

Mass Transfer Simulation Model for Justification Sodium Purification System Characteristics

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Abstract. Numerical simulation of a sodium cold traps performance characteristics is discussed within this paper. The method of consecutive heat and mass transfer simulation using custom open source CFD solver to determine the mass transfer and retain coefficients for the cold trap mock-up is discussed in this work. The new solver has been developed, which calculates fields of dissolved oxygen and suspended sodium oxide particles and the rate of their accumulation in the cold trap as well. It has been demonstrated that suggested methodology of CFD simulation allows one to analyze operational parameters of a sodium purification systems for nuclear facilities.

Key Words: sodium coolant, oxygen, purification, computational fluid dynamics.

1. Introduction

Almost any power equipment requires maintaining of coolant purity at the specific level to provide the most reliable and effective way of operation. Provision of the safe and reliable NPP operation with sodium fast reactor requires maintaining of the sodium coolant quality in regards of oxygen and hydrogen contents at the low level, since even a few parts per million of sodium oxide can have a deleterious effect on the performance and reliability of a fast reactor and its heat transfer system.

The main component of sodium coolant purification system is a cold trap. In a cold trap the sodium is cooled and impurities present in amounts exceeding their solubility at low (100 – 150 °C) temperatures. Cold traps are designed to promote controlled precipitation and to retain the precipitate in the trap [1].

Justification of cold trap operational parameters at the existing sodium fast reactors was performed at the beginning of fast reactor technology era based on experiments and semi-empirical calculations. Today's simulation technologies can be used to perform detailed computer analysis of cold trap performance taking in account accumulated experimental experience. But due to complexity of the heat and mass transfer processes effecting on each other and occurring in the cold trap simultaneously, there is a need in upgrading and validating standard calculation models incorporated in the existing codes.

The need in studying characteristics of purification trap considered within this simulation is driven by the need to sustain the number of the impurities at the reasonably low level for keeping equipment of the circuit from fouling and deterioration of heat transfer [2, 3].

The method of consecutive heat and mass transfer simulation using custom OpenFOAM solver [4] to determine the retention coefficient of the cold trap mock-up is discussed in this work.

2. Description of the simulation case, CAD model and mesh

Nowadays a number of approaches to simulate conjugated heat transfer are applied for different engineering design problems, including simulation of liquid metal coolant flow. Experience in mass transfer modeling inside cold trap using OpenFOAM software has been accumulated [5-7].

The simulation case was prepared based on CAD model created using Salome software and meshed using *snappyHex* mesher. The model is a cylinder ($R = 0.3$ m, $D = 1.85$ m) with inlet tube ($d_{in} = 15$ mm) immersed in it and asymmetrically located outlet pipe ($d_{out} = 25$ mm) at the top of the device (see FIG. 1).

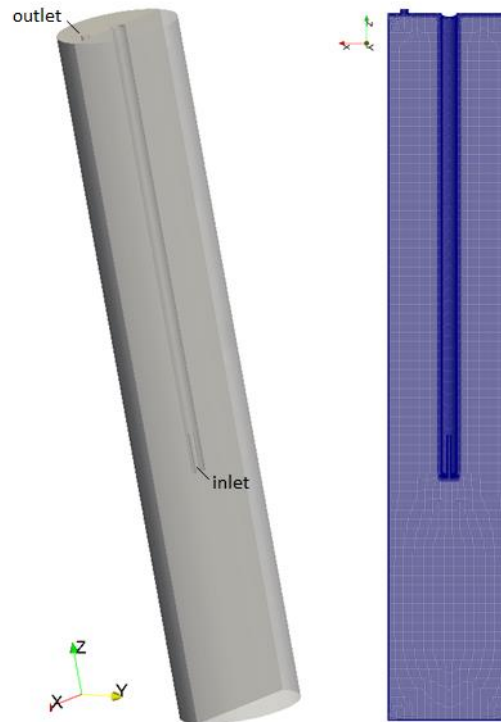


FIG. 1. Symmetrical half of the CAD model, and mesh of the model.

During the first stage of study a number of thermal hydraulic simulation runs was performed to determine optimal hexahedral mesh size of the model.

