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INFLUENCE OF CORIUM TEMPERATURE, CONCRETE COMPOSITION AND WATER INJECTION TIME ON CONCRETE ABLATION DURING MCCI: NEW INSIGHTS

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ABSTRACT

Molten corium, a mixture of molten nuclear fuel, cladding, thermo-hydraulic and structural elements, can originate in a nuclear plant accident after a reactor core meltdown. This un-cooled corium could penetrate through the reactor pressure vessel and cause concrete ablation via basement melt-through, a process known as Molten Corium Concrete Interaction (MCCI). The MCCI analysis because of its complex nature is still uncertain and needs thorough investigation of various parameters. In this study the use of CORQUENCH simulator is presented to model the molten corium, composition of concrete and heat transfer along with related chemical reactions. Using this modeling technique, the chemical reaction capabilities of CORQUENCH is successfully utilized enabling the modeling of interaction between molten corium and concrete. The developed model is validated against experimental data at PWR and BWR conditions. The results showed that the temperature of corium, composition of concrete and water injection time have a pronounced effect on mitigating ablation and reactor integrity in case of a nuclear accident. In addition, the composition of concrete was found to be the main controlling factor to mitigate ablation. An alternative to concrete is to utilize igneous rock (pyrolite) and this approach could lead to comparatively very low rates of ablation due to its high thermal resistant properties. Furthermore, the injection of water (as a cooling agent) into the reactor cavity should also be optimized to enhance corium quenching to avoid ablation via basement melt-through. The concrete ablation mechanisms during MCCI are very case-dependent on the concrete solidus, liquidus and ablation temperatures, respectively.

KEYWORDS:

Molten Corium; Concrete Ablation; Mitigation Scheme; Corium Temperature; Concrete Composition; Water Injection.
## Nomenclature

### Symbols

- \( A \) = Surface Area enhancement constant
- \( B \) = Temperature dependent constant
- \( c \) = Specific heat (J/kg-K)
- \( g \) = Acceleration due to gravity (m/s\(^2\))
- \( E \) = Activation energy (J/mol)
- \( h \) = Coefficient of heat transfer (W/m\(^2\)-K)
- \( H \) = Height (cm)
- \( j \) = Superficial velocity (cm/s)
- \( k \) = Thermal conductivity (W/m-K)
- \( L \) = Laplace constant
- \( n \) = Concentration (moles)
- \( P \) = System pressure (Mpa)
- \( q \) = Heat flux (W/m\(^2\))
- \( T \) = Temperature (K)
- \( V \) = Molten corium fraction
- \( Q \) = Volumetric heat of decay (W/m\(^3\))

### Greek Letters

- \( \mu \) = Viscosity (kg/m-s)
- \( \rho \) = Density (kg/m\(^3\))
- \( \sigma \) = Surface tension (N/m)
- \( \alpha \) = Coefficient of linear expansion (m/m-K)
- \( \delta \) = Thickness (cm)
- \( \varepsilon \) = Radiation emissivity
- \( \nu \) = Vapor phase

### Subscripts/Superscripts

- \( c \) = Continuous phase
- \( cr \) = Crust
- \( d \) = Dispersed phase
- \( frz \) = Freezing point
- \( g \) = Gas phase
- \( m \) = Molten corium
- \( k \) = solid species
- \( l \) = liquid
- \( r \) = Radial
- \( s \) = Slag
- \( sol \) = Solution state
- \( stef \) = Stefan-Boltzmann constant (5.67×10\(^{-8}\) w/m\(^2\)K\(^4\))
- \( tr \) = Transition
- \( w \) = water

### Abbreviations

- \( MCCI \) = Molten Corium concrete Interaction
- \( BWR \) = Boiling water reactor
- \( PWR \) = Pressurized water reactor
- \( ANL \) = Argonne National Laboratory
- \( SNL \) = Sandia National Laboratory
- \( LCS \) = Limestone /Common Sand Concrete
- \( MACE \) = Melt Attack and Coolability Experiment
1. INTRODUCTION

Tackling the ever-growing energy demand of the world is at the forefront of modern day engineering challenges. Scarcity of water resources around the globe and the limited fossil fuel reserves (Khurshid et al., 2020) has led to a paradigm shift towards alternative energy sources. With the renewable energy, still developing and far from being a reliable and cost-effective source, most of the developing countries are still relying heavily upon the nuclear power generation. The necessity of operating nuclear plants safely over extended periods of time in a cost-effective manner becomes an even bigger challenge as nuclear plants are designed with an operating lifespan of at least 40-50 years; generally operated for even longer periods of times (Cattant et al., 2008). The ageing materials and thermal hydraulic components inside the nuclear plants are constantly put under immense flow-induced-, thermal- and mechanical-fatigue. In case of a severe nuclear accident, the entire reactor core including fuel, cladding material, thermal-hydraulic components and supporting structure could melt and form a mixture called molten corium. This un-cooled corium could penetrate through the reactor pressure vessel and cause concrete ablation via basement melt-through, a process known as Molten Corium Concrete Interaction (MCCI). The MCCI analysis because of its complex nature is still uncertain and needs thorough investigation of various parameters. Since safety is of paramount importance, the nuclear power plants must take necessary action to mitigate the MCCI. Therefore, in this study the effects of corium temperature, composition of concrete and water injection time are looked upon from a practical perspective to mitigate ablation in nuclear power plants.

The characteristics and behavior of molten corium vary due to a number of factors such as time of water injection and the reactor cavity conditions (water filled or dry). The time after which the coolant (water) is introduced into the nuclear reactor controls the depth of ablation, reactor damage and long-term environmental effects. If in case the cavity of the reactor is pre-filled with coolant before the accident, the molten corium after its release will first interact with the coolant and then with the concrete. After the molten corium-coolant interaction, the corium will experience a fragmentation phenomenon and it could break up into debris of different sizes due to various cooling mechanisms that might take place in the reactor. The rate of heat transfer and its area could escalate with the spread of corium debris and produce significant quantity of steam. Thus, heat transferred by the water and its conversion into steam, initiates in the reactor cavity. However, this complex process could lead to explosion (steam) and spike problems that puts the reactor structure integrity at stake. If the corium disintegrates into fragments, the heavy particles could sink to the reactor bottom and form a particle bed (Bonnet et al., 2017; Farmer, 2018).

In order to estimate different mechanisms behind the formation and cooling of the particle bed, it is important to determine the size of particles, their stratification, bed porosity and permeability. It is essential to mention here that the various factors affecting particle bed formation are determined by the rate of its sedimentation and the different conditions controlling the deposition of disintegrated particles. Therefore, the ambiguity increases with the progress of each process. If in case, most of the heat is removed at an early stage, then the mechanism of cooling would become highly uncertain after the formation of the particle bed. Moreover, due to the current level of understanding, it is not possible to consider the uncertainties of this complex process, thus the pre-filled and relative particle bed formation is not considered in this research. During a reactor breach, corium could spread in an uncontrollable manner over the reactor bottom/sidewalls and the MCCI would initiate. In such cases, the ablation of concrete could take place in the early stages of the accident (Bonnet et al., 2017). Therefore, it is important to perform the MCCI calculations for nuclear power plants while the coolant is being introduced into the cavity of the reactor. Depending on the outcomes, the power plant design should have the ability to mitigate MCCI. Nevertheless, this is not possible to determine beforehand partly because of the scale of MCCI which varies depending upon a number of factors such as the cause of the accident, its type and severity, and partly on the different uncertainties, limitations and/or assumptions during the simulation process. Additionally, there is a need of MCCI data and results that are reliable. The objective of this research is to thus develop a model for different strategies of the mitigation of MCCI in real power plants. This research enables development of more robust MCCI mitigation strategies and related safety predictions. The proposed integrated strategy has the capability to model the molten corium concrete interaction with accuracy and reliability.

