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Thermal-Hydraulic Differential Sensitivity Theory

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**THERMAL-HYDRAULIC DIFFERENTIAL
SENSITIVITY THEORY**

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THERMAL-HYDRAULIC DIFFERENTIAL SENSITIVITY THEORY

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ABSTRACT

Differential sensitivity theory is applied to a non-linear, three-dimensional space- and time-dependent description of the thermal-hydraulic conservation equations. The resulting sensitivity equations, which are derived using adjoint functions, can be readily utilized for input parameter sensitivity analysis of large or long-running thermal-hydraulic computer codes without any prior engineering judgment. The procedure for applying this sensitivity theory is illustrated using several classical analytical problems.

INTRODUCTION

The application of various sophisticated sensitivity theories¹⁻⁴ to large thermal-hydraulic computer codes is very beneficial to the model developer, the analyst, and the experimentalist. The model developer uses sensitivity theory to identify important modeling parameters and to verify computer solutions. The analyst uses sensitivity theory to reduce the computational effort required to obtain sensitivity coefficients. Instead of using the direct method of rerunning a computer code to obtain a coefficient for a single input parameter, as few as two runs can provide sensitivities to all input parameters. The experimentalist uses sensitivity theory in conjunction with uncertainty theory to identify the important experimental parameters, thus yielding valuable information for the design or modification of experimental hardware.

The present work is an application of differential sensitivity theory (DST) (first introduced by Ohlow⁴ for a nonlinear thermal system problem) to a nonlinear, three-dimensional space and time description of the thermal-hydraulic conservation equations. This results in a general thermal-hydraulic DST description that will facilitate future applications of DST to any large or long-running thermal-hydraulic code. The mathematical details of deriving this description are given in Appendix A.

The application of DST to the thermal-hydraulic equations involves the development and solution of equations that are adjoint to the physical equations differentiated with respect to an arbitrary input parameter α . The physical and adjoint solutions are then integrated together to form the sensitivity $\frac{dR}{(d\alpha/\alpha)}$, where R is an important output quantity or response (e.g., a peak or average temperature, pressure, or velocity). The main advantage of DST over the direct method is that sensitivities for a many-parameter computer code are calculated from the information provided by only two computer code runs, a physical base case and its corresponding adjoint.

Based on the conservation equations given next, a thermal-hydraulic DST description is derived on pp. 3 through 12. The mechanics of applying this description to thermal-hydraulic problems is illustrated on pp. 12 through 25 using three analytical examples. Concluding discussion is provided on p. 25.

DERIVATION OF A THERMAL-HYDRAULIC SENSITIVITY DESCRIPTION

Physical Equations of Change

The thermal-hydraulic conservation equations for mass, momentum and thermal energy are given here for a single phase, single component system:

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \vec{v} \quad , \quad (1a)$$

$$\rho \frac{D\vec{v}}{Dt} = -\nabla P - \nabla \cdot \tau + \rho \vec{g} \quad , \quad (1b)$$

$$\rho C_p \frac{DT}{Dt} = -\nabla \cdot (k \nabla T) - \tau : \nabla \vec{v} + Q \quad . \quad (1c)$$

The quantities ρ , C_p , and k represent the physical properties of density, specific heat capacity, and thermal conductivity. The velocity vector, $\vec{v}$; static pressure, P ; and temperature, T ; represent the unknown dependent variables depending on time, space, and the various parameters appearing in Eqs. (1). The symmetric stress tensor, τ , and heat source, Q , are assumed to be functions of the dependent variables $\vec{v}$ and T . The vector $\vec{g}$ represents a known body force, which in most cases is gravity. Note that Fourier's law has been assumed for the conduction term in Eq. (1c), and also that compression work has been neglected. The reader is referred to Ref. 5 for a detailed derivation and description of Eqs. (1).

In general, the system parameters appearing in Eqs. (1) (e.g., ρ , C_p , k , Q , or the viscosity coefficients contained in the definition of τ) can depend on temperature and velocity, thus coupling these equations

into a nonlinear system of partial differential equations. This nonlinear dependence is taken into account in the sensitivity description presented below.

Definition of a Response Function

The first step in any sensitivity formulation is to identify an important "output" quantity called a response R . A general response is now defined having the integral form

$$R \equiv \int_t \int_V F [\vec{v}, P, T] dV dt, \quad (2)$$

where V and t represent the space and time domains. The arbitrary function F can be chosen to include delta or weight functions, so as to yield peak or average velocity, pressure or temperature responses. For example, if a peak pressure is desired at some point in time and space (i.e., t_0 and $\vec{r}_0$), then F would be chosen using delta functions as

$$F = P \delta(\vec{r} - \vec{r}_0) \delta(t - t_0), \quad (3)$$

which yields the response

$$R = \int_t \int_V P \delta(\vec{r} - \vec{r}_0) \delta(t - t_0) dV dt = P(\vec{r}_0, t_0). \quad (4)$$

Examples of other responses are given below.

In sensitivity theory the object is to calculate the sensitivity of R to some "input" parameter α . Therefore, Eq. (2) is differentiated with respect to giving

$$\frac{dR}{d\alpha} = \int_t \int_V \left[\vec{v} \cdot \frac{\partial \vec{v}}{\partial \alpha} + \frac{\partial F}{\partial P} \frac{\partial P}{\partial \alpha} + \frac{\partial F}{\partial T} \frac{\partial T}{\partial \alpha} \right] dV dt, \quad (5a)$$

where $\vec{v}_v$ is defined in analogy to the gradient ∇ as

$$\vec{v}_v \equiv \left(\frac{\partial}{\partial v_1}, \frac{\partial}{\partial v_2}, \frac{\partial}{\partial v_3} \right)^T. \quad (5b)$$

As discussed in Ref. 4, the use of Eq. (5a) to obtain sensitivity information for large codes can be quite expensive and time-consuming. Therefore, it is desirable to consider the alternate procedure described below.

Adjoint Equations of Charge

As mentioned in the Introduction, the application of DST to Eqs. (1) involves the development of equations which are adjoint to the differentiated form (with respect to an arbitrary parameter α) of the physical equations. The differentiation of system (1) and derivation of a corresponding adjoint system is only indicated here in general. A rigorous description of the derivation is given in Appendix A.

The adjoint equations of change corresponding to Eqs. (1) are obtained via the following steps:

- 1) All quantities in Eqs. (1) are assumed to be functions of the parameter α . Each equation is differentiated with respect to resulting in a linear system of differential equations featuring the new dependent variables $\frac{\partial \vec{v}}{\partial \alpha}$, $\frac{\partial P}{\partial \alpha}$, and $\frac{\partial T}{\partial \alpha}$. This system has the form

$$\underline{L} \left(\frac{\partial \vec{v}}{\partial \alpha}, \frac{\partial P}{\partial \alpha}, \frac{\partial T}{\partial \alpha} \right)^T = \vec{S}, \quad (6)$$

where $\underline{L}$ is a 3×3 matrix of differential operators operating on the dependent variable vector, and $\vec{S}$ is a source vector containing the explicit partial derivatives of the physical properties and parameters with respect to α .

- 2) Determine a differential matrix operator $\underline{L}^*$ that is adjoint to $\underline{L}$ from the definition

$$\int_t \int_V (\vec{f} \cdot \underline{L}^* \vec{g}) dV dt = \int_t \int_V (\vec{g} \cdot \underline{L} \vec{f}) dV dt + \text{boundary terms} , \quad (7)$$

where $\vec{f}$ and $\vec{g}$ are arbitrary vector functions. Use of this definition results in the following adjoint system corresponding to responding to Eq. (6):

$$\underline{L}^*(m^*, \vec{p}^*, H^*)^T = \vec{S}^* , \quad (8)$$

where m^* , $\vec{p}^*$, and H^* are labeled as adjoint mass, momentum and enthalpy functions, and are further discussed below. The quantity $\vec{S}^*$ is an adjoint source to be defined later. For the time being $\vec{S}^*$ is assigned the general form

$$\vec{S}^* \equiv (\vec{S}_T^*, S_p^*, S_T^*)^T . \quad (9)$$

It can be shown that the specific form of the equations corresponding to system (8) are

$$\begin{aligned} -\rho \nabla m^* &= \frac{D}{Dt} (\rho p^*) - (\nabla \vec{v}) \cdot (\rho \vec{p}^*) + \nabla \vec{v} : (\tau : \nabla \vec{p}^*) - \nabla \cdot \left[\nabla_{\nabla \vec{v}} (\tau : \nabla \vec{p}^*) \right] \\ &- H^* \left[\rho C_p \nabla T + \nabla_{\nabla \vec{v}} (\tau : \nabla \vec{v}) - \rho \vec{g} - \nabla_{\nabla \vec{v}} Q \right] + 2 \nabla \cdot (H^* \tau) + \vec{S}_T^* \end{aligned} \quad (10a)$$

$$-\nabla \cdot \vec{p}^* = S_p^* , \quad (10b)$$

$$\begin{aligned} -\rho C_p \left[\frac{DH^*}{Dt} + H^* \nabla \cdot \vec{v} \right] - k \nabla^2 H^* + H^* \frac{\partial \tau}{\partial T} : \nabla \vec{v} - H^* \frac{\partial Q}{\partial T} \\ = \frac{\partial \rho}{\partial T} \left[\frac{Dm^*}{Dt} - \frac{D\vec{v}}{Dt} \cdot \vec{p}^* \right] + \vec{g} \cdot \vec{p}^* + \frac{\partial \tau}{\partial T} : \nabla \vec{p}^* + S_T^* , \end{aligned} \quad (10c)$$

where the tensor operator $\nabla_{\nabla \vec{v}}$ has as components

$$\nabla_{\nabla \vec{v}} i j = \frac{\partial}{\partial (\partial v_i / \partial x_j)} . \quad (10d)$$

