Forschungszentrum Karlsruhe

Technik und Umwelt

Wissenschaftliche Berichte

FZKA 6481

Adjoint Sensitivity Analysis of the RELAP5/MOD3.2 Two-Fluid Thermal-Hydraulic Code System*

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*Von der Fakultät für Maschinenbau

der Universität Karlsruhe (TH)

genehmigte Dissertation

Forschungszentrum Karlsruhe GmbH, Karlsruhe

2000

ZUSAMMENFASSUNG

Diese Arbeit beschreibt die Implementierung der Adjungierten Sensitivitätsanalyse (*Adjoint Sensitivity Analysis Procedure*, ASAP) im nicht-gleichgewichtigen, nicht-homogenen Zwei-Flüssigkeiten-Modell des RELAP5/MOD3.2-Computercodes, variable Bohr-Konzentrationen sowie nicht-kondensierbare Gase mit berücksichtigt. Das Ergebnis dieser Implementierung ist das Adjungierte-Sensitivitäts-Modell (*Adjoint Sensitivity Model*, ASM-REL/TF), entwickelt sowohl für die Differential- als auch für die diskretisierten Gleichungen, die die Basis des Zwei-Flüssigkeiten-Modells mit nicht-kondensierbaren Komponenten bilden. Die geforderte Konsistenz zwischen diesen beiden Darstellungsarten wird ebenfalls behandelt.

Die Validierung des ASM-REL/TF wurde anhand von RELAP5/MOD3.2-Beispielaufgaben durchgeführt, die (i) nur die flüssige Phase, (ii) nur die Gas-Phase und (iii) eine zweiphasige Mischung (Wasser und Dampf) zum Gegenstand hatten. Die RELAP5/MOD3.2-Beispielaufgabe "Zwei Kreisläufe mit Pumpen" (“*Two-Loops with Pumps*”) wurde benutzt, um die Genauigkeit und Stabilität der numerischen Lösung des ASM-REL/TF zu überprüfen, wenn nur die flüssige Phase vorhanden ist. Für den Fall, daß ein Gemisch der flüssigen und gasförmigen Phase gegeben ist, wurde in gleicher Weise die ebenfalls mit RELAP5/MOD3.2 ausgelieferte Beispielaufgabe “Edwards Pipe” für die Validierung herangezogen. Zur Überprüfung von Genauigkeit und Stabilität bei reiner Gas-Phase wurden beide Beispielaufgaben ein zweites Mal herangezogen, wobei jedoch die jeweils vorhandenen Phasen durch reinen Dampf ersetzt wurden.

Die Ergebnisse, die mit diesen Rechnungen erzielt wurden, lassen die typischen Sensitivitäten der Verbindungsgeschwindigkeiten und Volumen-gemittelten Drücke in Abhängigkeit von Störungen in den Anfangsbedingungen erkennen und zeigen, daß die numerische Lösung des ASM-REL/TF ebenso robust, stabil und genau ist wie die ursprünglichen RELAP5/MOD3.2-Berechnungen. Darüber hinaus konnte die Lösung des ASM-REL/TF dazu genutzt werden, Sensitivitäten der Volumen-gemittelten Drücke in Abhängigkeit von Variationen im Pumpen-Kopf zu berechnen.

Zusätzlich zu der eben beschriebenen Implementierung und ihrer Validierung illustriert diese Arbeit die herausragende Rolle, die die Sensitivitäten in den thermodynamischen Eigenschaften des Wassers in der Sensitivitätsanalyse der Thermohydraulik-Codes für die Be-

rechnung von Leichtwasserreaktoren spielen. Anhand der allseits bekannten *ASME Steam Tables* (ASME Dampf-Tabelle, 1993), zeigt diese Arbeit typische analytische und numerische Ergebnisse für die Sensitivitäten der thermodynamischen Eigenschaften des Wassers in Abhängigkeit von Druck, Temperatur und den numerischen Parametern, die in den mathematischen Formulierungen dieser Eigenschaften auftauchen. Besondere Aufmerksamkeit ist hierbei den sehr großen Sensitivitäten gewidmet, die von den spezifischen isobaren Wärmekapazitäten von Flüssigkeit und Gas, C_{pf}, und C_{pg}, der spezifischen Flüssigkeitsenthalpie, h_f, dem spezifischen Gasvolumen, V_g, dem volumetrischen Expansionskoeffizienten für Gas, $ß_g$, und dem isothermen Gaskoeffizienten, k_g, an den Tag gelegt werden. Die Abhängigkeit von $ß_g$ und k_g vom *sensitivsten* Parameter stellt sich als *nicht-linear* heraus, während sich die Abhängigkeit von C_{pf}, C_{pg}, h_f, V_g vom *sensitivsten* Parameter als *linear* erweist, so daß die respektiven Sensitivitäten *exakt* die Effekte der Variation der entsprechenden Parameter vorhersagen.

Im Gegensatz dazu erweisen sich die Sensitivitäten des spezifischen Flüssigkeitsvolumens, V_f, des volumetrischen Expansionskoeffizienten für Flüssigkeiten, $ß_f$, der spezifischen Gasenthalpie, h_g, und des isothermen Kompressibilitätskoeffizienten für Flüssigkeiten, k_f, in Abhängigkeit von den Parametern, die in ihrer jeweiligen mathematischen Berechnung auftauchen, als ziemlich klein.

Diese Sensitivitäten sind essentiell für die korrekte Einordnung der einzelnen Parameter gemäß ihrer jeweiligen Bedeutung für das Endergebnis, für die Bewertung der Auswirkung der Nicht-Linearitäten, und, ganz generell, für die Durchführung umfassender Sensitivitäts- und Unsicherheitsanalysen der Thermohydraulik-Codes, die auf Wasser als Arbeitsflüssigkeit basieren.

ABSTRACT

This work presents the implementation of the Adjoint Sensitivity Analysis Procedure (ASAP) for the non-equilibrium, non-homogeneous two-fluid model, including boron concentration and non-condensable gases, of the RELAP5/MOD3.2 code. The end-product of this implementation is the Adjoint Sensitivity Model (ASM-REL/TF), which is derived for both the differential and discretized equations underlying the two-fluid model with non-condensable(s). The consistency requirements between these two representations are also highlighted. The validation of the ASM-REL/TF has been carried out by using sample problems involving: (i) liquid-phase only, (ii) gas-phase only, and (iii) two-phase mixture (of water and steam). Thus, the “Two-Loops with Pumps” sample problem supplied with RELAP5/MOD3.2 has been used to verify the accuracy and stability of the numerical solution of the ASM-REL/TF when only the liquid-phase is present. Furthermore, the “Edwards Pipe” sample problem, also supplied with RELAP5/MOD3.2, has been used to verify the accuracy and stability of the numerical solution of the ASM-REL/TF when both (i.e., liquid and gas) phases are present. In addition, the accuracy and stability of the numerical solution of the ASM-REL/TF have been verified when only the gas-phase is present by using modified “Two-Loops with Pumps” and the “Edwards Pipe” sample problems in which the liquid and two-phase fluids, respectively, were replaced by pure steam. The results obtained for these sample problems depict typical sensitivities of junction velocities and volume-averaged pressures to perturbations in initial conditions, and indicate that the numerical solution of the ASM-REL/TF is as robust, stable, and accurate as the original RELAP5/MOD3.2 calculations. In addition, the solution of the ASM-REL/TF has been used to calculate sample sensitivities of volume-averaged pressures to variations in the pump head.

This work also illustrates the role that sensitivities of the thermodynamic properties of water play for sensitivity analysis of thermal-hydraulic codes for light-water reactors. Using the well-known ASME Steam Tables (1993), this work presents typical analytical and numerical results for sensitivities of the thermodynamic properties of water to pressure, temperature, and the numerical parameters that appear in the mathematical formulation of these properties. Particular attention is given to the very large sensitivities displayed by the specific isobaric fluid and gas heat capacities, C_{pf}, and C_{pg}, the specific fluid enthalpy, h_f, the specific gas volume, V_g, the volumetric expansion coefficient for gas, $ß_g$, and the isothermal coefficient for gas, k_g. The dependence of $ß_g$, and k_g on the *most sensitive* parameters turns out to be *non-linear*, while the dependence of C_{pf}, C_{pg}, h_f, V_g on the *most sensitive* parameters turns out to

be *linear*, so the respective sensitivities predict *exactly* the effects of variations in the respective parameters. On the other hand, the sensitivities of the specific fluid volume, V_f, the volumetric expansion coefficient for fluid, $ß_f$, the specific gas enthalpy, h_g, and the isothermal coefficient of compressibility for fluid, k_f, to the parameters that appear in their respective mathematical formulae are quite small. Such sensitivities are essential for ranking the respective parameters according to their importance, for assessing the effects of nonlinearities and, more generally, for performing comprehensive sensitivity/uncertainty analyses of thermal-hydraulic codes which use water substance as the working fluid.

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NOTATION

- Lower-case Roman

$\underline{b}, \underline{f}^1, \underline{f}^2, \underline{g}^1, \underline{g}^2$ - vectors of sources in REL/CDE

h_f - specific fluid enthalpy

h_g - specific gas enthalpy

k_f - isothermal coefficient for fluid

k_g - isothermal coefficient for gas

v_g - gas velocity

v_f - fluid velocity

- Upper-case Roman

$\underline{\underline{A}}$ - matrix operator for REL/CDE

C_{pf} - specific isobaric fluid heat capacity

C_{pg} - specific isobaric gas heat capacity

$DR\left(\underline{\chi}^o, \underline{G}^o; \underline{\Phi}, \underline{\Gamma}\right)$ - sensitivity of the response R with respect of parameter variation Γ

$\underline{G} \equiv (g_1, \ldots, g_J)$ - vector of parameters

$G^{(n)}$, $H^{(n)}$ - matrix operators, components of FSM

P - the system pressure

$Q^{(n)}$ - the vector of sources for the discretized ASM

$R\left(\underline{\chi}, \underline{G}\right)$ - the response of interest

R_{pred} - predicted perturbed response

$R_{recal} \equiv R_i\left(\underline{\chi}^o + \underline{\Phi}, \underline{G}^o + \underline{\Gamma}\right)$ - the exact (recalculated) perturbed response

S – vector of inhomogeneous sources in the original REL/CDE

V_f - the fluid specific volume

V_g - the gas specific volume

U_f - the fluid specific internal energy

U_g - the gas specific internal energy

X_n - the total non-condensable mass fraction

X_{ni} - the non-condensable mass fraction for the i-th non-condensable species

$X^{(n)}$ - vector of variations of the final time-step variables

$X_I^{(n)}$ - vector of variations of the intermediate time-step variables

- Lowercase Greek

α_g - the void fraction

$ß_f$ - the volumetric expansion coefficient for fluid

$ß_g$ - the volumetric expansion coefficient for gas

$\underline{\chi} \equiv (\chi_1, \dots, \chi_9)$ - vector of state variables

$\underline{\chi}_d^{n+1} \equiv \left[(U_g)_k^{n+1}, (U_f)_k^{n+1}, (P)_k^{n+1}, (\alpha_g)_k^{n+1}, (X_n)_k^{n+1}, (X_{ni})_k^{n+1}, (\rho_b)_k^{n+1}, (v_g)_j^{n+1}, (v_f)_j^{n+1}, (\widetilde{U}_g)_k^{n+1}, (\widetilde{U}_f)_k^{n+1}, (\widetilde{\alpha}_g)_k^{n+1}, (\widetilde{X}_n)_k^{n+1} \right]$
- the vector of *discretized* state variables for volume k and/or junction j

ρ_b - the boron density

- Uppercase Greek

$\underline{\Gamma} \equiv (\gamma_1, \gamma_2, \dots, \gamma_J) \equiv (\delta g_1, \delta g_2, \dots, \delta g_J)$ - vector of parameter variations

$\underline{\Phi} \equiv (\Phi_1, \dots, \Phi_9) \equiv (\delta U_g, \dots, \delta v_f)$ - vector of variations of the state variables

$\underline{\Phi}^*(x,t) \equiv (\Phi_1^*(x,t), \dots, \Phi_9^*(x,t))$ - the vector of adjoint functions

$\underline{\Xi} \equiv (\Xi^{(0)}, \dots, \Xi^{(NF)})$ - the vector of discretized adjoint functions

$\underline{\Psi} \equiv \left[\left(\delta U_g \right)_k^{n+1}, \ldots, \left(\delta \tilde{X}_n \right)_k^{n+1} \right]$ - the variations in the vector of dependent variables $\underline{\chi}_d$

1 INTRODUCTION

The numerical simulation and analysis of light-water reactor (LWR) plant transients has progressed significantly through the coupling of three-dimensional neutron kinetics codes with reactor core and plant thermal-hydraulics codes. Such coupled code systems are now used both for normal operating conditions and for postulated accident scenarios. One of the most advanced code systems of this kind is the coupled RELAP5/PANBOX2/COBRA3 (R/P/C) code system[1,2], in which (i) the RELAP5 code simulates the thermal-hydraulic characteristics of LWR's by using a non-equilibrium, non-homogeneous two-phase flow model together with conservation equations for boron concentration and non-condensable gases (ii) the PANBOX code solves the diffusion-theory-based neutron kinetics equations in three-, one-, or zero-(point)-dimensions using the nodal expansion method, and (iii) the COBRA code computes the flow and enthalpy in the sub-channels of rod bundles for boiling and non-boiling conditions by including the effects of cross-flow mixing.

The implementation of efficient methods to analyze the sensitivity of results (responses) calculated with the R/P/C code system would represent a major development towards establishing a general-purpose code system for the analysis of postulated accident scenarios. To provide the R/P/C system with an efficient yet exhaustive sensitivity analysis capability, a research and development program has been initiated at the Institut für Reaktorsicherheit at Forschungszentrum Karlsruhe in cooperation with Siemens/KWU. The goal of this program is to implement the *local* Adjoint Sensitivity Analysis Procedure (ASAP) for nonlinear systems, originally developed by Cacuci[3-5], into the codes comprising the R/P/C system.

Sensitivity analysis should, in principle, be performed both locally and globally in the space spanned by the parameter variations. The objective of *local sensitivity analysis*[4-5] is to analyze the behavior of the system responses by calculating *sensitivities* around a chosen point or trajectory in the combined phase-space of parameters and state variables. Once these sensitivities are available, they can be used for: (a) ranking the importance of parameters as they affect the calculated response; (b) analyzing the effects of parameter variations on the response; (c) performing extensive uncertainty analysis; (d) prioritizing the introduction of improvements in the respective computer code; and (e) eliminating unimportant phenomena for later considerations in a *global* analysis. Note that the objective of *global analysis* subsequently developed by Cacuci[6] is to determine all of the system's critical points (bifurcations, turning points, response extrema) in the combined phase-space formed by the parameters, state variables, and adjoint variables, and subsequently analyze these critical points by local sensitivity analysis.

The purpose of this work is to present the main aspects of implementing the local ASAP for the non-equilibrium, non-homogeneous two-fluid flow model, including boron concentration and non-condensable gases, of the RELAP5/MOD3.2 code[7]. The main conceptual steps involved in this implementation of the *local* ASAP are the same as pioneered by Cacuci and Wacholder[8] in their work on applying the ASAP to the well-posed system of quasi-linear partial differential equations that describe transient one-dimensional, two-phase flow. Very few applications of the *local* ASAP (and no global sensitivity analysis applications) to two-phase flow problems have been reported in the open literature so far. Following the seminal work of Ref. 8, which also used the homogeneous equilibrium model of two-phase flow as an explicit paradigm, Cacuci et al[9]. and Wacholder et al[10]. presented an exact sensitivity analysis of a two-phase flow problem involving boiling transition between single-phase and two-phase flow. Later, Ounsy, Brun, and de Crecy[11] have applied Cacuci's ASAP to Burgers' equation as a paradigm for non-linear hyperbolic systems. Although they initially misapply the ASAP (by omitting to include, ab initio, the requisite shock condition as part of the set of equations defining the problem, and henceforth falsely concluding that the ASAP is not applicable to "non-linear hyperbolic problems"), they nevertheless come up with the correct results by including the shock condition explicitly, a posteriori. They also present several sensitivities calculated with the CATHARE code[11] .

This work is organized as follows: Sec. 2.1 presents briefly the so-called "Numerically Convenient Set of Differential Equations" (REL/CDE), which are obtained from the basic differential equations that underlie the non-homogeneous, non-equilibrium, one-dimensional two-fluid model. The REL/CDE are discretized using a staggered-mesh in the spatial direction, and either a one-step ("nearly-implicit") or a two-step ("semi-implicit") discretization procedure in time; the resulting set of nonlinear algebraic equations is presented in Sec. 2.2. As will be detailed in Sec. 3, the *local sensitivity analysis theory for nonlinear systems* developed by Cacuci[3-5] will be applied both to the Differential REL/CDE and to the Discretized REL/CDE. This two-tiered, parallel, approach is employed because:

(a) The ASAP is easier to implement and program using the Discretized REL/CDE, since the discretized geometry of RELAP5/MOD3.2 (i.e., the RELAP5 defined volumes, junctions, etc.) can be used directly, without additional modifications, which is a considerable advantage in view of the complex geometries modeled by RELAP5.