A lot of work has been done over the years on the nuclear thermal hydraulics and computational efforts to model these for example see Abed and Afgan, 2017; Wu et al., 2017a; Wu et al., 2017b; Bonnet et al., 2017; Wu et al., 2019; Kahil et al., 2019; Benhamadouche et al., 2020; Nguyen et al., 2020; Han et al., 2012; Revelly et al., 2020; D’Auria and Hassan, 2021. However, mitigating measures towards reactor safety and contingency plans have not received the much-needed attention. Thus, a number of researchers have recently performed various researches for nuclear power plants to develop strategies to mitigate MCCI and different factors affecting it. Since early 1980s, various MCCI experiments were performed for post-filled reactor cavity condition such as SWISS, WETCOR, ECOKATS-2, COTELS, MACE and MCCI, COMET-L3 and VULCANO. It is essential to mention that for pre-filled cavities conditions, the experiments were not performed because of steam explosion risk. The SWISS and WETCOR were performed at Sandia.
National Laboratory by Blose et al. (1987) and Blose et al. (1993); COTES by Kato et al. (1999), Nagasaka et al. (1999), Zhdanov et al. (1999), Maruyama et al. (2002). The ECOKATS-2 was experimented by Alsmeyer et al. (2005) in EU. The MACE was executed by Farmer et al. (2000) and (2001) and MCCI by Farmer et al. (2005); Lomperski and Farmer, (2006) and (2009) at Argonne National Laboratory (ANL). The COMET-L3 was performed by Miassoedov et al. (2010) and in VULCANO facility twelve molten corium concrete interaction experiments were performed by Journeau et al. (2012) with prototypic corium composition.

The benchmark study for MCCI was performed by Gencheva et al. (2013) on VVER1000 with different codes. They used the physical models in the codes for the molten corium cooling mechanism and found that the production of molten corium occurred in the post-flooded and dry reactor cavities. For Peach Bottom nuclear power plant, Bixler and Nathan (2013) executed the consequence studies and considered MCCI. Furthermore, Spengler et al. (2014) scaled up the issue of MCCI to reactor scale from a small-scale experiment. Moreover, different analytical computer codes were developed and utilized for analysis. Prediction of the cooling behavior and properties of molten corium are shown in Gardner and Bradley, 1993 (CORCON-Mod3); Cranga et al. 2005 (MAAP and MEDICIS); Bolshov and Strizhov, 2006 (SOCRAT); Spindler et al. 2006 (TOLBIAC-ICB code); Moiseenko et al. 2011; Parozzi et al. 2010 and Polidoro et al. 2013 (CORIMUM-2D); Farmer, 2010 and Farmer, 2018 (CORQUENCH). Additionally, Li and Yamaji, (2016) used the Moving Particle Semi-implicit (MPS) technique to simulate the MCCI experiments. They used the kernel function and the Lagrangian approach to trace the movement of particles in the dispersed phase. Similarly, Chai et al. (2017) performed MCCI numerical simulations based on the MPS method using different types of concretes. Recently, Chen et al. (2019) improved the original MPS methodology by including the explicit pressure calculation; this resulted in reduced computational costs and enhanced computational speeds.

In this study, CORQUENCH (Farmer, 2018) code was used to estimate and stimulate the different phenomena related to MCCI. This code has multi-nodal analysis capability, uses latest developed models including: molten-corium eruption model, molten corium-concrete heat transfer model, water ingestion model and a concrete ablation model. Farmer, (2010 and 2018) derived these models after performing different MCCI experiments. The Melt Attack and Coolability Experiment (MACE) program was executed by Farmer et al. (2000) and (2001) with the purpose to determine the quenching behavior of the corium under conditions analogous to a real nuclear power plant. They anticipated that corium quenching can be fully accomplished by introducing water to the molten corium. However, in a test named M-0, it was observed that a crust appeared on the water-cooled surface of the molten corium. They also determined that this crust blocked the direct contact of water and the molten corium to the reactor side wall. To verify these findings, observe the crust stability at actual conditions and to make the size of experiment similar to a reactor cavity, Farmer, (2010 and 2018) enlarged the experimental scale of M-0 to 120×120×20 cm in another test named M-3b. The MCCI research was initiated in 2002 and completed in 2010 at ANL. The main objective of MCCI research project was to provide the experimental data and to determine the different cooling mechanisms related to molten corium.

The developed MCCI experiments and the analysis of the results showed that the factor that immensely affects the safety of a reactor during the interaction of molten corium and concrete is the axial depth of ablation. Therefore, the ablation depth determined with developed model should be validated with the MCCI experimental data. From different MCCI experiments, CCI-2 and SURC-2 were selected to compare the results of the developed model with the experimental data because these experiments were performed at BWR and PWR conditions, respectively. Fig.1 shows the flowchart for molten corium concrete analysis where the MCCI regulatory requirements are considered to prevent the failure of the containment liner plate. Moreover, the axial depth of ablation was considered as the bench-mark factor for model validation. The analysis model can be effectively used to perform MCCI analysis for nuclear power plants and would help to determine various strategies to mitigate MCCI in actual nuclear power plants. The different results that are obtained from the developed model depends upon the different cooling mechanisms and the parameters used to model the MCCI phenomenon. Therefore, it is important to develop a comprehensive model to mimic MCCI experiments for detailed studies which could determine the different consequences of molten corium and concrete interaction that might occur during and after an actual nuclear core meltdown.

The layout of the current paper is as following. All modelling details related to concrete corium composition, concrete ablation and heat transfer are presented in section 2. The model validation/justification is then given in section 3. This is followed by results and discussions in section 4.
2. MODEL DESCRIPTION AND ANALYSIS

2.1 Modeling concrete and corium composition

The concrete used in nuclear power plants can be of one of the following kinds: limestone-based concrete, silica-based concrete, or basalt-based concrete. Depending upon the concrete aggregate composition, the CO₂ component of concrete has an important influence as it directly participates in the cooling of molten corium during the MCCI phenomenon. During MCCI when the temperature of contacted concrete exceeds 700 °C, limestone decomposes and releases CO₂ gas. This CO₂ helps in dragging the molten corium to the water pool and improves the transfer of heat from the molten corium to the water pool. In CORQUENCH, the properties and composition of the concrete can be specified. It was observed that a concrete with the capability of generating abundant amounts of CO₂ would definitely help in the cooling of molten corium.

The properties and composition of molten corium are the main parameters as they define the temperature, and the sources of heat in the molten corium. These heat sources include, the heat generated by the fission reaction, heat produced by the oxidation of molten corium, and the heat emitted by the chemical reaction between Silicon dioxide and Zirconium. The chemical reactions that are accounted for in the developed model are given in Table 1. This table provides the descriptions of various stoichiometric factors of the various reactions that are required to develop a relationship between the mass flow rate of the oxidizing agents (CO₂, H₂O, and SiO₂ which are released from the concrete into the molten corium) and the amount of metal ingestion. Table 1 also shows the reactions that lead to the formation of oxide. The molten corium energy conservation equation includes the terms of energy source and sink for concrete and overlying atmosphere. The conservation energy equation is given by (Farmer, 2018) as

\[
e = \frac{1}{m} \left\{ -me + \chi_{m,\text{UC}} \cdot m_{\text{dec}} - A_{b} h_{c}(T_{m} - T_{1}) - A_{b} h_{b}(T_{m} - T_{b}) - A_{b} h_{1}(T_{m} - T_{1}) + E_{H_{2}O}(A_{b} m_{b,H_{2}O} + A_{b} m_{s,H_{2}O} + E_{CO_{2}}(A_{b} m_{b,CO_{2}} + A_{b} m_{s,CO_{2}}) + E_{SiO_{2}}(A_{b} m_{b,SO_{2}} + A_{b} m_{s,SO_{2}})) + (1 - \chi_{\text{cng}}) \rho_{\text{con}} e_{\text{cond}}(A_{\eta} \eta_{b} + A_{\eta} \eta_{s} - A_{b} (\eta_{b} + \eta_{s} + \eta_{\text{mix}}) - (\eta_{b} + \eta_{s} + \eta_{\text{mix}}) A_{c} h_{m} + A_{b} m_{\text{ent}} e + m_{\text{core}} e_{\text{corem}} \right\}
\]

Where \( e \) is the melt zone specific enthalpy (J/kg), \( m \) is the mass of \( i^{th} \) constituent present in melt zone, \( \chi \) is the weight fraction, \( A_{b} \) is the base axial surface area (assumed equal to the top surface area), \( A_{s} \) is the radial surface area of melt in contact with the concrete, \( e_{\text{corem}} \) is the specific enthalpy of corium draining from the reactor vessel, \( e_{\text{cond}} \) is the concrete specific enthalpy at the decomposition temperature, \( T_{m} \) is the melt temperature, \( E_{H_{2}O} \) is the reaction heat for metals that are undergoing oxidation by \( H_{2}O \), \( E_{CO_{2}} \) is the reaction heat for metals that are undergoing oxidation by \( CO_{2} \), \( E_{SiO_{2}} \) is the reaction heat for Zr metal undergoing oxidation by \( SiO_{2} \), \( m_{\text{dec}} \) is the melt decay heat level (expressed as W/kg fuel), and \( h \) is the interfacial heat transfer coefficient.

