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**MODELLING THE INTERACTION OF A MOLTEN SEAL AND SOLID
PARTICLES USING SPH AND DEM SIMULATIONS: APPLICATION
FOR A PASSIVE NEW SCRAM SYSTEM FOR LMR**

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Abstract

A new shutdown system that does not rely on absorber rods, is being developed at SCK.CEN and UCL for application in Liquid Metal Reactors (LMR). The system consists of tubes filled with absorber particles. During normal operation, these particles are kept above the active core by means of a metallic melt seal. In case of an accident, the system is activated by the temperature increase in the coolant. This leads to melting of the metal seal, releasing the absorber particles into the core. The resulting flow of the particles has been studied both experimentally, and with Discrete Element Method (DEM) simulations. This paper focusses on the second important aspect of the safety system, being the melting and flowing of the metallic seal in interaction with the solid absorber particles moving through the molten seal.

Introduction

Because GEN IV reactors are designed to be safer than currently existing reactors, also the ability to shut down the chain reaction must be more reliable than in currently existing reactors. In PWR reactors there are two completely independent methods of shutting down the reactor. The first method is the insertion of safety and control bars by means of gravitation. The second method is the dilution of the neutron absorbing boric acid into the primary water. For liquid metal cooled GEN IV reactors this second method cannot be used because there are no liquid absorbers that can be diluted in liquid metal, and cleaning the liquid metal after a scram would be very expensive.

The purpose of this paper is presenting an alternative for the dilution of a neutron absorber into the primary coolant that can be used in a reactor cooled with liquid metal.

For safety reasons, the second method, also called secondary scram system, has to be as diverse as possible with respect to the primary system in order to reduce the probability for common cause failure modes. This includes that the activation signal for the secondary scram system cannot be shared with the primary system. The secondary system needs thus to be self-actuating, meaning that it does not require an external signal to activate. Since the primary scram system is already two or three times redundant, the common cause failure mode of an absence of the scram signal is already dominant. Adding a third system that also depends on the scram signal would not increase the reliability any further. Under normal circumstances

the primary scram system will protect the reactor core. It is not desirable that when the primary scram system activates as expected, that the secondary scram system also activates. The secondary scram system must therefore be acting fast enough to protect the reactor core, but slow enough to give the primary scram system time to work. Several existing concepts have already been proposed, and an overview can be found in [1].

1. Presented Concept.

The concept that is presented in this paper aims at combining the strong points of the currently existing concepts. The presented concept is shown in Figure 1. It consists of a tube with the same diameter as a fuel pin. In every fuel assembly such a tube is placed in the central position. The tube is divided into two sections by means of an aluminum seal. In the upper region, above the active core, neutron absorbing boron carbide particles are placed. In case of overpower and loss of coolant transients the seal will melt. The absorber balls are then no longer supported and fall down into the active core region and insert a large negative reactivity. The time available to do a scram before the reactor suffers damage depends very much on the type of transient. Also the time needed to melt the seal depends on the type of transient. Therefore it will have to be verified for all transients that the reactor is effectively protected by the secondary scram system. A solid absorber was selected here because liquid absorbing materials are rare and their negative reactivity effect is much lower compared to solid absorbers such as tantalum and boron carbide. A solid absorber has however the disadvantage that the flow of solid particles is not as well understood as the flow of liquids. Therefore the absorber particle flow study is an important aspect of study for this concept.

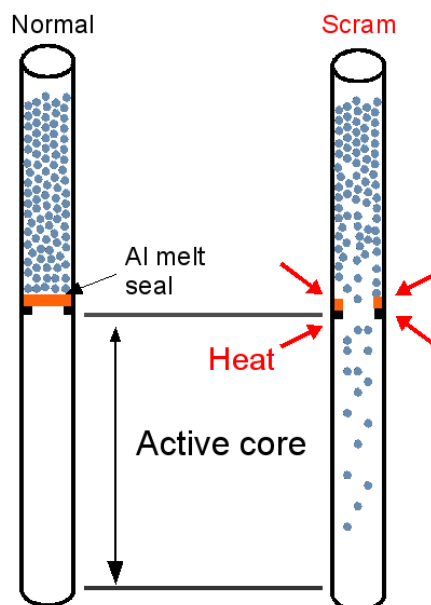


Figure 1: Conceptual drawing of the proposed concept.