(b) Implementing the ASAP for the Differential REL/CDE leads to the Differential Adjoint Sensitivity Model (ASM-REL/TF), as will be detailed in Sec.3.2.1, which is *not* discretized and therefore not readily solvable numerically. To discretize the Differential ASM-REL/TF is a time-consuming task, considering the complex geometry modeled in RELAP5.

(c) However, as will be discussed in Sec. 3.3, the Discretized ASM-REL/TF may not necessarily turn out to be consistent with the Differential ASM-REL/TF. As discussed in Sec. 3.3, the respective consistency must be ensured, and this can be done only if the Differential ASM-REL/TF is *also* available.

As is well known, this sensitivity analysis theory comprises two complementary aspects, namely the Forward Sensitivity Analysis Procedure (FSAP), and the Adjoint Sensitivity Analysis Procedure (ASAP). Correspondingly, Sec. 3.1.1 highlights the derivations underlying the application of the FSAP for the REL/CDE, while Sec. 3.1.2 highlights the FSAP for the Discretized REL/CDE. These derivations underscore the fact that the FSAP should be used only for the less usual situations when the number of results (or responses) of interest for sensitivity analysis exceeds the number of parameter variations to be considered. On the other hand, in the far more common situations encountered in practice, when the number of responses is less than the number of parameter variations, the ASAP must be used since, in view of the numerous parameters in RELAP5/MOD3.2, it is clear that the ASAP is the only practical way to perform a *complete* and *systematic sensitivity analysis* of the reactor plant transients calculated with this code. Underlying the ASAP are the Differential Adjoint Sensitivity Model (ASM-REL/TF), which comprises nine coupled differential equations that are *linear in the adjoint function,* and its discrete counterpart, the Discrete ASM-REL/TF, which comprises thirteen *linear algebraic equations* that result from the use of the RELAP5/MOD3.2 time discretization(s) and staggered-mesh spatial discretization procedures. The following fundamental characteristics of the ASAP have been highlighted during its implementation in the RELAP5/MOD3.2 two-fluid model: (a) the adjoint functions are independent of parameter variations; (b) the adjoint functions must be calculated anew for every response; (c) the ASM-REL/TF is linear in the adjoint function and may be solved by methods that are, in principle, independent of those used to solve the original, nonlinear equations; and (d) the adjoint functions depend (nonlinearly, in general) on the base-case solution, which must therefore be available prior to solving the ASM-REL/TF. The derivations underlying the application of the ASAP to the Differential REL/CDE are presented in Sec. 3.2.1, while the derivations underlying the application of the ASAP to the Discretized REL/CDE are presented in Sec. 3.2.2.

Section 3.3 highlights the fundamentally important aspect of *consistency between the differential and the corresponding discretized equations used for sensitivity analysis*. The indispensable a priori assumption must be that the original differential equations (in this case, the REL/CDE) are discretized consistently (in RELAP5/MOD3.2); otherwise, the base-case solution could not be calculated correctly. Starting from this indispensable assumption, the following consistency correspondences must be assured: (i) the Discretized Forward Sensitivity Model (FSM) must be consistent with the Differential FSM, if the FSAP is used; (ii) the Discretized Adjoint Sensitivity Model (ASM-REL/TF) must be consistent with the Differential ASM-REL/TF, if the ASAP is used; and (iii) the Discretized (representation of the) Response Sensitivity must be consistent with the Integral (representation of the) Response Sensitivity both for the FSAP and for the ASAP, in which the Integral and the Discretized Response Sensitivity are represented in terms of adjoint functions.

Section 4 presents typical results that illustrate the verification of the numerical solution of the ASM-REL/TF, for several sample problems that involve, respectively: (i) the liquid-phase only, (ii) the gas-phase only, and (iii) two-phase flow. Thus, Sec. 4.1 presents results that illustrate the verification of the numerical solution of the ASM-REL/TF when only the liquid-phase is present. The "Two-Loops with Pumps" sample problem supplied with RELAP5/MOD3.2 is used for this purpose. By replacing the liquid (water) by gas (pure steam) but keeping the respective geometry, a modified "Two-Loops with Pumps" sample problem is obtained and used, as described in Sec. 4.2, to verify the accuracy and stability of the numerical solution of the ASM-REL/TF when only the gas-phase is present. For the same verification purpose, a modified "Edwards Pipe" sample problem, in which only the gas-phase is present (thus describing the transient depressurization of a pipe filled with pure steam), is also used in Sec. 4.2. Finally, Sec. 4.3 illustrates the verification of the numerical solution of the ASM-REL/TF when both (i.e., liquid and gas) phases are present; the "Edwards Pipe" sample problem, as supplied with the RELAP5/MOD3.2 code, is employed for this verification.

This work also illustrates the role that sensitivities of the thermodynamic properties of water play for sensitivity analysis of thermal-hydraulic codes for light-water reactors. Using the well-known 1993 ASME Steam Tables[12], Sec. 5 presents typical analytical and numerical results for sensitivities of the thermodynamic properties of water to pressure, temperature, and the numerical parameters that appear in the mathematical formulation of these properties. Note that the explicit, exact expressions of all of these sensitivities have been obtained by using the symbolic computer language MAPLE V[13]. In particular, Sec. 5 highlights the very large sensitivities displayed by the specific isobaric fluid and gas heat capacities, C_{pf}, and C_{pg}, the specific fluid enthalpy, h_f, the specific gas volume, V_g, the volumetric expansion coefficient for gas, $ß_g$, and the isothermal coefficient for gas, k_g. In addition, Sec. 5 also presents the sensitivities of the remaining thermodynamic properties of water, namely: the specific fluid volume, V_f, the volumetric expansion coefficient for fluid, $ß_f$, the specific gas enthalpy, h_g, and the isothermal coefficient of compressibility for fluid, k_f. Finally, Sec. 6 summarizes and concludes this work by highlighting possible directions for future research.

2 THE RELAP5/MOD3.2 TWO-FLUID MODEL

The RELAP5/MOD3.2 code[7] simulates the thermal-hydraulic characteristics of light-water reactors (LWR) by using a non-homogeneous, non-equilibrium, one-dimensional two-fluid model, which consists of a system of nine coupled nonlinear partial differential equations describing the conservation of mass, momentum and energy for the liquid and gaseous phases, including non-condensable materials in the gaseous phase and boron concentration in the liquid field. These conservation equations are not solved directly in RELAP5/MOD 3.2; instead they are transformed into the so-called "Numerically Convenient Set of Differential Equations", abbreviated henceforth as REL/CDE, which comprises the "non-condensable density equations" (for each species, and for the total), the "vapor energy equation", the "liquid energy equation", the "difference density equation", the "sum density equation", the "difference momentum equation", the "sum momentum equation", and the "boron conservation equation".

2.1 The Numerically Convenient Set of Differential Equations (REL/CDE)

The explicit forms of the "Numerically Convenient Set of Differential Equations", abbreviated henceforth as REL/CDE, are:

the "non-condensable density equation":

$$\rho_g X_n \frac{\partial \alpha_g}{\partial t} + \alpha_g X_n \frac{\partial \rho_g}{\partial t} + \alpha_g \rho_g \frac{\partial X_n}{\partial t} + \frac{1}{A}\frac{\partial}{\partial x}\left(\alpha_g \rho_g X_n v_g A\right) = 0 \tag{2.1}$$

the "vapor energy equation":

$$\begin{aligned}
&\left(\rho_g U_g + P\right)\frac{\partial \alpha_g}{\partial t} + \alpha_g U_g \frac{\partial \rho_g}{\partial t} + \alpha_g \rho_g \frac{\partial U_g}{\partial t} + \frac{1}{A}\left[\frac{\partial}{\partial x}\left(\alpha_g \rho_g U_g v_g A\right) + P\frac{\partial}{\partial x}\left(\alpha_g v_g A\right)\right] = \\
&-\left(\frac{h_f^*}{h_g^* - h_f^*}\right) H_{ig}\left(T^s - T_g\right)\frac{P_s}{P} - \left(\frac{h_g^*}{h_g^* - h_f^*}\right) H_{if}\left(T^s - T_f\right) \\
&-\frac{P - P_s}{P} H_{gf}\left(T_g - T_f\right) + \left[\left(\frac{1+\varepsilon}{2}\right)h_g' + \left(\frac{1-\varepsilon}{2}\right)h_f'\right]\Gamma_w + Q_{wg} + DISS_g
\end{aligned} \tag{2.2}$$

the "liquid energy equation":

$$\begin{aligned}
&-\left(\rho_f U_f + P\right)\frac{\partial \alpha_g}{\partial t} + \alpha_f U_f \frac{\partial \rho_f}{\partial t} + \alpha_f \rho_f \frac{\partial U_f}{\partial t} + \frac{1}{A}\left[\frac{\partial}{\partial x}\left(\alpha_f \rho_f U_f v_f A\right) + P\frac{\partial}{\partial x}\left(\alpha_f v_f A\right)\right] \\
&= \left(\frac{h_f^*}{h_g^* - h_f^*}\right) H_{ig}\left(T^s - T_g\right)\frac{P_s}{P} + \left(\frac{h_g^*}{h_g^* - h_f^*}\right) H_{if}\left(T^s - T_f\right) + \frac{P - P_s}{P} H_{gf}\left(T_g - T_f\right) \\
&-\left[\left(\frac{1+\varepsilon}{2}\right)h_g' + \left(\frac{1-\varepsilon}{2}\right)h_f'\right]\Gamma_w + Q_{wf} + DISS_f .
\end{aligned} \tag{2.3}$$

the “difference density equation”:

$$\alpha_g \frac{\partial \rho_g}{\partial t} - \alpha_f \frac{\partial \rho_f}{\partial t} + \left(\rho_g + \rho_f\right)\frac{\partial \alpha_g}{\partial t} + \frac{1}{A}\frac{\partial}{\partial x}\left(\alpha_g \rho_g v_g A - \alpha_f \rho_f v_f A\right)$$
$$= -\frac{2\left[H_{ig}\frac{P_s}{P}\left(T^s - T_g\right) + H_{if}\left(T^s - T_f\right)\right]}{h_g^* - h_f^*} + 2\Gamma_w. \quad (2.4)$$

the “sum density equation”:

$$\alpha_g \frac{\partial \rho_g}{\partial t} + \alpha_f \frac{\partial \rho_f}{\partial t} + \left(\rho_g - \rho_f\right)\frac{\partial \alpha_g}{\partial t} + \frac{1}{A}\frac{\partial}{\partial x}\left(\alpha_g \rho_g v_g A + \alpha_f \rho_f v_f A\right) = 0. \quad (2.5)$$

the “sum momentum equation”:

$$\alpha_g \rho_g \frac{\partial v_g}{\partial t} + \alpha_f \rho_f \frac{\partial v_f}{\partial t} + \frac{1}{2}\alpha_g \rho_g \frac{\partial v_g^2}{\partial x} + \frac{1}{2}\alpha_f \rho_f \frac{\partial v_f^2}{\partial x} = -\frac{\partial P}{\partial x} + \rho_m B_x - \alpha_g \rho_g v_g FWG$$
$$- \alpha_f \rho_f v_f FWF - \Gamma_g\left(v_g - v_f\right). \quad (2.6)$$

the “difference momentum equation”:

$$\frac{\partial v_g}{\partial t} - \frac{\partial v_f}{\partial t} + \frac{1}{2}\frac{\partial v_g^2}{\partial x} - \frac{1}{2}\frac{\partial v_f^2}{\partial x} = -\left(\frac{1}{\rho_g} - \frac{1}{\rho_f}\right)\frac{\partial P}{\partial x} + -v_g FWG + v_f FWF +$$
$$\frac{\Gamma_g\left[\rho v_I - \left(\alpha_f \rho_f v_g + \alpha_g \rho_g v_f\right)\right]}{\alpha_g \rho_g \alpha_f \rho_f} - \rho_m FI\left(v_g - v_f\right) - C\frac{\rho_m^2}{\rho_g \rho_f}\frac{\partial\left(v_g - v_f\right)}{\partial t}. \quad (2.7)$$

the “mass conservation equation for each non-condensable component:

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g X_n X_{ni}\right) + \frac{1}{A}\frac{\partial}{\partial x}\left(\alpha_g \rho_g X_n X_{ni} v_g A\right) = 0 \quad (2.8)$$

where

$$X_{ni} = \frac{M_{ni}}{\sum_{i=1}^{N} M_{ni}} = \frac{M_{ni}}{M_n},$$

and where M_{ni} represents the mass of the i-th non condensable component in the gaseous phase, while M_n represents the total mass of non-condensable gas in the gaseous phase;

and, finally, the "boron conservation equation"

$$\frac{\partial \rho_b}{\partial t} + \frac{1}{A}\frac{\partial(\alpha_f \rho_f C_b v_f A)}{\partial x} = 0, \tag{2.9}$$

where the concentration parameter is defined as $C_b = \frac{\rho_b}{\rho_m(1-X)} = \frac{\rho_b}{\alpha_f \rho_f}$.

Equations (2.1) through (2.9) can be represented mathematically as the matrix-valued operator equation

$$\underline{N}(\underline{\chi}, \underline{G}) - \underline{S}(\underline{G}) = \underline{0}, \tag{2.10}$$

where $\underline{\chi} \equiv (\chi_1, \ldots, \chi_9)$ denotes a vector whose components are the nine dependent (i.e., state) variables in the REL/CDE system, as follows: the gas specific internal energy, $U_g \equiv \chi_1$, the fluid specific internal energy, $U_f \equiv \chi_2$, the pressure, $P \equiv \chi_3$, the void fraction, $\alpha_g \equiv \chi_4$, the total non-condensable mass fraction, $X_n \equiv \chi_5$, the non-condensable mass fraction for the i-th non-condensable species, $X_{ni} \equiv \chi_6$, the boron density, $\rho_b \equiv \chi_7$, the gas velocity, $v_g \equiv \chi_8$, and the fluid velocity, $v_f \equiv \chi_9$. It is important to note here that the two-fluid model equations depend on a large number of parameters, such as those entering in various correlations, initial and/or boundary conditions, formulae expressing the thermodynamic properties of water (the 1993 ASME Steam Tables[12]), and those describing the geometry of the problem under consideration, etc. These parameters are denoted in Eq. (2.10) by the J-component vector $\underline{G} \equiv (g_1, \ldots, g_J)$, where J denotes the total number of parameters in RELAP5/MOD3.2.

Note that Eq. (2.10) contains first-order derivatives in time and space; therefore, it must be supplemented with appropriate initial and boundary conditions, which are hereby denoted as

$$\underline{\chi}(x, t_o) = \underline{\chi}_{init}(x), \quad \text{for } t = t_o \text{ and all } x \qquad (2.11)$$

$$\underline{\chi}(x_o, t) = \underline{\chi}_{bound}(t), \quad \text{for } x = x_o \text{ and all } t > 0. \qquad (2.12)$$

At this stage, it is important to note that since Eq. (2.10) is nonlinear, it can, in principle, admit multiple solutions as well as discontinuous solutions that model shock waves. All of the considerations in this work, however, are restricted to those domains in phase (x, t) and parameter-space in which the solution of Eqs. (2.10) through (2.12) is unique. Bifurcations, shock waves, and all other physical phenomena that might lead to non-unique solutions are beyond the scope of this work.

2.2 The Discretized REL/CDE

In RELAP5/MOD3.2, the REL/CDE are discretized spatially using a staggered spatial mesh that defines the RELAP "volumes"; furthermore, two adjacent volumes are connected to each other by RELAP "junctions". The velocities are defined at junctions, while all other state variables are defined as volume-averaged variables. This spatial discretization procedure is illustrated in Fig. 1, below.