The composition of corium can be estimated by various initial circumstances, including the time of reactor failure, thermal power produced at the time of reactor failure, and the rate of corium oxidation. Moreover, the corium and its phase are controlled by concrete type and mass ablation, thus one needs to utilize the phase behavior relating to the type of concrete used in the reactor. In order to determine the corium decay heat with the CORQUENCH package, three different techniques can be used (1) User-defined corium power density for each layer: particle bed and crust (2) User-defined decay level of heat (3) ANSI/ANS-5.1 function. During the analysis of the experimental data, it was observed that main source of heat generation was the molten corium, this finding of the analysis shows that user-defined gross decay heat should be used. Thus, the heat produced from the particle bed and crust is defined as zero (Kim et al., 2019). However, in real power plants, technique (1) or (3) are usually applied to determine the decay heat that is produced from the molten corium. The various gases produced during concrete decomposition must be modeled along with the reactions between zirconium, silica, chromium, and iron.

During the interaction of molten corium with concrete, the viscosity of the corium is enhanced due to the inclusion of concrete into the corium. For oxidative melts with silica contents, Ramacciotti et al. (2001) proposed the use of Urbain correlation to determine the viscosity of the liquid. However, for solidification range, based on the published data they mentioned that the viscosity cannot be determined by a suspension viscosity model. In this study corium is assumed to consist of distinct oxide and metal phases, each of which is characterized by a solidus and liquidus temperature. The various gases produced during concrete decomposition must be modeled along with the reactions between zirconium, silica, chromium, and iron.

The model expresses the relationship between the mass flow rate of corium with concrete, the viscosity of the corium is enhanced due to the interaction of molten corium with concrete. The viscosity of the corium can be estimated by the models derived by Ishii and Zuber (1979) and Kunitz (1926) models. The corium viscosity defined by Farmer, 2018 reads as

\[
\mu = \mu_{c} \left( 1 - \frac{V_{\text{sol}}}{V_{\text{sol,max}}} \right)^{-2.5V_{\text{sol,max}}(\frac{\mu_{d} + \mu_{c}}{\mu_{d} + \mu_{c}} - 0.84\mu_{d} + \mu_{c})}
\]
\[
\mu = \mu_c \left[ \frac{\frac{1}{2} \nu_{sol}}{1 - \frac{\nu_{sol}}{\nu_{sol,max}}} \right]^{1/2}
\]

(3)

Where \( V_{sol,max} \) is the maximum fraction of the solid phase packing which is utilized to estimate the corium viscosity which is different from the fraction of solid that is used to assess the actual corium solids. Here, \( \mu_c \) is the viscosity of the continuous phase and \( \mu_d \) the viscosity of the dispersed phase which are estimated as

\[
\mu_c = V_{liq,m} \mu_m(T) + V_{liq,o} \mu_o(T)
\]

(4)

\[
\mu_d = V_{sol,m} \mu_m(T_{sol,m}) + V_{sol,o} \mu_o(T_{sol,o})
\]

(5)

It is worth mentioning here that in this study we considered two phases only, continuous (liquid) and dispersed (solid) phases. Thus, as the corium viscosity increases, its transition velocity decreases. Thus, it impedes the transfer of heat by reducing the corium coefficient of convective heat transfer. Similarly, high viscosity corium decreases the amount of molten corium that leaks through the crust vent holes. Thus, cooling efficiency is reduced.

2.2. Modeling concrete ablation

When the molten corium interacts with the cold concrete, a layer of crust is produced. This layer prohibits the transfer of heat. In the early phase, the concrete ablation would not initiate straightaway because the concrete surface temperature is less than its decomposition temperature. However, molten corium continuously generates the decay heat, and therefore the generated layer of crust liquefies again after some time and thus concrete ablation progresses (Cai et al., 2020). During this process, the layer of the crust can fail due to the either the weight applied by the heavy molten corium or the pressure produced by the generated gases during ablation. If the crust fails, the concrete surface is exposed to the molten corium, leading to high rates of ablation. OECD/MCCI has found this sequence of processes in CCI experiments (Farmer, 2018). It is important to mention here that Guillaumé et al. (2009) observed that concrete could even ablate without the formation of the crust. Nevertheless, it is quite challenging to determine the ablation of concrete because the formation and structure of crust changes depending upon the fact that the crust is permeable or impermeable.

The three different options provided by the CORQUENCH package to simulate the ablation of concrete include

1. Concrete dry-out model
2. Concrete dry-out transient model
3. Concrete ablation quasi-steady model. The first two models determine the heat transfer by conduction to the low temperature concrete, whereas, the quasi-steady model uses the traditional heat modeling approach, which does not calculate the heat conduction from the backside of the ablation front. Furthermore, the concrete dry-out model ignores the early transient surface heat-up, but the concrete dry-out transient model defines all the transitory phases. Thus, the best approach is to use the concrete dry-out transient model to estimate the crust growth and its failure mechanisms. For the crust structure, two different schemes can be considered at the corium-concrete boundary condition; either a crust that is considered permeable, leading to the development of a layer of slag at the upper surface of the molten corium or an impermeable crust for which a slag film develops at the bottom. For this latter impermeable case, the slag film interrupts the transfer of heat from the bottom side of the crust to the concrete where the distribution of temperature through the crust is defined as:

\[
T(x) = T_{s,l} - \left( \frac{T_{s,frz} - T_{s,l}}{\delta_s} + \frac{q_{sc}\delta_s}{2k_{sc}} \right) x - \frac{q_{sc}}{2k_{sc}} x^2
\]

(6)

where \( T(x = 0) = T_{s,l} \) and \( T(x = \delta_s) = T_{s,frz} \)

2.3 Heat transfer: molten corium to concrete

To calculate the coefficients of heat transfer from molten corium to concrete, Bradley’s slag film model (Bradley, 1988), gas film model or the Sevón correlation could be utilized. The Bradley’s slag film model is an improved form of Kutateladze-Malenkov’s heat transfer model (Kutateladze and Malenkov, 1978). This model determines the resistance caused by slag film generated in the MCCI phenomena where the coefficient of heat transfer in the axial direction is given as
where \( c_m \) is the molten corium specific heat, \( P \) is the system pressure, \( k_m \) is the molten corium thermal conductivity, \( j_0 \) is the transition velocity, and \( L_\lambda \) is the Laplace constant which reads as

\[
L_\lambda = \frac{\sigma_m}{\sqrt{\vartheta (\rho_m - \rho_g)}}
\]

Here \( \sigma_m \) is the molten surface tension, with \( \rho_m \) and \( \rho_g \) the densities of molten corium and sparging gas, respectively.

Another technique to determine the coefficient of heat transfer from molten corium is the gas film model, CORCON Mod3. This model assumes that a gas film which is generated with the decomposition of concrete covers the entire surface of the concrete. Thus, the transfer of heat between molten corium and the film occurs through radiation and convection. The formation of crust in the molten corium-film is calculated by solving the energy balance equation. The Sevón correlation (Sevón (2008)) is a third technique to determine the coefficient of heat transfer from the molten corium. The technique calculates the superficial gas velocity by using experimental data from MCCI (OECD based). It was observed that the coefficient of radial heat transfer varied depending upon the concrete type. However, the coefficients for axial heat transfer remain the same for both limestone and siliceous concretes. The coefficient for heat transfer in axial direction is a function of the gas superficial velocity which reads as

\[
h_x = 2906 \nu_g + 49
\]

In this study, the gas film model was not used, instead the Bradley and Sevón models were incorporated with the concrete dry-out transient model. Kim et al. (2019) compared these different models including Bradley model, gas film model and the Sevón model. They found that the Bradley model predicted low ablation depths compared to the Sevón heat transfer model. This is because the Bradley model is derived on the basis of experimental data generated through simulated nuclear material. In this model the crust effects at the interface are considered separately with no gas sparging effect. Therefore, the Sevón model is more convincing to use for the calculation of the molten-corium heat transfer coefficient.