Sensitivity Coefficient Formulation

Noting the mathematical definition of adjoint given by Eq. (7), the physical and adjoint operators $\underline{L}$ and $\underline{L}^*$ of Eqs. (6) and (8), respectively, can be related as

$$\begin{aligned} \int_t \int_V \left(\frac{\partial \vec{v}}{\partial \alpha}, \frac{\partial P}{\partial \alpha}, \frac{\partial T}{\partial \alpha} \right) \underline{L}^*(\vec{m}^*, \vec{p}^*, H^*)^T dV dt \\ = \int_t \int_V (\vec{m}^*, \vec{p}^*, H^*) \underline{L} \left(\frac{\partial \vec{v}}{\partial \alpha}, \frac{\partial P}{\partial \alpha}, \frac{\partial T}{\partial \alpha} \right)^T dV dt + BT, \end{aligned} \quad (11)$$

where BT represents the boundary terms that arise in application of the adjoint definition and are discussed on p. 12. The integrands in Eq. (11) can be replaced using Eqs. (6) and (8) to give

$$\int_t \int_V \vec{S}^* \cdot \left(\frac{\partial \vec{v}}{\partial \alpha}, \frac{\partial P}{\partial \alpha}, \frac{\partial T}{\partial \alpha} \right)^T dV dt = \int_t \int_V \vec{S}^* (\vec{m}^*, \vec{p}^*, H^*)^T dV dt + BT. \quad (12)$$

Inspection of Eq. (5a) and the LHS of Eq. (12) indicates that by specifying the adjoint source

$$\vec{S}^* = (\vec{S}_V^*, S_P^*, S_T^*)^T = \left(\vec{\nabla}_V F, \frac{\partial F}{\partial P}, \frac{\partial F}{\partial T} \right)^T, \quad (13)$$

the response sensitivity can be expressed in terms of the adjoint functions as

$$\frac{dR}{d\alpha} = \int_t \int_V \vec{S}^* \cdot (\vec{m}^*, \vec{p}^*, H^*)^T dV dt + BT. \quad (14)$$

It is important to recognize that the adjoint source $\vec{S}^*$ is determined solely from the particular response represented by Eq. (2).

The physical parameter source $\vec{S} = (S_m, \vec{S}_p, S_H)^T$ can be shown to have the elements

$$S_m = - \frac{D}{Dt} \left(\frac{\partial \rho}{\partial \alpha} \right) - \frac{\partial \rho}{\partial \alpha} \nabla \cdot \vec{v}, \quad (15a)$$

$$S_p^{\rightarrow} = \frac{\partial f}{\partial \alpha} \left[\vec{g} - \frac{D\vec{v}}{Dt} \right] - \nabla \cdot \frac{\partial \tau}{\partial \alpha} + \rho \frac{\partial \vec{g}}{\partial \alpha} , \quad (15b)$$

$$S_H = - \frac{\partial(\rho C_p)}{\partial \alpha} \frac{DT}{Dt} + \nabla \cdot \left(\frac{\partial k}{\partial \alpha} \nabla T \right) - \frac{\partial \tau}{\partial \alpha} : \nabla \vec{v} + \frac{\partial Q}{\partial \alpha} . \quad (15c)$$

Substitution of this source into Eq. (14) yields the final form for the response derivative

$$\begin{aligned} \frac{dR}{d\alpha} = \int_t \int_V \left\{ - m^* \left[\frac{D}{Dt} \left(\frac{\partial \rho}{\partial \alpha} \right) + \frac{\partial \rho}{\partial \alpha} \nabla \cdot \vec{v} \right] + \vec{p}^* \cdot \left[\frac{\partial \rho}{\partial \alpha} \left(\vec{g} - \frac{D\vec{v}}{Dt} \right) - \nabla \cdot \frac{\partial \tau}{\partial \alpha} + \rho \frac{\partial \vec{g}}{\partial \alpha} \right] \right. \\ \left. + H^* \left[- \frac{\partial(\rho C_p)}{\partial \alpha} \frac{DT}{Dt} + \nabla \cdot \left(\frac{\partial k}{\partial \alpha} \nabla T \right) - \frac{\partial \tau}{\partial \alpha} : \nabla \vec{v} + \frac{\partial Q}{\partial \alpha} \right] \right\} dV dt + BT . \quad (16) \end{aligned}$$

This equation expresses the response sensitivity to any thermal-hydraulic parameter as an integration of the physical and adjoint solutions.

Units for the adjoint functions can be inferred from Eq. (16) by noting that the three bracketed terms have the dimensions of mass, momentum, and enthalpy, respectively, multiplying inverse volume-time- $[\alpha]$. Therefore, to conserve dimensions in Eq. (16) m^* , $\vec{p}^*$, and H^* must have the dimensions of $[R]$ times inverse mass, momentum, and enthalpy, respectively. In SI units then, m^* is in $[R]/\text{kg}$, $\vec{p}^*$ is in $[R]/\text{kg-m/s}$, and H^* is in $[R]/\text{J}$.

As an example of the use of Eq. (16), consider a scale factor change in $k(T)$. Representing $k(T)$ as a constant scale factor times a temperature-dependent shape function,

$$k(T) = k_0 s(T) . \quad (17)$$

the sensitivity to the parameter k_0 is obtained by setting $\alpha = k_0$ in Eq. (16). All terms not involving the thermal conductivity vanish resulting in the sensitivity derivative

$$\frac{dR}{dk_0/k_0} = \int_t \int_v H^* \nabla \cdot (k \nabla T) dV dt \quad (18)$$

Other parameters appearing in Eq. (16) can be treated in an analogous manner. Also recognize that sensitivities to all parameters are readily available once the solutions to the physical system (1) and the adjoint system (10) are known.

Physical significance can be attached to the adjoint functions by examining the integrand terms of the sensitivity equation (16). The adjoints m^* , $\vec{p}^*$, and H^* are seen to represent the space and time importance of the various mass, momentum, and enthalpy transport terms in the determination of the sensitivity $\frac{dR}{d\alpha}$, hence the name "importance functions." Further discussion concerning the physical significance of the importance functions is given below.

Adjoint Boundary Terms

Application of the physical equations of change to a given problem requires the specification of physical boundary and time conditions. Application of the adjoint equations of change to the same problem requires specification of adjoint boundary and time conditions. These adjoint conditions are obtained by inspecting the residual boundary and time terms [BT, cf. Eq. (7)] resulting from the derivation for $\underline{L}^*$ on p. 7. These terms can be shown to have the form

$$\begin{aligned} BT = & - \int_v \left[m^* \frac{\partial \rho}{\partial T} \frac{\partial T}{\partial \alpha} + \rho \vec{p}^* \cdot \frac{\partial \vec{v}}{\partial \alpha} + H^* \rho C_p \frac{\partial T}{\partial \alpha} \right] \Big|_0^f dv \\ & - \int_t \oint_{\partial V} \left[\rho m^* \frac{\partial \vec{v}}{\partial \alpha} + \vec{v} m^* \frac{\partial \rho}{\partial T} \frac{\partial T}{\partial \alpha} + \left(\frac{\partial \vec{v}}{\partial \alpha} \cdot \nabla_{\vec{v}} \tau \right) \cdot \vec{p}^* \right. \\ & \left. + \rho \vec{v} \left(\vec{p}^* \cdot \frac{\partial \vec{v}}{\partial \alpha} \right) + \left(\nabla \frac{\partial \vec{v}}{\partial \alpha} : \nabla_{\vec{v}} \tau \right) \cdot \vec{p}^* - \frac{\partial \vec{v}}{\partial \alpha} \cdot (\nabla_{\vec{v}} \tau : \nabla \vec{p}^*) \right] dv dt \end{aligned}$$

$$\begin{aligned}
& + \vec{p}^* \frac{\partial \vec{p}}{\partial \alpha} + \vec{p}^* \cdot \frac{\partial \tau}{\partial T} \frac{\partial \vec{T}}{\partial \alpha} + 2H^* \tau \cdot \frac{\partial \vec{v}}{\partial \alpha} + H^* \rho C_p \vec{v} \frac{\partial T}{\partial \alpha} \\
& + k \nabla H^* \frac{\partial T}{\partial \alpha} - H^* \nabla \left(k \frac{\partial T}{\partial \alpha} \right) \cdot \vec{dA} dt, \quad (19)
\end{aligned}$$

where t_f is the final time of the physical transient, and $\vec{dA}$ is an outward pointing differential area vector normal to the surface ∂V which encloses the volume V .

