and core material melting and relocation.

- Core-concrete attack and ensuing aerosol generation.

- In-vessel and ex-vessel hydrogen production, transport, and combustion.

- Fission product release (aerosol and vapor), transport, and deposition, behavior of radioactive aerosols in the reactor containment building.

MELCOR can simulate the conditions in RPV and in coolant system for long period of time (up to several days) until conditions in the whole containment normalize. One problematic fission product is iodine-131 (half-life eight days). In acidic conditions most of the dissolved iodine is vaporized and can be released outside of the containment posing an environmental thread. This is why it is important to control the pH in the cooling system in the course of the accident. Injected buffer solutions (sodium pentaborate, trisodium phosphate) can be used to keep the pH neutral or alkaline in the pools but it becomes increasingly difficult to estimate the conditions in the aqueous pools as several acids and bases could be formed after the core melting. Nitric acid is formed from air and water due to irradiation from released fission products. Hydrochloric acid can be formed from organic materials like cables containing chlorine. Some fission products react with steam to form water soluble salts, like cesium hydroxide, which is a strong base.

Currently MELCOR code is not able to consider aqueous species and how they affect the pH in the pools. In earlier projects in VTT ChemSheet® [1] was coupled with MELCOR to calculate the equilibrium composition and the pH values of the pools. After MELCOR simulation the results from MELCOR are exported to text files containing temperatures, pressures and compositions of the pools at each time steps. The estimated formation rates of acids and dissolved salts from fission products are then coupled with these and the equilibrium compositions and the pH values of the pools are calculated with ChemSheet in Excel. Internally ChemSheet uses thermodynamic programming library, ChemApp®, for calculating the equilibrium composion of a thermodynamic system (gas, aqueous water and solids like fission products) by minimizing the Gibbs energy of the system.

The problem with ChemSheet model was that it needed to be tailored by hand for each MELCOR case and chemistry model separately which was time consuming process and susceptible to making errors. More advanced and properly validated software is required. Coupling of MELCOR data with thermodynamic calculation should be automated in code as much as possible. So a new simulation software, ChemPool, has been made. It is a Command Prompt program (it lacks user interface) using again ChemApp thermodynamic library for equilibrium calculation.

# 2 Thermodynamic data

Table 1 shows the thermodynamic system that has been used in the pH calculations. Thermodynamic system contains all the needed thermodynamic species and it provides the required species for the pH simulation. It contains a gas phase that uses Tsonopoulos model for non-ideal gas (for high pressure conditions), an aqueous water phase that uses Pitzer electrolyte model, and pure solid phases that are mainly used to input various acidic and basic salts and oxides into pools.

*Table 1 Thermodynamic system.*

| Phase | Constituent | B | C | Cl | Cs | H | I | N | Na | O | P | e- | H2O | HNO3 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Gas | H2O(g) | | | | | 2 | | | | 2 | | | 1 | |
| | N2(g) | | | | | | | 2 | | | | | | |
| | O2(g) | | | | | | | | | 2 | | | | |
| | H2(g) | | | | | 2 | | | | | | | | |
| | CO(g) | | 1 | | | | | | | 1 | | | | |
| | CO2(g) | | 1 | | | | | | | 2 | | | | |
| | CH4(g) | | 1 | | | 4 | | | | | | | | |
| | HI(g) | | | | | 1 | 1 | | | | | | | |
| | I2(g) | | | | | | 2 | | | | | | | |
| | HCl(g) | | | 1 | | 1 | | | | | | | | |
| | HNO3(g) | | | | | 1 | | 1 | | 3 | | | | 1 |
| | CsI(g) | | | | 1 | | 1 | | | | | | | |
| | CsOH(g) | | | | 1 | 1 | | | | 1 | | | | |
| | H3BO3(g) | 1 | | | | 3 | | | | 3 | | | | |
| Water | H2O(a) | | | | | 2 | | | | 1 | | | | |
| | B(OH)3(a) | 1 | | | | 3 | | | | 3 | | | | |
| | B(OH)4(-a) | 1 | | | | 4 | | | | 4 | | | | |
| | Cl(-a) | | | 1 | | | | | | | | 1 | | |
| | Cs(+a) | | | | 1 | | | | | | | -1 | | |
| | CsOH(a) | | | | 1 | 1 | | | | 1 | | | | |
| | H(+a) | | | | | 1 | | | | | | -1 | | |
| | I(-a) | | | | | | 1 | | | | | 1 | | |
| | I2(a) | | | | | | 2 | | | | | | | |
| | Na(+a) | | | | | | | | 1 | | | -1 | | |
| | OH(-a) | | | | | 1 | | | | 1 | | 1 | | |
| | N2(a) | | | | | | | 2 | | | | | | |
| | HNO3(a) | | | | | 1 | | 1 | | 3 | | | | 1 |
| | NH3(a) | | | | | 3 | | 1 | | | | | | |
| | NH4(+a) | | | | | 4 | | 1 | | | | -1 | | |
| | NO2(-a) | | | | | | | 1 | | 2 | | 1 | | 1 |
| | NO3(-a) | | | | | | | 1 | | 3 | | 1 | | 1 |
| | H2PO4(-a) | | | | | 2 | | | | 4 | 1 | 1 | | |
| | HPO4(-2a) | | | | | 1 | | | | 4 | 1 | 2 | | |
| | PO4(-3a) | | | | | | | | | 4 | 1 | 3 | | |
| | H3PO4(a) | | | | | 3 | | | | 4 | 1 | | | |
| | CO2(a) | | 1 | | | | | | | 2 | | | | |
| | CO3(-2a) | | 1 | | | | | | | 3 | | 2 | | |
| | HCO2(-a) | | 1 | | | 1 | | | | 2 | | 1 | | |
| | HCO3(-a) | | 1 | | | 1 | | | | 3 | | 1 | | |
| | NaCO3(-a) | | 1 | | | | | | 1 | 3 | | 1 | | |
| Solids | CsI(s) | | | | 1 | | 1 | | | | | | | |
| | CsOH(s) | | | | 1 | 1 | | | | 1 | | | | |
| | H3BO3(s) | 1 | | | | 3 | | | | 3 | | | | |
| | Na2O*2B2O3*10H2O(s) | 2 | | | | 20 | | | 2 | 17 | | | | |
| | Na2O*5B2O3*10H2O(s) | 5 | | | | 20 | | | 2 | 26 | | | | |
| | NaCl(s) | | | 1 | | | | | 1 | | | | | |
| | NaOH(s) | | | | | 1 | | | 1 | 1 | | | | |
| | Na3PO4(s) | | | | | | | | 3 | 4 | 1 | | | |
| | Na2HPO4(s) | | | | | 1 | | | 2 | 4 | 1 | | | |
| | NaH2PO4(s) | | | | | 2 | | | 1 | 4 | 1 | | | |
| | HCl(s) | | | 1 | | 1 | | | | | | | | |
| | HNO3(s) | | | | | 1 | | 1 | | 3 | | | | |
| Constraints | H2O(g)+ | | | | | | | | | | | | 1 | |
| | H2O(g)- | | | | | | | | | | | | -1 | |