2.4 Heat transfer from the upper surface molten corium

The various cooling mechanisms that play a part in molten corium cooling when water is injected include: corium bulk cooling, corium eruption, ingestion of water and crust breach. The corium bulk cooling is a process that takes place before the formation of crust on the surface of corium. The reason is that as soon as various gases are produced, they escalate MCCI and boiling is increased. For such extreme conditions, Farmer et al. (2000) determined the overall rate of heat transfer for the injected water and the radial heat transfer coefficient as

\[
q_{wat} = A \left( \frac{k_e \Delta T_{sat}}{\delta_{fb}} + q_r^{*} \right)
\]

\[
h_r = \sigma_{stef} \varepsilon_m (T_i^2 + T_s^2) (T_i + T_{sat})
\]

where \( \delta_{fb} \) stands for the gas film thickness composed of water vapors and various non-condensable gases produced during corium-concrete interaction and \( \Delta T_{sat} \) is the superheat surface comparative to the water saturation point.

If a stable crust forms, the molten corium remains isolated under the surface. For such a scenario, molten corium can only be cooled if coolant (water) flows through the crust cracks. The rate of heat transfer in this case is initially very small. However, if the crust breaks apart because of the produced gases, the permeability might increase. In such a scenario, the ingestion of water becomes extremely active and thermal boundary layer between the molten corium and the crust becomes thinner. This process can lead to a heat transfer enhancement due to conduction. Lompermj and Farmer, (2006) determined that the overall heat flux from the upper crust surface must decrease below the limits of crust dry-out and is given as
\[ q_{c,\text{dry}}^* \geq k_{t,c} \frac{(T_{t,\text{frz}} + T_{\text{sat}})}{\delta_t} + \left( \frac{\alpha_{t,c} \delta_t}{2} \right) \rho_v h_{1v} \] (12)

It is important to note that the crust permeability has an important effect on the estimation of the heat transfer through the injected water. Since crust permeability measured via experiments varies from case to case, it is thus better to revert to standard models. To determine dry-out limits for the crust, the following models are available. The first one is the Jones model that consists of the user-defined permeability of the crust to calculate the heat flux at dry-out (Jones et al., 1984). The second model is the improved Lister/Epstein model proposed by Lomperski and Farmer, (2006) which reads as

\[ q_{c,\text{dry}}^* = C_{\text{dry}} \left( \frac{\delta t}{2} \right)^{5/13} \left( \frac{h_{\text{crack}}}{\delta t} \right)^{4/13} \left( \frac{\alpha_{c,\text{exp}} [T_{t,\text{frz}} - (T_{\text{sat}} + \frac{\sigma_{t,f}}{\rho_{t,c} \rho_v})]}{\delta t} \right)^{15/13} \] (13)

where \( \sigma_{t,f} \) represents crust tensile strength and \( E_{t,y} \) is the crust elastic modulus.

In the MACE experiments, which used the LCS concrete, eruption of molten corium was observed. The gas generated during MCCS slipped to the upper most part of the created crust, thereby expanding the cracks. With the crack expansion, the molten corium came in direct contact with the injected water, forming a particle bed. This process led to the eruption of molten corium, thereby immensely increasing the heat transfer of water injection. Overall, the eruption of molten corium takes place when decay heat produced by the corium is more than the heat removal from the molten pool. Moreover, when molten corium erupts, its dispersal to the surroundings is estimated based on the assumption that the rate of molten corium entrainment is proportional to volumetric flow rate of the generated gases (Farmer, 2018), which reads as

\[ j_m = K_{\text{ent}} f \] (14)

The proportionality constant \( (K_{\text{ent}}) \) in the Equation (14) can be obtained by one of the three approaches; a user-specified function, a correlation from Ricou–Spalding entrainment rate (Ricou and Spalding, 1961) or via the ANL corium eruption model (Farmer, 2006). The \( K_{\text{ent}} \) in the Ricou–Spalding and corium molten eruption models read respectively as

\[ K_{\text{ent}} = E \left( \frac{\rho_b}{\rho_m} \right)^{1/2} \] Ricou-Spalding Model (15)

\[ K_{\text{ent}} = \frac{n_h N_h}{\rho_m} \] ANL corium eruption model (Farmer, 2006) (16)

where \( N_h \) stands for site density for the crust hole.

The M-3b experiments of Farmer (2018) revealed that both the Ricou–Spalding and ANL model predicted the same ablation depth. In the current study, the ANL corium model was utilized to calculate the corium entrainment coefficient. For this model, the mass flow rate of the corium through the crust vent hole and the amount of heat flux to the water can be determined by (Farmer, 2018) as

\[ m_h = \rho_m \mu_m \frac{\pi d_h^2}{4} = \frac{\pi \rho_m (\rho_{t,c} - \rho_m) d_h^2}{128 \mu_m} \] (17)

\[ q_{e,\text{m,sat}}^* = \rho_m j_m \Delta e_{m,sat} \] (18)

The Lipinski model (Lipinski, 1980) is used to determine the heat flux from the dry-out of the particle bed when it comes in contact with the coolant, given as

\[ q_{\text{bed,dry}}^* = \frac{0.756 \Delta e_{p}}{1 + \left( \frac{\rho_m}{\rho_f} \right)^{1/4}} \left( \frac{\rho_f \rho_{t,c} d_{\text{bed}}^3 h_{\text{bed}}}{\rho_{t,c} d_{\text{bed}}^3 h_{\text{bed}}} \right) \] (19)
On the basis of the CCM ANL experiment performed by Spencer et al. (1994), in the simulations, the particle size is considered as 0.28 cm with a bed porosity of 0.4 cm$^2$.

The FARO test findings obtained by Magallon and Huhtiniemi (2001) are representative of the fuel-coolant interaction experiments. Magallon, (2006) observed that the crust breach will take place with the increase in load after the water injection. In such a case, various cooling mechanisms can take place repeatedly as the molten corium comes in contact with the water. For modeling the formation of the crust top, two methodologies exist in the CORQUENCH package; in the first approach the crust breach is determined by assuming crust anchoring and crack formation, whereas in the second approach a floating crust is assumed. Both these approaches have the same underlying assumptions i.e.

- The transfer of heat throughout the formed crust is quasi-steady state
- The molten corium decay heat is distributed uniformly
- The thermal and physical properties of the crust remain constant

Yet another approach is to ignore the crust anchoring. The MACE experiments performed by Farmer et al. (2000) and (2001) reported that the anchoring of the crust will take place regardless of the size of the cavity, thus the first case is considered to model the crust top. The sizes of cavity in various MACE experiments such as M0, M1b, M3b, M4 were 30 cm$^2$, 50 cm$^2$, 120 cm$^2$, and 50 cm$^2$, respectively. It is important to mention here that due to the injection of water, thick crust could form and bond to the walls of reactor cavity. This crust will be not be stable in the typical 5 ~ 6 m span of most of the reactors. Thus, they would periodically fail, leading to renewed cooling (Farmer, 2018). Lomperksi et al. (2009) obtained the corium crust data and observed that this strength lies in the range of 1-3 MPa. However, when the breach of crust is determined by using the applied stresses on the crust, the anchoring of crust takes place around 180 min. Kim et al. (2019) also estimated that the molten corium will be quenched in about 180 minutes considering that the crust top floats on the surface of the molten corium. This process will lead to a decrease in the heat transfer of water injection and will cause the ablation rate to increase. Therefore, it is important to consider the formation of cracks and breaching of the crust in the model.

3. MODEL VALIDATION/JUSTIFICATION

Modeling the process of ablation is quite difficult and complex as it depends upon a number of factors such as

a) radioactive decay heat
b) molten corium mass flux from a failed reactor
c) chemical reactions between concrete decomposition gases (such as H$_2$O and CO$_2$) and metallic constituents of the molten corium (zirconium, silicon, chromium and iron)
d) chemical reactions between condensed phased zirconium and silicon dioxide
e) transfer of heat to concrete and slag
f) transfer of heat to the surroundings

It is therefore important to validate the developed model against the experimental data. This section of the paper presents the validation of the developed model in CORQUENCH.