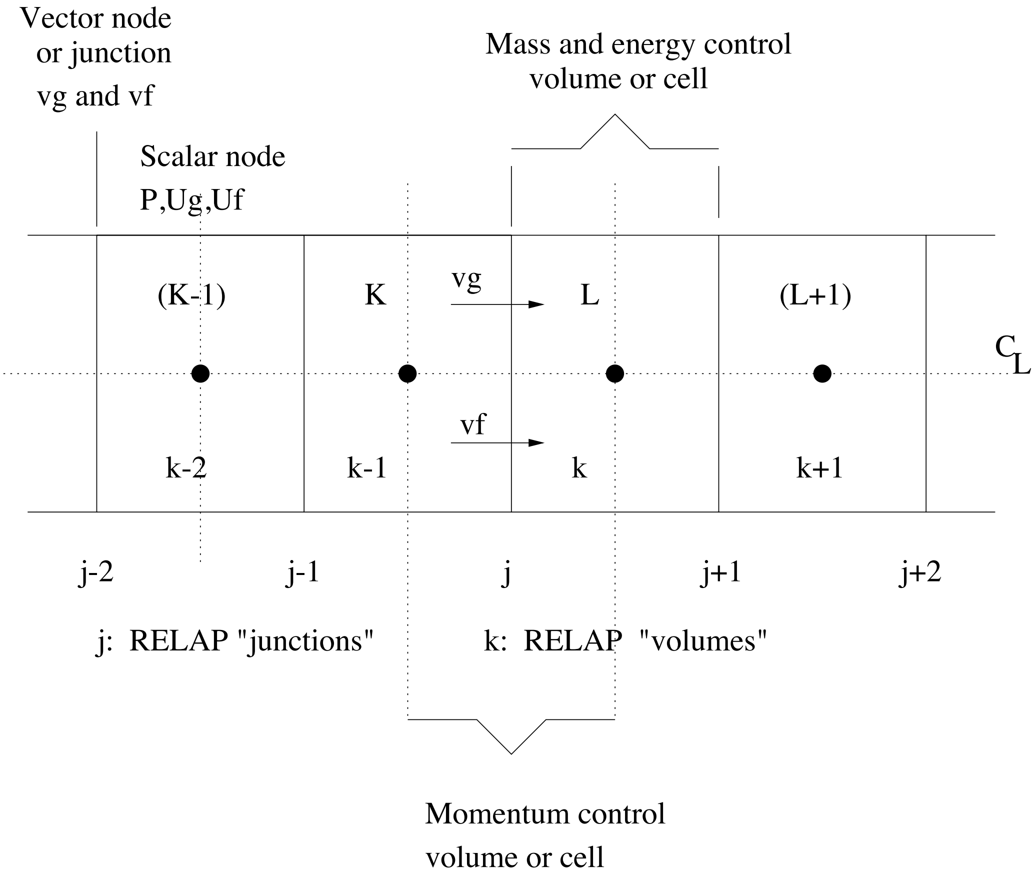

Fig. 1. Spatial discretization procedure (staggered mesh) for discretizing the REL/CDE

The Discretized REL/CDE equations for each cell are obtained by (i) integrating the mass and energy equations with respect to the spatial variable x, from a junction at x_j to the next junction at x_{j+1}, and (ii) integrating the momentum equations with respect to the spatial variable x, from a cell center x_K to the adjoining cell center x_L.

Two time-discretization procedures are implemented in RELAP5/MOD3.2; they are referred to as the nearly-implicit scheme, and the semi-implicit scheme, respectively. The nearly-implicit scheme is essentially a one-step integration procedure, while the semi-implicit scheme is a two-step integration procedure. Since the mathematical formalism of a one-step procedure can be formally considered to be a particular case of a two-step procedure, only the two-step procedure, i.e., the semi-implicit scheme, will be analyzed in this work.

In the semi-implicit scheme, the time advancement depends on the state of the fluid, in a control volume, for two successive time steps. The following four cases can occur in a control volume:

(a) “two-phase to two-phase”, where two-phase flow conditions exist at both the old (n) time-step, and the new (n+1) time step, respectively;

(b) “one-phase to one-phase”, where one-phase flow conditions (either pure gas or pure liquid) exist at both the old (n) time-step, and the new (n+1) time step, respectively;

(c) “two-phase to one-phase” (also referred to as “disappearance”), where two-phase flow conditions exist at the old (n) time-step, and one-phase flow conditions exist at the new (n+1) time-step, respectively;

(d) “one-phase to two-phase” (also referred to as “appearance”), where one-phase flow conditions exist at the old (n) time-step, and two-phase flow conditions exist at the new (n+1) time step, respectively.

After integration over x, from a junction at x_j to the next junction at x_{j+1}, the mass and energy equations yield a set of algebraic equations that can be written in matrix form as

$$\underline{\underline{A}}\,\underline{x} = \underline{b} + \underline{g}^1 v_{g,j+1}^{n+1} + \underline{g}^2 v_{g,j}^{n+1} + \underline{f}^1 v_{f,j+1}^{n+1} + \underline{f}^2 v_{f,j}^{n+1}, \tag{2.13}$$

where

$$\underline{\underline{A}} = \begin{bmatrix} A_{11} & A_{12} & 0 & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\ A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{bmatrix}, \qquad \underline{x} = \begin{bmatrix} \tilde{X}_{n,L}^{n+1} - X_{n,L}^{n} \\ \tilde{U}_{g,L}^{n+1} - U_{g,L}^{n} \\ \tilde{U}_{f,L}^{n+1} - U_{f,L}^{n} \\ \tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^{n} \\ P_{L}^{n+1} - P_{L}^{n} \end{bmatrix},$$

$$
\underline{b} = \begin{bmatrix} 0 \\ b_2 \\ b_3 \\ b_4 \\ 0 \end{bmatrix}, \quad \underline{g}^1 = \begin{bmatrix} g_1^1 \\ g_2^1 \\ 0 \\ g_4^1 \\ g_5^1 \end{bmatrix}, \quad \underline{g}^2 = \begin{bmatrix} g_1^2 \\ g_2^2 \\ 0 \\ g_4^2 \\ g_5^2 \end{bmatrix}, \quad \underline{f}^1 = \begin{bmatrix} 0 \\ 0 \\ f_3^1 \\ f_4^1 \\ f_5^1 \end{bmatrix}, \quad \underline{f}^2 = \begin{bmatrix} 0 \\ 0 \\ f_3^2 \\ f_4^2 \\ f_5^2 \end{bmatrix},
$$

for each time-step n, volume k and/or junction j; the symbols with tilda indicate quantities that are evaluated at an intermediate (provisional) time-step. All of the variables appearing in the components of the matrix $\underline{\underline{A}}$ and the vectors $\underline{b}, \underline{g}^1, \underline{g}^2, \underline{f}^1, \underline{f}^2$ are evaluated at old-time step, n. The expressions of these components are listed in Appendix A.

The sum momentum equation is integrated over x, from a cell center x_K to the adjoining cell center x_L, to obtain

$$
\begin{aligned}
&(\alpha_g\rho_g)_j^n(v_g^{n+1} - v_g^n)_j \Delta x_j + (\alpha_f\rho_f)_j^n(v_f^{n+1} - v_f^n)_j \Delta x_j + \frac{1}{2}(\dot{\alpha}_g\dot{\rho}_g)_j^n\left[(v_g^2)_L^n - (v_g^2)_K^n\right]\Delta t \\
&+ \frac{1}{2}(\dot{\alpha}_f\dot{\rho}_f)_j^n\left[(v_f^2)_L^n - (v_f^2)_K^n\right]\Delta t - \frac{1}{2}\left[(\dot{\alpha}_g\dot{\rho}_g)_j^n VISG_j^n - (\dot{\alpha}_f\dot{\rho}_f)_j^n VISF_j^n\right]\Delta t \\
&= -(1-\eta)(P_L - P_K)^{n+1}\Delta t + \left[(\rho_m)_j^n B_X - (\alpha_g\rho_g)_j^n FWG_j^n (v_g)_j^{n+1} - (\alpha_f\rho_f)_j^n FWF_j^n (v_f)_j^{n+1}\right. \\
&\left. - (\Gamma_g)_j^n (v_g - v_f)_j^{n+1}\right]\Delta x_j \Delta t - \left[(\dot{\alpha}_g\dot{\rho}_g)_j^n HLOSSG_j^n v_{g,j}^{n+1} - (\dot{\alpha}_f\dot{\rho}_f)_j^n HLOSSF_j^n v_{f,j}^{n+1}\right]\Delta t
\end{aligned}
\tag{2.14}
$$

Similarly, the difference momentum equation is also integrated over x from a cell center x_K to the adjoining cell center x_L to obtain

$$
\begin{aligned}
&\left[1 + C\rho_m^2/\left(\rho_g\rho_f\right)\right]_j^n\left[\left(v_g^{n+1} - v_g^n\right) - \left(v_f^{n+1} - v_f^n\right)\right]_j \Delta x_j + \frac{1}{2}\left[\left(\dot{\alpha}_g\dot{\rho}_g\right)/\left(\alpha_g\rho_g\right)\right]_j^n\left[\left(v_g^2\right)_L^n - \left(v_g^2\right)_K^n\right]\Delta t \\
&- \frac{1}{2}\left[\left(\dot{\alpha}_g\dot{\rho}_g\right)/\left(\alpha_g\rho_g\right)\right]_j^n \mathrm{VISG}_j^n \Delta t - \frac{1}{2}\left[\left(\dot{\alpha}_f\dot{\rho}_f\right)/\left(\alpha_f\rho_f\right)\right]_j^n\left[\left(v_f^2\right)_L^n - \left(v_f^2\right)_K^n\right]\Delta t \\
&+ \frac{1}{2}\left[\left(\dot{\alpha}_f\dot{\rho}_f\right)/\left(\alpha_f\rho_f\right)\right]_j^n \mathrm{VISF}_j^n \Delta t = -(1-\eta)\left[\left(\rho_g - \rho_f\right)/\left(\rho_g\rho_f\right)\right]_j^n \left(P_L - P_K\right)^{n+1}\Delta t - \Big\{\mathrm{FWG}_j^n\left(v_g\right)_j^{n+1} \\
&- \mathrm{FWF}_j^n\left(v_f\right)_j^{n+1} - \left(f_x\right)_j^n\left(\frac{1}{\alpha_g\rho_g} + \frac{1}{\alpha_f\rho_f}\right)_j^n\left[\left(f_{wg}\right)_j^n\left(v_g\right)_j^{n+1} - \left(f_{wf}\right)_j^n\left(v_f\right)_j^{n+1}\right] \qquad (2.15) \\
&- \left[\Gamma_g^n\left(\rho_m^n v_I^{n+1} - \alpha_f^n\rho_f^n v_g^{n+1} - \alpha_g^n\rho_g^n v_f^{n+1}\right)/\left(\alpha_g\rho_g\alpha_f\rho_f\right)^n\right]_j \\
&+ \left(\rho_m FI\right)_j^n\left(\left[1 + f_x\left(C_1 - 1\right)\right]_j^n\left(v_g\right)_j^{n+1} - \left[1 + f_x\left(C_0 - 1\right)\right]_j^n\left(v_f\right)_j^{n+1}\right)\Big\}\Delta x_j \Delta t \\
&- \left\{\left[\left(\dot{\alpha}_g\dot{\rho}_g\right)/\left(\alpha_g\rho_g\right)\right]_j^n \mathrm{HLOSSG}_j^n\left(v_g\right)_j^{n+1} - \left[\left(\dot{\alpha}_f\dot{\rho}_f\right)/\left(\alpha_f\rho_f\right)\right]_j^n \mathrm{HLOSSF}_j^n\left(v_f\right)_j^{n+1}\right\}\Delta t
\end{aligned}
$$

Equations (2.13) through (2.15) constitute a system of 13 coupled algebraic equations that can be represented in matrix form as

$$
\underline{N}\left(\underline{\chi}_d^{n+1}, \underline{G}\right) - \underline{S}\left(\underline{G}\right) = \underline{0} \qquad (2.16)
$$

For clarity, Eq. (2.16) displays only the most essential functional dependencies, namely those on the following quantities:

(i) $\underline{\chi}_d^{n+1} \equiv \Big[\left(U_g\right)_k^{n+1}, \left(U_f\right)_k^{n+1}, \left(P\right)_k^{n+1}, \left(\alpha_g\right)_k^{n+1}, \left(X_n\right)_k^{n+1}, \left(X_{ni}\right)_k^{n+1}, \left(\rho_b\right)_k^{n+1}, \left(v_g\right)_j^{n+1}, \left(v_f\right)_j^{n+1}, \left(\tilde{U}_g\right)_k^{n+1}, \left(\tilde{U}_f\right)_k^{n+1},$ $\left(\tilde{\alpha}_g\right)_k^{n+1}, \left(\tilde{X}_n\right)_k^{n+1}\Big]$, which represents the vector of *discretized* state variables for volume k and/or junction j; the first nine components of $\underline{\chi}_d^{n+1}$ are state variables at time-step (n+1), while the last four components (with tilda) represent state variables evaluated at an intermediate (provisional) time-step, between time-steps (n) and (n+1), respectively;

(ii) $\underline{G} \equiv \left(g_1, \ldots, g_J\right)$, which represents a J-component column vector whose components comprise all numerical parameters in RELAP5/MOD3.2 that are subject to variations; and

(iii) $\underline{S} \equiv (s_1, \ldots, s_{13})$, which represents a 13-component column vector whose components comprise all of the inhomogeneous source terms appearing in Eqs.(2.13) through (2.15).

The system of algebraic equations represented by Eq.(2.16) is solved to obtain (i) the pressure, the fluid and gas velocities at the new time step (n+1), and (ii) the intermediate time-step variables $(\tilde{U}_g)_k^{n+1}, (\tilde{U}_f)_k^{n+1}, (\tilde{\alpha}_g)_k^{n+1}, (\tilde{X}_n)_k^{n+1}$. For the cases (b) and (d) defined above, when one-phase conditions exist at the old time step (n), the intermediate time-step is actually skipped by setting $(\tilde{U}_g)_k^{n+1} \equiv (U_g)_k^{n+1}, (\tilde{U}_f)_k^{n+1} \equiv (U_f)_k^{n+1}, (\tilde{\alpha}_g)_k^{n+1} \equiv (\alpha_g)_k^{n+1}, (\tilde{X}_n)_k^{n+1} \equiv (X_n)_k^{n+1}$, so that the intermediate time-step variables are used directly at time-step (n+1). For the cases (a) and (c) defined above, when two-phase conditions exist at the old time-step (n), the non-expanded forms of the mass and energy equations are used to obtain $(U_g)_k^{n+1}, (U_f)_k^{n+1}, (\alpha_g)_k^{n+1}, (X_n)_k^{n+1}$. As an illustrative example, the calculation of $(U_g)_L^{n+1}$, for a volume L and time-step (n+1), is presented below; the calculation of the other three state variables are presented in Appendix A. Thus, to calculate $(U_g)_L^{n+1}$, the quantity $(\alpha_g \rho_g U_g)_L^{n+1}$ is calculated from the non-expanded form of the vapor energy equation

$$
\begin{aligned}
&V_L\left[(\alpha_g\rho_g U_g)_L^{n+1} - (\alpha_g\rho_g U_g)_L^{n}\right] + \left[\dot{\alpha}_{g,j+1}\left(\dot{\rho}_{g,j+1}\dot{U}_{g,j+1} + P_L\right)v_{g,j+1}^{n+1}A_{j+1} - \dot{\alpha}_{g,j}\left(\dot{\rho}_{g,j}\dot{U}_{g,j} + P_L\right)v_{g,j}^{n+1}A_j\right]\Delta t \\
&= -V_L P_L^n\left(\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^{n}\right) + \left\{-\left(\frac{h_f^*}{h_g^* - h_f^*}\right)_L^n \frac{P_{s,L}^n}{P_L^n} H_{ig,L}^n\left(\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}\right) - \left(\frac{h_g^*}{h_g^* - h_f^*}\right)_L^n H_{if,L}^n\left(\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1}\right)\right. \\
&\left. - \frac{P_L^n - P_{s,L}^n}{P_L^n} H_{gf,L}^n\left(\tilde{T}_{g,L}^{n+1} - \tilde{T}_{f,L}^{n+1}\right) + \Gamma_{w,L}^n\left[\left(\frac{1-\varepsilon}{2}\right)\left(h'_{f,L}\right)^n + \left(\frac{1+\varepsilon}{2}\right)\left(h'_{g,L}\right)^n\right] + Q_{wg,L}^n + DISS_{g,L}^n\right\} V_L \Delta t.
\end{aligned}
$$

The quantity $(\alpha_g \rho_g)_L^{n+1}$ is calculated next from the non-expanded form of the vapor density equation shown below:

$$V_L\left[(\alpha_g\rho_g)_L^{n+1} - (\alpha_g\rho_g)_L^n\right] + \left(\dot{\alpha}_{g,j+1}\dot{\rho}_{g,j+1}v_{g,j+1}^{n+1}A_{j+1} - \dot{\alpha}_{g,j}\dot{\rho}_{g,j}v_{g,j}^{n+1}A_j\right)\Delta t$$

$$= \left(- \frac{\frac{P_{s,L}^n}{P_L^n} H_{ig,L}^n \left(\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}\right) + H_{if,L}^n \left(\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1}\right)}{\left(h_{g,L}^*\right)^n - \left(h_{f,L}^*\right)^n} + \Gamma_{w,L}^n \right) V_L \Delta t.$$

Finally, the ratio of the results from the previous two operations is calculated to obtain $(U_g)_L^{n+1} = (\alpha_g\rho_g U_g)_L^{n+1} / (\alpha_g\rho_g)_L^{n+1}$.