Species have been selected from HSC® and FactSage® databases. Aqueous phase Pitzer interaction parameters were taken from VTT's in-house database and its data has been collected from various literature sources as shown in Table 2.

*Table 2 Sources for Pitzer parameters.*

| | |
|---|---|
| **Gas** | |
| H2O(g) | JANAF Thermochemical tables, 3rd ed., Chase et al., J. Phys. Chem. Ref. Data, 14(1) (1985) |
| Cl2(g) | JANAF Thermochemical tables, 3rd ed., Chase et al., J. Phys. Chem. Ref. Data, 14(1) (1985) |
| H2(g) | JANAF Thermochemical tables, 3rd ed., Chase et al., J. Phys. Chem. Ref. Data, 14(1) (1985) |
| HCl(g) | Thermodynamic Data of Pure Substances, Barin, VCH Verlags Gesellschaft, Weinheim, 1993 |
| N2(g) | JANAF Thermochemical tables, 3rd ed., Chase et al., J. Phys. Chem. Ref. Data, 14(1) (1985) |
| O2(g) | Thermodynamic Data of Pure Substances, Barin, VCH Verlags Gesellschaft, Weinheim, 1993 |
| **Water** | |
| H2O | JANAF Thermochemical tables, 3rd ed., Chase et al., J. Phys. Chem. Ref. Data, 14(1) (1985) |
| B(OH)3(a) | Shock et al., Geochim. Cosmochim Acta 53 (1989) 2157-2183 |
| B(OH)4(-a) | The NBS Tables of Chemical Thermodynamic Properties, Bailey et al., J. Phys. Chem. Ref. Data, 11(Supl2) (1982) |
| Cl(-a) | Shock et al., Geochim. Cosmochim Acta 52 (1988) 2009-2036 |
| H(+a) | Definition |
| Na(+a) | Shock et al., Geochim. Cosmochim Acta 52 (1988) 2009-2036 |
| OH(-a) | Shock et al., Geochim. Cosmochim Acta 52 (1988) 2009-2036 |
| **Solids** | |
| Na2O*2B2O3*10H2O | Thermodynamic Data of Pure Substances, Barin, VCH Verlags Gesellschaft, Weinheim, 1993 |
| NaOH | Thermodynamic Properties of Inorganic Substances, 2nd ed., Knacke et al., Springer-Verlag, 1991 |
| **Ionic interactions** | |
| H-Na-Cl | Thermodynamics (3. ed), Pitzer, McGraw-Hill, 1995 |
| H-Cl | Pitzer, Pure & Appl. Chem., 58 (1986) 1599-1610 |
| H-Na | Thermodynamics (3. ed), Pitzer, McGraw-Hill, 1995 |
| Cl-OH-Na | Harvey et al., Geochim. Cosmochim. Acta 48 (1984) 723-751 |
| Cl-OH | Harvey et al., Geochim. Cosmochim. Acta 48 (1984) 723-751 |
| Na-OH | Pitzer, Pure & Appl. Chem., 58 (1986) 1599-1610 |
| Na-Cl | Thermodynamics (3. ed), Pitzer, McGraw-Hill, 1995 |