3.1 Validation with experimental data in concrete ablation

To validate the capability of the developed model in providing the insights into the concrete ablation, a set of experimental concrete ablation data was selected. In this research, the results of the developed model were compared with two sets of experimental work (1) CCI-2 from OECD/MCCI performed by Farmer et al. (2005) and (2) SURC-2 from NRC-SNL performed by Cupus (1992). The various concrete and corium properties for each of CCI-2 are given in Tables 2 and 3 and for SURC-2 are given in Tables 4 and 5. To match the results of the developed model with experimental data, different parameters were tuned including the coefficient to diffusion, dispersitivity and thermal diffusion.

3.2 CCI-2 from OECD/MCCI

The CCI-2 was part of the OECD/MCCI test, it was performed for a 2-D rectilinear 50 cm square cavity. The concrete was made up of limestone/common sand concrete (LCD) with 400 kgs of total mass of the molten corium at BWR conditions. The test was executed for 300 mins under dry cavity conditions and then waterfloode. Figures 2
through 5 present comparisons of molten corium temperature, location of ablation front and heat flux predictions against the experimental data.

For the CCI-2 experiments, Figs. 2 and 3 present the ablation depth in the axial and the radial directions respectively. Ablation depth was used for the comparisons here since this parameter determines the integrity of the reactor containment. From these figures it can be observed that the abrupt concrete ablation takes place as soon as molten corium interacts with concrete at the beginning of the cycle (during the dry phase). However, the developed model shows that the ablation takes place from zero and increases linearly to 25.4, 22.2 and 20.5 cm respectively for the three tested cases; quasi-steady concrete decomposition model, concrete dry-out model with crust formation, and concrete dry-out model without crust formation. It can also be observed that the results predicted by quasi-steady concrete decomposition model (Case 1) are closest to the experimental data. The rate of decrease in the ablation (reducing slope of the ablation curves both for the experimental and the numerical results) is due to the decrease in heat conduction to concrete as the heat energy is consumed by concrete ablation. Thus, the overall trend is that of a gradual reduction of further concrete ablation for all cases in both the axial and the radial directions. It is also evident form the behavior of all the models shown in Figs. 2 and 3 that the ablation stops after a certain amount of time after the injection of water (at 300 mins).

The top surface heat flux of molten corium is an important parameter, which is shown in Fig. 4. Experimental measurements during the CCI-2 tests and the numerical models all show that the surface heat flux remains almost zero before the injection of water (300 min). In the experiments as soon as water is injected, there is a sharp spike in the surface heat flux which then continues to decrease till it becomes zero again. However, for all the tested models, after the water injection, there is a delayed initial spike in the heat flux at 305 mins, after which it becomes constant at 378 KW/m² till 424 mins. This high prediction of heat flux data causes the discrepancy between CCI-2 data and the predicted model findings as was observed in Figs. 2 and 3. It is speculated that in the numerical simulations after the injection of water, a crust is formed on the surface of molten corium (at 305 minutes). After passing this point, the thickness of the crust increases by the continuous injection of water until the corium is quenched at 424 minutes. As soon as MCCI stops and a safe coolable state is achieved, the trend of the experimental data and the predicted model of ablation depth becomes similar (zero ablation rate) as the total amount of the heat flux is the same, as was observed in Figs. 2 and 3.

Modelled molten corium temperature prediction comparisons with the experimental data of CCI-2 (Farmer, 2018) are shown in Fig. 5. The figure shows an overall good match between experimental and simulation results, especially for the concrete dry-out model with crust formation that gives the best match. It is observed that for the Cases 2 and 3, the molten corium temperature drops promptly till 75 mins before the water is injected. However, for the experimental tests and the Case 1 this behavior was not observed. With the water injection, the experimental measurements show a gradual increase in the corium temperature from 1818 K (at 300 mins) to 1873 K (at 350 mins), after which point it starts to decrease till 1690 K. However, the developed models show that the corium temperature continues to drop after the injection of water at 300 minutes; from 1818 K to 1670 K. These findings are in line with the previous observations when one compares Fig. 4 in conjunction with Fig. 5; the heat flux in the simulations is constant beyond 310 K (Fig. 4) which leads to the continues decrease in temperature (Fig. 5).

3.3 SURC-2 from NRC-SNL

The SURC-2 test is a 1-D cylindrical cavity experiment with 40 cm diameter performed for molten corium concrete interaction. This test was performed at PWR conditions under dry cavity to provide data for the modelling of different thermal-hydraulic processes and various fission products. The SURC-2 was a reactor experiment performed on oxide core material. The SURC differs from the other tests as it is a cylindrical configuration with sidewalls of MgO inserts. The heat source for the molten corium was done with rungs of tungsten susceptor placed at various axial locations inside the experimental vessel. The initial set maximum temperatures and composition of corium for SURC-2 are given in Table 4 with the composition and properties of the concrete basement listed in Table 5. The analysis shows that the composition is basaltic concrete. Figs. 6 to 9 show comparisons of the modelled results against the experimental measurements for molten corium temperature, location of the ablation front, gas superficial velocity and the heat flux for this test case. It can be observed that the predictions of the molten corium temperature in the early stages of the test are slightly different to the experimental measurements, however, the trend is similar (see Fig. 6). It is speculated that the corium temperature would increase with the oxidation of Zirconium and thus the molten corium solidus temperature could increase. It is important to mention here that for the simulations, the core-cladding mixture solidus and liquidus temperatures are taken based on the assumption that the mixture is fully oxidized (UO₂-ZrO₂). Ultimately, the concentration of solid estimated from the Uranium-Zirconium-oxide phase diagram reaches the predicted concentration of solids with the oxidized phase diagram including the effect of the products
formed by concrete decomposition. After reaching to this point, the concentration of the solid decreases with
generation of slag into the molten corium. Thus, the overall results and its affects would decrease if the concentration
of free zirconium in the molten corium is reduced at the initial molten corium concrete interaction that starts ablation.
Modelling molten corium concrete interaction is a complicated process with many unknown and complex phenomena
going on in the whole process. Numerical predictions will thus always show some discrepancies due to the underlying
assumptions of the uncertain and/or unknown physical processes; in the current scenario, discrepancies in the molten
corium temperature predictions in the early phases. However, with the given data and modelling/physical parameter
assumptions, the results show that the molten corium temperature, concentration of ablation and its overall prediction
in the present study are done in a reasonable fashion with an acceptable accuracy.

4. RESULTS AND DISCUSSIONS

An integrated model is developed to simulate the interaction of molten corium and concrete as described in the
previous sections. To determine the validity of the developed model and its results, a detailed sensitivity analysis was
carried out for the molten corium temperature, composition of concrete and water injection time. It should be noted
here that the values used for these described parameters are within the range of typical experimental conditions. The
details of the data for the model analysis are listed in Tables 2-4. The simulations ran for a certain period of time (425
mins) with constant parameters using the dry-out concrete model with crust formation. This model was chosen for the
prediction of changes in the ablation depth, heat flux and the temperature of molten corium as it gave the best overall
match with the experimental data. The developed model was validated with the experimental data of CC1-2 and
SURC-2. According to the modelling results, the initial set maximum temperature of corium plays an important role.
It can be seen from the Fig. 10 that with an increase in the initial set maximum temperature of molten corium both the
ablation rate and the total depth increases. Sensitivity analysis and the validity of the results also show that after the
injection of water, a stable crust is almost always formed on the surface of the molten corium, regardless of the size
of the experimental bed. However, as the bed size increases it loses its mechanical strength. Thus, at a reactor scale, a
breach of crust could occur depending upon the size of the reactor cavity and the mechanism of corium cooling.

4.1. CORIUM TEMPERATURE EFFECT

Fig. 10 shows the effect of molten corium temperature on the depth of concrete ablation. In the current study,
water was injected at 300 minutes. It is evident from the results that the before the water injection (300 minutes),
the ablation depth of concrete increases linearly. It can also be noted that both the ablation depth and the rate of
ablation increase as the temperature of the corium is increased; ablation depth increases from 16.8 cm to 22.2 cm as
the corium temperature is increased from 2,000 K to 2,300 K. However, after the injection of water the ablation rate
decreases to zero. This can be seen by the attained constant plateau of ablation depth around 350 minutes. Interestingly,
the present simulation results show that both the time and the rate of reduction of ablation depth remains the same for
all molten corium temperatures. These results prove that by reducing the temperature of corium, it would be possible to
successfully mitigate concrete ablation and its spread.