3 DETERMINISTIC SENSITIVITY ANALYSIS OF THE TWO-FLUID MODEL IN RELAP5/MOD3.2

Many results, customarily referred to as “responses”, $R(\underline{\chi}, \underline{G})$, calculated by RELAP5/MOD3.2 can be generally represented in the integral form

$$R(\underline{\chi}, \underline{G}) \equiv \int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx F[\underline{\chi}(x,t), \underline{G}(x,t)] \tag{3.1}$$

In particular, this integral form can be used to represent either instantaneous or averaged (in space and/or time) values of the dependent variables; for example, setting $F(\underline{\chi}, \underline{G}) = \delta_{ij}\delta(x - x_1)\delta(t - t_1) \cdot \underline{\chi}(x,t)$ in Eq. (3.1), where δ_{ij} represents the Kronecker-delta functional while $\delta(x - x_1)$ and $\delta(t - t_1)$ denote Dirac-delta functionals, yields the instantaneous value of the i-th dependent variable at the point (x_1,t_1) in space-time, namely $R(\underline{\chi}, \underline{G}) = \chi_i(x_1, t_1)$. On the other hand, setting $F(\underline{\chi}, \underline{G}) = \delta_{ij} \cdot \underline{\chi}(x,t)$ in Eq. (3.1), yields the space-time averaged value of the i-th dependent variable, namely $R(\underline{\chi}, \underline{G}) = \int_{t_0}^{t_f} dt \int_{x_0}^{x_f} dx \chi_i(x,t)$.

Conceptually, the REL/CDE are solved using base-case (or nominal) parameter values, denoted here by $\underline{G}^o$, to obtain the base-case (or nominal) solution $\underline{\chi}^o$. In turn, the base-case (nominal) solution and parameter values are used to obtain the base-case (nominal) response value $R^o(\underline{\chi}^o, \underline{G}^o)$. The base-case (nominal) parameter values $\underline{G}^o \equiv (g_1^o, \ldots, g_J^o)$ are customarily determined from experimental data; consequently, their numerical values are not known exactly but are known only within some bounds (e.g., tolerances, variations); these bounds can be represented by the vector $\underline{\Gamma} \equiv (\gamma_1, \gamma_2, \ldots, \gamma_J) \equiv (\delta g_1, \delta g_2, \ldots, \delta g_J)$, whose components are the respective parameter variations δg_j.

When the parameter variations $\underline{\Gamma} \equiv (\gamma_1, \gamma_2, \ldots, \gamma_J) \equiv (\delta g_1, \delta g_2, \ldots, \delta g_J)$ are introduced in Eqs. (2.10) and (3.1), the corresponding "perturbed" solution becomes $\underline{\chi}^o + \underline{\Phi}$, satisfying the perturbed system

$$\underline{N}(\underline{\chi}^o + \underline{\Phi}, \underline{G}^o + \underline{\Gamma}) - \underline{S}(\underline{G}^o + \underline{\Gamma}) = \underline{0}\,, \qquad (3.2)$$

while the perturbed response would become $R(\underline{\chi}^o + \underline{\Phi}, \underline{G}^o + \underline{\Gamma})$, where $\underline{\Phi} \equiv (\Phi_1, \ldots, \Phi_9) \equiv (\delta U_g, \ldots, \delta v_f)$ denotes the nine-component vector of variations in the respective components of $\underline{\chi}$. In principle, the above equation could be solved repeatedly, for each vector of variations $\underline{\Gamma} \equiv (\gamma_1, \gamma_2, \ldots, \gamma_J) \equiv (\delta g_1, \delta g_2, \ldots, \delta g_J)$ of interest, to obtain exactly perturbed solution $\underline{\chi}^o + \underline{\Phi}$, but such a procedure would become impractical when many variations δg_i must be considered.

The objective of *local sensitivity analysis*[3-5] is to analyze the behavior of the system responses locally around a chosen point or trajectory in the combined phase-space of parameters and state variables. On the other hand, the objective of *global sensitivity analysis*[6] is to determine all of the system's critical points (namely, bifurcations, turning points, extrema) in the combined phase-space formed by the parameters, state variables, and adjoint variables, and subsequently analyze these critical points by local sensitivity analysis. The most general and fundamental concept for the definition of the *local sensitivity*[4,5] of a response to parameter variations is the Gateaux (G-) differential. By definition, the G-differential $DP(\underline{e}^o;\underline{h})$ of an operator $P(\underline{e})$ at $\underline{e}^o$ with increment $\underline{h}$ is

$$DP(\underline{e}^o;\underline{h}) \equiv \lim_{\varepsilon \to 0} \varepsilon^{-1}\left[P(\underline{e}^o + \varepsilon \underline{h}) - P(\underline{e}^o) \right] = \frac{d}{d\varepsilon}\left\{ P(\underline{e}^o + \varepsilon \underline{h}) \right\}_{\varepsilon=0}, \tag{3.3}$$

for all (i.e., arbitrary) vectors $\underline{h}$, and scalar ε. The G-differential $DP(\underline{e}^o;\underline{h})$ is related to the total variation $\left[P(\underline{e}^o + \underline{h}) - P(\underline{e}^o) \right]$ through the relationship

$$P(\underline{e}^o + \underline{h}) - P(\underline{e}^o) = DP(\underline{e}^o;\underline{h}) + W(\underline{h}), \quad \text{with } \lim_{\varepsilon \to 0}\left[W(\varepsilon \underline{h})/\varepsilon \right] = 0. \tag{3.4}$$

It is important to note here that in most practical cases the G-differential $DP(\underline{e}^o;\underline{h})$ is linear in $\underline{h}$; in such cases, Eq. (3.4) indicates that the terms in $W(\underline{h})$ are of second- and higher-order in $\|\underline{h}\|$.

Applying Eq.(3.3) to Eq. (3.1), while noting that $\underline{e} = (\underline{\chi}, \underline{G})$, $\underline{e}^o = (\underline{\chi}^o, \underline{G}^o)$, and $\underline{h} = (\underline{\Phi}, \underline{\Gamma})$, yields the sensitivity $DR(\underline{\chi}^o, \underline{G}^o; \underline{\Phi}, \underline{\Gamma})$ of the response defined in Eq. (3.1) as

$$\begin{aligned} DR(\underline{\chi}^o, \underline{G}^o; \underline{\Phi}, \underline{\Gamma}) &\equiv \frac{d}{d\varepsilon}\left\{ \int_{t_o}^{t_f} dt \int_{x_o}^{x_f} dx F\left[\underline{\chi}^o + \varepsilon \underline{\Phi}, \underline{G}^o + \varepsilon \underline{\Gamma} \right] \right\}_{\varepsilon=0} \\ &= \int_{t_o}^{t_f} dt \int_{x_o}^{x_f} dx (\partial F/\partial \underline{G})^o \underline{\Gamma}(x,t) + \int_{t_o}^{t_f} dt \int_{x_o}^{x_f} dx (\partial F/\partial \underline{\chi})^o \underline{\Phi}(x,t). \end{aligned} \tag{3.5}$$

For the response $R(\underline{\chi}, \underline{G})$ defined in Eq.(3.1), Eq.(3.4) takes on the form

$$R(\underline{\chi}^o + \underline{\Phi}, \underline{G}^o + \underline{\Gamma}) = R(\underline{\chi}^o, \underline{G}^o) + DR(\underline{\chi}^o, \underline{G}^o; \underline{\Phi}, \underline{\Gamma}) + O\left(\|\underline{\Phi}\|^2 + \|\underline{\Gamma}\|^2 \right), \tag{3.6}$$

indicating that the exact value of the perturbed response, $R\left(\underline{\chi}^{o}+\underline{\Phi},\underline{G}^{o}+\underline{\Gamma}\right)$, namely the response-value that would be obtained by (exact) recalculations using perturbed values, is predicted by the sensitivity $DR\left(\underline{\chi}^{o},\underline{G}^{o};\underline{\Phi},\underline{\Gamma}\right)$ to first-order accuracy in $\|\underline{\Phi}\|$ and $\|\underline{\Gamma}\|$.

3.1 Implementation of the Forward Sensitivity Analysis Procedure (FSAP) in RELAP5/MOD3.2

This Section presents the implementation of the Forward Sensitivity Analysis Procedure for Nonlinear Systems (FSAP), as originally developed by Cacuci[3-5] , for the two-fluid model of RELAP5/MOD3.2. Thus, Sec. 3.1.1 below presents the implementation of the FSAP for the "Numerically Convenient Set of Differential Equations" (REL/CDE) represented by Eq. (2.10), while Sec. 3.1.2 describes the implementation of the FSAP for the set of algebraic equations represented by Eq. (2.16), obtained by discretizing the REL/CDE using the semi-implicit time-discretization scheme and the staggered-mesh spatial discretization scheme that was described in Sec. 2.2.

3.1.1 Implementation of the FSAP for REL/CDE

As Eq. (3.5) indicates, the sensitivity $DR\left(\underline{\chi}^{o},\underline{G}^{o};\underline{\Phi},\underline{\Gamma}\right)$ can be calculated once the function $\underline{\Phi}$ is determined. *To first-order accuracy in* $\|\underline{\Gamma}\|$, $\underline{\Phi}$ *is the solution of the Forward Sensitivity Model (FSM),* ***obtained by taking the G-differentials of the Differential REL/CDE***. In the following, the derivation of the FSM is illustrated by presenting the calculations of the respective G-differentials for a typical "momentum-like"-conservation equation, a typical "density-like"-conservation equation, and a typical "energy-like"-conservation equation. For example, the G-differential of the "sum momentum equation" is obtained by calculating the expression

$$
\begin{aligned}
&\frac{d}{d\varepsilon}\Big\{\Big[\left(\alpha_g^o+\varepsilon\delta\alpha_g\right)\rho_g\left(X_n^o+\varepsilon\delta X_n, U_g^o+\varepsilon\delta U_g, P^o+\varepsilon\delta P; g_j^o+\varepsilon\delta g_j\right)\frac{\partial}{\partial t}\left(v_g^o+\varepsilon\delta v_g\right)+\\
&\left(1-\alpha_g^o-\varepsilon\delta\alpha_g\right)\frac{\partial}{\partial t}\left(v_f^o+\varepsilon\delta v_f\right)\cdot\rho_f\left(U_f^o+\varepsilon\delta U_f, P^o+\varepsilon\delta P; g_j^o+\varepsilon\delta g_j\right)+\\
&\frac{1}{2}\left(\alpha_g^o+\varepsilon\delta\alpha_g\right)\cdot\rho_g\left(X_n^o+\varepsilon\delta X_n, U_g^o+\varepsilon\delta U_g, P^o+\varepsilon\delta P; g_j^o+\varepsilon\delta g_j\right)\frac{\partial}{\partial x}\left(v_g^o+\varepsilon\delta v_g\right)^2+\\
&\frac{1}{2}\left(1-\alpha_g^o-\varepsilon\delta\alpha_g\right)\rho_f\left(U_f^o+\varepsilon\delta U_f, P^o+\varepsilon\delta P; g_j^o+\varepsilon\delta g_j\right)\frac{\partial}{\partial x}\left(v_f^o+\varepsilon\delta v_f\right)^2\\
&+\frac{\partial}{\partial x}\left(P^o+\varepsilon\delta P\right)\Big]\Big\}_{\varepsilon=0}=\frac{d}{d\varepsilon}\Big\{E_6\big(X_n^o+\varepsilon\delta X_n, U_g^o+\varepsilon\delta U_g, U_f^o+\varepsilon\delta U_f, \alpha_g^o+\varepsilon\delta\alpha_g,\\
&P^o+\varepsilon\delta P, v_g^o+\varepsilon\delta v_g, v_f^o+\varepsilon\delta v_f; g_j^o+\varepsilon\delta g_j\big)\Big\}_{\varepsilon=0}
\end{aligned}
$$

where $E_6\left(\underline{\chi},\underline{G}\right)$ is defined as

$$
E_6\left(\underline{\chi},\underline{G}\right)\equiv\rho_m B_x-\alpha_g\rho_g FWG\, v_g-\alpha_f\rho_f FWF\, v_f-\Gamma_g\left(v_g-v_f\right),
$$

and where FWG, FWF, and Γ_g are nonlinear algebraic functions of the dependent variables $\underline{\chi}$ and parameters $\underline{G}$.

Performing the differentiation operations in the above equation yields

$$\left(\alpha_g^o\left[\frac{\partial v_g^o}{\partial t}+\frac{1}{2}\frac{\partial\left(v_g^o\right)^2}{\partial x}\right]\left(\frac{\partial\rho_g}{\partial X_n}\right)_o-\left(\frac{\partial E_6}{\partial X_n}\right)_o\right)\delta X_n+\left(\alpha_g^o\left[\frac{\partial v_g^o}{\partial t}+\frac{1}{2}\frac{\partial\left(v_g^o\right)^2}{\partial x}\right]\left(\frac{\partial\rho_g}{\partial U_g}\right)_o-\left(\frac{\partial E_6}{\partial U_g}\right)_o\right)\delta U_g$$

$$+\left(\alpha_f^o\left[\frac{\partial v_f^o}{\partial t}+\frac{1}{2}\frac{\partial\left(v_f^o\right)^2}{\partial x}\right]\cdot\left(\frac{\partial\rho_f}{\partial U_f}\right)_o-\left(\frac{\partial E_6}{\partial U_f}\right)_o\right)\delta U_f$$

$$+\left(\rho_g^o\left[\frac{\partial v_g^o}{\partial t}+\frac{1}{2}\frac{\partial\left(v_g^o\right)^2}{\partial x}\right]-\rho_f^o\left[\frac{\partial v_f^o}{\partial t}+\frac{1}{2}\frac{\partial\left(v_f^o\right)^2}{\partial x}\right]-\left(\frac{\partial E_6}{\partial\alpha_g}\right)_o\right)\delta\alpha_g$$

$$+\left(\alpha_g^o\left[\frac{\partial v_g^o}{\partial t}+\frac{1}{2}\frac{\partial\left(v_g^o\right)^2}{\partial x}\right]\left(\frac{\partial\rho_g}{\partial P}\right)_o+\alpha_f^o\left[\frac{\partial v_f^o}{\partial t}+\frac{1}{2}\frac{\partial\left(v_f^o\right)^2}{\partial x}\right]\left(\frac{\partial\rho_f}{\partial P}\right)_o-\left(\frac{\partial E_6}{\partial P}\right)_o\right)\delta P+\frac{\partial}{\partial x}(\delta P)+$$

$$+\alpha_g^o\rho_g^o\left(\frac{\partial}{\partial t}\left(\delta v_g\right)+\frac{\partial}{\partial x}\left(v_g^o\cdot\delta v_g\right)\right)-\left(\frac{\partial E_6}{\partial v_g}\right)_o\delta v_g+\alpha_f^o\rho_f^o\cdot\left(\frac{\partial}{\partial t}\left(\delta v_f\right)+\frac{\partial}{\partial x}\left(v_f^o\cdot\delta v_f\right)\right)-\left(\frac{\partial E_6}{\partial v_f}\right)_o\delta v_f$$

$$=\left(\frac{\partial E_6}{\partial A}\right)_o\delta A+\left(\frac{\partial E_6}{\partial g_j}\right)_o\delta g_j-\left(\alpha_g^o\left[\frac{\partial v_g^o}{\partial t}+\frac{1}{2}\frac{\partial\left(v_g^o\right)^2}{\partial x}\right]\left(\frac{\partial\rho_g}{\partial g_j}\right)_o+\alpha_f^o\left[\frac{\partial v_f^o}{\partial t}+\frac{1}{2}\frac{\partial\left(v_f^o\right)^2}{\partial x}\right]\left(\frac{\partial\rho_f}{\partial g_j}\right)_o\right)\delta g_j.$$

As a further example, the G-differential of the “sum density equation” is calculated by performing the differentiation shown in the following equation:

$$\frac{d}{d\varepsilon}\left\{\left(\alpha_g^o+\varepsilon\delta\alpha_g\right)\frac{\partial}{\partial t}\rho_g\left(X_n^o+\varepsilon\delta X_n,U_g^o+\varepsilon\delta U_g,P^o+\varepsilon\delta P;g_j^o+\varepsilon\delta g_j\right)\right.$$

$$+\left(1-\alpha_g^o-\varepsilon\delta\alpha_g\right)\frac{\partial}{\partial t}\rho_f\left(U_f^o+\varepsilon\delta U_f,P^o+\varepsilon\delta P;g_j^o+\varepsilon\delta g_j\right)$$

$$+\left(\rho_g\left(X_n^o+\varepsilon\delta X_n,U_g^o+\varepsilon\delta U_g,P^o+\varepsilon\delta P;g_j^o+\varepsilon\delta g_j\right)-\rho_f\left(U_f^o+\varepsilon\delta U_f,P^o+\varepsilon\delta P;g_j^o+\varepsilon\delta g_j\right)\right)$$

$$\frac{\partial}{\partial t}\left(\alpha_g^o+\varepsilon\delta\alpha_g\right)+\frac{1}{A^o+\varepsilon\delta A}\left\{\frac{\partial}{\partial x}\left[\left(\alpha_g^o+\varepsilon\delta\alpha_g\right)\left(v_g^o+\varepsilon\delta v_g\right)\left(A^o+\varepsilon\delta A\right)\right.\right.$$

$$\rho_g\left(X_n^o+\varepsilon\delta X_n,U_g^o+\varepsilon\delta U_g,P^o+\varepsilon\delta P;g_j^o+\varepsilon\delta g_j\right)$$

$$\left.\left.\left.\left(1-\alpha_g^o-\varepsilon\delta\alpha_g\right)\rho_f\left(U_f^o+\varepsilon\delta U_f,P^o+\varepsilon\delta P;g_j^o+\varepsilon\delta g_j\right)\left(v_f^o+\varepsilon\delta v_f\right)\left(A^o+\varepsilon\delta A\right)\right]\right\}\right\}_{\varepsilon=0}=0$$