Thermodynamic data has been validated with a separate ChemSheet model that uses the same thermodynamic system in its calculations. In this model the pH values at different temperatures and compositions are calculated and verified against measured pH values (that have been collected from literature). Figure 2 shows the correlation between the calculated and the measured pH values.
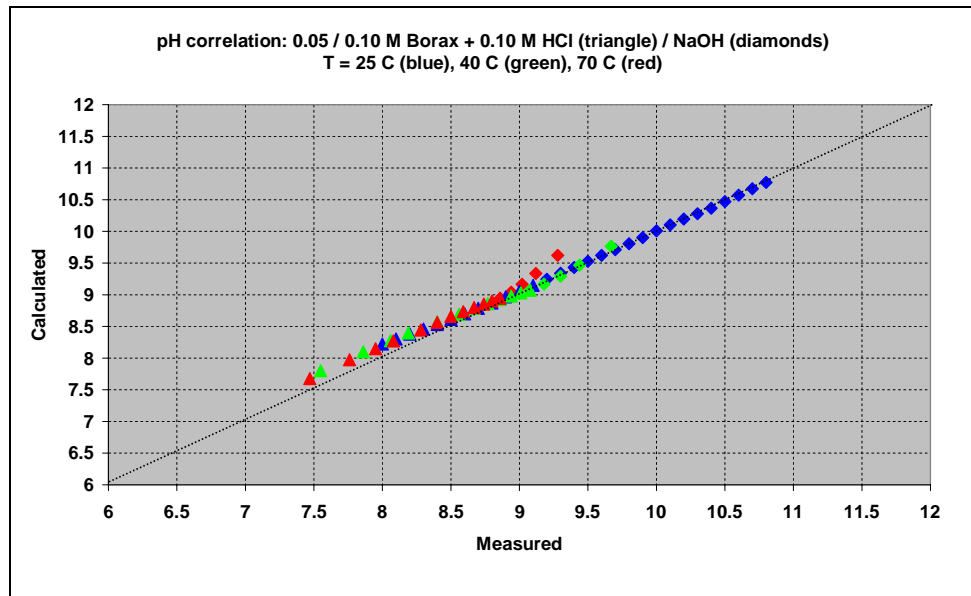


*Figure 2 Correlation between the calculated and the measured pH values.*

Also solubilities of some gas species have been validated. Figure 3 shows the measured and calculated solubilities of $N_2$ into water at different pressures.
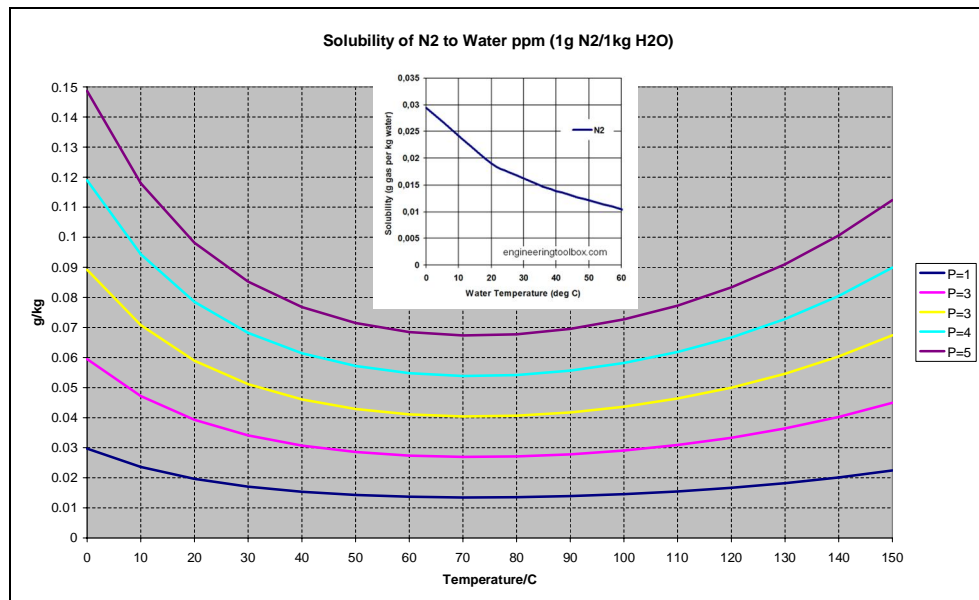


*Figure 3 Solubility of N2 into water at different pressures.*

In MELCOR the chemical species are defined as Materials (like water vapour ($H_2O(g)$), water ($H_2O(a)$), nitrogen gas ($N_2(g)$), ..) and Classes (like fission products CsI(s) and CsOH(s)). These same species are also found from the thermodynamic system used by ChemPool. Table 3 shows how the species are mapped from MELCOR to ChemPool.