The concept is self-actuating but it is not resettable. Because this system is placed in every assembly it has a distributed character similar to the dissolution of boric acid. Due to the flow like behaviour of the absorber balls, it is less prone to failure due to channel

deformation/blocking than the absorber rods even though this issue has to be investigated. Estimations of the neutronic impact and the reactivity worth of the scram system on the XT-ADS core have been done[2]. Several absorber materials have been considered, however the most efficient material proved to be 90% enriched Boron Carbide.

Understanding the particle flow was a first priority in assessing the feasibility of this safety system. Experiments using high speed camera optical flow measurements and simulation using the Discrete Element Method (DEM) have been done[2]. This work is still ongoing and this paper focusses on the simulation of the melting of the aluminum seal and the consequential particle flow that interacts with the molten aluminum. First an overview of the required algorithms is given, followed by some validation results and finally some preliminary combined results.

2. Simulation Requirements.

The interactions of the liquid metal seal with the particles that pass through will be vital to determine whether or not the secondary scram system will work reliably under all circumstances, therefore complete understanding of the entire process is desired. This section describes the algorithms used to simulate the entire process. First of all the particle flow is described by the DEM approach, a method where every individual absorber particle is simulated accurately. Next, the seal is simulated both in solid as well in solid state by the Smoothed Particle Hydrodynamics (SPH) [3] method. This is a particle based mesh-less method. The liquid is represented by individual particles, and properties of the liquid in between the particles can be estimated by using an interpolation method. Using a particle based method has two significant advantages over a classical mesh-based CFD computation. Firstly representing a free surface flow such as the melting of the seal is a problem that is very well suited for the SPH method[3]. A second advantage is that interaction between the seal and the particle can be done in a very natural way due to fact that they are both represented by particles. The regular SPH model has been extended by a heat conduction equation to model the heat transfer from the liquid metal coolant at the boundary of the tube, towards the melt seal.

2.1 Discrete Element Method Simulation.

In order to be able to predict the absorber particle flow the Discrete Element Method (DEM) is used [4]. DEM is a numerical technique used for modeling the motion of colliding objects. The method is summarized in Figure 2. After the problem is initialized with the starting positions and velocities of the particles, the simulation loop can start.

The first step in this loop is to determine which particles are in contact with each other and how deep they penetrate each other. The next step consists of calculating the contact forces for each particle starting from the given penetration of the other particles in the considered particle. The Kono-Kuwabara-Hertz [5] model is used to give a relation between the amount of penetration and the contact force. The normal force in this contact model is a function of the normal penetration u_n [m] and the normal penetration velocity $\dot{u}_n$ [m/s]. The normal penetration is the amount of overlap between the two particles in that time step projected on the normal of the contact surface. In case of two spheres, the normal of the contact surface is the vector connecting the two centers of the spheres. The normal contact force is thus given by:

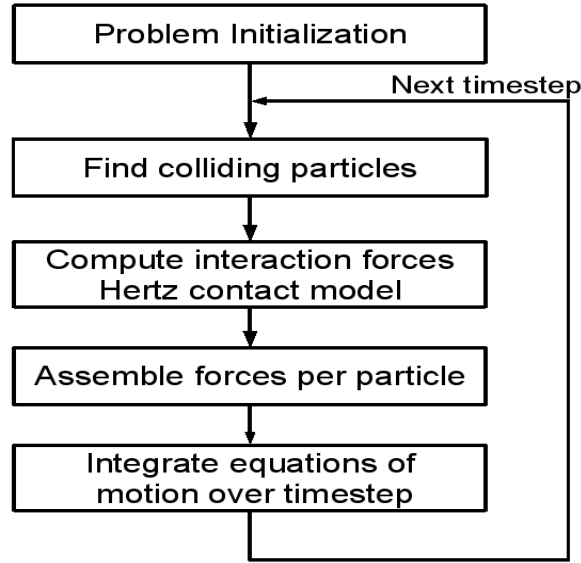


Figure 2: Schematic representation of the DEM algorithm

$$f_n = k \cdot \sqrt{r_{eff}} \cdot u_n (u_n - A \cdot \dot{u}_n) \quad (1)$$

$$r_{eff} = \frac{r_1 \cdot r_2}{r_1 + r_2} \quad (2)$$

where k is the contact stiffness [$\text{N/m}^{5/2}$], A is the viscoelastic damping coefficient [$1/\text{s}$] and r_1 and r_2 are the radii of respectively particle 1 and 2 taking part in the collision. For the interaction between the wall and the particles, the same Kono-Kuwabara-Hertz model is used. Tangential forces could be modeled analogously to normal forces however since bodies can slide against each other the model is extended with a friction law. The magnitude of the tangential force f_t is given by:

$$f_t = -\min(k_t \cdot u_t + A \dot{u}_t, \mu f_n) \quad (3)$$

Where u_t is the tangential penetration, $\dot{u}_t$ the tangential penetration velocity, k_t the tangential stiffness, which has been assumed identical to the normal stiffness, also the viscoelastic damping coefficient A has been assumed identical. The friction factor μ has in reality two values. One 'static' friction factor when the two bodies do not slide over each other and one 'dynamic' friction factor when the two bodies slide over each other. In general the dynamic friction factor is lower than the static friction factor.

The next step is to sum all forces working on a particle and combine them into one force acting on the center of gravity and one moment.

The final step is to integrate these forces to new positional and rotational velocities of the particles and integrate the positional and rotational velocities to respectively new positions and orientations using Newtons motion laws.

The DEM simulations are done using the existing but adapted “DEMeter” [6] software developed at the Katholieke Universiteit Leuven (KUL).

It is important that the simulation software can accurately simulate blocking flows. This might seem like a trivial requirement, however most implementations of the DEM method use spherical particles as elementary particles. They have the advantage that they are very simple and can therefore be processed very quickly. However, because perfect spheres have no resistance to rolling, and therefore can always “roll” loose no matter how high the friction factor is.

The approach taken here is to use a combination of two simple spheres as elementary particles in the simulation with a small offset in their centre point. The two spheres form together a single rigid body as shown exaggerated in Figure 3. The advantage is that the computationally simple spheres can still be used while the rotational movement is prevented in a single direction.

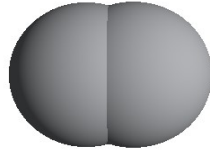


Figure 3: "Double Sphere" particles used in the simulation that have a resistance against rolling in a single direction.

2.2 Liquid/Solid Seal Smoothed Particle Hydrodynamics formulation

The liquid seal is simulated using the Smoothed Particle Hydrodynamics (SPH) method [3]. The SPH equations are obtained from the continuum equations of a liquid by interpolating from a set of points. The interpolation is done using interpolation kernels, which are analytic functions which can be differentiated without a grid. The SPH equations describe the motion of the points which can be thought of as particles.

The simulation scheme is very similar to the DEM scheme, except that no longer penetrations, but distances are computed between the SPH particles.

The momentum equation for particle *a* becomes:

$$\frac{dv_a}{dt} = - \sum m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \Pi_{ab} \right) \nabla_a W_{ab} + F_a \quad (4)$$

With *P* the pressure, *m* the mass, *v* the velocity, ρ the density of particles, F_a is a body force working on particle “a”, in our case gravity. Π_{ab} represents the bulk and shear friction term. W_{ab} is the interpolation kernel function of the distance between the two particles, and ∇_a denotes the gradient of the kernel taken with respect to the coordinates of particle “a”.

For free surface flows where the density drops discontinuously at the interface, the rate of change in the density is calculated rather than the density itself. Starting from the continuity equation:

$$\frac{d\rho}{dt} = -\nabla \cdot (\rho \mathbf{v}) + \mathbf{v} \cdot \nabla \rho \quad (5)$$

Using the SPH interpolation kernels for the right hand side, the rate of change of the density of particle a becomes:

$$\frac{d\rho_a}{dt} = \sum m_b (\mathbf{v}_a - \mathbf{v}_b) \cdot \nabla_a W_{ab} \quad (6)$$

The density of the particles is then updated by integrating (6) over time. Surface tension is not implemented yet but several possible implementations [7] exist and can be added when required.

The implementation of these equations in the DEMeter program have been successfully validated against a standard literature reference case [3] where a drop of water is compressed.

