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

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Background – Thermal stratification in nuclear systems

➢ Thermal stratification
  ❖ Formation of stratified layers of coolant with a large temperature gradient

➢ Nuclear systems involved
  ❖ High-Temperature Gas-Cooled Reactors (HTGR)
  ❖ Small-Modular Boiling-Water Reactors (SMBWR)
  ❖ Pool-type Sodium-Cooled Fast Reactors (SFR)
  ❖ ...

➢ Concerns
  ❖ Leads to neutronic and thermal-hydraulic instabilities
  ❖ Causes thermal fatigue crack growth
  ❖ Impedes natural circulation
Background – Development of the 1-D TS model (1)

The Thermal Stratification Testing Facility (TSTF)

- Cylindrical
  - H=150 cm
  - D=32 cm
- Sodium

CFD modeling and simulation

![Temperature Distribution](image)

1-D TS model

\[ \rho_{amb} c_{p,amb} \frac{\partial T_{amb}}{\partial t} + \rho_{amb} c_{p,amb} \bar{u}_x \frac{\partial T_{amb}}{\partial z} - \frac{\partial}{\partial z} \left( k_{amb} \frac{\partial T_{amb}}{\partial z} \right) = \frac{N_{jet}}{A_{amb}} c_{p,jet} \rho_{jet} Q_{jet}' (T_{jet} - T_{amb}) \]
Background – Development of the 1-D TS model (2)

\[ \rho_{amb}c_{p,amb}\frac{\partial T_{amb}}{\partial t} + \rho_{amb}c_{p,amb}\frac{\partial T_{amb}}{\partial z} - \frac{\partial}{\partial z}\left( k_{amb}\frac{\partial T_{amb}}{\partial z} \right) = \frac{N_{jet}}{A_{amb}}c_{p,jet}\rho_{jet}Q'_{jet}(T_{jet} - T_{amb}) \]

Jet volumetric flow rate

Jet temperature

Heat capacity of the ambient fluid

Thermal conductivity of the ambient fluid

Test conditions

\[ T_{jet} = 200^\circ C \]
\[ T_{amb} = 250^\circ C \]
\[ Q_{jet} = 0.38 \text{ L/s} \]

The Thermal Stratification Testing Facility (TSTF)
To investigate the sensitivity of the temperature gradient of the ambient fluid in the test section, which serves as a good quantitative metric (figure of merit - FOM) reflecting the severity of the thermal stratification phenomenon, with respect to four parameters.

**Parameters considered**
- Jet volumetric flow rate $Q_{jet}$
- Jet temperature $T_{jet}$
- Heat capacity of the ambient fluid $C_{p,amb}$
- Thermal conductivity of the ambient fluid $k_{c,amb}$

**Method employed**
- Conventional forward sensitivity method
- Advanced adjoint sensitivity method
Outline

- Sensitivity analysis with conventional forward sensitivity method
- Sensitivity analysis with adjoint sensitivity method
- Additional findings from the sensitivity analysis
- Uncertainty quantification by using the adjoint sensitivities
- Summary and conclusions
Forward sensitivity method

1-D thermal stratification model

\[ S_{\theta r} = \frac{\delta J}{J_0} \frac{\theta_0}{\Delta \theta} = J(T(\theta_0 + \Delta \theta)) - J(T(\theta_0)) \frac{\theta_0}{J_0} \]

where \( \theta = Q_{\text{jet}}, T_{\text{jet}}, C_{p,\text{amb}}, \text{or } k_{c,\text{amb}} \)

Minimal computational expense

- Nominal condition \( \times 1 \)
- Variation introduced \( \times 4 \)
- 5 in total

Temperature distribution \( T \)

Temperature gradient distribution \( J \)

Relative sensitivity \( S_r \)
Can we avoid repetitively solving the 1-D system?
Adjoint sensitivity method - theory

\[ \delta J(T) = \frac{dJ(T)}{dT} \delta T \]

- Repetitively solving 1-D TS model for different \( \delta T \)
- Cast 1-D TS model into the residual form: \( F(T, \theta) = 0 \)

\[ \delta F(T, \theta) = 0 = \frac{\partial F(T, \theta)}{\partial T} \delta T + \frac{\partial F(T, \theta)}{\partial \theta} \delta \theta \]

\[ \delta J(T) = \left( \frac{dJ(T)}{dT} + \Phi^T \frac{\partial F(T, \theta)}{\partial T} \right) \delta T + \Phi^T \frac{\partial F(T, \theta)}{\partial \theta} \delta \theta \]

\[ \delta J(T) = \Phi^T \frac{\partial F(T, \theta)}{\partial \theta} \delta \theta \] (This is true when \( \frac{dJ(T)}{dT} + \Phi^T \frac{\partial F(T, \theta)}{\partial T} = 0 \) → the adjoint equation)

\[ \Phi^T = -\frac{dJ(T)}{dT} \left( \frac{\partial F(T, \theta)}{\partial T} \right)^{-1} \]

\( \delta J \): A variation in temperature gradient
\( \delta T \): A variation in temperature
\( \delta \theta \): A variation in the input parameters
Adjoint sensitivity method - application