*Table 3. Mapping of MELCOR Materials and Classes to ChemPool species.*

| Type | Name/ID | Chemapp name | Description |
|------|---------|--------------|-------------|
| Material | POOL | H2O/H2O | MELCOR default material - water in pool |
| Material | FOG | H2O/H2O | MELCOR default material - water ingas as fog |
| Material | H2O-VAP | Gas/H2O(g) | MELCOR default material - water vapor |
| Material | N2 | Gas/N2(g) | MELCOR optional material |
| Material | O2 | Gas/O2(g) | MELCOR optional material |
| Material | H2 | Gas/H2(g) | MELCOR optional material |
| Material | CO | Gas/CO(g) | MELCOR optional material |
| Material | CO2 | Gas/CO2(g) | MELCOR optional material |
| Material | CH4 | Gas/CH4(g) | MELCOR optional material |
| CLASS | 2 | CsOH | MELCOR default class |
| CLASS | 16 | CsI | MELCOR default class |
| CLASS | CH3I | CH3I | iodine pool model class |
| CLASS | HCL | HCl | iodine pool model class |
| CLASS | HNO3 | HNO3 | iodine pool model class |
| CLASS | IM | - | iodine pool model class |
| CLASS | HBO2 | H3BO3 | iodine pool model class |
| CLASS | HPO4 | Na3PO4 | iodine pool model class |
| CLASS | LIBO | - | |
| REACTION | | Any Chemapp species | ChemPool source term |

## 3 Methods

### 3.1 Simulation model
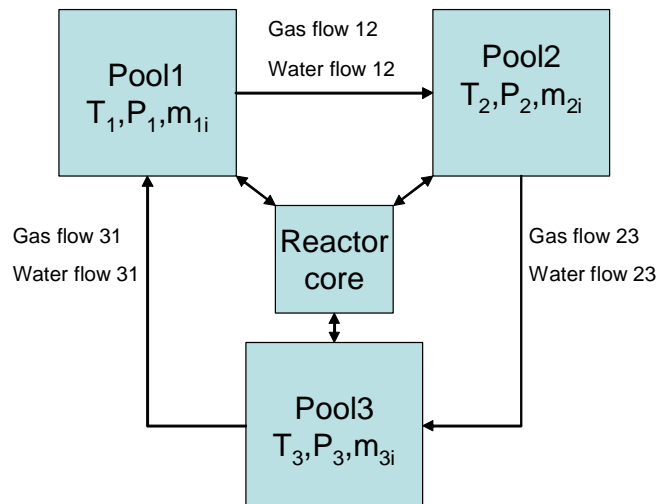
Figure 4 shows a simple network of pools.



*Figure 4 Example layout of a simple pool system.*

Temperature, T, pressure, P, and masses, $m_i$, of materials and classes (i.e. species) at different time steps are read from the external datafile generated by MELCOR. Then species like $HNO_3$ and HCl can be added to those pools after which their equilibrium compositions and pH values are calculated. And now that MELCOR also calculates the flow rates between the pools, ChemPool is also able use that information in order to calculate how these additional species flow between the

pools by assuming that the pools are ideally stirred tanks, i.e. concentrations of species in pool are uniform (simplifying assumption).

All hydrodynamic material, together with its associated energy, in a MELCOR calculation resides in control volumes. Hydrodynamic material includes the coolant (water), vapor and fog, and non-condensable gases.

## 3.2 Control volume

The contents of each control volume are divided between pool and an atmosphere (Figure 5). The pool fills the lower part of the control volume and the atmosphere the remainder. When using non-equilibrium mode MELCOR calculates energy and mass transfer between the pool and atmosphere as conduction / convection / radiation and boiling / flashing.
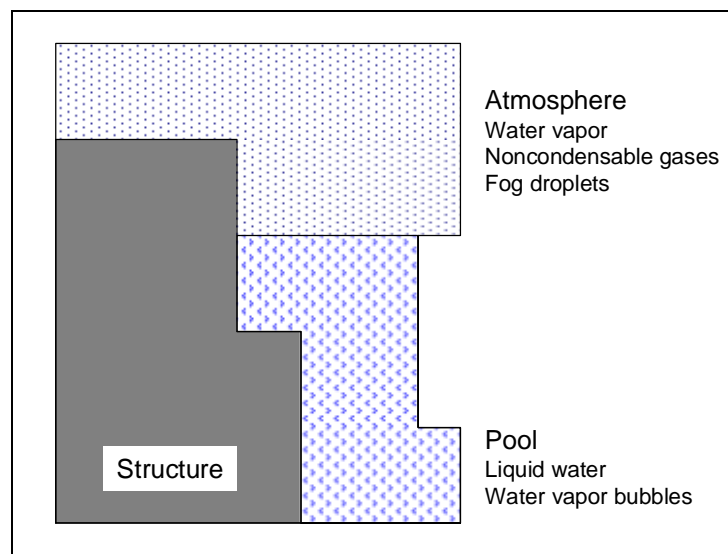