For the solid seal a simple spring damper model is used. When the particles become solid the distance between them is stored as reference distance and following equation is used to model the solid behaviour:

$$F_a = -k(|ab| - |ab|_{ref}) - A \cdot \mathbf{v}_{ab} \quad (7)$$

Where $|ab|$ is the distance between particle “a” and “b” and $|ab|_{ref}$ the reference distance. The stiffness is determined by k, and A is a viscous damping factor.

It is clear that this model will not yield a very accurate description of the mechanical properties of the metal seal, since k and A are not related to a physical parameter. However the function of the solid seal is only to keep the particles in their initial position, with a very small mechanical loading, so the exact amount of bending of the seal is not relevant for this simulation.

2.3 Solid particle interaction with molten seal.

The solid particles interact both mechanically as well as by exchanging heat with the seal. The colder particles might cool down the seal again and re-solidify it when passing through the seal causing a particle blockage.

For the mechanical interaction a simple truncated Lennard-Jones repulsion barrier is used. If necessary this model can be expanded with a more accurate model that also takes into account the possible cohesion between the absorber particles and the molten aluminum. However initial experiments have shown that cohesion between the molten aluminum and the particles is very low.

The thermal interaction of the absorber particles with the seal is computed in the same way as for SPH seal particles using the formulation given in section 2.4

2.4 Smoothed Particle Hydrodynamics Energy Equation.

Because the heat conduction equation involves second derivatives it is necessary to choose an SPH form with care. If this is not done, the disorder that often occurs with SPH particles in a problem involving motion will result in second derivatives with large errors. The following formulation[8] is therefore used:

$$\frac{dE}{dt} = \sum \frac{m_b}{\rho_a \rho_b} \frac{4 \cdot \kappa_a \kappa_b}{(\kappa_a + \kappa_b)} (T_a - T_b) F_{ab} \quad (8)$$

With:

$$rF(r, h) = \nabla W(r, h) \quad (9)$$

Where $\nabla W(r, h)$ is the gradient of the interpolation kernel, r is the distance between the two particles, h the interpolation length, κ the thermal diffusivity, ρ the density, T the temperature and m the mass of a particle. This form is shown[9] to be insensitive to discontinuities of up to 10^3 in the thermal diffusivity.

To close the set of equations we still need an equation of state relating the energy to the temperature of the liquid. For alloys or non-pure metals the equation of state used is:

$$LF = \frac{T - T_s}{T_l - T_s} \quad (10)$$

$$E = LF \cdot L + C_p \cdot T \quad (11)$$

Where LF is the liquid fraction or the mass of the liquid phase, divided by the total mass, T_s the solidification temperature, T_l the liquidification temperature, L the latent heat of melting/solidification.

In order to verify the implementation of the SPH energy transport equation, the simulation results for a simple case have been compared to the analytical solution. This test case is the “quenching” of a cylinder. This transient heat conduction problem has an analytical solution given by:

$$T(t, r) = \frac{2T_0}{b} \sum \frac{J_0(\lambda_i)}{\lambda_i J_1(\lambda_i b)} e^{-\alpha \lambda_i^2 t} \quad (12)$$

Where T_0 is the initial temperature, b the radius of the cylinder, α the diffusivity and λ_i the solutions of the equation:

$$J_0\left(\frac{x}{b}\right) = 0 \quad (13)$$

For a cylinder with a radius of 3mm and an initial temperature of 200°C the evolution of the temperature is shown in Figure 4 in the solid line. The solution of the SPH energy equation is also plotted in Figure 4 as dots. As illustrated the agreement is very good between the analytical solution and the SPH method.

