A lumped parameter modelling of particle generation from Na-pool fires in SFR containments

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ABSTRACT

Modelling of sodium-evaporation and formation of sodium-oxide aerosols from a sodium-pool fire is of fundamental importance for the assessing of the radiological consequences in Sodium-cooled Fast Reactors severe accidents. This paper summarizes the derivation of a simple model to estimate the amount and size of particles being generated from Na-pool fires and its performance assessment, once implemented in an integral severe accident tool (ASTEC-Na), against available large-scale separate effect tests. The model has been transposed in analytical correlations which implementation in lumped-parameter severe accident codes is straightforward. According to the comparisons to data set, the correlations do not adversely impact the code estimates with respect to other more empirical alternative approaches and, in addition, the correlations remove any need of user-defined ad-hoc parameters in the input deck concerning Na-based particles behaviour, as other alternates do. Regarding code behaviour, the model predictions yield the same order of magnitude both in terms of suspended aerosol concentration and diameter as data and capture the reliable measured data trends.

1. Introduction

In case of a severe accident in a Sodium Fast Reactor (SFR), sodium-based particles may be considered as key carriers of the radiological and chemical threat of any potential release to the environment. Their formation from sodium (Na) pool and/or spray fires strongly depends on processes such as sodium vaporization, chemical reactions with the surrounding gas, nucleation/condensation and primary particle agglomeration. Therefore, a full-scope risk assessment of SFRs would require analytical tools in which a suitable modelling of Na-based particle generation is properly accounted for, which points to the need to build a multidisciplinary model coupling thermal hydraulics, chemical reactivity of Na species and compounds and particle dynamics (Yamaguchi and Tajima, 2009). The final outcomes of any Na-based aerosol generation model are particle concentration, size and composition.

Since the early 70s last century, Na burning and Na-based aerosol behaviour and their chemical composition have been the subject of experimental research projects conducted in facilities like PLUTON (Lhiaubet et al., 1990) and JUPITER (Malet et al., 1990) in France,

CSTF in the USA (Hilliard et al., 1977, 1979; McCormack et al., 1978; Souto et al., 1994), FAUNA in Germany (Cherdron et al., 1985, 1990; Cherdron and Jordan, 1980, 1983) and ATF in India (Baskaran et al., 2011; Subramanian et al., 2009; Subramanian and Baskaran, 2007). As for pool-fire modelling, Beiriger et al. (1973) achieved a major milestone in the field by developing the SOFIRE code, a tool focused on fire energetics to model the whole SFR severe accident scenario by assuming that Na−O₂ reactions take place on the pool surface (i.e., surface approach). Later on, Sagae and Suzuoki (1985), inspired by Newman (1983), developed an alternative model based on Na diffusion to the gas atmosphere from a hot pool (over 800 °C) and its subsequent reactions of Na and O₂ in gas phase (flame sheet approach). Miyake et al. (1991), Lee and Choi (1997), or more recently Yamaguchi and Tajima (2003) or Takata et al. (2003) included the vapour-phase sodium-combustion modelling in several combustion codes (SPM, SOPA, SPHINCS or AQUA-SF code respectively).

The above mentioned computer codes have mostly focused on pool-fire energetics and thermal-hydraulics (Murata et al., 1993) so that particle modelling has received much less attention and usually built on major hypotheses not thoroughly proved. The SOFIRE code, for
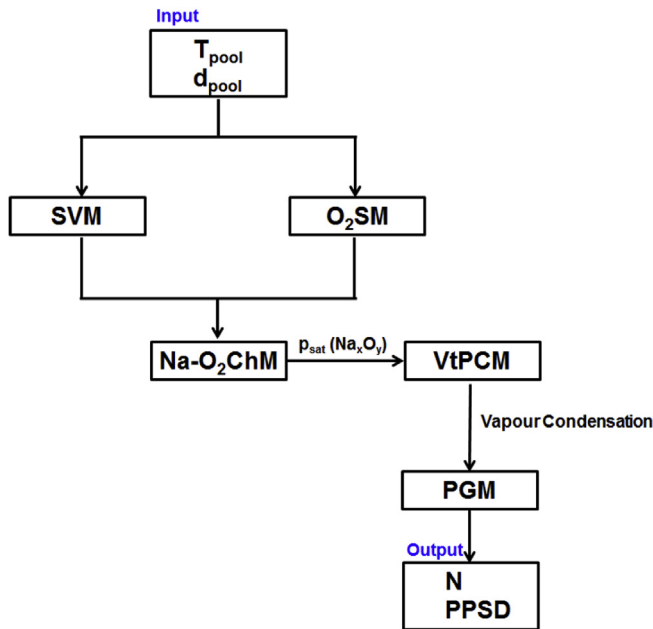

Fig. 1. PG model diagram.

example, assumes that all sodium oxides (Na_xO_y) produced become particles of a given size with no specific consideration of particle formation kinetics or primary-particle size. The CONTAIN-LMR code (Murata et al., 1993), which is heavily inspired by SOFIRE regarding Na combustion, requires the user to set a particle seed size and to introduce a number of parameters that heavily control both Na-based particle generation and subsequent behaviour (Herranz et al., 2017).

