Sensitivity Analysis of the 1-D Thermal Stratification Model via Forward and Adjoint Methods

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INTRODUCTION

Thermal stratification is a phenomenon that has been continuously investigated during the development of the Gen-IV reactors. Being possible to occur in a wide range of reactor designs, thermal stratification brings uncertainties to the reactor safety in different ways, including leading to both neutronic and thermal-hydraulic instabilities, causing damages to both reactor vessel and in-vessel components, and impeding the establishment of natural circulation in accidental scenarios [1]. The study of thermal stratification in liquid-metal-cooled reactors (LMRs), among other reactor designs, is especially indispensable due to its large impact. In order to prevent the formation of thermal stratification or to mitigate the damages caused by it, an efficient 1-D model to predict the formation of the stratified layers in LMRs was recently developed in our research group [2]. Satisfactory performance of the 1-D model has been demonstrated against both experimental data acquired in the Thermal Stratification Experimental Facility (TSTF) [3, 4] and the Gallium Thermal-hydraulic Experiment (GaTE) facility [5, 6].

In this paper, parameter sensitivity analysis (SA) were performed to the 1-D model to enhance our understanding on the thermal stratification phenomenon. Both the conventional forward SA method and the more advanced adjoint SA method were considered in the study. The most significant difference between these two methods is the computational cost. Assuming that we have a time-space-dependent model with *n* inputs and *m* outputs as shown in Figure 1, and we hope to view the sensitivity of each output to each input, we then need to solve the full system for at least *n+1* times by using the forward method, and at least *m+1* times by using the adjoint method. Therefore, compared with the forward method, the adjoint method is more efficient when the number of outputs is small and the number of input parameters is large [7].

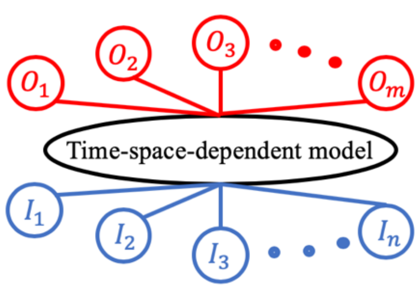

Figure 1. Schematic of a time-space-dependent model with multiple I/O parameters.

The accuracy of the sensitivities obtained is verified by comparing the results obtained from both methods. The most influencing factor that impact the severity of the thermal-stratification phenomenon is also determined through the SA.

1-D THERMAL STRATIFICATION MODEL

Eq.(1) was developed in in our previous study [2] to predict the temperature profile of the ambient fluid in a thermally stratified large enclosure such as the coolant tank,

$$\rho_{amb}c_{p,amb}\frac{\partial T_{amb}}{\partial t}+\rho_{amb}c_{p,amb}\frac{Q_{jet}}{A_{amb}}\frac{\partial T_{amb}}{\partial z}-\frac{\partial}{\partial z}\left(k_{amb}\frac{\partial T_{amb}}{\partial z}\right)=\frac{c_{p,jet}\rho_{jet}}{A_{amb}}Q'_{jet}\left(T_{jet}-T_{amb}\right). \quad (1)$$

In the equation $\rho_{amb}, c_{p,amb}, A_{amb}$, T_{amb} and k_{amb} represent the mass density, heat capacity, surface area, temperature, and the effective thermal conductivity of the ambient fluid, respectively. $\rho_{jet}, c_{p,jet}, Q_{jet}, T_{jet}$ and Q'_{jet} represent the mass density, heat capacity, volumetric flow rate, temperature, and the linear volumetric dispersion rate of impinging jet, respectively. A correlation between the effective thermal conductivity of the ambient, k_{amb}, and the static one, $k_{c,amb}$, was established and validated in our previous publication [4].

The test conditions of one of the experiments performed in the TSTF was used as the reference in this study. In this reference transient, the cylindrical test section of the TSTF, with a height of about 150 cm and a diameter of about 32 cm, was initially filled with sodium at 250 ℃. A jet of sodium at 200 ℃ was injected into the test section from the bottom of the tank, at the beginning of the transient, with a volumetric flow rate of $Q_{jet} = 0.38$ L/s. The ambient fluid temperature profile predicted by Eq (1) is plotted in Figure 2, which shows that the predicted temperature of the ambient fluid converged to that of the jet at around 300 s elapsed time.