Similarly, the G-differential of the “liquid energy equation” is obtained by calculating the expression

$$
\begin{aligned}
&\frac{d}{d\varepsilon}\Bigg\{-\Big[\rho_f\left(U_f^0+\varepsilon\delta U_f, P^0+\varepsilon\delta P; g_j^0+\varepsilon\delta g_j\right)\left(U_f^0+\varepsilon\delta U_f\right)+P^0+\varepsilon\delta P\Big]\frac{\partial}{\partial t}\left(\alpha_g^0+\varepsilon\delta\alpha_g\right)\\
&+\left(1-\alpha_g^0-\varepsilon\delta\alpha_g\right)\left(U_f^0+\varepsilon\delta U_f\right)\frac{\partial}{\partial t}\rho_f\left(U_f^0+\varepsilon\delta U_f, P^0+\varepsilon\delta P; g_j^0+\varepsilon\delta g_j\right)\\
&+\left(1-\alpha_g^0-\varepsilon\delta\alpha_g\right)\rho_f\left(U_f^0+\varepsilon\delta U_f, P^0+\varepsilon\delta P; g_j^0+\varepsilon\delta g_j\right)\frac{\partial}{\partial t}\left(U_f^0+\varepsilon\delta U_f\right)\\
&+\frac{1}{A^0+\varepsilon\delta A}\Bigg\{\frac{\partial}{\partial x}\Big[\left(1-\alpha_g^0-\varepsilon\delta\alpha_g\right)\rho_f\left(U_f^0+\varepsilon\delta U_f, P^0+\varepsilon\delta P; g_j^0+\varepsilon\delta g_j\right)\left(U_f^0+\varepsilon\delta U_f\right)\cdot\\
&\left(v_f^0+\varepsilon\delta v_f\right)\left(A^0+\varepsilon\delta A\right)+\left(P^0+\varepsilon\delta P\right)\frac{\partial}{\partial x}\Big[\left(1-\alpha_g^0-\varepsilon\delta\alpha_g\right)\left(v_f^0+\varepsilon\delta v_f\right)\left(A^0+\varepsilon\delta A\right)\Big]\Bigg\}\Bigg\}_{\varepsilon=0}\\
&=\frac{d}{d\varepsilon}\Big\{E_3\Big(X_n^0+\varepsilon\delta X_n, U_g^0+\varepsilon\delta U_g, U_f^0+\varepsilon\delta U_f, \alpha_g^0+\varepsilon\delta\alpha_g, P^0+\varepsilon\delta P, v_g^0+\varepsilon\delta v_g, v_f^0+\varepsilon\delta v_f;\\
&g_j^0+\varepsilon\delta g_j\Big)\Big\}_{\varepsilon=0}
\end{aligned}
$$

where

$$
\begin{aligned}
E_3\left(\underline{\chi},\underline{G}\right)\equiv&\left(\frac{h_f'}{h_g'-h_f'}\right)H_{ig}\left(T^s-T_g\right)+\left(\frac{h_g'}{h_g'-h_f'}\right)H_{if}\left(T^s-T_f\right)\\
&-\left[\left(\frac{1+\varepsilon}{2}\right)h_g^s+\left(\frac{1-\varepsilon}{2}\right)h_f^s\right]\Gamma_w+Q_{wf}+DISS_f,
\end{aligned}
$$

and where H_{if}, Γ_w, Q_{wf} and $DISS_f$ are nonlinear algebraic functions of the dependent variables $\underline{\chi}$ and parameters $\underline{G}$.

The G-differentials of the remaining equations comprising the REL/CDE are calculated similarly. Collecting all of the G-differentiated REL/CDE yields the FSM for the two-fluid model, which can be represented in the form

$$\sum_{n=1}^{9}\left\{\frac{\partial}{\partial t}\left[S_{mn}(x,t)\Phi_n(x,t)\right]+\frac{1}{A^o(x)}\frac{\partial}{\partial x}\left[A^o(x)T_{mn}(x,t)\Phi_n(x,t)\right]+U_{mn}(x,t)\ \Phi_n(x,t)\right\}$$
$$\equiv \underline{\underline{L}}\underline{\Phi} \tag{3.7}$$
$$=\sum_{j=1}^{J}Q_{mj}(x,t)\Gamma_j(x,t),\quad \text{for } m=1,\ldots 9.$$

where the vector-valued function $\underline{\Phi}\equiv(\Phi_1,\ldots,\Phi_9)\equiv(\delta U_g,\ldots,\ \delta v_f)$ is subject to the known initial-time condition $\underline{\Phi}(x,t_o)=\Delta\underline{\chi}(x,t_o)$, for all x, and the known boundary condition $\underline{\Phi}(x_o,t)=\Delta\underline{\chi}(x_o,t)$ at x_o for all t, respectively.

The expressions for the quantities $S_{mn}(x,t)$, $T_{mn}(x,t)$, $U_{mn}(x,t)$ and $Q_{mj}(x,t)$ introduced in the above equation have been obtained by symbolic computer calculus using MAPLE V[13]. Since the quantities $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$ appear on the left-side of Eq. (3.7), they will also appear in the expression of the ASM-REL/TF, as will be shown in the sequel in Sec. 3.2; for this reason, their explicit formulae are presented in Appendix B.

The solution of Eq. (3.7) could, in principle, be used in Eq.(3.6) to calculate the sensitivity $DR(\underline{\chi}^o,\underline{G}^o;\underline{\Phi},\underline{\Gamma})$, since the error in obtaining $\underline{\Phi}\equiv(\Phi_1,\ldots,\Phi_9)$ from Eq. (3.7) is of second-order in $\|\underline{\Gamma}\|$. Note, however, that Eq. (3.7) would need to be solved anew (i.e., repeatedly) for each Γ_i, which is impractical if there are many Γ_i. Thus, *the Forward Sensitivity Analysis Procedure (FSAP) is computationally just as expensive as performing repeatedly the exact recalculations* by solving Eq. (3.2) with the RELAP5/MOD3.2 code system, and then recalculating the exact perturbed response $R(\underline{\chi}^o+\underline{\Phi},\underline{G}^o+\underline{\Gamma})$.

3.1.2 Implementation of the FSAP for the Discretized REL/CDE

A result (response) calculated by RELAP5/MOD3.2 can be generally represented in discretized form as

$$R\left(\underline{\chi}_d, \underline{G}\right) = \sum_{n=0}^{NF} \sum_{j=1}^{NJ} \sum_{k=1}^{NV} F_{jk}^n \left(\underline{\chi}_d, \underline{G}\right) \tag{3.8}$$

where NF, NJ, and NV denote, respectively, the total number of time steps, the total number of junctions, and the total number of volumes in the problem under consideration.

When the parameter variations $\underline{\Gamma} \equiv (\gamma_1, \gamma_2, \ldots, \gamma_J) \equiv (\delta g_1, \delta g_2, \ldots, \delta g_J)$ are considered in Eqs. (2.16) and (3.8), the corresponding "perturbed" solution would become $\underline{\chi}_d^o + \underline{\Psi}$, satisfying the perturbed system

$$\underline{N}\left(\underline{\chi}_d^o + \underline{\Psi}, \underline{G}^o + \underline{\Gamma}\right) - \underline{S}\left(\underline{G}^o + \underline{\Gamma}\right) = \underline{0}\ , \tag{3.9}$$

while the perturbed response would become $R\left(\underline{\chi}_d^o + \underline{\Psi}, \underline{G}^o + \underline{\Gamma}\right)$, where $\underline{\Psi} \equiv \left[\left(\delta U_g\right)_k^{n+1}, \ldots, \left(\delta \widetilde{X}_n\right)_k^{n+1}\right]$ denotes the corresponding variations in the vector of dependent variables $\underline{\chi}_d$.

Applying Eq. (3.3) to (3.8) yields the following expression for the sensitivity DR of R to variations $\underline{\Gamma}$ (in $\underline{G}$ around $\underline{G}^o$) and $\underline{\Psi}$ (in $\underline{\chi}_d$ around $\underline{\chi}_d^o$) :

$$DR = \sum_{n=0}^{NF} \sum_{j=1}^{NJ} \sum_{k=1}^{NV} \left[\sum_{v=1}^{13} \frac{\partial F_{jk}^n}{\partial \chi_{d,v}} \Psi_v + \sum_{\alpha=1}^{J} \frac{\partial F_{jk}^n}{\partial G_\alpha} \Gamma_\alpha \right] \equiv DR\left(\underline{\Psi}\right) + DR\left(\underline{\Gamma}\right) \tag{3.10}$$

where $DR(\underline{\Gamma})$ represents the “direct effect” term while $DR(\underline{\Psi})$ represents the “indirect effect” term.

The indirect effect term $DR(\underline{\Psi})$ can be calculated only after having obtained $\underline{\Psi}$, which can be obtained, to first order in $\|\underline{\Gamma}\|$, by taking the G-differential of Eq.(2.16) to obtain the Discrete FSM, and subsequently solving this system. To derive the Discrete FSM, it is convenient to introduce the following notations:

for variations in the volume-averaged dependent variables, over a volume k = 1,...,NV, at time-step n, n = 1,..,NF, the following notations are introduced:

$$\left(X_k^1\right)^n \equiv \left(\delta U_g\right)_k^n,\ \left(X_k^2\right)^n \equiv \left(\delta U_f\right)_k^n,\ \left(X_k^3\right)^n \equiv \left(\delta P\right)_k^n,\ \left(X_k^4\right)^n \equiv \left(\delta \alpha_g\right)_k^n,$$
$$\left(X_k^5\right)^n \equiv \left(\delta X_n\right)_k^n,\ \left(X_k^6\right)^n \equiv \left(\delta X_{ni}\right)_k^n,\ \left(X_k^7\right)^n \equiv \left(\delta \rho_b\right)_k^n ;$$

for variations in the dependent variables defined at junctions j = 1,...,NJ, at time-step n, the following notations are introduced:

$$\left(Y_k^1\right)^n \equiv \left(\delta v_g\right)_j^n,\ \left(Y_k^2\right)^n \equiv \left(\delta v_f\right)_j^n ;$$

for variations in the volume-averaged, intermediate-time-step variables, for a volume k = 1,...,NV, at time-step n, the following notations are introduced:

$$\left(Z_k^1\right)^n \equiv \left(\delta \tilde{U}_g\right)_k^n,\ \left(Z_k^2\right)^n \equiv \left(\delta \tilde{U}_f\right)_k^n,\ \left(Z_k^3\right)^n \equiv \left(\delta \tilde{\alpha}_g\right)_k^n,\ \left(Z_k^4\right)^n \equiv \left(\delta \tilde{X}_n\right)_k^n .$$

It is also convenient to denote the total number of volume-averaged dependent variables by M_1, and the total number of intermediate-time-step variables by M_2, at any time step n; note that $4 \le M_1 \le 7$ and $0 \le M_2 \le 4$. Note also that the quantities $\left(X_k^1\right)^n, \ldots, \left(X_k^7\right)^n, \left(Y_k^1\right)^n, \left(Y_k^2\right)^n, \left(Z_k^1\right)^n, \ldots, \left(Z_k^4\right)^n$ are actually components of $\underline{\Psi}$; they were introduced in order to simplify the notation in the derivations to follow below, aimed at eliminating the intermediate-time variables.

Applying the definition of the G-differential to Eq. (3.9) and using the above notations yields the following matrix representation of the Discrete FSM:

$$\sum_{\nu=1}^{M_1}\left[BV_{\mu\nu}^{n-1}X_\nu^n + CV_{\mu\nu}^{n-1}X_\nu^{n-1}\right] + \sum_{\nu=1}^{2}\left[DV_{\mu\nu}^{n-1}Y_\nu^n + EV_{\mu\nu}^{n-1}Y_\nu^{n-1}\right] + \sum_{\nu=1}^{M_2}\left[TV_{\mu\nu}^{n-1}Z_\nu^n\right] = FV_{\mu\nu}^{n-1},$$

for $\mu = 1,\ldots,M_1$; $n = 1,\ldots,NF$;

$$\sum_{\nu=1}^{M_1}\left[BJ_{\mu\nu}^{n-1}X_\nu^n + CJ_{\mu\nu}^{n-1}X_\nu^{n-1}\right] + \sum_{\nu=1}^{2}\left[DJ_{\mu\nu}^{n-1}Y_\nu^n + EJ_{\mu\nu}^{n-1}Y_\nu^{n-1}\right] = FJ_{\mu\nu}^{n-1},$$

for $\mu = 1,2$; $n = 1,\ldots,NF$;

$$\sum_{\nu=1}^{M_1}\left[BI_{\mu\nu}^{n-1}X_\nu^n + CI_{\mu\nu}^{n-1}X_\nu^{n-1}\right] + \sum_{\nu=1}^{2}\left[DI_{\mu\nu}^{n-1}Y_\nu^n + EI_{\mu\nu}^{n-1}Y_\nu^{n-1}\right] + \sum_{\nu=1}^{M_2}\left[TI_{\mu\nu}^{n-1}Z_\nu^n\right] = FI_{\mu\nu}^{n-1},$$

for $\mu = 1,\ldots,M_2$; $n = 1,\ldots,NF$ (3.11)

The various matrices and vectors appearing in the above Discrete FSM are defined as follows:

$$FV_\mu^n \equiv \begin{bmatrix} (fv)_1^\mu \\ \vdots \\ (fv)_{NV}^\mu \end{bmatrix}_{(NV\times 1)}; \; FJ_\mu^n \equiv \begin{bmatrix} (fj)_1^\mu \\ \vdots \\ (fj)_{NJ}^\mu \end{bmatrix}_{(NJ\times 1)}; \; FI_\mu^n \equiv \begin{bmatrix} (fi)_1^\mu \\ \vdots \\ (fi)_{NV}^\mu \end{bmatrix}_{(NV\times 1)};$$

$$X_\mu^n \equiv \begin{bmatrix} X_1^\mu \\ \vdots \\ X_{NV}^\mu \end{bmatrix}_{(NV\times 1)}; \; Y_\mu^n \equiv \begin{bmatrix} Y_1^\mu \\ \vdots \\ Y_{NJ}^\mu \end{bmatrix}_{(NJ\times 1)}; \; Z_\mu^n \equiv \begin{bmatrix} Z_1^\mu \\ \vdots \\ Z_{NV}^\mu \end{bmatrix}_{(NV\times 1)};$$

$$BV_{\mu\nu}^n \equiv \left[(bv)_{ij}^{\mu\nu}\right]_{(NV\times NV)}; \quad CV_{\mu\nu}^n \equiv \left[(cv)_{ij}^{\mu\nu}\right]_{(NV\times NV)}; \; DV_{\mu\nu}^n \equiv \left[(dv)_{ij}^{\mu\nu}\right]_{(NV\times NJ)};$$

$$EV_{\mu\nu}^n \equiv \left[(ev)_{ij}^{\mu\nu}\right]_{(NV\times NJ)}; \quad TV_{\mu\nu}^n \equiv \left(diag\left\{(tv^{\mu\nu})_k^n\right\}\right)_{NV\times NV}; \quad TI_{\mu\nu}^n \equiv \left(diag\left\{(ti^{\mu\nu})_k^n\right\}\right)_{NV\times NV};$$

$$BJ_{\mu\nu}^n \equiv \left[(bj)_{ij}^{\mu\nu}\right]_{(NJ\times NV)}; \quad CJ_{\mu\nu}^n \equiv \left[(cj)_{ij}^{\mu\nu}\right]_{(NJ\times NV)}; \; DJ_{\mu\nu}^n \equiv \left[(dj)_{ij}^{\mu\nu}\right]_{(NJ\times NJ)};$$

$$EJ_{\mu\nu}^n \equiv \left[(ej)_{ij}^{\mu\nu}\right]_{(NJ\times NJ)}; \; BI_{\mu\nu}^n \equiv \left[(bi)_{ij}^{\mu\nu}\right]_{(NV\times NV)}; \quad CI_{\mu\nu}^n \equiv \left[(ci)_{ij}^{\mu\nu}\right]_{(NV\times NV)};$$

$$DI_{\mu\nu}^n \equiv \left[(di)_{ij}^{\mu\nu}\right]_{(NV\times NJ)}; \quad EI_{\mu\nu}^n \equiv \left[(ei)_{ij}^{\mu\nu}\right]_{(NV\times NJ)};$$

The vectors on the right-side of Eqs. (3.11) represent the $\underline{\Gamma}$-dependent terms that result from the application of the definition of the G-differential to Eq. (2.16). All of the components entering the definitions of the matrices appearing on the left-side of Eqs. (3.11) and vectors appearing on the right-side of Eqs. (3.11) have been obtained explicitly using the symbolic computer language MAPLE V, and have been programmed accordingly, but will not be reproduced here because of their lengthy and cumbersome expressions.