Due to the attention that Source Term is being given in the frame of Gen. IV SFR (Girault et al., 2015, 2017) designs to achieve better assessments of SFR potential risks and/or more efficient development of engineered safety features, an *ad-hoc* particle generation model from Na-pool fires has been built by Garcia et al. (2016). The model consists of a suite of individual models for Na vaporization (diffusion layer approach), O_2 transport by air natural circulation (3D flow pattern modelling), $Na-O_2$ chemical reactions (instantaneous reactions and energy of reaction) and vapour-to-particle conversion of Na-oxides (i.e., nucleation and/or condensation). Fig. 1 shows a simplified flowchart of the coupling of individual models. By characterizing sodium pools through temperature and diameter, a Sodium Vaporization Model (SVM) calculates the vaporized Na from the surface. Highly turbulent conditions foreseen in the close vicinity of the sodium reaction zone together with the O_2 supply to the reaction region require a 3D Computational Fluid Dynamics (CFD) approach to be used. By using FLUENT (ANSYS Inc., 2008), the O_2 natural circulation and the $Na-O_2$ chemical reactions are modelled (O_2 Supply Model, O_2SM; $Na-O_2$ Chemical Model, $Na-O_2$ChM). Then, a Vapour-to-Particle Conversion model (VtPCM) calculates particle generation by homogeneous nucleation and particle growth by condensation of the formed sodium oxides. As a result, the Particle Generation (PG) model produces the total number of generated particles (N) and the Primary Particle Size Distribution (PPSD) during an in-containment sodium pool fire. The authors partially validated the model with data from Newman and Payne (1978) and showed a consistent model response in terms of burning rate. However, as stated above, such an agreement requires capturing the 3D natural circulation that feeds the $Na-O_2$ reaction layer and the associated turbulence foreseen right above such a reaction region.

The current international trend in the development of SFR severe accident codes is to take advantage of the commonalities with LWR ones, so that the main code architecture and programming is adopted,

and just modifications to account for those phenomena that are specific of SFRs are to be included. This was, for example, the strategy in the European JASMIN project of the 7th Framework Programme of EURATOM. Nevertheless, this approach is not free of drawbacks, like the fact that the description of some of those specific phenomena might require variables not included in the original code. In other words, once a model describing a phenomenon is developed and validated, it might still require some further work to make it compatible with the code structure and language. This is the main focus of the present paper: transposing the PG formulation introduced above into a form ready to be implemented in any lumped-parameter code to be used for SFR severe accident analysis such as MELCOR/CONTAIN-LMR (Louie and Humphries, 2016) and/or ASTEC-Na (Girault et al., 2015, 2017). Finally the performance of the ASTEC-Na code with the proposed correlations implemented is analysed by comparing its predictions with some of the most credited experiments on aerosol behaviour in SFR containments.

2. Zero-D particle generation modelling

As mentioned above, particle generation from a Na-pool fire is associated with substantial gradients of temperature, Na_xO_y vapours and oxygen concentrations as well as turbulent agitation in the region right over the thin reaction layer set up next to the pool surface. Thus, the use of a 3D approach to capture the entire picture of particle generation seems to be recommendable. Nevertheless, using 3D computational fluid dynamics in analysis of Beyond Design Basis Accidents (BDBAs) at present is unsuitable, due to the lack of validation of these tools in SFR accident conditions, and impractical, since the necessary computing resources and the number of scenarios to be explored would render this approach too onerous. Therefore, a zero-D (lumped) approach is to be developed based on the work by Garcia et al. (2016).

In order to turn the chosen 3D model into a consistent 0D version, some qualitative criteria have been adopted:

- The 0D response to major environmental variables (i.e., pool temperature, oxygen concentration, over-pool gas velocity and composition, etc.) should follow the same trends shown by the original 3D model;
- The quantitative deviations of the 0D predictions with respect to the 3D estimates should be within the uncertainty range of the latter in the main output variables of the model (i.e., particle generation rate and primary-particle size distribution);
- The final formulation of the 0D model should be compatible with architecture and variables available in integral lumped-parameter codes to be used for SFR severe accident analyses (i.e., MELCOR-Na and/or ASTEC-Na).

2.1. Zero-D model

2.1.1. Fundamental equations

In addition to the qualitative criteria introduced above, the 0D adaptation of the PG model is based on the preservation of the total number of particles formed in the active nucleation volume (i.e., the region over the pool in which Na-oxides are supersaturated) in the 3D model, i.e.,:

$$N_{3D} = \sum_i \left(\int_{\Delta t} J_i^{CNT}(T_i, p_{v_i}) \cdot dt \right) \cdot v_i \equiv N_{0D} = \left(\int_{\Delta t} J^{CNT}(\overline{T}, \overline{p}_v) \cdot dt \right) \cdot V_{PG} \tag{1}$$

In Eqn. (1), the number of generated particles (N_{3D}) in the active volume is given by the integration over time of the nucleation rate in all the cells forming the active volume (summation running over subindex i). As shown at the right side of the equation, the 0D approximation requires a characteristic nucleation rate that keeps the major Classical Nucleation Theory dependencies and relies on average gas properties