*Figure 5 Control volume.*

## 3.3 Flow path

Flow path defines the geometry and characteristics of connections between control volumes, through which the control volume contents may be transported (Figure 6). No material resides in flow paths.
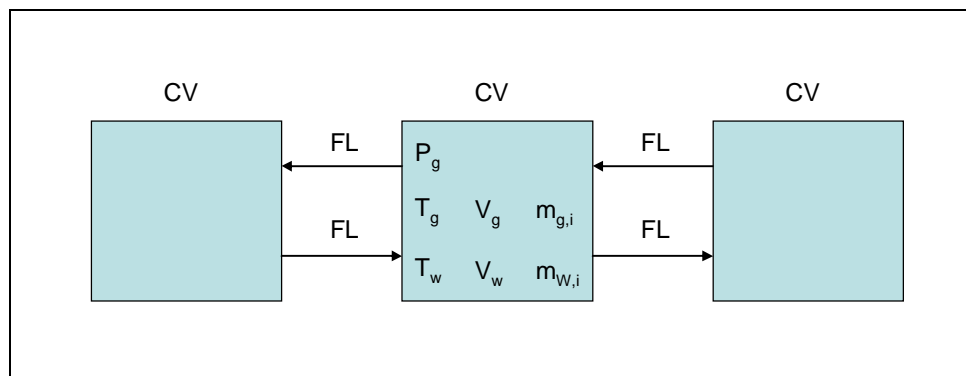


*Figure 6 Network of control volumes and flow paths.*

Equation of conservation of mass of component in control volume:

$$\frac{dm_i}{dt} = \sum_j w_i^j FL^j + R_i \qquad (1)$$

where m is mass of component in a control volume, w is mass fraction of component in a flow in flow path, FL is total flow rate in a flow path and Ri is formation rate of component in a control volume. The mass fraction of component in flow is same as the mass fraction of component in the control volume from which the flow originates (source control volume). If flow rate is positive then the flow direction is from specified source control volume to specified destination control volume. If flow rate is negative then the flow direction is reversed (actual source control volume is same as the specified destination control volume). Total flow rates at each time step are calculated by MELCOR.

## 3.4    Simulation algorithm

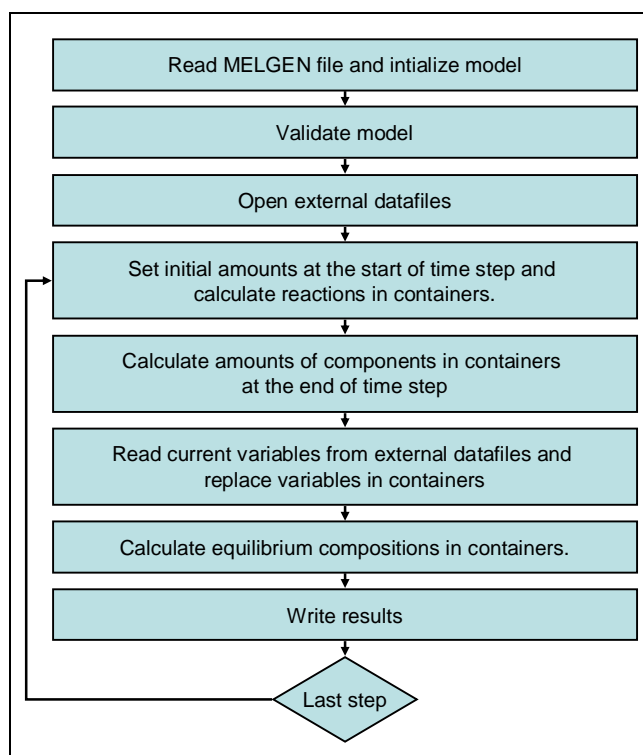Figure 7 shows the simulation algorithm.



*Figure 7 Simulation algorithm.*

ChemPool reads input data from four files. First file is MELCOR configuration file that is used by ChemPool to construct the complete flowsheet (that same that MELCOR uses), i.e. to read all the control volumes in the scenario and the connections between them. It also contains the definitions of the chemical components in the control volumes.  Second file is ChemPool configuration file that contains ChemPool specific information, i.e. information about the components (positions and time dependent formation rates) that are not part of the MELCOR simulation, like acids formed from fissions products or buffer solutions added to neutralize the acids.  It also contains information about the results that will be written by ChemPool program (pH, amounts, mass-fractions,

concentrations of selected components in selected control volumes). Third file is the external data-file written by MELCOR, that contains temperature, pressure, masses of components and total mass flow rates of gas and water between the control volumes at each time step. Fourth file contains the definitions and specifications of the thermodynamic system used in the equilibrium and pH calculation