3. Development of custom mass transfer solver for sodium cold-trap simulation

Since there was no ready-to-use solver for transient simulation of both dissolved impurities and precipitated particulates in sodium, custom OpenFOAM transport solver was developed first with verification and validation stages followed after that.

The base equation for impurity transport in flowing coolant has the following form:

$$\frac{dC_i}{d\tau} + \text{div}(vC) - \text{div}(D \cdot \text{grad}C) = 0 \quad .$$

The custom OpenFOAM solver designed to consider crystallization process of dissolved impurity due to coolant temperature decrease has the following form of impurity transport equation:

$$\frac{dC_i}{d\tau} + \text{div}(vC_i) - \text{div}\left(\left(\frac{\nu}{Sc} + \frac{\nu_t}{Sc_t}\right)\text{grad}C_i\right) = Q_i,$$

where C – impurity concentration, ppm; and index « i » means dissolved and crystallized phases; v – coolant velocity, m/s; ν и ν_t – viscosity and turbulent viscosity, m²/s; Sc и Sc_t – Schmidt number and turbulent Schmidt number; Q – source of concentration in the cell (dissolution of crystallization), ppm.

Custom computational model considers additional phenomena, such as:

- if there is supersaturation in the given cell (C_p) and the value of concentration in this cell is less than impurity concentration of saturation at the same cell ($C < C_s$), the value of saturated impurity concentration set equal to concentration of impurity saturation and surplus of concentration transforms to particulate phase with concentration C_p .
- reverse process of impurity dissolution.

To realize the first phenomenon and make two phases transformation to each other possible, the source Q are implemented in both transport equations, for dissolved impurities and for particulate. When temperature in cell are high enough to dissolve additional amount of impurity concentration, particulate phase C_p transforms to dissolved impurity C (i.e. $Q_C = -Q_{C_p}$) and vice versa.

Desupersaturation of C_p occurs at the cooled wall due to crystallization of impurities in mass exchange surface process. The new amount of impurities is driven to the surface by the diffusion through the boundary layer. Process of depositions (in the form of crystals) dissolution on the mass exchange surface occurs by diffusion through the boundary layer of impurities from the wall to the bulk sodium.

If the concentration at the boundary is less than saturation concentration, and concentration of impurity in the flow is less than saturation, than zero gradient condition is true for the boundary.

4. Verification of the custom solver developed

It's obvious that any changes put in default solver have to be validated and verified first, so validation of the custom solver based on experimental data of mass transfer in pipes preceded the simulation runs.

Experimental data was obtained at the sodium test facility comprised by tube with flowing sodium cooled down from outside [8]. Due to cooling supersaturation of sodium occurred and deposits accumulated at the wall. After experiment the test section was cut by pieces and particulates collected from the surface of each sample was measured. Comparison of experimental and simulation data was perform at different Re numbers, for both turbulent and for laminar regimes.

The scheme of the simulation domain is presented at the FIG. 2. The model is a 3D hexahedral mesh of the channel. It has the same diameter as experimental test section, but also includes inlet and outlet stabilization sections.

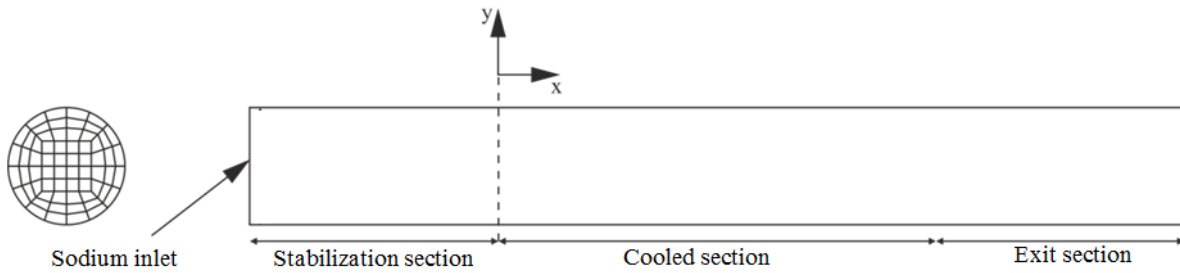


FIG. 2. Schematic picture of calculation model.