The effects of initial set maximum molten corium temperatures on the surface heat flux are shown in Fig. 11. It
can be observed from this figure that before the water injection (at 300 mins), the surface heat flux prediction is
lowest for the highest initial set maximum temperature case, i.e., 2300 K. This low trend of the surface heat flux is
due to the high rate of ablation at this 2300 K temperature. For the other initial set maximum corium temperatures, as
the rate of ablation is low, the heat flux is slightly higher. However, with the injection of water, the ablation stops for
all the cases. This is apparent from the same trend of surface heat flux after 300 mins for all the initial set maximum
temperature cases.

Fig. 12, which presents the thermal behavior of molten corium at different initial set maximum temperatures,
reinforces these findings. It can be observed from this figure that at the highest initial set maximum temperature of
2,300 K, the temperature of molten corium drops linearly until waterflooding (300 minutes). Once again this happens
because of the high rate of ablation. It is reasoned that the exothermic reactions taking place in the reactor during the
MCCI, lead to the production of inflamable gases such as H₂ and CO. It thus becomes very important to determine
the exact initial set maximum temperature as these gases govern the ablation rate and can lead to explosions.

The effect of initial set maximum corium temperature on molten corium viscosity during MCCI is presented in
Fig. 13. After the initial variation in viscosity (before 40 mins) which is due to a difference in the initial set maximum
corium temperatures, all tested cases show a gradual increase which is due to the inclusion of concrete/slag as the
ablation takes place. After about 120 mins all cases show the same trend till the point of water injection (300 mins).
It is thus concluded that higher temperatures favor higher ablation rates which increase the corium viscosity due to the increase in concentration of slag formation.

Figs. 14 and 15 show the production of hydrogen and carbon monoxide at various corium temperature during molten corium concrete interaction. It is important to mention here that the design, concrete composition, corium composition and other parameters were kept constant except the initial set maximum corium temperature which was varied. It is observed from these figures that the temperature has a significant effect on the production of hydrogen and carbon monoxide gases. Both of these gases seem to be produced at an increased rate as the initial set maximum corium temperature is increased. Thus, it is concluded that the temperature of molten corium plays a critical role in the production of these explosive gases and should be controlled to mitigate the effects of molten corium.

### 4.2. CONCRETE COMPOSITION EFFECT

The effects of concrete composition on its ablation in the presence of molten corium was tested at an initial set maximum temperature at 2,150 K. The base case of concrete composition (Case 1) was with limestone/common sand (LCS) concrete. This composition was changed to silica-based concrete (Case 2) and then to Igneous rock (Case 3). The composition of both limestone-based concrete and silica-based concrete was taken from Farmer (2018), CCI-5 and CCI-2, respectively. The composition of igneous rock named pyrolite (Case 3) was taken from Andrault et al. (2011). Andrault et al. (2011) estimated the melting behavior of this rock for chondritic mantle because of related composition. It is important to mention here that all other parameters such as corium temperature, corium mass and boundary conditions were kept constant. It was found that the solidus, liquidus and ablation temperatures played a very important role in the mitigation of concrete ablation as will be shown later. The detailed compositions and properties for all the 3 cases are given in Table 6.

Figs. 16 through 20 show the effects of concrete composition and various parameters. Fig. 16 shows the predicted ablation depth for all the three compositions. It can be observed that for Case 1 (limestone-based concrete) and Case 2 (silica-based concrete), the maximum ablation depth was found to be 20.5 and 22.2 cm respectively. However, for the Case 3 (Igneous rock (pyrolite)), the ablation rate was zero. This is not only due to the inherit material property of this specific rock which has high solidus and liquidus temperatures but also because of the reasons listed below. These findings demonstrate, that the best strategy to control the spread of nuclear radiation in an event of a core meltdown is to use a pool containment made up of material that is non-ablative at high temperatures.

i. The surface heat flux for pyrolite remains very low and there is no peak (heat flux) after the injection of water at 300 minutes as can be observed for LCS and silica-based concrete in Fig. 17.

ii. The generation of hydrogen gas is lowest for pyrolite, with a maximum of 293 moles of hydrogen gas. However, for LCS and Silica based concrete the amount of hydrogen generation is 1,000 and 1,050 moles, respectively as shown in Fig. 18.

iii. Pyrolite during its interaction with molten corium produces zero carbon monoxide and carbon dioxide at shown in Figs. 19 and Fig. 20 respectively. This is because the concentration of carbon in igneous rock is zero. However, LCS and silica-based concrete contains significant percentage of carbon by weight as listed in Table 6.

iv. Pyrolite has high thermal resist properties (solidus temperature of 4,150 K and liquidus temperature of 4,725 K at a core-mantle boundary pressure of 135 GPa. This pressure is too high, thus pyrolite cannot be implemented in an actual reactor but it is still better than concrete). For this Case 3 (Igneous rock), crust forms on the surface of the molten corium which only becomes thicker and stronger with time, leading to a thorough containment of molten corium. Therefore, when water is injected at 300 minutes, it is unable to come in direct contact with the molten core; only interacting with the surface of the crust. Thus, no spike or peak was observed for the surface heat flux for this Case 3 in Fig. 17. Furthermore, for the other cases (1 and 2), the formed crust was thin, weak and unstable. Therefore, after the injection of water, the molten core directly comes in contact with the water leading to the spikes in the surface heat flux as observed in Fig. 17.

v. Additionally, it is important to mention that we kept the initial set maximum temperature of the corium at 2150K and used the compositions of cementing material as shown in Table 6. The suggested material has high thermal resist properties (solidus temperature of 4,150 K and liquidus temperature of 4,725 K). The heat will continuously generate and does not transfer outside. Thus, the corium temperature would increase. However, in this case the corium temperature did not increase to level of 4000 K (ablation temperature) which is approximately double of the initial set temperature of corium. Thus, the suggested material resisted ablation for this specific corium composition.
It can also be observed from Fig. 16 that the ablation is low for Case 1 (LCS-based concrete) compared to Case 2 (silica-based concrete). This is due to the high amounts of CO$_2$ gas generation that is the result of interaction of molten corium with the LCS based concrete (see Fig. 20). The produced CO$_2$ helps in cooling by dragging the molten corium towards the water pool, thereby improving the heat transfer. On the basis of results shown in Figs. 16 to 20, it is suggested to use pyrolite or other materials which have high temperature resist properties. This approach has the capability to reduce concrete ablation and minimize the risk of reactor breach in case of major nuclear accident.

4.3. WATER INJECTION TIME EFFECT

In the previous section, we recommended to utilize concrete with certain composition to mitigate MCCI. However, if the concrete composition cannot be changed then the best possible method to mitigate the MCCI is to inject water into the reactor cavity. The effect of water injection time on the axial depth of ablation is shown in Fig. 21. In this figure the zero minute shows the time at which molten corium comes in contact with the reactor cavity (top of the cold concrete); initiation of the MCCI. Here the time of water injection is described as the amount of time lapsed after the MCCI initiation. To reduce the complexity, we considered that water reached the base of the reactor as soon as it is injected. Thus, it is evident from Fig. 21 that the quenching of molten corium occurred much rapidly if water is injected within 100 mins of breach. In a real accident the reactor damage could increase/elevate to total destruction of the site if the water is not able to reach the base of the reactor in time due to any of the operational problems.

It is evident from the results presented in Figs. 21 through 26 that the time needed to quench the molten corium is controlled by the injection time of water. The plots show the trends of ablation depth, molten corium temperature, surface heat flux and production of gases (such as hydrogen, carbon monoxide and carbon dioxide) of the reactor cavity with different water injection times. When water is introduced into the reactor at 100 mins after the accident, a temporary local ablation depth control is achieved at 6.35 cm (from 100 to 140 mins). However, due to the high temperature of corium the depth of concrete ablation starts increasing again (140 mins till 240 mins) when it finally plateaus off to 10 cm. For the other cases of water injection time (200, 300 and 400 mins) a similar trend was observed but without a local plateau as can be seen in Fig. 21. When one looks at the production of hydrogen, carbon monoxide and carbon dioxide gases in Figs. 22 to 24, it becomes apparent that the longer one waits for the water injection the more these gases will be produced, favoring higher rates of ablation.