The terms appearing in Eq. (19) represent either adjoint boundary and time conditions or sensitivity coefficients to the physical boundary and time conditions. However, which terms become conditions and which become sensitivities is determined by the physical conditions and the knowledge that the response derivative must be independent of unknown values of $\frac{\partial \vec{v}}{\partial \alpha}$, $\frac{\partial \vec{p}}{\partial \alpha}$, and $\frac{\partial T}{\partial \alpha}$. For example, suppose a physical problem has the initial conditions for temperature and velocity of T_0 and $\vec{v}_0$, respectively. Choosing adjoint time conditions at t_f for m^* , $\vec{p}^*$ and H^* to be zero so as to eliminate the unknown values of $\frac{\partial \vec{v}}{\partial \alpha}$, $\frac{\partial \vec{p}}{\partial \alpha}$, and $\frac{\partial T}{\partial \alpha}$ at t_f , the volume integral in Eq. (19) simplifies to the physical initial condition sensitivities:

$$\begin{aligned}
\text{BT (volume integral)} = & \int_V \left[\left(m^* \frac{\partial \rho}{\partial T} + \rho C_p H^* \right) \right]_{t=0} \frac{\partial T_0}{\partial \alpha} \\
& + \rho \vec{p}^* \Big|_{t=0} \cdot \frac{\partial \vec{v}_0}{\partial \alpha} \Big] dV. \quad (20)
\end{aligned}$$

The same procedure applies in deriving adjoint boundary conditions from the surface-time integrals in Eq. (19). This is best illustrated using specific examples as done on pp. 12 through 25.

Rules for Applying the Adjoint Equations of Change

When applying the adjoint system (10) to a specific thermal-hydraulic problem that does not contain all the conservation equations

and space-time dependence represented by the physical system (1), there are two rules that must be adhered to: the rule of equivalent dependence and the rule of correspondence.

The rule of equivalent dependence states that the set of independent variables describing the physical solution is identical to the set describing the adjoint solution. For example, in the steady boundary-layer flow over a heated flat plate, the velocity and temperature solutions are functions of the space coordinates x and y only. Therefore, the corresponding adjoint mass, momentum, and enthalpy solutions will be functions of x and y only.

It can be seen from the derivation of the adjoint system (10), that each adjoint variable corresponds to exactly one physical equation in system (1). Furthermore, each adjoint equation directly corresponds to one physical dependent variable in system (1). The specific associations are depicted in Table 1. Thus, a rule of correspondence is

Table 1. Matrix Description for Applying the Rule of Correspondence

Equation Name	Equation No.	Dependent Variables									
		v_1	v_2	v_3	P	T	m^*	p_1^*	p_2^*	p_3^*	H^*
Continuity	(1a)						x				
$\hat{e}_1$ -Momentum	(1b) $\hat{e}_1$							x			
$\hat{e}_2$ -Momentum	(1b) $\hat{e}_2$								x		
$\hat{e}_3$ -Momentum	(1b) $\hat{e}_3$									x	
Energy	(1c)										x
v_1 -Adjoint	(10a) $\hat{e}_1$	x									
v_2 -Adjoint	(10a) $\hat{e}_2$		x								
v_3 -Adjoint	(10a) $\hat{e}_3$			x							
P -Adjoint	(10b)				x						
T -Adjoint	(10c)					x					

established which allows simplification of system (1) to also result in simplification of system (10). In other words, this rule is used to eliminate irrelevant adjoint variables and equations for a specific problem. For example, recall that the boundary-layer equations for the flat plate include continuity, $\bar{e}_1$ -momentum, and energy, which are solved for the dependent variables v_1 , v_2 , and T . Locating these physical equations on the LHS of Table 1 and moving horizontally indicates m^* , p^* , and H^* are the three relevant adjoint variables. Locating the physical dependent variables at the top of Table 1 and moving vertically indicates that the $\bar{e}_1$ and $\bar{e}_2$ components of Eq. (10a) and Eq. (10c) are the three relevant adjoint equations. Further illustration of the above two rules and the use of Table 1 are given below.

APPLICATION OF THERMAL-HYDRAULIC DIFFERENTIAL SENSITIVITY THEORY

The purpose of this section is to illustrate the procedure for applying Eqs. (10), (13), (16), and (19) to specific thermal-hydraulics problems. The simple analytical examples presented below are not as complex as real-world applications, but are useful in demonstrating application of the theory.

Couette Flow

Consider the fully developed, steady laminar flow of oil between two horizontal plates of separation L . The lower plate has a maintained temperature of T_0 and a horizontal velocity of u_0 ; similar conditions exist for the upper plate and are specified as T_L and u_L . All dependent variables are independent of the flow direction coordinate x . It can be shown for this problem that the general equations of change simplify to

$$0 = \frac{d^2 u}{dy^2} , \quad (21a)$$

$$0 = \mu \left(\frac{dT}{dy} \right)^2 + k \frac{d^2 T}{dy^2} . \quad (21b)$$

Using the boundary conditions described above, Eqs. (21) have the solution

$$u = u_o + (u_L - u_o) \frac{y}{L} . \quad (22a)$$

$$T = T_o + (T_L - T_o) \frac{y}{L} + \frac{1}{2} \frac{\mu}{k} (u_L - u_o)^2 \left[\frac{y}{L} - \left(\frac{y}{L} \right)^2 \right] . \quad (22b)$$

To determine how small changes in the parameters k , μ , T_o , T_L , u_o , and u_L affect the oil temperature between the plates, a DST analysis of Eqs. (21) is carried out using the average oil temperature as a response. The adjoint equations of change for Couette flow are obtained by simplifying system (10) with the rules of equivalent dependence and correspondence. Since Couette flow depends only upon y , the same is true for the adjoint problems. Equations (21) contain only the x -momentum and energy equations, solved for velocity u and temperature T . Table 1 indicates that the adjoint problem contains only the $\hat{e}_x$ component of Eq. (10a) and Eq. (10c); these are solved for the adjoint variables p_x^* and H^* . The resulting adjoint system then simplifies to

$$0 = \mu \frac{d^2 p_x^*}{dy^2} - 2\mu \frac{du}{dy} \frac{dH^*}{dy} + S_u^* , \quad (23a)$$

$$0 = k \frac{d^2 H^*}{dy^2} + S_T^* . \quad (23b)$$

Adjoint boundary conditions for Eqs. (23) are determined by simplifying Eq. (19), as mentioned on pp. 9 and 10. The volume integrals vanish since Couette flow is steady. The remaining terms can then be reduced to

$$\begin{aligned}
 BT = t_f A \left[\nu \frac{d}{dy} \left(\frac{\partial u}{\partial \alpha} \right) p_x^* - \nu \frac{\partial u}{\partial \alpha} \frac{dp_x^*}{dy} + 2H^* \nu \frac{du}{dy} \frac{\partial u}{\partial \alpha} \right. \\
 \left. - k \frac{dH^*}{dy} \frac{\partial T}{\partial \alpha} + H^* \frac{d}{dy} \left(k \frac{\partial T}{\partial \alpha} \right) \right] \Big|_0^L. \quad (24)
 \end{aligned}$$

Since second derivatives of both p_x^* and H^* appear in Eqs. (23), each of these variables must have exactly two boundary conditions. Recalling that these conditions must eliminate the unknown values of $\frac{\partial u}{\partial \alpha}$ and $\frac{\partial T}{\partial \alpha}$ from Eq. (24) while retaining known values as sensitivities, the boundary conditions are

$$p_x^* = 0 \text{ and } H^* = 0 \text{ at } y = 0, L. \quad (25)$$

Applying these conditions to Eq. (24) gives the result

$$B1 = -t_f A \left[\nu \frac{dp_x^*}{dy} \frac{\partial u}{\partial \alpha} + k \frac{dH^*}{dy} \frac{\partial T}{\partial \alpha} \right]_0^L, \quad (26)$$

where t_f is some arbitrary final time (unimportant for steady Couette flow), and A is the plate area such that $L \cdot A$ is the volume V between the plates.

Simplification of Eq. (16) combined with Eq. (26) yields the Couette sensitivities

$$\begin{aligned}
 \frac{dR}{d\alpha} = t_f A \left[\int_0^L H^* \left[\frac{\partial k}{\partial \alpha} \frac{d^2 T}{dy^2} + \frac{\partial u}{\partial \alpha} \left(\frac{du}{dy} \right)^2 \right] dy \right. \\
 \left. - \nu \frac{dp_x^*}{dy} \frac{\partial u}{\partial \alpha} \Big|_0^L - k \frac{dH^*}{dy} \frac{\partial T}{\partial \alpha} \Big|_0^L \right]. \quad (27)
 \end{aligned}$$

For an average temperature response, Eq. (2) assumes the specific form

$$R = \int_0^{t_f} \int_V \frac{1}{V t_f} T \, dV \, dt = \int_0^L \frac{1}{L} T \, dy = \bar{T}, \quad (28)$$

and F becomes the integrand of Eq. (28) [comp. Eq. (2)]. Determination of the adjoint sources S_u^* and S_T^* via Eq. (13) yields

$$S_u^* = \frac{\partial F}{\partial u} = 0 \text{ and } S_T^* = \frac{\partial F}{\partial T} = \frac{1}{v_{zf}}. \quad (29)$$

Solution of Eqs. (23) using these adjoint sources and the conditions given by Eq. (25) is seen to be

$$p_x^* = -\frac{L}{kAt_f} (u_L - u_o) \left[\frac{1}{6} \frac{y}{L} - \frac{1}{2} \left(\frac{y}{L} \right)^2 + \frac{1}{3} \left(\frac{y}{L} \right)^3 \right], \quad (30a)$$

$$H^* = \frac{1}{2} \frac{L}{kAt_f} \left[\frac{y}{L} - \left(\frac{y}{L} \right)^2 \right]. \quad (30b)$$

The physical and adjoint solutions, using the parametric values for engine oil given in Table 2, are presented in Figs. 1. Figure 1a shows typical Couette velocity and temperature profiles, and Fig. 1b shows the corresponding adjoint momentum and enthalpy functions.