## 4    Results

### 4.1    ChemPool program

ChemPool has been developed by using Microsoft Develper Studio Environment and Fortran 90 compiler. ChemPool is divided into number of Fortran modules:

- MModel          Specifications for pH simulation model
- MContainer      Specifications for container (control volume in MELCOR - CV)
- MConnector      Specifications for connector (flow path in MELCOR - FL)
- MDatafile       Specifications for datafile (external datafile in MELCOR - EDF)
- MVariable       Specifications for variable (control function in MELCOR - CF)
- MNuclides       Specifications for variable (radionuclides in MELCOR - RN)
- Mclass          Specifications for class (decay heat in MELCOR - DCH)
- MFluid          Specifications for conditions of thermodynamic system (temperature, pressure and amounts of phase constituents)
- MSystem         Specifications for thermodynamic system (components, phases and phase constituents)
- MReaction       Specifications for reaction sources (like formation of HCl from fission products)
- MTable          Specifications for table (tabular function in MELCOR - TF)
- MParser         Specifications for parsing MELGEN/MELCOR input file
- MScanner        Specifications for reading tokens from MELGEN / MELCOR input file
- MChars          Specifications for characters
- MError          Specifications for error

Figure 8 shows how the modules are dependent on each other. Arrows show the direction of dependencies between the modules. In Fortran module a dependency is shown with USE statement. For example MParser module uses MModel and MScanner modules.
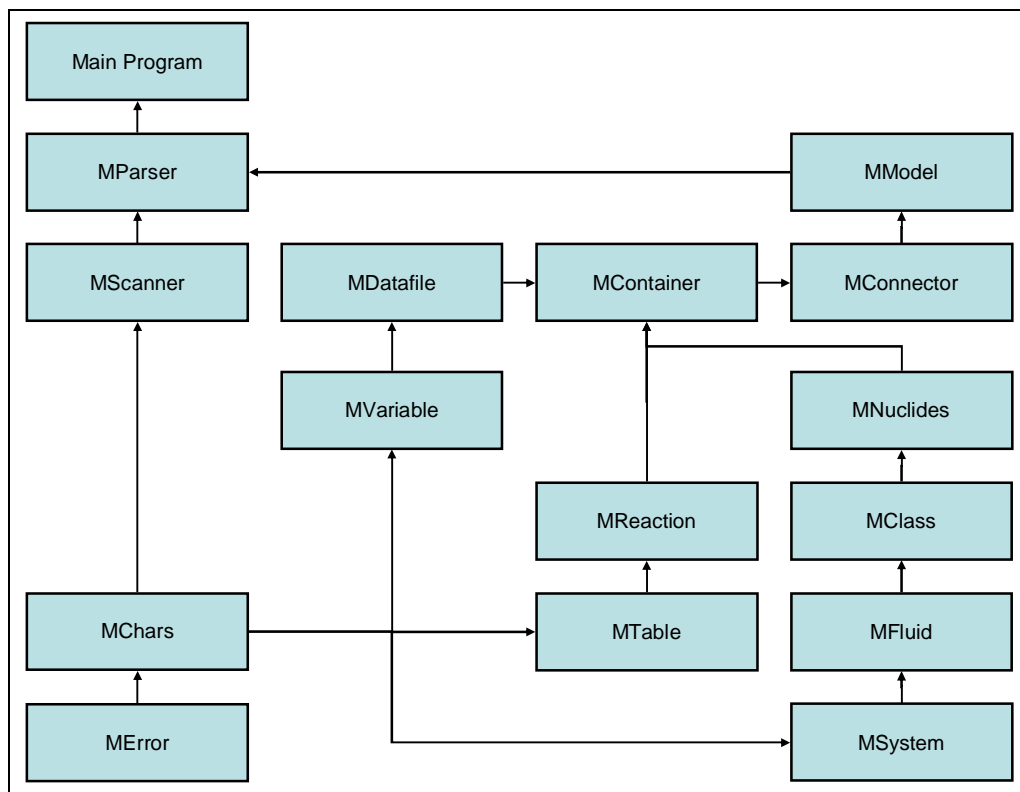