The algebraic system represented by Eq. (3.11) can be written in a more compact form by introducing the partitioned matrices:

$$\begin{bmatrix} BV_{11} & \cdots & BV_{1,M_1} & DV_{11} & DV_{12} \\ \vdots & & \vdots & \vdots & \vdots \\ BV_{M_1,1} & \cdots & BV_{M_1,M_1} & DV_{M_1,1} & DV_{M_1,2} \\ BJ_{11} & \cdots & BJ_{1,M_1} & DJ_{11} & DJ_{12} \\ BJ_{21} & \cdots & BJ_{2,M_1} & DJ_{21} & DJ_{22} \end{bmatrix}^{(n)}_{(M_1+2)\times(M_1+2)} \equiv B_1^{(n)} ;$$

$$\begin{bmatrix} BI_{11} & BI_{1,M_1} & DI_{11} & DI_{12} \\ \vdots & \vdots & \vdots & \vdots \\ BI_{M_2,1} & BI_{M_2,M_1} & DI_{M_2,1} & DI_{M_2,2} \end{bmatrix}^{(n)}_{M_2\times(M_1+2)} \equiv B_2^{(n)} ;$$

$$\begin{bmatrix} TV_{11} & \cdots & TV_{1,M_2} \\ \vdots & & \vdots \\ TV_{M_1,1} & \cdots & TV_{M_1,M_2} \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \end{bmatrix}^{(n)}_{(M_1+2)\times M_2} \equiv T_1^{(n)} ; \quad \begin{bmatrix} TI_{11} & \cdots & TI_{1,M_2} \\ \vdots & & \vdots \\ TI_{M_2,1} & \cdots & TI_{M_2,M_2} \end{bmatrix}^{(n)}_{M_2\times M_2} \equiv T_2^{(n)} ;$$

$$\begin{bmatrix} CV_{11} & \cdots & CV_{1,M_1} & EV_{11} & EV_{12} \\ \vdots & & \vdots & \vdots & \vdots \\ CV_{M_1,1} & \cdots & CV_{M_1,M_1} & EV_{M_1,1} & EV_{M_1,2} \\ CJ_{11} & \cdots & CJ_{1,M_1} & EJ_{11} & EJ_{12} \\ CJ_{21} & \cdots & CJ_{2,M_1} & EJ_{21} & EJ_{22} \end{bmatrix}^{(n)}_{(M_1+2)\times(M_1+2)} \equiv C_1^{(n)} ; \quad \begin{bmatrix} X_1 \\ \vdots \\ X_{M_1} \\ Y_1 \\ Y_2 \end{bmatrix}^{(n)} \equiv X^n ;$$

$$\begin{bmatrix} CI_{11} & CI_{1,M_1} & EI_{11} & EI_{12} \\ \vdots & \vdots & \vdots & \vdots \\ CI_{M_2,1} & CI_{M_2,M_1} & EI_{M_2,1} & EI_{M_2,2} \end{bmatrix}^{(n)}_{M_2\times(M_1+2)} \equiv C_2^{(n)}\,; \quad \begin{bmatrix} Z_1 \\ \vdots \\ Z_{M_2} \end{bmatrix}^{(n)} \equiv X_I^{(n)}\,;$$

and introduce them in Eq. (3.11) to obtain the following system of matrix equations:

$$\begin{cases} B_1^{(n-1)} X^{(n)} + T_1^{(n-1)} X_I^{(n)} = F_1^{(n-1)} - C_1^{(n-1)} X^{(n-1)} \\ B_2^{(n-1)} X^{(n)} + T_2^{(n-1)} X_I^{(n)} = F_2^{(n-1)} - C_2^{(n-1)} X^{(n-1)} \end{cases} \tag{3.12}$$

As shown in Appendix C, the matrix $T_2^{(n-1)}$ in Eq. (3.12) is always nonsingular, and therefore admits an inverse $\left[T_2^{(n-1)}\right]^{-1}$; the procedure to calculate $\left[T_2^{(n-1)}\right]^{-1}$ is also presented in Appendix C. The matrix $\left[T_2^{(n-1)}\right]^{-1}$ is used in Eq. (3.12) above to eliminate the vector of "intermediate-time" unknowns, $X_I^{(n)}$. The result of this elimination is the following system of matrix equations:

$$\begin{cases} G^{(n-1)} X^{(n)} + H^{(n-1)} X^{(n-1)} = K^{(n-1)}, \quad \text{for } n = 1,\ldots,NF \\ X^{(0)} = K^{init}, \end{cases} \tag{3.13}$$

where K^{init} is a vector that contains the (known) perturbations in the initial conditions, and where the matrices $G^{(n-1)}$, $H^{(n-1)}$, and $K^{(n-1)}$ are defined as follows:

$$G^{(n-1)} \equiv B_1^{(n-1)} - T_1^{(n-1)}\left[T_2^{(n-1)}\right]^{-1} B_2^{(n-1)}, \;\; H^{(n-1)} \equiv C_1^{(n-1)} - T_1^{(n-1)}\left[T_2^{(n-1)}\right]^{-1} C_2^{(n-1)},$$

and $K^{(n-1)} \equiv F_1^{(n-1)} - T_1^{(n-1)}\left[T_2^{(n-1)}\right]^{-1} F_2^{(n-1)}$, respectively.

3.2 Implementation of the Adjoint Sensitivity Analysis Procedure (ASAP) in RELAP5/MOD3.2

This Section presents the implementation of the Adjoint Sensitivity Analysis Procedure for Nonlinear Systems (ASAP), as originally developed by Cacuci[4,5], for the two-fluid model of RELAP5/MOD3.2. Thus, Sec. 3.2.1 presents the implementation of the ASAP for the Differential REL/CDE, while Sec. 3.2.2 describes the implementation of the ASAP for Discretized REL/CDE.

3.2.1 Implementation of the ASAP for REL/CDE

The Adjoint Sensitivity Analysis Procedure (ASAP) relies[4] on the fact that the FSM represented by Eq. (3.7) is linear in $\underline{\Phi}$. It is therefore possible to introduce the vector $\underline{\Phi}^*(x,t) \equiv \left(\Phi_1^*(x,t),\ldots,\Phi_9^*(x,t)\right)$ of adjoint functions by taking the inner product of $\underline{\Phi}^*$ with Eq. (3.7) to obtain

$$\left\langle \underline{\Phi}^*, \underline{\underline{L}}\underline{\Phi} \right\rangle = \left\langle \underline{\underline{M}}\underline{\Phi}^*, \underline{\Phi} \right\rangle + \left\{ P\left[\underline{\Phi}, \underline{\Phi}^*\right] \right\}, \tag{3.14}$$

where: (i) the angular brackets denote the inner product $\left\langle \underline{a}, \underline{b} \right\rangle \equiv \int_{t_o}^{t_f} dt \int_{x_o}^{x_f} dx\, \underline{a}(x,t) \cdot \underline{b}(x,t)$, (ii) $\underline{\underline{M}}$ is the formal adjoint of $\underline{\underline{L}}$, and (iii) $\left\{ P\left[\underline{\Phi}, \underline{\Phi}^*\right] \right\}$ denotes the bilinear concomitant evaluated on the surface, in space-time, of the computational domain (x,t). In practice, the right-side of Eq. (3.14) is obtained by first performing the vector-multiplication between $\underline{\Phi}^*$ and $\underline{\underline{L}}\underline{\Phi}$, and then by integrating the resulting differential equations by parts over x and t such as to transfer all of the differentiation operations from the components of $\underline{\Phi}$ to the components of $\underline{\Phi}^*$.

Following the ASAP guidelines[4] to obtain the ASM-REL/TF, the following sequence of operations is performed in Eq. (3.14): (i) set $\underline{\underline{M}}\,\underline{\Phi}^* = (\partial F/\partial \underline{\chi})^o$; (ii) eliminate the unknown values $\underline{\Phi}(x,t_f)$ and $\underline{\Phi}(x_f,t)$ by imposing $\underline{\Phi}^*(x,t_f) = \underline{0}$ and $\underline{\Phi}^*(x_f,t) = \underline{0}$ as "final-time" and, respectively, "boundary" conditions for $\underline{\Phi}^*$; and (iii) use the known initial and boundary conditions for $\underline{\Phi}$. This sequence of operations transforms Eq. (3.14) to

$$\left\langle (\partial F/\partial \underline{\chi})^o, \underline{\Phi} \right\rangle = \left\langle \underline{\Phi}^*, \underline{\underline{L}}\,\underline{\Phi} \right\rangle + \int_{x_o}^{x_f} \underline{\Phi}^*(x,t_o)\left[\underline{\underline{S}}(x,t_o) \bullet \Delta\underline{\chi}(x,t_o)\right] dx + \int_{t_o}^{t_f} \underline{\Phi}^*(x_o,t)\left[\underline{\underline{T}}(x_o,t) \bullet \Delta\underline{\chi} \qquad (3.15)$$

where the vector-valued adjoint function $\underline{\Phi}^*$ satisfies the following system of equations:

$$\sum_{n=1}^{9} \left\{ -S_{nm}\,\partial \Phi_n^*/\partial t - A^o(x) T_{nm}\,\partial\left(\Phi_n^*/A^o\right)/\partial x + U_{nm}(x,t)\,\Phi_n^*(x,t) \right\} = (\partial F/\partial \chi_m)^o,\ m = 1,.. \qquad (3.16)$$

and where $\underline{\Phi}^*$ is subject to the final-time conditions $\underline{\Phi}^*(x,t_f) = \underline{0}$, for all x, and the boundary conditions $\underline{\Phi}^*(x_f,t) = \underline{0}$, for all t. *Equation* (3.16) *together with the respective boundary and initial conditions for the adjoint function* $\underline{\Phi}^*(x,t)$ *are referred to as the Adjoint Sensitivity Model (ASM-REL/TF).*

Comparing Eqs. (3.5) and (3.15) reveals that the sensitivity DR can now be expressed in terms of the adjoint function $\underline{\Phi}^*$ as

$$\begin{aligned} DR\left(\underline{\chi}^o, \underline{G}^o; \underline{\Phi}, \underline{\Gamma}; \underline{\Phi}^*\right) &= \sum_{j=1}^{J} \int_{x_o}^{x_f} dx \int_{t_o}^{t_f} dt\, (\partial F/\partial \gamma_j)^o \Gamma_j + \int_{t_o}^{t_f} dt \int_{x_o}^{x_f} dx\, \underline{\Phi}^* \bullet \left(\underline{\underline{Q}}\,\underline{\Gamma}\right) \\ &+ \int_{x_o}^{x_f} \underline{\Phi}^*(x,t_o)\left[\underline{\underline{S}}(x,t_o) \bullet \Delta\underline{\chi}(x,t_o)\right] dx + \int_{t_o}^{t_f} \underline{\Phi}^*(x_o,t)\left[\underline{\underline{T}}(x_o,t) \bullet \Delta\underline{\chi}(x_o,t)\right] dt. \end{aligned} \qquad (3.17)$$

Equation (3.16) reveals the following important characteristics regarding the ASAP:

the ASM-REL/TF does not depend on the parameter variations Γ_j; hence, *the adjoint function* $\underline{\Phi}^*$ *is independent of parameter variations*, too;

the source for (i.e., the right-side of) the ASM-REL/TF depends on the response R; hence, $\underline{\Phi}^*$ *must be calculated anew for every R*;

the ASM-REL/TF is *linear in* $\underline{\Phi}^*$; hence, the numerical methods for calculating $\underline{\Phi}^*$ need not be the same as originally used for calculating the base-case solution $\underline{\chi}^o$ of the nonlinear original system described by Eq. (2.10). (Particularizing this conclusion to our code system, the implication is that the numerical methods for solving the ASM-REL/TF need *not* be the same as the original numerical methods used in RELAP5/MOD3.2). In many cases, it is easier to calculate the adjoint function $\underline{\Phi}^*$, which results from the solution of a *linear* system, rather than the original calculation of $\underline{\chi}^o$, which results from the solution of a *nonlinear* system;

the ASM-REL/TF depends (in general, nonlinearly) on the base-case (nominal) solution $\underline{\chi}^o$ through the quantities $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$; hence, *the adjoint function* $\underline{\Phi}^*$ *depends, in general nonlinearly, on the base-case solution* $\underline{\chi}^o$, too. Thus, *the base-case solution* $\underline{\chi}^o$ *must be available prior to solving the ASM-REL/TF*. Furthermore, the programming strategy for solving the ASM-REL/TF must be intertwined efficiently with the programming in the original code (in this case, RELAP5/MOD3.2) in order to optimize the calculation of $\underline{\Phi}^*$ by minimizing memory requirements and CPU-time for its calculation. It is important to note here that *if the original system were linear (such as would occur, for example, for neutron and/or radiation transport problems), then the ASM-REL/TF would not only be linear, too, but would in addition be independent of the base-case solution, and could therefore be calculated independently of it*.

From the characteristics described in items (a) through (d) above, it follows that *the Adjoint Sensitivity Analysis Procedure (ASAP) should be used whenever the number of parameter variations* Γ_j *exceeds the number of responses R of interest;* this is generally the case in practice. The reverse case, when the number of responses R exceeds the number of parameter variations Γ_j, occurs rather seldom in practice. Should such a case occur, however, the FSAP might be used for sensitivity analysis, if it already exists in the respective code; otherwise, direct recalculations should be performed, since they would require no additional programming.

3.2.2 Implementation of the ASAP for the Discretized REL/CDE

The (Discrete) ASM-REL/TF corresponding to the (Discrete) FSM represented by Eq.(3.13) is obtained by introducing the respective adjoint, vector-valued, function via the scalar (inner) product of two vectors in a finite-dimensional Euclidean space. This inner product is formed by writing Eq.(3.13) as a single (partitioned) matrix equation, and by multiplying this matrix equation on the left by a yet undefined partitioned column-vector $\underline{\Xi} \equiv \left(\Xi^{(0)},\ldots,\Xi^{(NF)}\right)$, with components $\Xi^{(n)}$ of the same size and structure as $X^{(n)}$, to obtain an expression of the form $\Xi^T AX \equiv \sum_{n=0}^{NF} \Xi^{(n)} A^{(n)} X^{(n)}$, where A represents a matrix composed of the corresponding matrices $G^{(n)}$ and $H^{(n)}$. The (Discrete) ASM-REL/TF is then obtained by transposing the inner product $\Xi^T AX$ to obtain $X^T A^T \Xi$, and by setting this expression to be equal to the indirect effect term, as follows:

$$
\begin{aligned}
DR\left(\underline{\Psi}\right) &\equiv X^T A^T \Xi = X^T Q = \sum_{n=0}^{NF} X^{(n)} Q^{(n)} \\
&= \Xi^T AX = \Xi^T K = \sum_{n=0}^{NF} \Xi^{(n)} K^{(n)}
\end{aligned}
\qquad (3.18)
$$

The source $Q^{(n)}$ appearing in Eq.(3.18) is determined by the quadrature scheme chosen to calculate numerically the system response R in Eq.(3.8). From the identification $X^T A^T \Xi = X^T Q = \sum_{n=0}^{NF} X^{(n)} Q^{(n)}$, it follows that the (Discrete) ASM-REL/TF is given by the system of matrix equations

$$\begin{cases} \left[G^{(NF-1)}\right]^T \Xi^{(NF)} = Q^{(NF)}, \quad \text{for } n = NF \\ \left[G^{(n-1)}\right]^T \Xi^{(n)} + \left[H^{(n)}\right]^T \Xi^{(n+1)} = Q^{(n)}, \quad \text{for } n = NF-1,\ldots,1 \\ \Xi^{(0)} + \left[H^{(0)}\right]^T \Xi^{(1)} = Q^{(0)}, \quad \text{for } n = 0 \end{cases} \tag{3.19}$$

In view of Eqs.(3.10) and (3.18), it follows that the sensitivity DR of the response R is given in terms of the adjoint function $\underline{\Xi} \equiv \left(\Xi^{(0)},\ldots,\Xi^{(NF)}\right)$ by the following expression

$$DR \equiv DR(\underline{\Gamma}) + DR(\underline{\Psi}) = DR(\underline{\Gamma}) + \sum_{n=0}^{NF} \Xi^{(n)} K^{(n)} \tag{3.20}$$

Note that the (Discrete) ASM-REL/TF represented by Eq.(3.19) must be solved backwards in time, starting, in principle, from the final time-step NF. In practice, however, the calculation of the vector-valued adjoint function $\underline{\Xi} \equiv \left(\Xi^{(0)},\ldots,\Xi^{(NF)}\right)$ commences backwards in time only from the time-step, n, at which the source terms $Q^{(n)}$ are non-zero. Furthermore, just as for the Differential ASM-REL/TF represented by Eq.(3.16), Eq.(3.19) reveals that (a) *the adjoint function* $\underline{\Xi}$ *is independent of parameter variations*; (b) $\underline{\Xi}$ *must be calculated anew for every R*; (c) *the ASM-REL/TF is linear in* $\underline{\Xi}$, and (d) *the adjoint function* $\underline{\Xi}$ *depends (nonlinearly, in general) on the base-case solution* $\underline{\chi}_d^o$*, which must therefore be available prior to solving the ASM-REL/TF*.