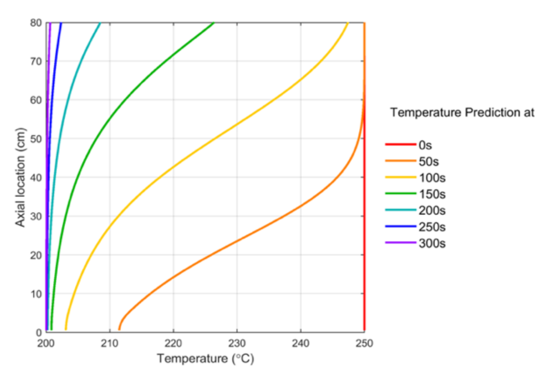

Figure 2. Temperature profiles predicted in the reference transient at different elapsed times.

Because the temperature gradient of the ambient fluid best reflects the severity of the thermal stratification phenomenon in the tank, it is considered as the figure of merit in the SA procedure. The temperature gradients at different times of the reference transient were calculated and shown in Figure 3. The discontinuities appeared in temperature gradient curves were caused by an Upper Instrumentation Structure (UIS), which was installed in the tank to emulate the in-vessel components and blocked the impinging jet. Because of the nearly uniform temperature profiles at both the beginning and the end of the transient, the corresponding temperature gradients were small.

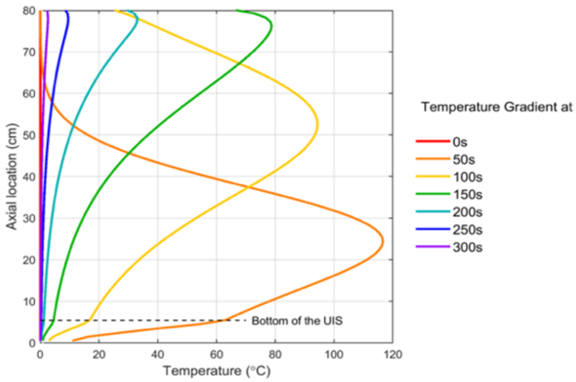

Figure 3. Temperature gradient for the reference transient at different elapsed times.

SENSITIVITY ANALYSIS

In this section, we investigated the sensitivities of the ambient fluid temperature gradient to four different parameters, including jet volumetric flow rate Q_{jet}, jet temperature T_{jet}, heat capacity of the ambient fluid $C_{p,amb}$, and static thermal conductivity of the ambient fluid $k_{c,amb}$. The calculations of the sensitivities through both the forward sensitivity method and the adjoint sensitivity method are introduced in the following two subsections.

Forward sensitivity methods

We introduced small perturbations into each of the four parameters around their nominal values, and calculated the corresponding variation in temperature gradient of the ambient fluid. By using the forward sensitivity method, the absolute sensitivity of the ambient fluid temperature gradient to different parameters can be calculated by the center difference scheme as follows

$$S_\theta = \frac{\delta J}{\delta \theta} = \frac{J(T(\theta_0+\Delta\theta))-J(T(\theta_0-\Delta\theta))}{2\Delta\theta}, \quad (2)$$

where J represents the temperature gradient, T represents the predicted temperature, $\theta = Q_{jet}, T_{jet}, C_p, or\ k_c$, and θ_0 represents its nominal value. The relative sensitivities of temperature gradient to each of the four parameters, calculated as

$$S_r = \frac{\delta J}{\delta \theta}\frac{\theta_0}{J_0} = S_\theta \frac{\theta_0}{J_0}, \quad (3)$$

were further calculated at 100 s elapsed time, by using a $\frac{\Delta\theta}{\theta_0} = 10^{-9}$ to guarantee the convergence, as shown in Figure 4. The resultant relative sensitivities will be compared to those calculated with adjoint sensitivity method in the following subsection for verification.