Table 2. Couette Flow Sensitivity Results

Parameter α	Nominal Value	DST $\frac{dT}{d\alpha/\alpha}$ K	Direct $\frac{dT}{d\alpha/\alpha}$ K
k	0.131W/m-K	-0.286	-0.286
μ	4.49mPa-s	0.286	0.286
T_o	400K	0.500	0.500
T_L	400K	0.500	0.500
u_o	0	0	0
u_L	10m/s	0.571	0.571

Fig. 1a. Couette flow velocity and temperature profiles.

Fig. 1b. Couette flow adjoint momentum and enthalpy profiles.

As mentioned on the preceding page, interpretation of the adjoint solutions can only be inferred from the sensitivity coefficients appropriate for the physical problem. For example, Eq. (27) for Couette flow yields the viscosity sensitivity coefficient

$$\frac{d\bar{T}}{d\nu/\nu} = t A \int_0^L H^* \nu \left(\frac{du}{dy} \right)^2 dy \quad (31)$$

Here H^* represents the importance of viscous heating upon the average temperature, and as physical intuition may suggest, the enthalpy adjoint in Fig. 1b indicates that viscous heating has the most impact upon $\bar{T}$ at $y/L = 1/2$. Similar interpretations for H^* and p_x^* can be obtained from the other coefficients in Eq. (27).

Table 2 presents Couette flow sensitivity results for the average oil temperature. The

first two columns list the sensitivity parameters and their nominal values. The last two columns give the numerical sensitivities using Eq. (27) and direct method calculations via Eqs. (22b) and (28), respectively. Obviously, the identical values in the two columns serve to validate DST. Note that for engine oil the velocity of the upper plate (or rotation of a bearing) gives the largest sensitivity.

Lumped Heat Capacity

Consider a tungsten electric-lamp filament in a deep space environment radiating at a temperature T_0 . At time zero, electric power is switched off and the filament cools according to the Stefan-Boltzmann law. Applying a lumped heat capacity analysis to the filament, it can be shown that the general energy equation, Eq. (1c), simplifies to

$$\rho C_p \frac{dT}{dt} = - \frac{1}{V} A \epsilon \sigma T^4, \quad (32)$$

where A is the surface area of the filament which has an emissivity of ϵ . Using the initial condition given above, the filament temperature as a function of time is

$$T = [T^{-3} + \gamma t]^{-\frac{1}{3}}, \quad (33a)$$

where

$$\gamma = \frac{3A\epsilon\sigma}{V\rho C_p}. \quad (33b)$$

To determine how small changes in the parameters A , V , ϵ , ρ , C_p , and T affect the cooling of the filament, a DST analysis of Eqs. (33) is implemented. The particular response of interest is the temperature when the filament is cool enough to touch, i.e., 298K.

The adjoint equations of change for lumped heat capacity are obtained via system (10), and by using the rules of equivalent dependence and correspondence. The filament problem depends only upon time; hence, the same is true for the adjoint problem. The filament problem contains only the energy equation solved for temperature T . Table 1 indicates that the adjoint problem should contain only Eq. (10c), solved for adjoint variable H^* . Simplification reduces this equation to

$$-\rho C_p \frac{dH^*}{dt} - H^* \frac{\partial Q}{\partial T} = S_T^* \quad (34)$$

An adjoint time condition for Eq. (34) is obtained by simplifying Eq. (19). All surface integrals vanish since lumped capacity is space independent, and the remaining volume integrals simplify to

$$BT = -H^* V \rho C_p \left. \frac{\partial T}{\partial \alpha} \right|_0^{t_f} \quad (35)$$

Evaluation of Eq. (35) at the lower limit gives a term involving $\frac{\partial T_0}{\partial \alpha}$, which is determined from the known initial condition T_0 . Since $\frac{\partial T}{\partial \alpha}$ at $t = t_f$ is not known, this term must be eliminated by the following choice of the adjoint time condition:

$$H^*(t = t_f) = 0. \quad (36)$$

Combining Eqs. (16) and (35) then yields the lumped heat capacity sensitivity formulation

$$\frac{dR}{d\alpha} = V \int_0^{t_f} H^* \left[-\frac{\partial(\rho C_p)}{\partial \alpha} \frac{\partial T}{\partial t} + \frac{\partial Q}{\partial \alpha} \right] dt + H^* V \rho C_p \frac{\partial T_c}{\partial \alpha} \quad (37)$$

Assuming the filament temperature at some final time is the desired response, i.e.,

$$R = \int_0^{t_f} \int_V F(t, \mathbf{r}) dV dt = T(t_f) \quad , \quad (38)$$

then F is the integrand of Eq. (38) as defined by Eq. (2). Solving for the adjoint source S_T^* via Eq. (13) yields

$$S_T^* = \frac{\partial F}{\partial T} = \frac{1}{V} \delta(t - t_f) \quad . \quad (39)$$

Solution of Eq. (34) using this adjoint source and the condition given by Eq. (36) can be finally obtained as

$$H^* = \frac{1}{V\rho C_p} \left[\frac{T_0^{-3} + \gamma t}{T_0^{-3} + \gamma t_f} \right]^{1/3} \quad . \quad (40)$$

A cylindrical tungsten filament of diameter 1 mm and length 1 cm is assumed to have the initial temperature and material properties listed in the first two columns of Table 3. The time required for the filament to cool from T_0 to room temperature is $t_f = 366s$.

Table 3. Lumped Heat Capacity
Sensitivity Results

Parameter α	Nominal Value	DST $\frac{dT(t_f)}{d\alpha/\alpha}$ K	Direct $\frac{dT(t_f)}{d\alpha/\alpha}$ K
ρ	19.3Mg/m ³	99.2	99.2
C_p	134J/kg-K	99.2	99.2
A	0.314cm ²	-99.2	-99.2
ϵ	0.390	-99.2	-99.2
T_0	3600K	0.169	0.169
V	7.85mm ³	99.2	99.2

Figure 2 presents the physical and adjoint solutions given by Eqs. (33) and (40) over the time interval zero to t_f . The temperature drops sharply over the first hundred seconds, and then levels off. The adjoint enthalpy is approximately linear over the entire transient, increasing in absolute value as t_f is approached.

The last two columns of Table 3 include the sensitivity of $T(t_f)$ to the various problem parameters. Obviously, the identical values in these columns serve to validate DST. The T_0 -sensitivity indicates that the exactness of T_0 has negligible impact upon $T(t_f)$. This is supported by observing the flatness of the Fig. 2 temperature solution in the region near t_f and the near zero value of the adjoint importance function at $t = 0$. Other sensitivities in Table 3 have equal magnitude as might be expected after inspection of Eq. (33).

Fig. 2. Lumped heat capacity temperature and adjoint enthalpy time solutions.

An Irrotational Vortex

Consider a steady irrotational vortex (described in cylindrical geometry) which exhibits flow symmetry about the vertical z -axis and is independent of the z coordinate. Such an idealized flow field reasonably approximates the velocity components and pressure gradients of a

tornado. The pressure and velocity are measured at some radius r_0 in the flow field providing the boundary conditions $P(r_0)$, $v_r(r_0)$, and $v_\theta(r_0)$. Here v_r and v_θ are the radial and tangential velocity components, respectively. The continuity and momentum equations describing this vortex can be obtained by simplifying Eqs. (1) to give

$$\frac{d}{dr} (r v_r) = 0 \quad , \quad (41a)$$

$$v_r \frac{dv_r}{dr} - \frac{1}{r} v_\theta^2 = - \frac{1}{\rho} \frac{dP}{dr} \quad , \quad (41b)$$

$$v_r \frac{dv_\theta}{dr} + \frac{1}{r} v_r v_\theta = 0 \quad . \quad (41c)$$

Using the measured information given above, the velocity and pressure solutions to Eqs. (41) are

$$v_r = v_r(r_0) \frac{r_0}{r} \quad , \quad (42a)$$

$$v_\theta = v_\theta(r_0) \frac{r_0}{r} \quad , \quad (42b)$$

$$P = P(r_0) - \frac{1}{2} \rho \left[v_r^2(r_0) + v_\theta^2(r_0) \right] \left[\left(\frac{r_0}{r} \right)^2 - 1 \right] \quad . \quad (42c)$$

A DST analysis of Eqn. (41) is now carried out to determine how small changes in the air density and measured information affect the pressure difference $P_{atm} - P(r')$. This difference describes the net force on the walls of a hermetically sealed house located at radius r' in the tornado, ($r' < r_0$).