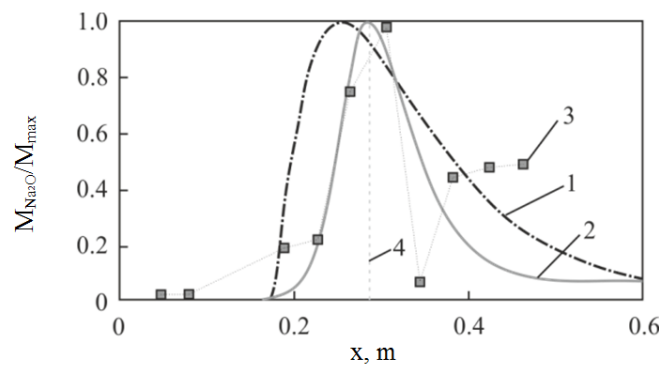
For comparison of simulation results analytical solution for simplified mass transfer was used – decrease of concentration in the channel per time unit equals to the mass of generated depositions:

$$\frac{d\Sigma C}{dx} = -\frac{j\Pi}{G},$$

where ΣC – impurity concentration ($C + C_p$), ppm; x – coordinate, m; j – impurity flux at the wall, $\text{kg/m}^2\text{s}$; Π – perimeter, m; G – sodium flowrate, kg/s .

Concentration of oxygen at the inlet of test section equals to 100 ppm. Temperature data were measured by a special movable thermal couple.

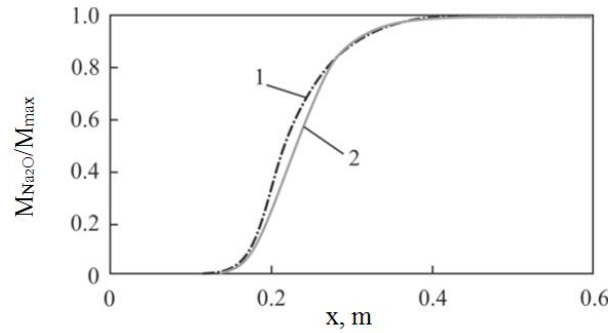
As comparison of simulation results and experimental data at the FIG. 3 (regime parameters: $Re = 42000$; diffusion coefficient $D = 7 \cdot 10^{-5} \text{ m}^2/\text{s}$; turbulent diffusion coefficient $D_t = 100 \cdot D$) shows in regimes with supersaturation of ~ 100 ppm at the test section, the function of the accumulated depositions has the maximum around the middle of the channel. In simulation the temperature at the wall was calculated and integral value over the channel section was used to calculate supersaturation. In experiment there was no inlet stabilization section considered, but in simulation it was implemented.



1 – analytical solution; 2 – simulation results using custom OpenFOAM solver;
3 – experimental data; 4 – coordinate of the depositions maximum

FIG. 3. Results of simulation, analytical solution and experimental data ($Re = 42000$)

At the FIG. 4 comparison of analytical solution and simulation result is presented ($Re = 2420$; $D = 5 \cdot 10^{-8} \text{ m}^2/\text{s}$; $Sc = 10$).



1 – analytical solution; 2 – simulation results using custom OpenFOAM solver

FIG. 4 Results of simulation and analytical solution ($Re = 2420$)

As one can see, there is a good agreement between analytical solution and simulation results obtained with *OpenFOAM* software at both low and high Re numbers.

The important thing to mention is effective diffusion coefficient for case with highly turbulent flow was deliberately chosen slightly higher than presented in literature [9] or sodium self-diffusion coefficient, since reference data are valid only for stagnant sodium and temperatures higher, than those measured at experiment. Significant effect on effective diffusion coefficient brings not only temperature rise, but growth of deposited particles diameter as well.

5. Mass transfer simulation results and discussion

Simulation of cold trap described earlier was performed with verified OpenFOAM solver. Cold trap is conventionally divided on three zones: settler section, section of final cooling down zone and filters section). Sodium inlet located at the middle part of the trap, sodium is pumped through thermally isolated tube, so coolant flows from the top consequently through the inlet at the middle and then turns up to the outlet passing the cooled wall and filter mesh zone. That way effective combination of forced and natural convection is taking place inside the device. Sodium flowrate provided sodium residence time in trap around 15 min.