Fig. 25 shows the effect of water injection time on the temperature of the molten corium. It can be observed from this figure that temperature of the molten corium immediately drops with the injection of water at various injection times. Though for all injection time trends are similar, the 100 mins injection time trend is somewhat different. One can observe that after the injection of water, the temperature first decreases from 2,000 K (at 100 mins) to 1,650 K (at 140 mins), but then gradually increases (from 140 to 240 mins) to plateau off at 1,800 K. This behavior is completely in line with the ablation trend shown in Fig. 21 where for the 100 mins water injection case, ablation was locally stopped between 100 and 140 mins when the temperature was falling, reinitiated when temperature increased from 140 to 240 mins and then finally plateaued off to 10 cm at 240 mins. Similarly, for the other water injection time cases, 200, 300 and 400 mins, as there was no local increase in temperature, no local ablation plateau was observed. In fact for these cases once the water was injected, the temperature of the corium decreased accompanied with a gradual decrease in the ablation gradient till it plateaued off to a constant value. For a better understanding of these phenomena, the ablation depth periods are superimposed over the corium temperature trends in Fig. 25.

The important factor that should be considered during the concrete ablation after the flooding of reactor cavity is the rate of decrease in surface heat flux of the molten corium. The results shown in Fig. 26 depict that with the injection of water, the surface heat flux spikes, this is most probably due to the water changing its phase and removing immense amounts of heat when it first comes in contact with the hot corium. Once the initial heat is removed the surface heat flux tends to gradually decrease. Similar trends were observed for all cases with different water injection times, 200, 300 and 400 mins. However, the spike (local increase) in the heat flux was more pronounced for the latter cases as the molten corium temperature reached higher due to the delay in the water injection time. The performed sensitivity analysis for flooding the reactor cavity at different water injection times thus provides useful data, which can improve confidence in computations for MCCI mitigation, by providing reliable data through the use of the COREQUENCH simulator.

5. SUMMARY AND CONCLUSIONS

In this study the effect of molten corium on concrete ablation was successfully simulated from a chemical reaction’s perspective. It was shown that the CORQUENCH simulator could be used as an effective tool to predict the risk and safety in the design of a nuclear reactor, and envisage inherit design resilience of a nuclear reactor during
a possible molten corium and concrete interaction (MCCI). It was found that the concrete composition and its properties play a vital role in the MCCI process; where a high temperature corium can cause more damage and high rates of ablation. Comparison of various concrete compositions lead to the conclusion that pyrolite, an igneous rock, is a better candidate for the concrete composition than limestone/common sand concrete (LCS) or silica-based concrete as it shows almost zero ablation. Simulations were also performed to mitigate MCCI, by flooding the reactor cavity with water at various injection times (100, 200, 300 and 400 mins). Significant differences in the ablation depths, surface heat flux and gas production were observed for water injection after 100 mins, compared to the other cases. An earlier water injection leads to lower concrete ablation, low production of gases and overall, more heat removal from the system. Based on this it is concluded that water flooding should be done as soon as possible once a reactor meltdown takes place. This will not only stop the local damage but will also help with the containment of the melt pool breach through MCCI.

**Limitations and Future Work.** One of the limitations of this work is that it does not capture the change in solidus and liquidus temperature of the suggested material with the change in pressure behaviour as a result of the MCCI. This is because of the limited reported data on solidus and liquidus temperature in the literature. In addition, this work used one type of material that is pyrolite at a certain pressure. Therefore, the findings of this study hold for the pressure conditions used in this work, which is more into ablation at high-pressure conditions. For future work, laboratory work will be conducted to further validate the observations from the literature and the numerical work. Furthermore, sensitivity analysis and optimization studies of reactor-scale predictions will be performed.

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Table 1. Chemical reactions (Oxidation) utilized in CORQUENCH (Farmer, 2018)

<table>
<thead>
<tr>
<th>Chemical Reactions (oxidation)</th>
<th>Constituent $i$</th>
<th>$\gamma_i^{SiO_2}$</th>
<th>$\gamma_i^{H_2O}$</th>
<th>$\gamma_i^{CO_2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zr$+2$H$2$O$\rightarrow$ZrO$2$+2H$2$</td>
<td>Zr</td>
<td>$-F_{cond}(1+F_{Si})M_{Zr}$</td>
<td>$-F_{Zr}M_{Zr}$</td>
<td>$-F_{Zr}M_{Zr}$</td>
</tr>
<tr>
<td>Zr$+2$CO$2$→ZrO$2$+2CO</td>
<td>ZrO$2$</td>
<td>$F_{cond}(1+F_{Si})M_{ZrO_2}$</td>
<td>$F_{Zr}M_{ZrO_2}$</td>
<td>$F_{Zr}M_{ZrO_2}$</td>
</tr>
<tr>
<td>Si$+2$H$2$O→SiO$2$+2H$2$</td>
<td>Si</td>
<td>$F_{cond}M_{Si}$</td>
<td>$F_{Si}M_{Si}$</td>
<td>$F_{Si}M_{Si}$</td>
</tr>
<tr>
<td>Si$+2$CO$2$→SiO$2$+2CO</td>
<td>SiO$2$</td>
<td>$-F_{cond}$</td>
<td>$F_{Si}M_{SiO_2}$</td>
<td>$F_{Zr}M_{SiO_2}$</td>
</tr>
<tr>
<td>Zr$+SiO_2→ZrO_2+Si(i)$ $(T\leq2784)$</td>
<td>Cr</td>
<td>0</td>
<td>$2F_{Cr}^{M_{Cr}}$</td>
<td>$2F_{Cr}^{M_{Cr}}$</td>
</tr>
<tr>
<td>Zr$+2$SiO$2→ZrO_2+2SiO(g)(T &gt; 2784)$</td>
<td>Cr$_2$O$_3$</td>
<td>0</td>
<td>$3F_{Cr}^{M_{CrO_3}}$</td>
<td>$3F_{Cr}^{M_{CrO_3}}$</td>
</tr>
<tr>
<td>Fe$+H_2O→FeO+H_2$</td>
<td>Fe</td>
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<td>$F_{Fe}^{M_{FeO}}$</td>
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<tr>
<td>Fe$+CO_2→FeO+CO$</td>
<td>FeO</td>
<td>0</td>
<td>$F_{Fe}^{M_{FeO}}$</td>
<td>$F_{Fe}^{M_{FeO}}$</td>
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Table 2. CCI-2: Composition of concrete and its properties (Farmer, 2018)

<table>
<thead>
<tr>
<th>Composition of concrete (wt. %)</th>
<th>Component</th>
<th>CCI-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$_2$</td>
<td>30.42</td>
<td></td>
</tr>
<tr>
<td>CaO</td>
<td>26.42</td>
<td></td>
</tr>
<tr>
<td>SiO$_2$</td>
<td>22.01</td>
<td></td>
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<tr>
<td>MgO</td>
<td>11.71</td>
<td></td>
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<tr>
<td>H$_2$O</td>
<td>4.46</td>
<td></td>
</tr>
<tr>
<td>Al$_2$O$_3$</td>
<td>2.54</td>
<td></td>
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<tr>
<td>Fe$_2$O$_3$</td>
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<td></td>
</tr>
<tr>
<td>K$_2$O</td>
<td>0.56</td>
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</tr>
<tr>
<td>Na$_2$O</td>
<td>0.32</td>
<td></td>
</tr>
<tr>
<td>TiO$_2$</td>
<td>0.14</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Properties of Concrete</th>
<th>CCI-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{solidus}$ (K)</td>
<td>1393</td>
</tr>
<tr>
<td>$T_{liquidus}$ (K)</td>
<td>1568</td>
</tr>
<tr>
<td>Tablation (K)</td>
<td>1500</td>
</tr>
<tr>
<td>Fraction H$_2$O liberated</td>
<td>1.00</td>
</tr>
<tr>
<td>Fraction CO$_2$ liberated</td>
<td>1.00</td>
</tr>
</tbody>
</table>
Table 3. CCI-2: Composition of corium and its temperature (Farmer, 2018)