Again, the adjoint equations of change are obtained via system (10) and by using the rules of equivalent dependence and correspondence. The vortex problem depends only upon the radius r ; hence, the same is true for the adjoint problem. The vortex problem contains continuity, $\hat{e}_r$ -momentum, and $\hat{e}_\theta$ -momentum equations solved for velocities v_r , v_θ , and pressure P . Table 1 indicates that the adjoint problem should contain the $\hat{e}_r$ and $\hat{e}_\theta$ components of Eq. (10a) and Eq. (10b), solved for the adjoint variables m^* , p_r^* , and p_θ^* . Simplification of these adjoint equations yields

$$-\rho \frac{dm^*}{dr} = \rho \left(v_r \frac{dp_r^*}{dr} - \frac{1}{r} v_\theta p_\theta^* \right) - \rho \left(p_r^* \frac{dv_r}{dr} + p_\theta^* \frac{dv_\theta}{dr} \right) + S_{v_r}^* \quad (43a)$$

$$0 = \rho \left(r \frac{dp_\theta^*}{dr} + \frac{1}{r} v_\theta p_r^* \right) - \rho \left(\frac{1}{r} v_r p_\theta^* - \frac{1}{r} v_\theta p_r^* \right) + S_{v_\theta}^* \quad (43b)$$

$$-\frac{d}{dr} (r p_r^*) = r S_p^* \quad (43c)$$

Adjoint boundary conditions are next obtained by simplifying Eq. (19). The volume integrals vanish since the vortex is steady, and the remaining surface integrals reduce to

$$BT = -t_f 2\pi r_o L \left[\rho m^* \frac{\partial v_r}{\partial \alpha} + \rho v_r \left(p_r^* \frac{\partial v_r}{\partial \alpha} + p_\theta^* \frac{\partial v_\theta}{\partial \alpha} \right) + p_r^* \frac{\partial P}{\partial \alpha} \right]_0^{r_o} \quad (44)$$

An inspection of Eqs. (43) indicates that a boundary condition is required for each adjoint function m^* , p_r^* , and p_θ^* . Recalling that these conditions must eliminate the unknown values of $\frac{\partial v_r}{\partial \alpha}$, $\frac{\partial v_\theta}{\partial \alpha}$, and $\frac{\partial P}{\partial \alpha}$ from Eq. (44) while retaining known values as sensitivities, the following adjoint conditions are chosen:

$$m^*(0) = 0, \quad p_r^*(\infty) = 0, \quad \text{and} \quad p_\theta^*(0) = 0, \quad (45)$$

which in combination with Eqs. (16) and (44) yield the vortex response derivative

$$\begin{aligned} \frac{dR}{d\alpha} = & -t_f 2\pi L \left[\int_0^{r_0} \frac{\partial \rho}{\partial \alpha} \vec{r} p^* \cdot \frac{D\vec{v}}{Dt} dr \right. \\ & \left. + r_0 \left[\rho m^* \frac{\partial v_r}{\partial \alpha} + \rho v_r \left(p_r^* \frac{\partial v_r}{\partial \alpha} + v_\theta^* \frac{\partial v_\theta}{\partial \alpha} \right) + p_r^* \frac{\partial P}{\partial \alpha} \right]_{r_0} \right]. \quad (46) \end{aligned}$$

The pressure response discussed above can be represented as

$$R = \int_0^{t_f} \int_V \frac{\delta(r-r')}{2\pi r' L t_f} dV dt = P(r'), \quad (47)$$

implying [via Eqs. (2) and (13)] the necessary adjoint sources to be

$$S_{v_r}^* = 0, \quad S_{v_\theta}^* = 0, \quad S_P^* = -\frac{(r-r')}{2\pi r' L t_f}. \quad (48)$$

Solution of Eqs. (43) using this adjoint source and the boundary conditions (45) can be obtained as

$$m^* = \frac{v_r(r_0)}{2\pi r_0 L t_f} \left(\frac{r_0}{r'} \right)^2 U(r - r'), \quad (49a)$$

$$p_r^* = \frac{-1}{2\pi r_0 L t_f} \frac{r_0}{r} U(r - r'), \quad (49b)$$

$$p_\theta^* = \frac{1}{2\pi r_0 L t_f} \frac{v_\theta}{v_r} \left[\frac{r r_0}{r'^2} - \frac{r_0}{r} \right] U(r - r'), \quad (49c)$$

where $U(r - r')$ is a unit step function.

A small tornado is measured at $r_0 = 50$ m to have the velocities and pressure given in the first two columns of Table 4. Figures 3a and

Table 4. Inviscid Tornado Sensitivity Results

Parameter α	Nominal Value	DST $\frac{dP(r')}{d\alpha/\alpha}$ Pa	Direct $\frac{dP(r')}{d\alpha/\alpha}$ Pa
ρ	0.710g/m ³	-17.2	-17.2
$v_r(r_0)$	-4.88m/s	-0.406	-0.406
$v_\theta(r_0)$	44.7m/s	-34.0	-34.0
$P(r_0)$	3000Pa	3000	3000

It presents the physical and adjoint solutions given by Eqs. (42) and (49) shown over 50 m of radius. The velocities and pressure are observed to rapidly increase moving from r_0 to the vortex center. The adjoint functions vary in different fashions but all drop to zero for $r < r'$, thus linking the response $P(r')$ to the vortex boundary conditions at r_0 .

Fig. 3a. Inviscid tornado velocity and pressure profiles.

Fig. 3b. Inviscid tornado adjoint mass and momentum profiles.

Table 4 also presents $P(r')$ sensitivities to the various problem parameters in the last two columns. Recognizing that if $P(r')$ decreases, the net force $[P_{atm} - P(r')]$ increases, Table 4 shows the air density to have sizable sensitivity. This implies a cold air vortex is more destructive than a hot air vortex holding all other parameters constant.

SUMMARY AND CONCLUDING DISCUSSION

A thermal-hydraulic differential sensitivity theory represented by Eqs. (10), (13), (16), and (19) was derived. The procedure for applying these equations to large or long-running computer programs for the purpose of obtaining input parameter sensitivities includes the following steps:

- 1) Identify the physical equations and their dependent variables,
- 2) Obtain the appropriate adjoint equations via Table 1,
- 3) Specify a response (the important output quantity),
- 4) Solve the physical and adjoint equations using the adjoint source which corresponds to the response, and the appropriate adjoint boundary conditions (see p. 9),
- 5) Integrate (fold) the physical and adjoint solutions together to obtain all the parameter sensitivities via Eq. (16).

The above procedure is illustrated on pp. 11 through 24 using the analytical problems of Couette flow, lumped heat capacity, and irrotational flow. The sensitivity coefficients thus obtained can then be used in a subsequent uncertainty analysis, response surface construction, or for other purposes.

Thermal-hydraulic DST has been successfully applied to the single phase portion of the fast reactor safety code MELT-IIIA.^{6,7} This code

models the transient, one-dimensional, multi-region, two-phase, multi-component turbulent flow of sodium in parallel coolant channels, and has roughly 65 input parameters. Obviously, a direct method sensitivity analysis would require 66 MELT runs to calculate sensitivities to the entire input field. A DST analysis requires only two runs to calculate the same sensitivities--one base case run and its corresponding adjoint. For this MELT example, a computational savings of 97% is thus realized, disregarding the additional code development necessary to program the adjoint option.

Modification of thermal-hydraulic DST to include the complexities of compressible or two-phase flow is straightforward using the approach outlined above. Work of this nature is currently being performed by the authors, working with the fast reactor safety code VENUS-II.⁶

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**APPENDIX A. DERIVATION OF THE ADJOINT SYSTEM
FOR THE THERMAL HYDRAULIC CONSERVATION EQUATIONS**

In order to apply DST to system (1), it is necessary to differentiate each equation with respect to the arbitrary parameter α . For notational convenience, define the new variables

$$\vec{\psi} \equiv \frac{\partial \vec{v}}{\partial \alpha}, \quad \pi \equiv \frac{\partial P}{\partial \alpha}, \quad \phi \equiv \frac{\partial T}{\partial \alpha}.$$

Differentiation of Eq. (1a) produces

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{\partial \rho}{\partial T} \phi \right) + \vec{\psi} \cdot \nabla \rho + \vec{v} \cdot \nabla \left(\frac{\partial \rho}{\partial T} \phi \right) + \frac{\partial \rho}{\partial T} \phi \nabla \cdot \vec{v} + \rho \nabla \cdot \vec{\psi} \\ + \frac{\partial}{\partial t} \left(\frac{\partial \rho}{\partial \alpha} \right) + \vec{v} \cdot \nabla \left(\frac{\partial \rho}{\partial \alpha} \right) + \frac{\partial \rho}{\partial \alpha} \nabla \cdot \vec{v} = 0, \end{aligned}$$

which can be expressed in the form

$$\frac{D}{Dt} \left(\frac{\partial \rho}{\partial T} \phi \right) + \nabla \cdot (\rho \vec{\psi}) + \phi \left(\frac{\partial \rho}{\partial T} \nabla \cdot \vec{v} \right) = \frac{-D}{Dt} \left(\frac{\partial \rho}{\partial \alpha} \right) - \frac{\partial \rho}{\partial \alpha} \nabla \cdot \vec{v}. \quad (A.1)$$