3.3 Consistency Between the Differential/Integral and the Discretized Representations in Sensitivity Analysis

This section highlights the fundamentally important aspect of *consistency between the differential and the corresponding discretized equations used for sensitivity analysis*. In this context, *consistency means that the discretized representation converges to the corresponding differential and/or integral representation in the limit as* $\Delta x_j \to 0$ *and* $\Delta t \to 0$. A priori, it must be assumed that the original systems of differential equations (in this case, the REL/CDE) has been discretized consistently, i.e., Eq.(2.16) represents a consistent discretization of Eq. (2.10). This is an indispensable assumption, of course, since if it were false, then one could not calculate the base-case solution correctly. Similarly, it must also be assumed that Eq.(3.8) represents a consistent discretization of the response represented by Eq.(3.1). Starting from these essential assumptions, the following consistency correspondences must be assured:

(a) the Discretized FSM represented by Eq. (3.11) must be consistent with the Differential FSM represented by Eq. (3.7);

(b) the Discretized ASM-REL/TF represented by Eq. (3.19) must be consistent with the Differential ASM-REL/TF represented by Eq. (3.16);

(c) the Discretized Response Sensitivity represented by Eq.(3.10), the Integral Response Sensitivity represented by Eq.(3.5), the Integral Response Sensitivity represented by Eq.(3.17) in terms of adjoint functions, and the Discretized Response Sensitivity represented by Eq.(3.20) in terms of adjoint functions, must all be consistent with each other.

If item (a) above turns out to be false, i.e., if the Discretized FSM represented by Eq. (3.11) turns out to be *inconsistent* with the Differential FSM represented by Eq. (3.7), then the *a priori assumption* that the original nonlinear differential equations (in this case, the REL/CDE) have been discretized consistently *must be carefully re-examined*. If this a priori assumption is still confirmed to be correct, then the Discretized FSM represented by Eq. (3.11) must be discarded from further consideration. Two possibilities arise at this juncture:

(a.1) if the implementation of the FSAP is necessary, then the Differential FSM represented by Eq. (3.7) must be discretized in a consistent manner, to enable its subsequent numerical solution; note that the Differential FSM represented by Eq. (3.7) can be discretized, in principle, independently of the original discretization procedures used to discretize the original nonlinear differential equations (in this case, the REL/CDE), or

(a.2) if the implementation of the FSAP is not necessary, then item (b) described above must be verified.

If item (b) above turns out to be false, i.e., if the Discretized ASM-REL/TF represented by Eq. (3.19) turns out to be *inconsistent* with the Differential ASM-REL/TF represented by Eq. (3.16), then the Discretized ASM-REL/TF represented by Eq. (3.19) must be discarded; instead, the Differential ASM-REL/TF represented by Eq. (3.16) must be discretized consistently, and subsequently solved numerically. The considerations of consistency outlined so far are depicted in the flow-chart shown in Fig. 2 below.

Finally, if item (c) above turns out to be false, then the Integral Response Sensitivity represented in terms of adjoint functions, cf. Eq.(3.17), must be discretized in a consistent manner to enable its correct numerical calculation. In closing, it is important to note that the *fundamental hypothesis* underlying all of the consistency considerations in this section is that *the differential and/or integral forms (i.e., the Differential FSM, ASM-REL/TF, and Integral-Response-representation)* are the forms that *contain/model physical reality*; thus, it is *the discretized forms* that *must conform to, and represent consistently, the differential/integral forms*, rather then the other way around.

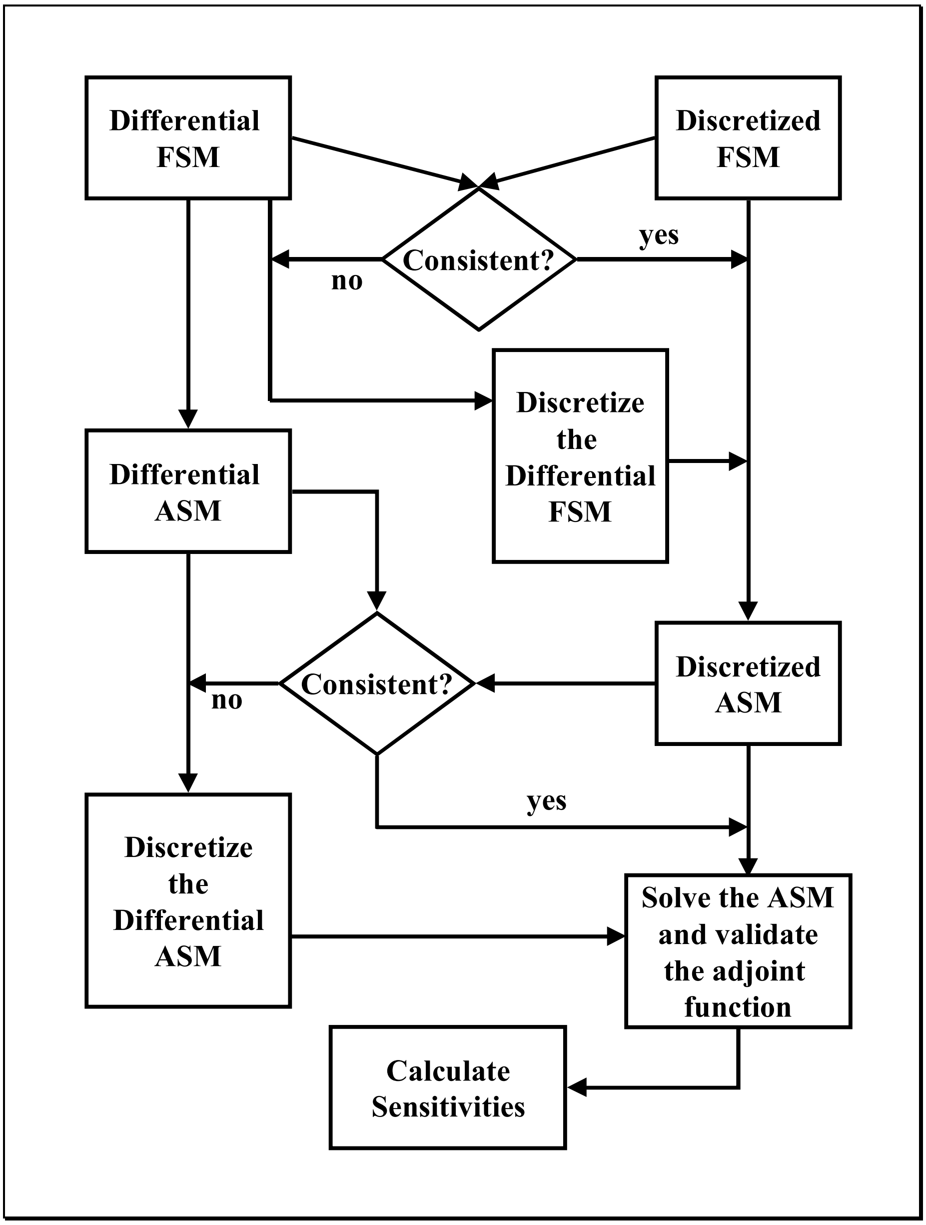

Fig. 2. Required consistencies between the differential and discretized formulations of FSM and ASM-REL/TF

4 VALIDATION OF THE ADJOINT SENSITIVITY MODEL FOR THE RELAP5/MOD3.2 TWO-FLUID MODEL

A very important use of Eq.(3.17) is for validating the computation of the adjoint function $\underline{\Phi}^*$. For example, by choosing the response R_i to denote the i-th REL/CDE dependent variable at some discrete point (x_1, t_f) in space-time, by setting $\underline{\Gamma} = \underline{0}$, $\Delta\underline{\chi}(x_o, t) = \underline{0}$, and $\Delta\underline{\chi}(x, t_o) = [0, ..., \delta(x - x_1)\Delta\chi_i(x, t_o), ...0]$ in Eq.(3.17), i.e., by effecting solely a variation in the initial conditions of the i-th dependent variable in the REL/CDE, the following expression is obtained:

$$DR_i\left(\underline{\chi}^o, \underline{G}^o; \underline{\Phi}, \underline{\Gamma}; \underline{\Phi}^*\right) = \Phi_i^*(x_1, t_o)\, S_{ii}(x_1, t_o)\Delta\chi_i(x_1, t_o) \quad (4.1)$$

The above expression reveals that the sensitivity DR_i can be used to validate the i-th component of the adjoint function $\underline{\Phi}^*$, as follows: (i) on the one hand, Eq.(3.16) is solved to obtain the adjoint function, and then perform the multiplication on the right-side of Eq. (4.1) to obtain DR_i; the sensitivity DR_i would then be added to the nominal response value $R_i^o\left(\underline{\chi}^o, \underline{G}^o\right)$ to obtain the *predicted perturbed response*, R_{pred}, as indicated by Eq.(3.6); (ii) on the other hand, the *exact perturbed response* is recalculated $R_{recal} \equiv R_i\left(\underline{\chi}^o + \underline{\Phi}, \underline{G}^o + \underline{\Gamma}\right)$, for the perturbation $\Delta\chi_i(x_1, t_o)$. Recall that, according to Eq.(3.6), the values of R_{recal} and R_{pred} agree with each other up to second order perturbations in the system parameters. Therefore, by deliberately selecting the perturbation $\Delta\chi_i(x_1, t_o)$ to be so small as to render the effects of higher-order terms negligible in Eq.(3.6), the value of R_{pred} should agree closely with the value of R_{recal} if the adjoint function Φ_i^* had been accurately computed. On the contrary, if the computation of the respective adjoint function was not accurate, then R_{pred} would differ from R_{recal}, no matter how small one selected the variation $\Delta\chi_i(x_1, t_o)$.

The programming considerations for implementing the ASAP in RELAP5/MOD3.2 are highlighted in Appendix A. In particular, it is important to note that the ASM-REL/TF is solved by calling, at each time-step, the subroutine DSLUGM[14], which is a generalized minimum residual (GMRES) iterative sparse-matrix solver that uses incomplete LU factorization for preconditioning non-symmetric linear systems.

4.1 Validation of the ASM-REL/TF for Liquid-Phase Using the "Two-Loops With Pumps" RELAP5/MOD3.2 Sample Problem

Using the concepts outlined above, the accuracy and stability of the numerical solution of the ASM-REL/TF for the liquid-phase have been verified by using the "Two Loops With Pumps" sample problem supplied with the RELAP5/MOD3.2 code. This problem models two, mostly identical, closed loops containing 19 pipe-volumes and a pump-volume. For the first loop, the pipe-volumes are numbered consecutively from 101 to 119, while the pump-volume has number 201 and connects pipe-volumes 101 and 119; similarly, the second loop consists of pipe-volume numbers 301 to 319, with pump-volume 401 connecting pipe-volumes 301 and 319. Each loop is filled with fluid, and has friction and an orifice.

At the start of the transient, the water in the first loop is at zero (initial) velocity, but the pump is rotating in the positive direction. Thus, the pump trip is initially false, and the pump angular velocity is constant at the initial value until the pump trip becomes true. With the pump rotating at a constant angular velocity but the water at rest, the head is high and the water is accelerated. As the velocity of the water increases, wall friction and area change losses increase because these losses depend on the velocity of water. At the same time, the pump head obtained from the homologous data will decrease as the volumetric flow increases. A steady state is reached when the pump head and the loss effects balance. This steady state is reached after about 14.5 seconds from initiating the transient; at this time, the fluid velocity attains a value that remains constant for the next 5.5 seconds. At about 20 sec., the pump is tripped and therefore the pump speed and fluid velocities begin to decrease.

For the second loop, the initial angular rotational velocity for the (second) pump is zero; a pump motor torque curve, corresponding to an induction motor, is used. From the curve, the torque is positive at zero angular velocity; the torque increases slowly as the velocity increases, up to a value that is slightly below the synchronous speed. Then, the torque decreases sharply to zero at the synchronous speed, where the developed torque matches the frictional torque and the torque imposed by the water. While the net torque is positive, the water is accelerated. Once the second pump approaches synchronous speed, the transient behavior of the second becomes similar to that of the first loop.

To verify the stability and accuracy of the numerical solution of the ASM-REL/TF, various variations in the initial conditions have been considered for the pressures in the volumes and, respectively, velocities at the junctions comprising the respective loops. *Note that such perturbations do not correspond to actual physical processes, but are introduced numerically as mathematical means to verify the accuracy and stability of the numerical solution of the ASM-REL/TF.* To facilitate the comparisons between the results (sensitivities) predicted by the ASM-REL/TF and the corresponding exact recalculations, the numerical values presented in the various tables below were deliberately not rounded off, but were displayed with all the decimals printed by RELAP5.

For the results reported in this section, the fluid used in the "Two-Loops With Pumps" sample problem described above is single-phase water. To ensure that the fluid remains in the liquid-phase throughout the transient, the initial conditions were P_{init}=1.56E+7 Pa and $T_{f,init}$=555K. The solution of the ASM-REL/TF was then verified by effecting various perturbations in the initial pressures and velocities, as well as in the pump head, by calculating the respective predicted responses, and by comparing these predictions with exact recalculations.

TABLE I "Two-Loops With Pumps" – liquid-phase: influence of perturbations in the initial pressure in volume 301 (adjacent to the pump) on the pressure in same volume.

Perturbation	Transient Duration / No. of time steps	Nominal Value (N/m^2)	P_{pred}-P^o	P_{recal}-P^o
1% of the initial pressure	0.05 sec. / 5 t.s.	1.56259E+7	7391.4	7400
	0.2 sec. / 20 t.s.	1.56259E+7	7391.5	7400
	0.5. sec. / 52 t.s.	1.56263E+7	7391.5	7300
	5. sec. / 144 t.s.	1.56549E+7	7392.0	7400
	20. sec. / 294 t.s.	1.73607E+7	7440.8	7500
5% of the initial pressure	0.05 sec. / 5 t.s.	1.56259E+7	36957	36600
	0.2 sec. / 20 t.s.	1.56259E+7	36958	36600
	0.5. sec. / 52 t.s.	1.56263E+7	36958	36600
	5. sec. / 144 t.s.	1.56549E+7	36960	36600
	20. sec. / 294 t.s.	1.73607E+7	37204	36900
10% of the initial pressure	0.05 sec. / 5 t.s.	1.56259E+7	73914	72400
	0.2 sec. / 20 t.s.	1.56259E+7	73915	72500
	0.5. sec. / 52 t.s.	1.56263E+7	73915	72400
	5. sec. / 144 t.s.	1.56549E+7	73920	72300
	20. sec. / 294 t.s.	1.73607E+7	74408	73000

The behavior of the volume-averaged pressure in volume 301 (adjacent to the pump) to various perturbations in the initial values of the pressure in the same volume are presented in Fig. 3 and TABLE I. These results are typical for the pressure sensitivities to variations in the initial pressures for all of the other loop-volumes, as well. The values presented for P_{recal} are obtained by re-running the entire transient using the respective perturbed initial condition. As noted from the results in Fig. 3 and TABLE I, the solution of the ASM-REL/TF, which is used to obtain P_{pred}, is very accurate and stable, practically coinciding with the exact recalculations for the entire duration of the transient (294 time steps).