*Figure 8 ChemPool modules.*

Main program uses MParser module (Figure 10) to read and parse MELGEN/MELCOR input files. MParser module constructs the simulation model by setting the structures in TModule structure (Figure 9).

```
type TModel
    type(TTables)     :: Tables
    type(TReactions)  :: Reactions
    type(TMaterials)  :: Materials
    type(TClasses)    :: Classes
    type(TNuclides)   :: Nuclides
    type(TDatafiles)  :: Datafiles
    type(TContainers) :: Containers
    type(TConnectors) :: Connectors
end type
```
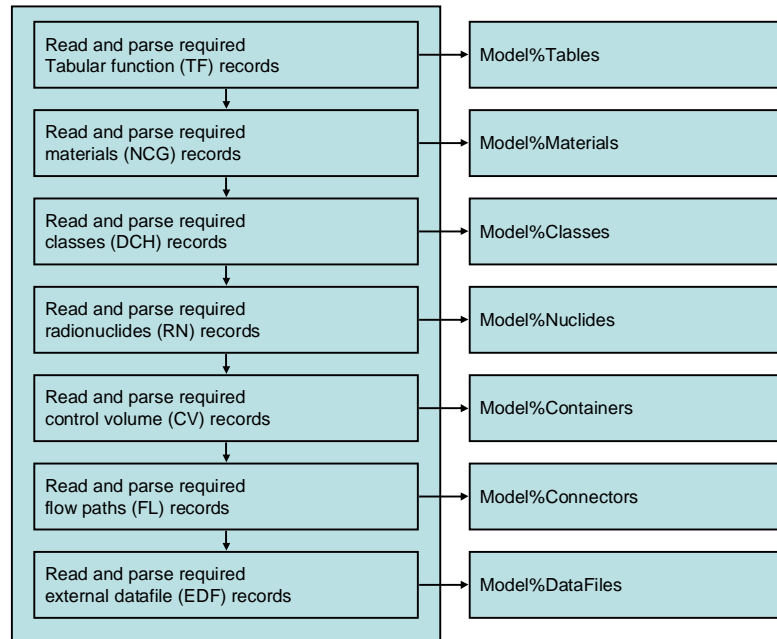
*Figure 9 TModel structure.*

*Figure 10 Parse routine in MParser module constructs the model variables.*

The main program uses MModel to do the simulation and finally to write the requested results.

## 4.2 ChemPool results

ChemPool has been tested with one Olkiluoto 1 case. MELCOR saved values of following variables at each time step to an external datafile.

For each pool/container:

- Time [s]
- Gas temperature [K]
- Gas pressure [Pa]
- Water temperature [K]
- $H_2O(a)$ [kg]
- CsI(a) [kg]
- CsOH(a) [kg]
- $N_2(g)$ [kg]
- $H_2O(g)$ [kg]
- $O_2(g)$ [kg]
- $H_2(g)$ [kg]
- $CO_2(g)$ [kg]
- CO(g) [kg]
- $CH_4(g)$ [kg]

For each flow/connector:

- Time [s]
- Water flow rate [kg/s]
- $N2(g)$ [kg/s]
- $H2O(g)$ [kg/s]
- $O2(g)$ [kg/s]
- $H2(g)$ [kg/s]
- $CO2(g)$ [kg/s]
- $CO(g)$ [kg/s]
- $CH4(g)$ [kg/s]

These value were the read by ChemPool program. Table 4 shows the ChemPool definitions for $HNO_3$ formations in Pedestal and $HNO_3$ formations in Wetwell and Pedestal. These values are taken from separate dose rate calculations.

*Table 4. ChemPool definitions for HCl and HNO3 formation rates.*

```
TF71000   'HCl Pedestal' 4  1.0  0.0
*         Time [s]  Formation rate [kg/s]
TF71010   0.00000      0.0
TF71011   3600.00      0.652778
TF71012   3780.00      0.0
TF71013   100800.      0.0
*
TF72000   'HNO3 WetWell' 6  1.0  0.0
*         Time [s]  Formation rate [kg/s]
TF72010   0.00000      0.0
TF72011   3600.00      0.000107395
TF72012   10800.0      0.000122311
TF72013   21600.0      9.6954E-05
TF72014   43200.0      7.8309E-05
TF72015   100800.      0.0
*
TF73000   'HNO3 Pedestal' 6  1.0  0.0
*         Time [s]  Formation rate [kg/s]
TF73010   0.00000      0.0
TF73011   3600.00      6.06016E-05
TF73012   10800.0      6.13687E-05
TF73013   21600.0      5.36976E-05
TF73014   43200.0      5.75331E-05
TF73015   100800.      0.0
```

These records are only table definitions containing time steps and rate values in given time intervals.

Table 5 shows how these rates are actually mapped to specific species and pools.

*Table 5. ChemPool definitions for HCl and HNO3 pool locations.*

```
****************************************************************
*
* REACTIONS
*
****************************************************************
*
CP10100 HCL  400 710  * name (32 chars), CV no, TF no 300 Drywell
CP10200 HNO3 200 720  * name (32 chars), CV no, TF no 200 Wetwell
CP10300 HNO3 400 730  * name (32 chars), CV no, TF no 400 Pedestal
```