Similarly, Eqs. (1b) and (1c) are differentiated and rearranged to get

$$\begin{aligned} \rho \left(\frac{D\vec{\psi}}{Dt} + \vec{\psi} \cdot \nabla \vec{v} \right) + \nabla \cdot \left[\nabla_{\vec{v}} \tau \cdot \vec{\psi} + \nabla_{(\nabla \vec{v})} \tau : \nabla \vec{\psi} \right] + \nabla \pi \\ + \phi \frac{D\rho}{Dt} \left(\frac{D\vec{v}}{Dt} - \vec{g} \right) + \nabla \cdot \left(\frac{\partial \tau}{\partial T} \phi \right) = \frac{\partial \rho}{\partial \alpha} \left(\vec{g} - \frac{D\vec{v}}{Dt} \right) - \nabla \cdot \frac{\partial \tau}{\partial \alpha} + \rho \frac{\partial \vec{g}}{\partial \alpha}, \quad (A.2) \end{aligned}$$

$$\begin{aligned} \vec{\psi} \cdot \left[\rho c_p \nabla T + \nabla_{\vec{v}} \tau : \nabla \vec{v} - \rho \vec{g} - \nabla_{\vec{v}} Q \right] + \nabla \vec{\psi} : \left[\tau^T + \nabla_{(\nabla \vec{v})} \tau : \nabla \vec{v} \right] + \phi \left(\frac{\partial (\rho c_p)}{\partial T} \right. \\ \left. \frac{DT}{Dt} + \frac{\partial \tau}{\partial T} : \nabla \vec{v} - \frac{\partial \rho}{\partial T} (\vec{v} \cdot \vec{g}) - \frac{\partial Q}{\partial T} \right) + \rho c_p \frac{D\phi}{Dt} - \nabla^2 (k\phi) = \frac{\partial \rho}{\partial \alpha} (\vec{v} \cdot \vec{g}) \\ - \frac{\partial (\rho c_p)}{\partial \alpha} \frac{DT}{Dt} + \nabla \cdot \left(\frac{\partial k}{\partial \alpha} \nabla T \right) - \frac{\partial \tau}{\partial \alpha} : \nabla \vec{v} + \rho \left(\vec{v} \cdot \frac{\partial \vec{g}}{\partial \alpha} \right) + \frac{\partial Q}{\partial \alpha}. \quad (A.3) \end{aligned}$$

Equations (A.1) - (A.3) are simplified by defining the following coefficient functions and source terms, which are known completely once the original system (1) has been solved.

$$s_1 \equiv -\frac{D}{Dt} \left(\frac{\partial \rho}{\partial \alpha} \right) - \frac{\partial \rho}{\partial \alpha} \nabla \cdot \vec{v}$$

$$\vec{s}_2 \equiv \frac{\partial \rho}{\partial \alpha} \left(\vec{g} - \frac{D\vec{v}}{Dt} \right) - \nabla \cdot \frac{\partial \tau}{\partial \alpha} + \rho \frac{\partial \vec{g}}{\partial \alpha}$$

$$s_3 \equiv \frac{\partial \rho}{\partial \alpha} (\vec{v} \cdot \vec{g}) - \frac{\partial(\rho c_p)}{\partial \alpha} \frac{DT}{Dt} + \nabla \cdot \left(\frac{\partial k}{\partial \alpha} \nabla T \right) - \frac{\partial \tau}{\partial \alpha} : \nabla \vec{v} + \rho \left(\vec{v} \cdot \frac{\partial \vec{g}}{\partial \alpha} \right) + \frac{\partial Q}{\partial \alpha}$$

$$\vec{A} \equiv \rho c_p \nabla T + \nabla \cdot \tau : \nabla \vec{v} - \rho \vec{g} - \nabla \cdot \vec{Q}$$

$$B \equiv \tau^T + \nabla \cdot (\nabla \vec{v}) \tau : \nabla \vec{v}$$

$$C \equiv \frac{\partial(\rho c_p)}{\partial T} \frac{DT}{Dt} + \frac{\partial \tau}{\partial T} : \nabla \vec{v} - \frac{\partial \rho}{\partial T} (\vec{v} \cdot \vec{g}) - \frac{\partial Q}{\partial T}$$

Using these definitions, Eqs. (A.1) - (A.3) reduce to

$$\frac{D}{Dt} \left(\frac{\partial \rho}{\partial T} \phi \right) + \nabla \cdot (\rho \vec{\psi}) + \phi \left(\frac{\partial \rho}{\partial T} \nabla \cdot \vec{v} \right) = s_1, \quad (A.4a)$$

$$\begin{aligned} \rho \left(\frac{D\vec{\psi}}{Dt} + \vec{\psi} \cdot \nabla \vec{v} \right) + \nabla \cdot \left[\vec{\psi} \cdot \nabla \tau + \nabla \vec{\psi} : \nabla (\nabla \vec{v}) \tau \right] + \nabla \pi \\ + \phi \frac{\partial \rho}{\partial T} \left(\frac{D\vec{v}}{Dt} - \vec{g} \right) + \nabla \cdot \left(\frac{\partial \tau}{\partial T} \phi \right) = \vec{s}_2, \end{aligned} \quad (A.4b)$$

$$\vec{\psi} \cdot \vec{A} + \nabla \vec{\psi} : B + \phi C + \rho c_p \frac{D\phi}{Dt} - \nabla^2(k\phi) = s_3. \quad (A.4c)$$

Next, the operators occurring in system (A.4) are represented symbolically as follows:

$$L_{11} \vec{\psi} = \nabla \cdot (\rho \vec{\psi})$$

$$L_{12} \pi = 0$$

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$$L_{13}\phi = \frac{D}{Dt} \left(\frac{\partial \rho}{\partial T} \phi \right) + \phi \left(\frac{\partial \rho}{\partial T} \nabla \cdot \vec{v} \right)$$

$$L_{21}\vec{\psi} = \rho \left(\frac{D\vec{\psi}}{Dt} + \vec{\psi} \cdot \nabla \vec{v} \right) + \nabla \cdot \left[\vec{\psi} \cdot \nabla \vec{\tau} + \nabla \vec{\psi} : \nabla (\nabla \vec{v}) \vec{\tau} \right]$$

$$L_{22}\pi = \nabla \pi$$

$$L_{23}\phi = \phi \frac{\partial \rho}{\partial T} \left(\frac{D\vec{v}}{Dt} - \vec{g} \right) + \nabla \cdot \left(\frac{\partial \tau}{\partial T} \phi \right)$$

$$L_{31}\vec{\psi} = \vec{\psi} \cdot \vec{A} + \nabla \vec{\psi} : B$$

$$L_{32}\pi = 0$$

$$L_{33}\phi = C\phi + \rho c_p \frac{D\phi}{Dt} - \nabla^2(k\phi) \quad .$$

Using this notation, system (A.4) can be expressed by the single matrix equation

$$L X = s \quad , \quad (A.5)$$

where L is an operator matrix with elements L_{ij} ; X is the vector of dependent variables, $X = (\vec{\psi}, \pi, \phi)^T$; and s is the vector of source terms, $s = (s_1, \vec{s}_2, s_3)^T$.

It is now necessary to introduce adjoint functions m^* , $\vec{p}^*$, and H^* , corresponding to Eqs. (A.4a), (A.4b), and (A.4c), respectively. Adjoint operators L_{ij}^* can be obtained for each operator L_{ij} using simple vector analysis and the Divergence Theorem. These operators are determined to be (see Appendix B for details):

$$L_{11}^* m^* = -\rho \nabla m^*$$

$$L_{12}^* m^* = 0$$

$$L_{13}^* m^* = - \frac{\partial \rho}{\partial T} \frac{Dm^*}{Dt}$$

$$L_{21}^* \vec{p}^* = - \frac{D(\rho \vec{p}^*)}{Dt} + \nabla \vec{v} \cdot (\rho \vec{p}^*) - \nabla \cdot \tau^T : \nabla \vec{p}^* + \nabla \cdot \left[\nabla (\nabla \vec{v}) \tau^T : \nabla \vec{p}^* \right]$$

$$L_{22}^* \vec{p}^* = - \nabla \cdot \vec{p}^*$$

$$L_{23}^* \vec{p}^* = - \frac{\partial \tau^T}{\partial T} : \nabla \vec{p}^* + \vec{p}^* \cdot \left(\frac{D\vec{v}}{Dt} - \vec{g} \right) \frac{\partial \rho}{\partial T}$$

$$L_{31}^* H^* = H^* \vec{A} - \nabla \cdot (H^* \vec{B})$$

$$L_{32}^* H^* = 0$$

$$L_{33}^* H^* = CH^* - (\rho c_p \nabla \cdot \vec{v}) H^* - \frac{D}{Dt} (\rho c_p H^*) - k \nabla^2 H^* .$$