<table>
<thead>
<tr>
<th>Composition of corium (kg)</th>
<th>Component</th>
<th>CCI-2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>UO$_2$</td>
<td>242.48</td>
</tr>
<tr>
<td></td>
<td>ZrO$_2$</td>
<td>99.60</td>
</tr>
<tr>
<td></td>
<td>Cr</td>
<td>25.64</td>
</tr>
<tr>
<td></td>
<td>SiO$_2$</td>
<td>13.56</td>
</tr>
<tr>
<td></td>
<td>CaO</td>
<td>12.52</td>
</tr>
<tr>
<td></td>
<td>MgO</td>
<td>4.56</td>
</tr>
<tr>
<td></td>
<td>Al$_2$O$_3$</td>
<td>1.64</td>
</tr>
<tr>
<td></td>
<td>Zr</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>Fe</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>400.0</td>
</tr>
</tbody>
</table>

| Temperature (K)           | Initial set molten corium temperature | 2150 |
|                          | Upper structure temperature             | 750  |

Table 4. SURC-2: Composition of corium and its temperature (Farmer, 2018)

<table>
<thead>
<tr>
<th>Composition of corium (kg)</th>
<th>Component</th>
<th>SURC-2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>UO$_2$</td>
<td>140.9</td>
</tr>
<tr>
<td></td>
<td>ZrO$_2$</td>
<td>46.1</td>
</tr>
<tr>
<td></td>
<td>Zr</td>
<td>16.9</td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>203.9</td>
</tr>
</tbody>
</table>

| Temperature (K)           | Initial set molten corium temperature | 2600 |
|                          | Upper structure temperature             | 900  |

Table 5. SURC-2: Composition of concrete and its properties (Farmer, 2018)

<table>
<thead>
<tr>
<th>Composition of concrete (wt. %)</th>
<th>Component</th>
<th>SURC-2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SiO$_2$</td>
<td>57.90</td>
</tr>
<tr>
<td></td>
<td>CaO</td>
<td>13.80</td>
</tr>
<tr>
<td></td>
<td>Al$_2$O$_3$</td>
<td>7.20</td>
</tr>
<tr>
<td></td>
<td>H$_2$O</td>
<td>5.00</td>
</tr>
<tr>
<td></td>
<td>Fe$_2$O$_3$</td>
<td>4.40</td>
</tr>
<tr>
<td></td>
<td>MgO</td>
<td>4.00</td>
</tr>
<tr>
<td></td>
<td>K$_2$O</td>
<td>3.80</td>
</tr>
<tr>
<td></td>
<td>CO$_2$</td>
<td>1.50</td>
</tr>
<tr>
<td></td>
<td>Na$_2$O</td>
<td>1.40</td>
</tr>
<tr>
<td></td>
<td>TiO$_2$</td>
<td>0.80</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Properties of Concrete</th>
<th>T$_{\text{solidus}}$ (K)</th>
<th>1350</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>T$_{\text{liquidus}}$ (K)</td>
<td>1650</td>
</tr>
<tr>
<td></td>
<td>T$_{\text{ablation}}$ (K)</td>
<td>1500</td>
</tr>
<tr>
<td></td>
<td>Fraction H$_2$O liberated</td>
<td>0.68</td>
</tr>
<tr>
<td></td>
<td>Fraction CO$_2$ liberated</td>
<td>1.00</td>
</tr>
</tbody>
</table>
### Table 6. Composition of various concrete

<table>
<thead>
<tr>
<th>Component</th>
<th>LCS</th>
<th>Silica</th>
<th>Pyrolite</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO₂</td>
<td>22.01</td>
<td>57.90</td>
<td>45.1</td>
</tr>
<tr>
<td>CaO</td>
<td>26.42</td>
<td>13.80</td>
<td>3.1</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>2.54</td>
<td>7.20</td>
<td>3.3</td>
</tr>
<tr>
<td>MgO</td>
<td>11.71</td>
<td>4.00</td>
<td>38.1</td>
</tr>
<tr>
<td>K₂O</td>
<td>0.56</td>
<td>3.80</td>
<td>--</td>
</tr>
<tr>
<td>Na₂O</td>
<td>0.32</td>
<td>1.40</td>
<td>--</td>
</tr>
<tr>
<td>TiO₂</td>
<td>0.14</td>
<td>0.80</td>
<td>--</td>
</tr>
<tr>
<td>H₂O</td>
<td>4.46</td>
<td>5.00</td>
<td>0.25</td>
</tr>
<tr>
<td>CO₂</td>
<td>30.42</td>
<td>1.50</td>
<td>--</td>
</tr>
<tr>
<td>Fe₂O₃</td>
<td>1.42</td>
<td>4.40</td>
<td>--</td>
</tr>
<tr>
<td>FeO</td>
<td>--</td>
<td>--</td>
<td>8.0</td>
</tr>
</tbody>
</table>

### Properties of Concrete

<table>
<thead>
<tr>
<th>Property</th>
<th>LCS</th>
<th>Silica</th>
<th>Pyrolite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tₗ(liquidus) (K)</td>
<td>1568</td>
<td>1523</td>
<td>4725</td>
</tr>
<tr>
<td>Tₗ(liquidus) (K)</td>
<td>1500</td>
<td>1450</td>
<td>4400</td>
</tr>
<tr>
<td>Fraction H₂O liberated</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Fraction CO₂ liberated</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>
Fig. 1 Flowchart for molten corium concrete interaction analysis

Fig. 2 Comparison of axial ablation depth experimental data (CCI-2) with model prediction
Fig. 3 Comparison of radial ablation depth experimental data (CCI-2) with model prediction

Fig. 4 Comparison of surface heat flux experimental data (CCI-2) with model prediction
Fig. 5 Comparison of molten corium temperature experimental data (CCI-2) with model prediction

Fig. 6 Comparison of molten corium temperature experimental data (SURC-2) with model prediction
Fig. 7 Comparison of location of ablation front experimental data (SURC-2) with model prediction

Fig. 8 Comparison of Gas superficial velocity experimental data (SURC-2) with model prediction
Fig. 9 Comparison of heat flux experiments data (SURC-2) with model prediction

Fig. 10 Effect of corium temperature on ablation depth during molten corium concrete interaction
Fig. 11 Effect of corium temperature on surface heat flux during molten corium concrete interaction

Fig. 12 Effect of corium temperature on thermal behavior of molten corium during molten corium concrete interaction
Fig. 13 Effect of corium temperature on viscosity of molten corium during molten corium concrete interaction

Fig. 14 Effect of corium temperature on hydrogen production during molten corium concrete interaction
Fig. 15 Effect of corium temperature on carbon monoxide production during molten corium concrete interaction

![Graph showing carbon monoxide production vs. time for different corium temperatures.]

- 2000 K
- 2050 K
- 2150 K
- 2200 K
- 2250 K
- 2300 K

Injection time: 300 min

Fig. 16 Effect of concrete composition on ablation depth during molten corium concrete interaction

![Graph showing ablation depth vs. time for different concrete compositions.]

- Case 1: LCS based
- Case 2: Silica Based
- Case 3: Igneous rock

Injection time: 300 min
Fig. 17 Effect of concrete composition on surface heat flux during molten corium concrete interaction.

Fig. 18 Effect of concrete composition on hydrogen gas production during molten corium concrete interaction.
Fig. 19 Effect of concrete composition on carbon monoxide (CO) gas production during molten corium concrete interaction

Fig. 20 Effect of concrete composition on carbon dioxide (CO$_2$) gas production during molten corium concrete interaction
Fig. 21 Effect of water injection time on concrete ablation depth during molten corium concrete interaction

Fig. 22 Effect of water injection time on hydrogen (H₂) production during molten corium concrete interaction
Fig. 23 Effect of water injection time on carbon monoxide (CO) production during molten corium concrete interaction

Fig. 24 Effect of water injection time on carbon dioxide (CO₂) production during molten corium concrete interaction
Fig. 25 Effect of water injection time on molten corium temperature during molten corium concrete interaction

Fig. 26 Effect of water injection time on surface heat flux during molten corium concrete interaction