Figure 11 and Figure 12 show the calculated pH values as function of time with the given HCl and $HNO_3$ formation rates and with H2O(g), N2(g), O2(g), H2(g), CO(g), CO2(g) H2O(a), CsOH(s), CSI(s) masses calculated by MELCOR.
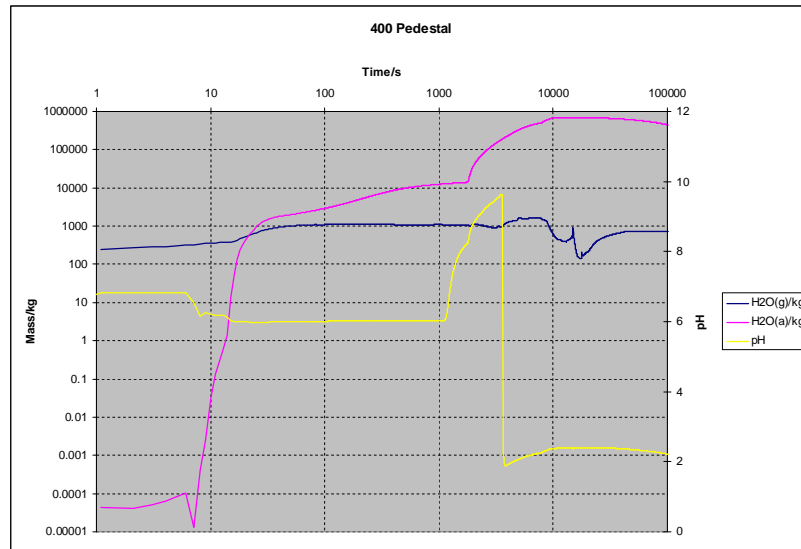


*Figure 11 Water vapour and water mass and pH in Pedestal.*
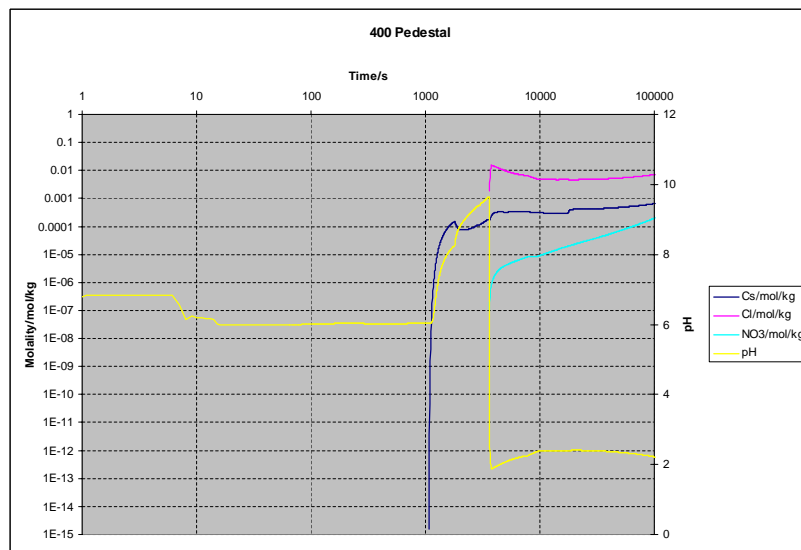


*Figure 12 Cesium (CsOH), Chlorium(HCl), Nitrate ion (HNO3) and pH in Pedestal.*

## 5 Conclusions

There are some simplifying assumptions like assuming all the pools to be ideally stirred tanks so that all the dissolved species are instantly spread into pools, or that species in atmosphere and pool are in equilibrium with each other (or those additional species that are not handled by MELCOR). But still ChemPool can be used quite effortlessly to add calculation of pH chemistry to MELCOR simulations. For example an existing MELCOR model only needs to be calculated once again so that it creates the external datafile containing the parameters required by ChemPool. After that ChemPool can be calculated several times with different formation rates and pool locations of acids, and to test with different neutralizing solutions for example.

## 6 Summary

In severe accident scenario the water vaporized by the melting core flows through compartments where it condenses again. Hydrochloric acid can be formed from organic materials containing chlorine. Cesium hydroxide and cesium iodine are formed from released fission products. Controlling the pH in the containment is important as in acidic conditions radioactive iodine could be formed and released into atmosphere. Injected buffer solutions can be used to keep the pH neutral or alkaline in the pools. Currently MELCOR code is not able to consider aqueous species and how they affect the pH in the pools. ChemPool is a new program to be used with MELCOR to calculate the equilibrium composition and the pH values of the pools. After MELCOR simulation the results from MELCOR are exported to external datafile containing the temperatures, the pressures and the compositions of the pools at each time steps. The estimated formation rates of acids and dissolved salts from fission products are then coupled with these and the equilibrium compositions and the pH values of the pools are calculated with ChemPool. Internally ChemPool uses thermodynamic programming library, ChemApp®, for calculating the equilibrium composition of a thermodynamic system (gas, aqueous water and solids like fission products) by minimizing the Gibbs energy of the system. ChemPool is an easy to use tool for adding simulation of pH chemistry to a MELCOR simulation.

## References

1. Hack, K., Petersen, S., Koukkari, P. and Penttilä, K., "CHEMSHEET an Efficient Worksheet Tool for Thermodynamic Process Simulation", Microstructures, Mechanical Properties and Processes, Bréchet Y., Wiley (Ed.), EUROMAT, Vol. 3, 1999, pp 323-330.