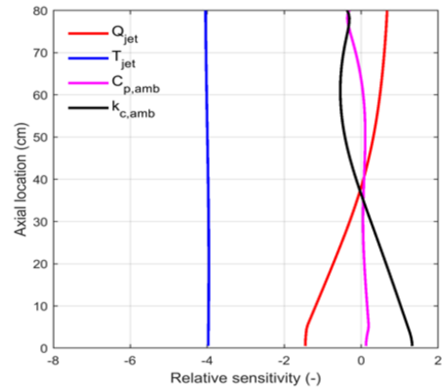

Figure 4. Relative sensitivities of temperature gradient to θ, calculated at 100 s elapsed time.

Adjoint sensitivity methods

Considering a non-linear system $\boldsymbol{N}(\boldsymbol{x},\boldsymbol{\theta}) = \boldsymbol{0}$, $\boldsymbol{x}$ is the variable that needs to be solved, and $\boldsymbol{\theta}$ is the variable on which $\boldsymbol{x}$ is dependent. $\boldsymbol{J}(\boldsymbol{x})$ is the variable of interest, which is dependent only on $\boldsymbol{x}$. By using the adjoint sensitivity method, $\delta\boldsymbol{J}(\boldsymbol{x})$ can be expressed as

$$\delta\boldsymbol{J}(\boldsymbol{x}) = \frac{d\boldsymbol{J}(x)}{dx}\delta\boldsymbol{x}. \quad (4)$$

For the non-linear system $\boldsymbol{N}$, we have

$$\delta\boldsymbol{N}(\boldsymbol{x},\boldsymbol{\theta}) = \boldsymbol{0} = \frac{\partial \boldsymbol{N}(x,\theta)}{\partial x}\delta\boldsymbol{x} + \frac{\partial \boldsymbol{N}(x,\theta)}{\partial \theta}\delta\boldsymbol{\theta}. \quad (5)$$

By introducing the vector of Lagrangian multipliers, $\boldsymbol{\Phi}^T$, Eq. (4) can also be written as

$$\delta\boldsymbol{J}(\boldsymbol{x}) = \frac{d\boldsymbol{J}(x)}{dx}\delta\boldsymbol{x} + \boldsymbol{\Phi}^T\left(\frac{\partial \boldsymbol{N}(x,\theta)}{\partial x}\delta\boldsymbol{x} + \frac{\partial \boldsymbol{N}(x,\theta)}{\partial \theta}\delta\boldsymbol{\theta}\right). \quad (6)$$

In order to cancel out the term $\delta\boldsymbol{x}$, we need

$$\frac{d\boldsymbol{J}(x)}{dx} + \boldsymbol{\Phi}^T\frac{\partial \boldsymbol{N}(x,\theta)}{\partial x} = \boldsymbol{0}, \quad (7)$$

which is referred to as the "adjoint equation" of the forward equation governing the system, and thus Eq. (6) becomes

$$\delta\boldsymbol{J}(\boldsymbol{x}) = \boldsymbol{\Phi}^T\frac{\partial \boldsymbol{N}(x,\theta)}{\partial \theta}\delta\boldsymbol{\theta}. \quad (8)$$

By combining Eq. (7) and Eq. (8), we can get the final expression of $\delta\boldsymbol{J}(\boldsymbol{x})$ as a function of $\delta\boldsymbol{\theta}$:

$$\delta\boldsymbol{J}(\boldsymbol{x}) = -\frac{d\boldsymbol{J}(x)}{dx}\left(\frac{\partial \boldsymbol{N}(x,\theta)}{\partial x}\right)^{-1}\frac{\partial \boldsymbol{N}(x,\theta)}{\partial \theta}\delta\boldsymbol{\theta}. \quad (9)$$

In this sensitivity analysis of interest, $\boldsymbol{J}$ is the temperature gradient, $\boldsymbol{x}$ is the predicted temperature, and $\boldsymbol{\theta}$ is the four parameters investigated. By introducing the system of the 1-D thermal stratification model, expressed in Eq. (1), into Eq (9), the absolute sensitivity of the ambient fluid temperature gradient to different parameters were calculated. The relative sensitivities of temperature gradient to each of the four parameters were further calculated according to Eq. (3). The differences between the sensitivities calculated by using both methods are plotted in Figure 5. The discrepancies for Q_{jet}, T_{jet}, $C_{p,amb}$, and $k_{c,amb}$, were less than 0.02, 0.05, 0.01, and 0.02, respectively. The forward sensitivity method and the adjoint sensitivity method therefore mutually verified as the differences were negligible compared to the predicted sensitivities plotted in Figure 4.