Now, letting L^* be the matrix of adjoint operators,

$$L^* = \begin{bmatrix} L_{11}^* & L_{12}^* & L_{13}^* \\ L_{21}^* & L_{22}^* & L_{23}^* \\ L_{31}^* & L_{32}^* & L_{33}^* \end{bmatrix} ,$$

and letting y be the vector of adjoint variables $y = (m^*, \vec{p}^*, H^*)^T$, then

$$\begin{aligned} \langle y^T L X \rangle &= \langle m^* (L_{11}^* \vec{\psi} + L_{13}^* \phi) + \vec{p}^* (L_{21}^* \vec{\psi} + L_{22}^* \pi + L_{23}^* \phi) + H^* (L_{31}^* \vec{\psi} + L_{33}^* \phi) \rangle \\ &= \langle \vec{\psi} \cdot (L_{11}^* m^* + L_{21}^* \vec{p}^* + L_{31}^* H^*) + \pi (L_{22}^* \vec{p}^* + \phi (L_{13}^* m^* + L_{23}^* \vec{p}^* + L_{33}^* H^*)) \rangle \\ &= \langle x^T (L^*)^T y \rangle + BT , \end{aligned} \quad (A.6)$$

where $\langle f \rangle = \int_t \iiint_V f \, dV \, dt$, and BT represents the boundary terms, given by

$$\begin{aligned}
BT = & - \int_V \left[m^* \frac{\partial p}{\partial T} \frac{\partial T}{\partial \alpha} + \rho \vec{p}^* \cdot \frac{\partial \vec{v}}{\partial \alpha} + H^* \rho c_p \frac{\partial T}{\partial \alpha} \right]_0^{t_f} dv \\
& - \int_t \oint_{\partial V} \left[\rho m^* \frac{\partial \vec{v}}{\partial \alpha} + \vec{v} m^* \frac{\partial \rho}{\partial T} \frac{\partial T}{\partial \alpha} + \left(\frac{\partial \vec{v}}{\partial \alpha} \cdot \nabla_{\vec{v}} \right) \cdot \vec{p}^* \right. \\
& + \rho \vec{v} \left(\vec{p}^* \cdot \frac{\partial \vec{v}}{\partial \alpha} \right) + \left(\nabla \frac{\partial \vec{v}}{\partial \alpha} : \nabla_{\vec{v}} \right) \cdot \vec{p}^* - \frac{\partial \vec{v}}{\partial \alpha} \cdot \left(\nabla_{\vec{v}} \nabla : \nabla \vec{p}^* \right) \\
& + \vec{p}^* \frac{\partial p}{\partial \alpha} + \vec{p}^* \cdot \frac{\partial \tau}{\partial T} \frac{\partial T}{\partial \alpha} + 2H^* \tau \cdot \frac{\partial \vec{v}}{\partial \alpha} + H^* \rho c_p \vec{v} \frac{\partial T}{\partial \alpha} \\
& \left. + k \nabla H^* \frac{\partial T}{\partial \alpha} - H^* \nabla \left(k \frac{\partial T}{\partial \alpha} \right) \right] \cdot \vec{n} dA dt .
\end{aligned}$$

A quick inspection of Eq. (A.6) reveals that it corresponds exactly to Eq. (11), which is the desired result.

A6

APPENDIX B. DERIVATION OF ADJOINT OPERATORS

$$\text{I. } \underline{L_{11}\vec{\psi} = \nabla \cdot (\rho\vec{\psi})} \quad .$$

$$\begin{aligned} \int_t \iiint_V m^* \nabla \cdot (\rho\vec{\psi}) d\vec{x} dt &= \int_t \iiint_V [\nabla \cdot (\rho m^* \vec{\psi}) - \rho \vec{\psi} \cdot \nabla m^*] d\vec{x} dt \\ &= \int_t \oint_{\partial V} \rho m^* \vec{\psi} \cdot \vec{n} dA dt - \int_t \iiint_V \psi \cdot (\rho \nabla m^*) d\vec{x} dt \quad . \end{aligned}$$

Therefore, $L_{11}^* m^* = -\rho \nabla m^*$, and

$$\int_t \iiint_V m^* L_{11} \vec{\psi} d\vec{x} dt = \int_t \iiint_V \vec{\psi} \cdot L_{11}^* m^* d\vec{x} dt + \int_t \oint_{\partial V} \rho m^* \vec{\psi} \cdot \vec{n} dA dt \quad .$$

$$\text{II. } \underline{L_{13}\phi = \frac{D}{Dt} \left(\phi \frac{\partial \rho}{\partial T} \right) + \phi \left(\frac{\partial \rho}{\partial T} \nabla \cdot \vec{v} \right)} \quad .$$

$$\begin{aligned} \int_t \iiint_V m^* \left[\frac{\partial}{\partial t} \left(\phi \frac{\partial \rho}{\partial T} \right) + \nabla \cdot \left(\phi \frac{\partial \rho}{\partial T} \vec{v} \right) \right] d\vec{x} dt \\ = \iiint_V m^* \phi \frac{\partial \rho}{\partial T} \Big|_0^{t_f} d\vec{x} - \int_t \iiint_V \phi \frac{\partial \rho}{\partial T} \frac{\partial m^*}{\partial t} d\vec{x} dt \\ + \int_t \iiint_V \left[\nabla \cdot \left(m^* \phi \frac{\partial \rho}{\partial T} \vec{v} \right) - \phi \frac{\partial \rho}{\partial T} \vec{v} \cdot \nabla m^* \right] d\vec{x} dt \\ = \iiint_V m^* \phi \frac{\partial \rho}{\partial T} \Big|_0^{t_f} d\vec{x} + \int_t \oint_{\partial V} m^* \phi \frac{\partial \rho}{\partial T} \vec{v} \cdot \vec{n} dA dt \\ - \int_t \iiint_V \phi \left(\frac{\partial \rho}{\partial T} \frac{\partial m^*}{\partial t} + \frac{\partial \rho}{\partial T} \vec{v} \cdot \nabla m^* \right) d\vec{x} dt \end{aligned}$$

Therefore, $L_{13}^* m^* = - \frac{\partial \rho}{\partial T} \frac{Dm^*}{Dt}$, and $\int_t \iiint_V m^* L_{13}^* \phi \, d\vec{x} dt = \int_t \iiint_V \phi \, L_{13}^* m^* \, d\vec{x} dt$

$$+ \iiint_V m^* \phi \frac{\partial \rho}{\partial T} \bigg|_0^{t_f} d\vec{x} + \int_t \oint_{\partial V} m^* \phi \frac{\partial \rho}{\partial T} \vec{v} \cdot \vec{n} \, dAdt \quad .$$

III. $L_{21} \vec{\psi} = \rho \left(\frac{D\vec{\psi}}{Dt} + \vec{\psi} \cdot \nabla \vec{v} \right) + \nabla \cdot \left[\vec{\psi} \cdot \nabla \vec{\tau} + \nabla \vec{\psi} : \nabla (\nabla \vec{v}) \vec{\tau} \right] \quad .$

A. $\int_t \iiint_V \vec{p}^* \cdot \left(\rho \frac{\partial \vec{\psi}}{\partial t} \right) d\vec{x} dt$

$$= \iiint_V \rho \vec{p}^* \cdot \vec{\psi} \bigg|_0^{t_f} d\vec{x} - \int_t \iiint_V \vec{\psi} \cdot \frac{\partial (\rho \vec{p}^*)}{\partial t} d\vec{x} dt \quad .$$

B. $\int_t \iiint_V \vec{p}^* \cdot (\rho \vec{v} \cdot \nabla \vec{\psi}) \, d\vec{x} dt$

$$= \int_t \iiint_V \left[\nabla \cdot \left[\rho \vec{v} (\vec{p}^* \cdot \vec{\psi}) \right] - (\vec{p}^* \cdot \vec{\psi}) \nabla \cdot (\rho \vec{v}) - (\rho \vec{v} \cdot \nabla \vec{p}^*) \cdot \vec{\psi} \right] d\vec{x} dt$$

$$= \int_t \oint_{\partial V} \rho \vec{v} (\vec{p}^* \cdot \vec{\psi}) \cdot \vec{n} \, dAdt - \int_t \iiint_V \vec{\psi} \cdot \left[\vec{p}^* \nabla \cdot (\rho \vec{v}) + (\rho \vec{v} \cdot \nabla \vec{p}^*) \right] d\vec{x} dt$$

C. $\int_t \iiint_V \vec{p}^* \cdot (\rho \vec{\psi} \cdot \nabla \vec{v}) \, d\vec{x} dt = \int_t \iiint_V \vec{\psi} \cdot (\nabla \vec{v} \cdot \rho \vec{p}^*) \, d\vec{x} dt \quad .$