The space-time discretized form of 1-D thermal stratification model:

\[
\rho_{amb} c_{p,amb} \frac{\partial T_{amb}}{\partial t} + \rho_{amb} c_{p,amb} u_z \frac{\partial T_{amb}}{\partial z} - \frac{\partial}{\partial z} \left( k_{amb} \frac{\partial T_{amb}}{\partial z} \right) = \frac{N_{jet}}{A_{amb}} c_{p,jet} \rho_{jet} \frac{\partial T_{amb}}{\partial t} Q'_{jet} (T_{jet} - T_{amb})
\]

\[
\rho_{n,m-1} c_{p,n,m-1} \frac{T_{n,m-1} - T_{n,m-2}}{\Delta t} + \rho_{n,m-1} c_{p,n,m-1} u_{z,n} \frac{T_{n,m-1} - T_{n,m-2}}{\Delta z} - \frac{2}{\Delta z} k_{n,m-1} \left( \frac{T_{n+1,m-1} - T_{n,m-1}}{2\Delta z} - \frac{T_{n,m-1} - T_{n-1,m-1}}{2\Delta z} \right) = \frac{1}{A_{amb,n}} c_{p,jet} \rho_{jet} \frac{\partial T_{amb}}{\partial t} Q'_{jet,n} (T_{jet} - T_{n,m-1}^{m-1})
\]

\[
F_{n}^{m} = A_{n,n-1}^{m} T_{n,m-1}^{n} + A_{n,n}^{m} T_{n,m}^{m} + A_{n,n+1}^{m} T_{n+1,m}^{m} - B_{n}^{m} T_{n,m-1}^{m-1} - C_{n}^{m} = 0
\]

\[
F(T, \theta) = 0 \text{ with } (M + 1) \times N \text{ equations } (M + 1) \text{ time steps and } N \text{ spatial steps (300 time steps and 83 spatial steps)}
\]

\[
\text{Expressions of } \frac{\partial F(T, \theta)}{\partial T}, \frac{\partial F(T, \theta)}{\partial \theta}, \text{ and } \frac{dJ(T)}{dT}
\]

\[
\text{Calculation of } \Phi^{T} = - \frac{dJ(T)}{dT} \cdot \left( \frac{\partial F(T, \theta)}{\partial T} \right)^{-1}
\]

\[
\text{Calculation of } \delta J(T) = \Phi^{T} \frac{\partial F(T, \theta)}{\partial \theta} \delta \theta
\]

\[
\text{Absolute sensitivity } S^{m} = (\Phi^{m})^{T} \frac{\partial F(T, \theta)}{\partial \theta} \text{ at time step } m
\]

Are we confident about the application process?
Adjoint sensitivity method - verification

Minimal computational expense
- Nominal condition $\times 1$
- Computation of matrices $\times 1$
  - $\frac{\partial F(T,\theta)}{\partial \theta}$
  - $\frac{dJ(T)}{dT}$
  - $\frac{\partial F(T,\theta)}{\partial T}$
  - $\Phi^T$
- 2 in total (compared to 5 in total for forward method)

The adjoint method is more efficient when $N_{output}$ is small and $N_{input}$ is large (Wang, 2013).

<table>
<thead>
<tr>
<th>Parameter investigated</th>
<th>Max. abs. difference in $S_T$</th>
<th>Forward method</th>
<th>Adjoint method</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_{jet}$</td>
<td>0.02</td>
<td>-1.45</td>
<td>-1.47</td>
</tr>
<tr>
<td>$T_{jet}$</td>
<td>0.04</td>
<td>-3.96</td>
<td>-4.00</td>
</tr>
<tr>
<td>$C_{p, amb}$</td>
<td>0.01</td>
<td>0.13</td>
<td>0.14</td>
</tr>
<tr>
<td>$k_{c, amb}$</td>
<td>0.03</td>
<td>1.33</td>
<td>1.36</td>
</tr>
</tbody>
</table>
Change of temperature gradient caused by

- $Q_{jet}$, $C_{p,amb}$, and $k_{c,amb}$
  - Positive or negative
- $T_{jet}$
  - Always negative

Sensitivity of Max temperature gradient

- $150 \, ^\circ C/m$ for $Q_{jet}$
- $-730 \, ^\circ C/m$ for $T_{jet}$
- $-30 \, ^\circ C/m$ for $C_{p,amb}$
- $-120 \, ^\circ C/m$ for $k_{c,amb}$

Additional findings from the adjoint sensitivity analysis
What else to do with these sensitivity information?
Uncertainties quantification

- **Deterministic method with adjoint sensitivities**
  - uncertainty of a response
  - uncertainty of the $m$th input parameter
  $$\sigma_R^2 = \sum_m (s_m \sigma_m)^2$$
  - adjoint sensitivity of the response to the $m$th input parameter

- **Verification of the correctness**
  - Uncertainty of predicted temperature gradient at 100s elapsed time
  - $Q_{jet}$ (±3%), $T_{jet}$ (±3%), $C_{p,amb}$ (±3%), $k_{c,amb}$ (±5%)
  - Monte Carlo method with 500,000 realizations

- **Comparison of the computational cost**
  - Adjoint sensitivity method $\rightarrow$ equivalent to 2 times
  - Monte Carlo method $\rightarrow$ at least 20,000 times
Summary and conclusions

- Performed a sensitivity study of the temperature gradient
  - Conventional forward method ⇔ Advanced discrete adjoint method
  - Mutual verification of the correctness of both methods
  - Advanced discrete adjoint method is \(~50\%\) computational costly

- Investigated four parameters
  - $Q_{jet}$ sensitivity (+/-), max 150 °C/m
  - $T_{jet}$ sensitivity (-), max -730 °C/m
  - $C_{p,amb}$ sensitivity (+/-), max -30 °C/m
  - $k_{c,amb}$ sensitivity (+/-), max -120 °C/m

- Performed an uncertainty quantification of the temperature gradient
  - Deterministic method with adjoint sensitivities ⇔ Monte Carlo method
  - Mutual verification of the correctness of both methods
  - Deterministic method with adjoint sensitivities is \(~0.01\%\) computational costly
References