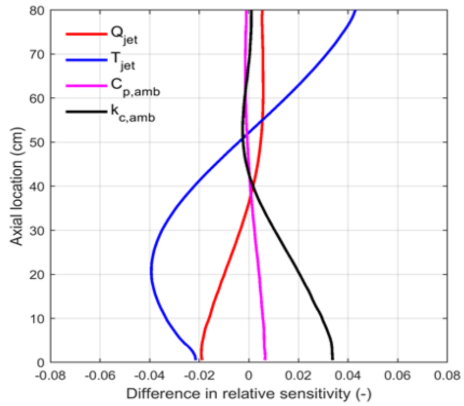

Figure 5. Differences in the relative sensitivities predicted through the forward and the adjoint methods.

RESULTS

The predicted temperature gradient of the ambient fluid calculated at different axial locations throughout the experiment is shown in Figure 6. The peak of the temperature gradient appeared around the bottom of the tank at the beginning of the experiment, and moved upward with an increasing elapsed time.

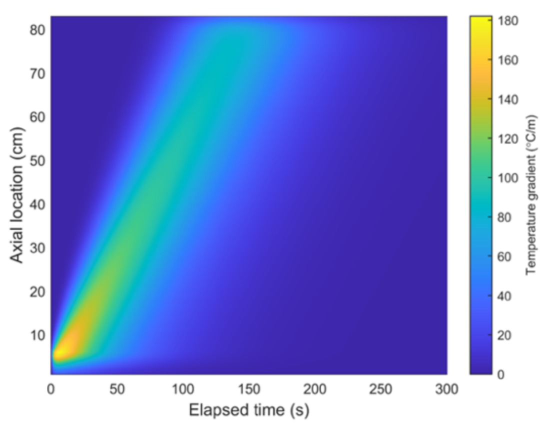

Figure 6. Predicted temperature gradient at different axial locations throughout the experiment.

Semi-relative sensitivities to the four parameters, in the sense of an absolute change in the temperature gradient caused by a relative change in the parameter, defined as

$$S_{sr} = \frac{\delta J}{\delta \theta}\theta_0 = S_\theta \theta_0 \,, \qquad (10)$$

were calculated by using the adjoint sensitivity method.

Semi-relative sensitivity of temperature gradient to Q_{jet} is plotted in Figure 7 as an example. In general, perturbations in Q_{jet}, $C_{p,amb}$, and $k_{c,amb}$ could introduce either positive or negative changes to the temperature gradient of the ambient fluid, depending on the axial location and the elapsed time, while an increase in T_{jet} always decreased the temperature gradient. Moreover, the impact of T_{jet} on the temperature gradient was much higher than the other three parameters.

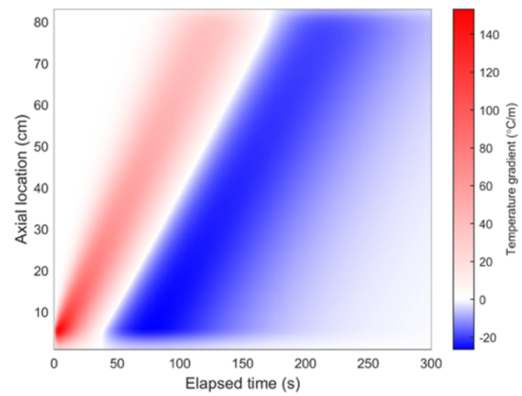

Figure 7. Semi-relative sensitivity of temperature gradient to Q_{jet} at different axial locations throughout the experiment.

CONCLUSIONS

Sensitivity analysis to the 1-D thermal stratification model was performed to identify the model parameter that impacts the temperature gradient the most using both forward and adjoint sensitivity methods. It was found that the jet temperature T_{jet}, among the four parameters investigated, has the largest impact on the temperature gradient. Future study will use the sensitivity information to quantify the prediction uncertainties associated with these parameters.

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