D. $\int_t \iiint_V \vec{p}^* \left[\nabla \cdot (\vec{\psi} \cdot \nabla \vec{\tau}) \right] d\vec{x} dt$

$$= \int_t \iiint_V \left[\nabla \cdot \left[(\vec{\psi} \cdot \nabla \vec{\tau}) \cdot \vec{p}^* \right] - (\vec{\psi} \cdot \nabla \vec{\tau}^T) : \nabla \vec{p}^* \right] d\vec{x} dt$$

$$= \int_t \oint_{\partial V} \left[(\vec{\psi} \cdot \nabla \vec{\tau}) \cdot \vec{p}^* \right] \cdot \vec{n} \, dAdt - \int_t \iiint_V \vec{\psi} \cdot (\nabla \vec{\tau}^T : \nabla \vec{p}^*) \, d\vec{x} dt \quad .$$

$$\begin{aligned}
E. \int_t \iiint_V \vec{p}^* \cdot \left\{ \nabla \cdot \left[\nabla \vec{\psi} : \nabla_{(\nabla \vec{v})} \tau \right] \right\} d\vec{x} dt \\
= \int_t \iiint_V \left\{ \nabla \cdot \left[(\nabla \vec{\psi} : \nabla_{(\nabla \vec{v})} \tau) \cdot \vec{p}^* - \vec{\psi} \cdot (\nabla_{(\nabla \vec{v})} \tau^T : \nabla \vec{p}^*) \right] \right. \\
\left. + \vec{\psi} \cdot \left[\nabla \cdot (\nabla_{(\nabla \vec{v})} \tau^T : \nabla \vec{p}^*) \right] \right\} d\vec{x} dt \\
= \int_t \oint_{\partial V} \left[(\nabla \vec{\psi} : \nabla_{(\nabla \vec{v})} \tau) \cdot \vec{p}^* - \vec{\psi} \cdot (\nabla_{(\nabla \vec{v})} \tau^T : \nabla \vec{p}^*) \right] \cdot \vec{n} dA dt \\
+ \int_t \iiint_V \vec{\psi} \cdot \left[\nabla \cdot (\nabla_{(\nabla \vec{v})} \tau^T : \nabla \vec{p}^*) \right] d\vec{x} dt .
\end{aligned}$$

Therefore,

$$L_{21} \vec{p}^* = - \frac{D(\rho \vec{p}^*)}{Dt} + \nabla \vec{v} \cdot (\rho \vec{p}^*) - \nabla_{\vec{v}} \tau^T : \nabla \vec{p}^* + \nabla \cdot \left[\nabla_{(\nabla \vec{v})} \tau^T : \nabla \vec{p}^* \right] ,$$

and

$$\begin{aligned}
\int_t \iiint_V \vec{p}^* \cdot L_{21} \vec{\psi} d\vec{x} dt &= \int_t \iiint_V \vec{\psi} \cdot L_{21}^* \vec{p}^* d\vec{x} dt \\
&+ \int_t \oint_{\partial V} \left[(\vec{\psi} \cdot \nabla_{\vec{v}} \tau) \cdot \vec{p}^* \right] \cdot \vec{n} dA dt + \iiint_V \rho \vec{p}^* \cdot \vec{\psi} \Big|_0^{t_f} d\vec{x} \\
&+ \int_t \oint_{\partial V} \rho \vec{v} (\vec{p}^* \cdot \vec{\psi}) \cdot \vec{n} dA dt + \int_t \oint_{\partial V} \left[(\nabla \vec{\psi} : \nabla_{(\nabla \vec{v})} \tau) \cdot \vec{p}^* \right. \\
&\left. - \vec{\psi} \cdot (\nabla_{(\nabla \vec{v})} \tau^T : \nabla \vec{p}^*) \right] \cdot \vec{n} dA dt .
\end{aligned}$$

IV. $L_{22} \pi = \nabla \pi$.

$$\begin{aligned}
\int_t \iiint_V \vec{p}^* \cdot \nabla \pi d\vec{x} dt &= \int_t \iiint_V \left[\nabla \cdot (\pi \vec{p}^*) - \pi \nabla \cdot \vec{p}^* \right] d\vec{x} dt \\
&= \int_t \oint_{\partial V} \pi \vec{p}^* \cdot \vec{n} dA dt - \int_t \iiint_V \pi \nabla \cdot \vec{p}^* d\vec{x} dt .
\end{aligned}$$

Therefore, $L_{22}^* \vec{p}^* = -\nabla \cdot \vec{p}^*$, and

$$\int_t \iiint_V \vec{p}^* L_{22}^* \pi \, d\vec{x} dt = \int_t \iiint_V \pi L_{22}^* \vec{p}^* \, d\vec{x} dt + \int_t \oint_{\partial V} \pi \vec{p}^* \cdot \vec{n} \, dA dt.$$

V. $L_{23} \phi = \phi \frac{\partial \rho}{\partial T} \left(\frac{D\vec{v}}{Dt} - \vec{g} \right) + \nabla \cdot \left(\frac{\partial \tau}{\partial T} \phi \right)$.

$$\begin{aligned} \int_t \iiint_V \vec{p}^* \cdot \left[\nabla \cdot \left(\frac{\partial \tau}{\partial T} \phi \right) \right] d\vec{x} dt &= \int_t \iiint_V \left[\nabla \cdot \left(\phi \vec{p}^* \cdot \frac{\partial \tau}{\partial T} \right) - \phi \frac{\partial \tau}{\partial T} : \nabla \vec{p}^* \right] d\vec{x} dt \\ &= \int_t \oint_{\partial V} \left(\phi \vec{p}^* \cdot \frac{\partial \tau}{\partial T} \right) \cdot \vec{n} \, dA dt - \int_t \iiint_V \phi \left[\frac{\partial \tau}{\partial T} : \nabla \vec{p}^* \right] d\vec{x} dt \end{aligned}$$

Therefore, $L_{23}^* \vec{p}^* = -\frac{\partial \tau}{\partial T} : \nabla \vec{p}^* + \vec{p}^* \cdot \left(\frac{D\vec{v}}{Dt} - \vec{g} \right) \frac{\partial \rho}{\partial T}$, and

$$\int_t \iiint_V \vec{p}^* \cdot L_{23} \phi \, d\vec{x} dt = \int_t \iiint_V \phi L_{23}^* \vec{p}^* \, d\vec{x} dt + \int_t \oint_{\partial V} \left(\phi \vec{p}^* \cdot \frac{\partial \tau}{\partial T} \right) \cdot \vec{n} \, dA dt.$$

VI. $L_{31} \vec{\psi} = \vec{A} \cdot \vec{\psi} + \nabla \vec{\psi} : \vec{B}$.

$$\begin{aligned} \int_t \iiint_V H^* (\nabla \vec{\psi} : \vec{B}) \, d\vec{x} dt &= \int_t \iiint_V \left[\nabla \cdot (H^* \vec{B} \cdot \vec{\psi}) - \vec{\psi} \cdot (\nabla \cdot (H^* \vec{B})) \right] d\vec{x} dt \\ &= \int_t \oint_{\partial V} (H^* \vec{B} \cdot \vec{\psi}) \cdot \vec{n} \, dA dt - \int_t \iiint_V \vec{\psi} \cdot (\nabla \cdot (H^* \vec{B})) \, d\vec{x} dt. \end{aligned}$$

Therefore, $L_{31}^* H^* = \vec{A} H^* - \nabla \cdot (H^* \vec{B})$, and

$$\int_t \iiint_V H^* L_{31} \vec{\psi} \, d\vec{x} dt = \int_t \iiint_V \vec{\psi} \cdot L_{31}^* H^* \, d\vec{x} dt + \int_t \oint_{\partial V} (H^* \vec{B} \cdot \vec{\psi}) \cdot \vec{n} \, dA dt.$$

VII. $L_{33} \phi = C\phi + \rho C_p \frac{D\phi}{Dt} - \nabla^2 (k\phi)$.

$$\begin{aligned} \int_t \iiint_V H^* \left(\rho C_p \frac{\partial \phi}{\partial t} + \rho C_p \vec{v} \cdot \nabla \phi \right) d\vec{x} dt &= \int_t \iiint_V \left[\nabla \cdot (H^* \rho C_p \phi \vec{v}) - \phi \nabla \cdot (H^* \rho C_p \vec{v}) \right] d\vec{x} dt \\ &+ \iiint_V H^* \rho C_p \phi \Big|_0^t d\vec{x} - \int_t \iiint_V \phi \frac{\partial}{\partial t} (H^* \rho C_p) \, d\vec{x} dt \end{aligned}$$

$$\begin{aligned}
&= - \int_t \iiint_V \phi \left[\nabla \cdot (H^* \rho C_p \vec{v}) + \frac{\partial}{\partial t} (H^* \rho C_p) \right] d\vec{x} dt \\
&\quad + \iiint_V H^* \rho C_p \phi \Big|_0^{t_f} d\vec{x} + \int_t \oint_{\partial V} (H^* \rho C_p \phi \vec{v}) \cdot \vec{n} dA dt \\
&\quad - \int_t \iiint_V H^* \nabla^2 (k\phi) d\vec{x} dt = - \int_t \iiint_V k\phi \nabla^2 H^* d\vec{x} dt \\
&\quad + \int_t \oint_{\partial V} \left[k\phi \nabla H^* - H^* \nabla (k\phi) \right] \cdot \vec{n} dA dt .
\end{aligned}$$

Therefore, $L_{33}^* H^* = CH^* - \frac{\partial}{\partial t} (\rho C_p H^*) - \nabla \cdot (H^* \rho C_p \vec{v}) - k \nabla^2 H^*$, and

$$\begin{aligned}
\int_t \iiint_V H^* L_{33}^* \phi d\vec{x} dt &= \int_t \iiint_V \phi L_{33}^* H^* d\vec{x} dt \\
&\quad + \iiint_V H^* \rho C_p \phi \Big|_0^{t_f} d\vec{x} + \int_t \oint_{\partial V} (H^* \rho C_p \phi \vec{v}) \cdot \vec{n} dA dt \\
&\quad + \int_t \oint_{\partial V} \left[k\phi \nabla H^* - H^* \nabla (k\phi) \right] \cdot \vec{n} dA dt .
\end{aligned}$$