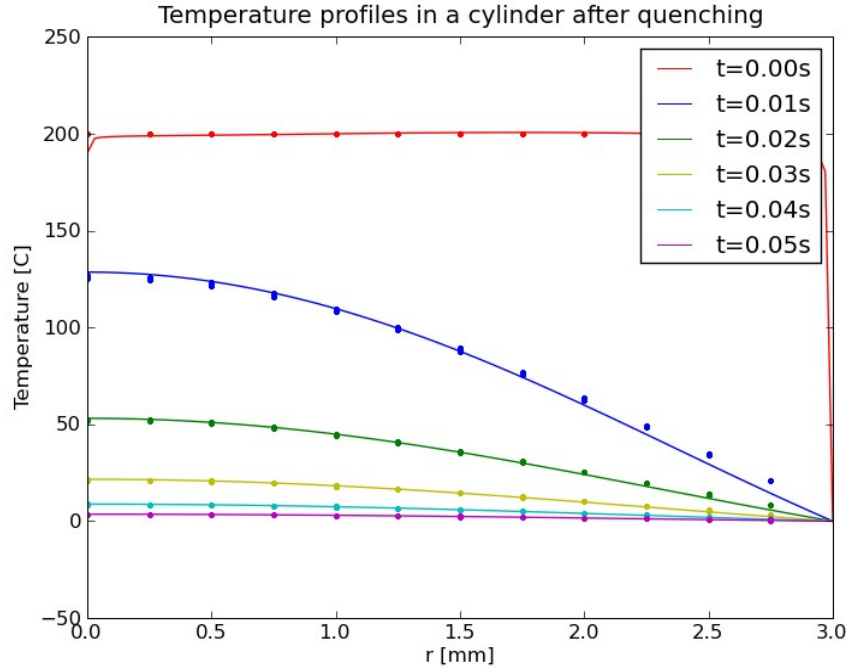


Figure 4: Temperature evolution in quenched cylinder as a function of distance from the center for different times.

3. Results

With the presented simulation tools a simulation of the melting seal alone, without any solid particles has been done using 40 000 liquid particles in a cone shape of 6mm outer diameter and a height of 2mm. Two different cases are shown in Figure 5 and Figure 6. In the first case (Figure 5) the seal is initially at 200°C, quite far from the melting temperature range which is between 650°C and 690°C. The wall has a constant temperature of 1000°C. It can be seen that the edges of the seal start to melt first, starting to flow and fall down under the influence of gravity. Because of the seal deformation, the heat conduction cross section with the wall decreases and the seal partially re-solidifies during drop down. When the seal releases completely, it is however fully liquid. However the original shape of the seal is still recognizable.

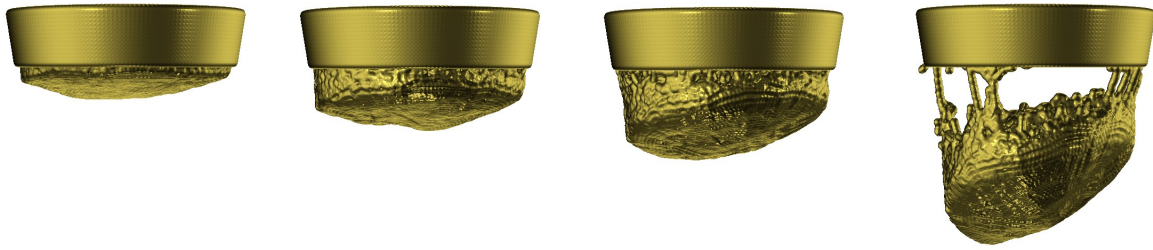


Figure 5: Seal melt with initial temperature at 200°C

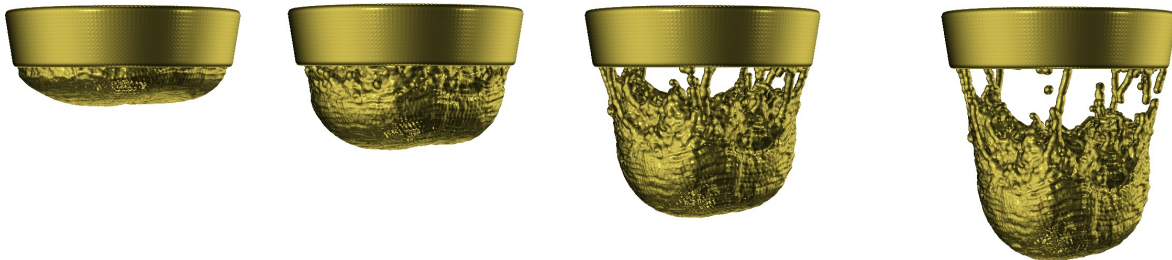


Figure 6: Seal melt with initial temperature at 600°C

The second case shows an aluminum seal with an initial temperature of 600°C, and also a wall temperature of 1000°C. In this case heat conduction is fast enough to completely melt the seal before any significant drop of the seal occurs. The flow pattern has a more parabolic shape.