In a result of simulation the values of calculated and measured mass transfer coefficients were obtained and compared against each other (see Table I). Discrepancy between calculated coefficient and those obtained from experiment can be explained by increase of effective diffusion coefficient during experiment run due to growth of deposited particulates size and porosity of the depositions layer, which hasn't been considered in simulation (only temperature effect has been considered).

TABLE I: COMPARISON OF CALCULATED AND MEASURED MASS TRANSFER COEFFICIENTS.

Regime	α_{exp}	α_{sim}
Accumulation	0.33 m/h	0.35 m/h
Dissolution	0,09 m/h	0,043 m/h

Retention coefficient β of cold trap was calculated as a slope ratio of the curve ($f(x) = \beta \cdot \ln(y) + A$):

$$f\left(\frac{G \cdot \tau}{M}\right) = \ln\left(\frac{\Sigma\bar{C}(\tau) - C_s(T)}{\Sigma\bar{C}(0) - C_s(T)}\right).$$

Performance of cold trap is an amount of impurity retained or accumulated by the device in the unit of time and determined by formula:

$$\Delta P = \beta \cdot G(\Sigma\bar{C} - C_s(T_{\min})),$$

where $\Sigma C(\tau)$ – average concentration of oxygen (the sum of dissolved concentration and particulates) in the cold trap, ppm; G – sodium flowrate through the cold trap, kg/s; M_{Na} – sodium mass in cold trap, kg.

Calculated retention coefficient is equal to 0.9, which agreed with values obtained for «clean» cold traps just started operation and haven't accumulated any impurities yet [1]. During operation process retention coefficient of cold trap increases due to growth of particulates size accumulated at the wall and thus area available for precipitation increase as well.

So as a common recommendation for mass transfer simulation in sodium equipment it should be mentioned that diffusion coefficient depends not only temperature, but on time of operation as well.

Dependence of diffusion coefficient on temperature available in literature [9]:

$$D_{O-\text{Na}} = 0.213 \cdot \exp\left(\frac{-78570}{RT}\right), \text{ cm}^2/\text{s};$$

where R – gas constant, $8.31 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$; T – temperature, K.

In the temperature range of the phenomena considered within this study (150 – 250 °C) this formula give extrapolated values in the range between $10^{-11} - 10^{-10} \text{ m}^2/\text{s}$ ($Sc = 4 \div 60$). But they seem to be underestimated since experiments were carried out at temperatures 700 – 750 °C and gave values 2 – 3 orders of magnitude higher. It's not clear how valid extrapolation of this experimental data to such a low temperatures is. Since the result of simulation is sensitive in regards of diffusion coefficient provided, it's very important to review and update all available experimental data for sodium heat and mass transfer experience to get reliable predictions. In this view NAPRO project managed by IAEA is very promising initiative to put all available information on sodium coolant research up to date [10].

It is also worth noting, that usually in sodium trap both sodium oxide and sodium hydroxide present, which can interact with each other chemically and have a different mechanism of precipitation [11]. Their interaction could raise efficiency of purification, but at this stage of the work authors considered only oxygen transport.

6. Conclusion

The method of consecutive heat and mass transfer simulation using custom OpenFOAM solver to determine the retention coefficient of the cold trap mock-up is described in this work. It has been demonstrated that suggested methodology allows one to extend conventional convective heat transfer simulation possibilities of CFD code with mass transfer simulation features to study parameters of sodium cold traps with different geometries.

In the result of performed simulations the distributions of velocity, pressure, temperature and concentration of both dissolved and particulate phases inside the cold trap were obtained as

well as the rate of impurity accumulation. Predicted information helps to analyze operational parameters of purification systems for sodium facilities.

Spacial distribution of dissolved impurity and particulates inside the purification trap was obtained during custom solver verification process. Analysis of dissolved and precipitated concentration fields allowed obtaining mass transfer characteristics of the device.

Mass transfer CFD simulations require a number of additional input data, such as mass transfer coefficient, saturation concentration and diffusion coefficient vs temperature dependencies, and concentration of impurity at the inlet of computational domain. The result of simulation is sensible in regards of the input data provided, so it's important to bring all available reference data on sodium research to up-to-date condition.

7. Acknowledgment

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