Finally a complete simulation including the absorber particles using a 6mm tube filled up to 0.1m with 10 000 particles with a diameter of 0.5mm and 40 000 liquid particles is shown in Figure 7. The solid ring at the end of the tube that remains stationary during the entire simulation are the boundary SPH particles that represent the solid wall.

Unfortunately it is very hard to qualitatively match this simulation to an experiment due to the difficulties to obtain numerical experimental data. In the future an experimental verification will be done by filming an identical experiment and performing an optical tracking method and visually compare the experiment to the simulation.

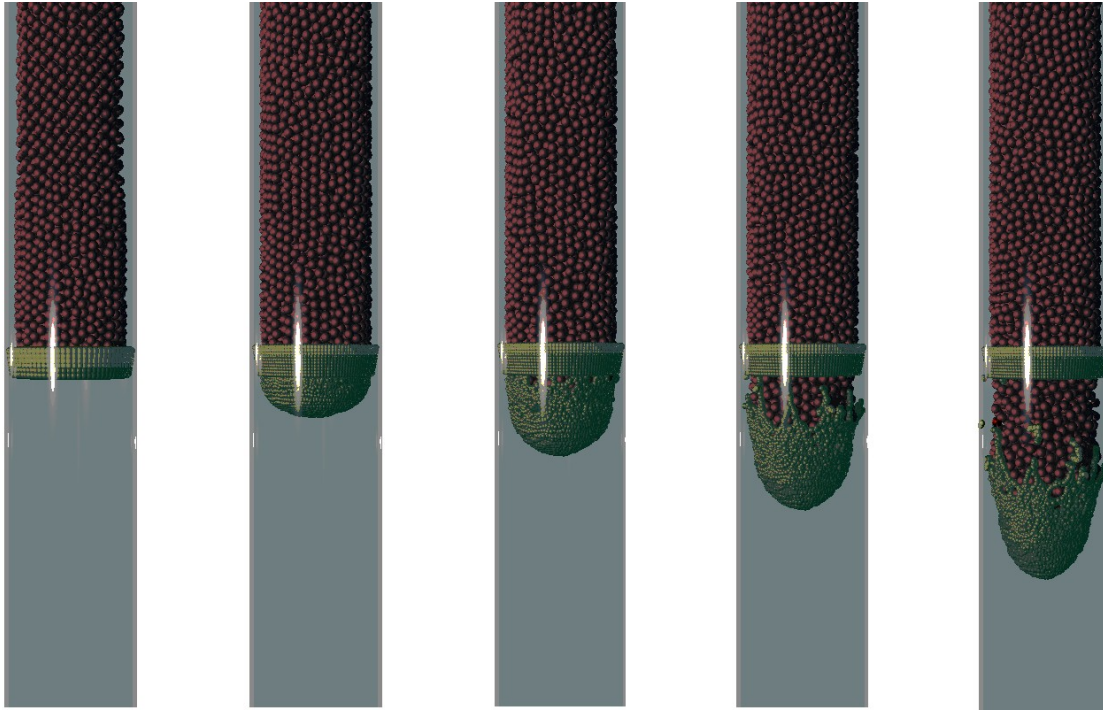


Figure 7: Fast melting seal, with absorber particles interaction.:

4. Conclusion

In this paper the challenges in simulating a new concept for a secondary scram system for liquid metal cooled nuclear reactors have been outlined. The system consists out of a tube filled with absorber particles that are kept above the core by means of melt seal. In case of an accident the temperature of the melt seal will increase up to the point where it melts, releasing the particles in the core. It is of primary concern that the particles do not block, neither when flowing alone in the tube, or when in contact with the, partially, molten seal. The tools to simulate the particles, seal, and interaction between the seal and the particles have been presented. Although not every tool has been fully validated yet, some preliminary simulations of the melting seal and a melting seal interacting with the absorber particles have been demonstrated. Further validation, of the tool, and more in particular the absorber particle simulation and the interaction between the particles and the molten seal, are needed. Experiments are planned to validate these last issues. In the near future, when validations will be completed, sensitivity studies will be performed in order to check the effect of the seal shape and size together with the particle size and shape distribution. Finally the full scale apparatus of a single SCRAM-pin will be simulated.

5. References

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