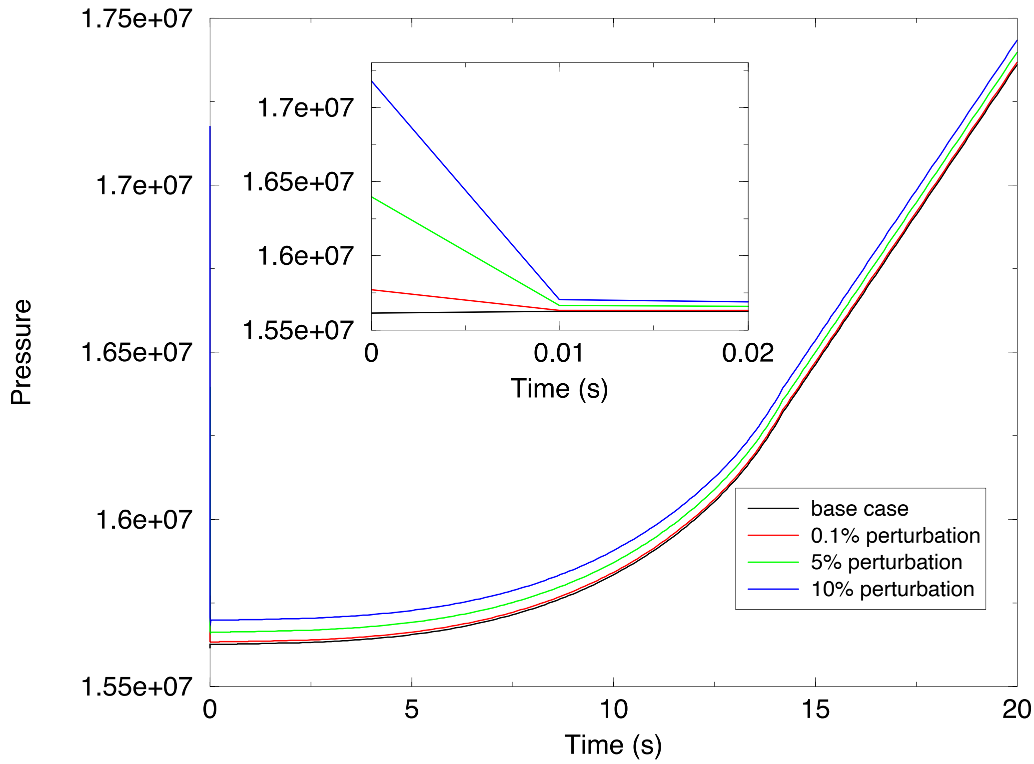

Fig. 3. “Two-Loops With Pumps” – liquid-phase: influence of perturbations in the initial pressure in volume 301 (adjacent to the pump) on the pressure in same volume.

TABLE II “Two-Loops With Pumps” – liquid-phase: influence of perturbations in the initial velocity in junction 301 (adjacent to the pump) on the velocity in same junction.

Perturbation In initial velocity (j301)	Transient duration / nr. of time steps	Nominal value v_{fj}^{o} (j301) (m/s)	$v_{fj,pred} - v_{fj}^{o}$	$v_{fj,recal} - v_{fj}^{o}$
3.048*10^{-2} m/s (0.1 ft/s) at t = 0	0.05 sec. / 5 t.s.	1.20631E-5	1.50766E-3	1.50840E-3
	0.1 sec. / 10 t.s.	1.13544E-4	1.60894E-3	1.60889E-3
	0.2 sec. / 20 t.s.	9.80435E-4	2.467843E-3	2.47489E-3
	0.5 sec. /50 t.s.	1.60002E-2	1.74949E-2	1.74856E-2
	1.0 sec. /100 t.s.	.12428	.12559	.12550
.9144 m/s (3 ft/s) at t = 0	0.05 sec. / 5 t.s.	1.20631E-5	.44879E-1	.44507E-1
	0.1 sec. / 10 t.s.	1.13544E-4	.44975E-1	.44186E-1
	0.2 sec. / 20 t.s.	9.80435E-4	.45822E-1	.44432E-1
	0.5 sec. /50 t.s.	1.60002E-2	.60609E-1	.57258E-1
	1.0 sec. /100 t.s.	.12428	.16369	.15583

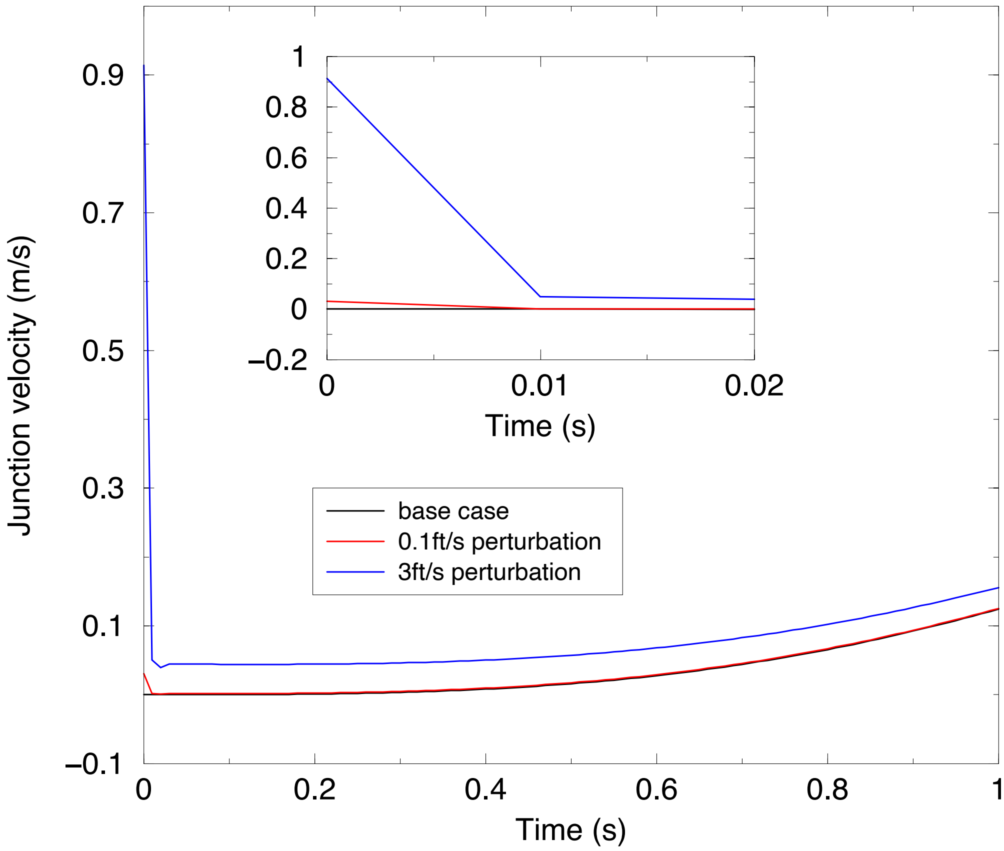

Fig. 4. “Two-Loops With Pumps” – liquid-phase: influence of perturbations in the initial velocity in junction 301 (adjacent to the pump) on the velocity in same junction.

The influence of perturbations of 0.1ft/s and 3ft/s, respectively, in the initial velocity (0.0 ft/s) in junction 301 on the subsequent time-dependent behavior of the velocity in the same junction (301) are depicted in Fig. 4 and TABLE II, respectively. The effects of the perturbations in the initial velocity are noticeable during the early stages of the transient only, but then diminish quickly in time. Note that the results obtained using the ASM-REL/TF for the 0.1ft/s perturbation are practically indistinguishable from the exact recalculations, thus confirming the robustness, stability, and accuracy of the respective numerical solution of the ASM-REL/TF. The nonlinear effects are more prominent for the 0.9144m/s (3 ft/s) perturbation, particularly at early time values, but these effects also diminish in time and converge to the respective steady state values, as would be expected.

TABLE III Predicted and RELAP5-recalculated velocity in junction 305 (perturbations in the initially zero velocity in the same junction)

Perturbation in initial velocity (j305)	Transient duration / nr. of time steps	Nominal value (m/s) v_{fj}^{o} (j305)	$v_{fj,pred} - v_{fj}^{o}$	$v_{fj,recal} - v_{fj}^{o}$
$3.048*10^{-2}$ m/s (0.1 ft/s) at t = 0	0.05 sec. / 5 t.s.	9.76885E-6	1.50596E-3	1.50601E-3
	0.1 sec. / 10 t.s.	1.12958E-4	1.60825E-3	1.60821E-3
	0.2 sec. / 20 t.s.	9.79162E-4	2.47356E-3	2.47352E-3
	0.5 sec. /50 t.s.	1.59969E-2	1.74817E-2	1.74821E-2
	1.0 sec. /100 t.s.	.12427	.12556	.12550
	5.0 sec./142 t.s.	1.6241	1.6241	1.6241
	10.0 sec./192 t.s.	2.9979	2.9979	2.9979
	20.0 sec./292 t.s.	4.4761	4.4761	4.4761
$3.048*10^{-1}$ m/s (1 ft/s) at t = 0	0.05 sec. / 5 t.s.	9.76885E-6	1.4971E-2	1.49366E-2
	0.1 sec. / 10 t.s.	1.12958E-4	1.5065E-2	1.49976E-2
	0.2 sec. / 20 t.s.	9.79162E-4	1.5923E-2	1.57965E-2
	0.5 sec. /50 t.s.	1.59969E-2	3.0848E-2	3.0646E-2
	1.0 sec. /100 t.s.	.12427	.13722	.13603
	5.0 sec./142 t.s.	1.6241	1.6241	1.6241
	10.0 sec./192 t.s.	2.9979	2.9979	2.9979
	20.0 sec./292 t.s.	4.4761	4.4761	4.4761
.9144 m/s (3 ft/s) at t = 0	0.05 sec. / 5 t.s.	9.76885E-6	4.4896E-2	4.4499E-2
	0.1 sec. / 10 t.s.	1.12958E-4	4.4971E-2	4.4180E-2
	0.2 sec. / 20 t.s.	9.79162E-4	4.5811E-2	4.4426E-2
	0.5 sec. /50 t.s.	1.59969E-2	6.0453E-2	5.72603E-2
	1.0 sec. /100 t.s.	.12427	.16138	.15582
	5.0 sec./142 t.s.	1.6241	1.6241	1.6240
	10.0 sec./192 t.s.	2.9979	2.9979	2.9978
	20.0 sec./292 t.s.	4.4761	4.4761	4.4761

The results presented above in Tables I and II and Figs. 3 and 4, respectively, are typical for perturbations in all of the volume-averaged pressures and junction-velocities of the "Two-Loops With Pumps Problem". Additional results that illustrate this general trend are presented in TABLE III and TABLE IV, and in Figs. 5 and 6. Thus, TABLE III and Fig. 5 present results for the sensitivities of the time-dependent velocity in junction 305 to perturbations (of 0.1ft/s, 1ft/s, 3ft/s) in the initial velocity (0.0ft/s) at this junction. Furthermore, TABLE IV and Fig. 6 present the sensitivities of the time-dependent velocity at junction 103 in loop 1 to perturbations from zero in the initial velocity at this junction. Recall that the perturbations introduced numerically in the volume-averaged pressures and junction velocities serve only as mathematical means to verify the accuracy and stability of the numerical solution of the ASM-REL/TF, and are irrelevant to actual physical processes. Nevertheless, the results obtained indicate that the numerical method for solving the ASM-REL/TF is as accurate, robust, and stable as the original numerical methods used in RELAP5/MOD3.2 for solving liquid-phase problems.

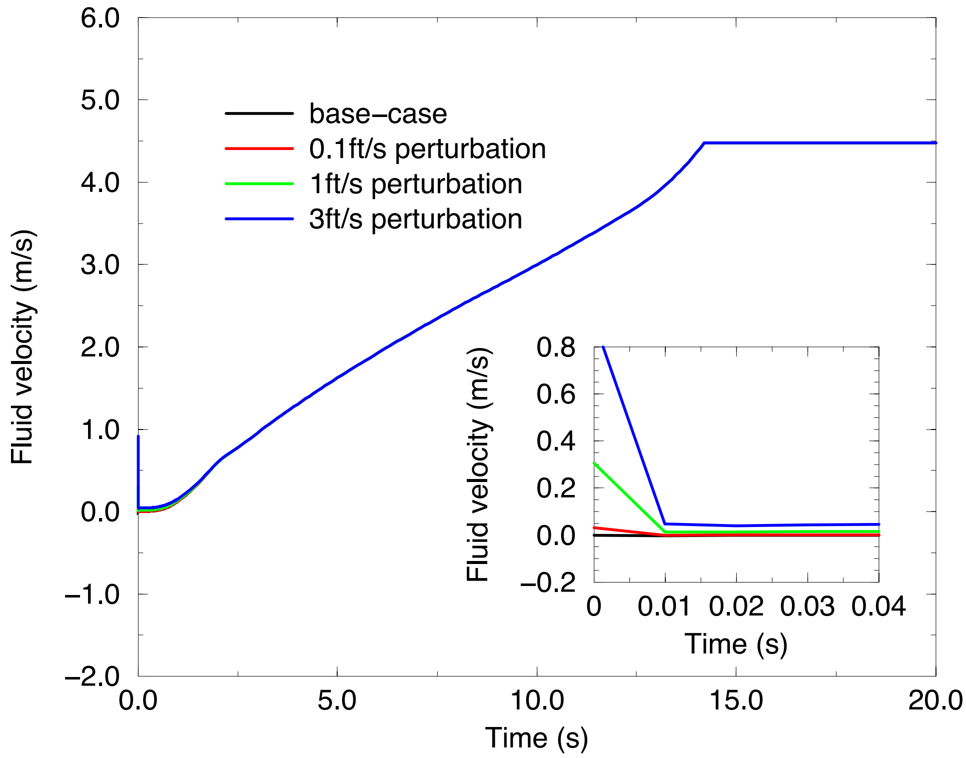

Fig. 5. Influence of perturbations in the initial junction velocity (j305) on the velocity in the same junction

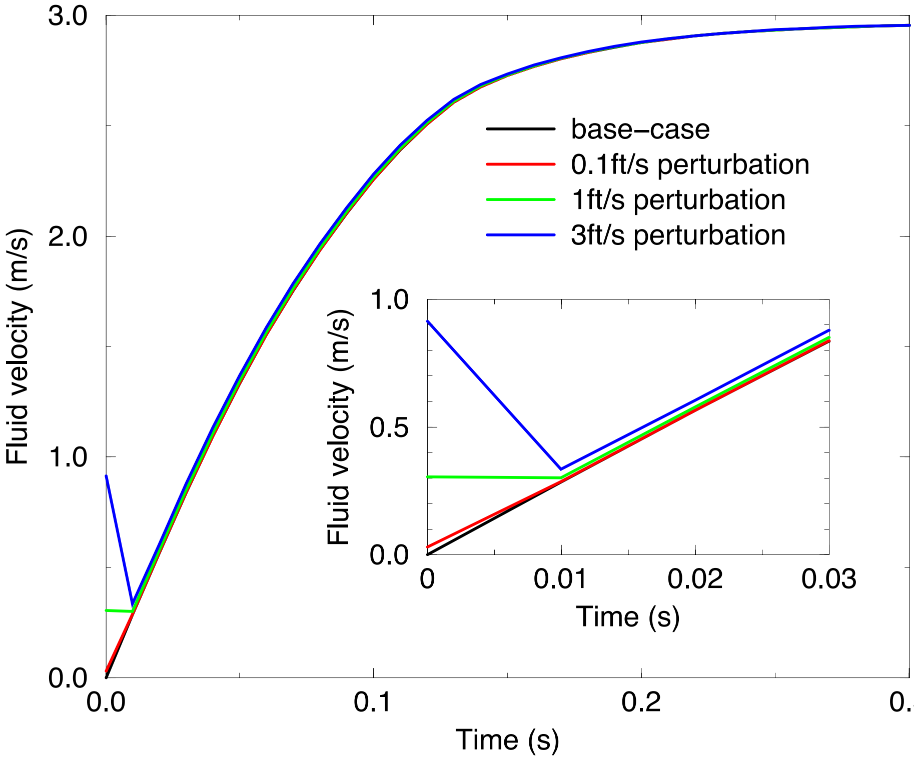

Fig. 6. Influence of initial conditions on the fluid velocity at junction 103

As example of a perturbation that does have physical meaning within the liquid-filled "Two-Loops With Pumps Problem", the ASM-REL/TF has been used to obtain the sensitivity of the pressure in the loops to variations in the pump head. Typical results for such sensitivities are presented in TABLE V, which, in particular, shows the time-dependent (100 time-steps) sensitivity of the pressure in Vol. 101 (adjacent to the pump in Loop 1) to a small (1%) and, respectively, large (10%) variation in the pump head. These results show that the pressure variations predicted by the ASM-REL/TF for the 1%-perturbations in the pump head are very close to, albeit somewhat larger than, the exactly recalculated pressures. For the larger (10%) pump head variations, the nonlinear effects become stronger, leading to a more marked over-prediction of the exactly recalculated results by the ASM-REL/TF-calculated sensitivities.

TABLE IV Predicted and RELAP5-recalculated fluid velocity at junction 103 (perturbations in initial conditions at the same junction)

Perturbation in initial velocity (j103)	Transient duration / nr. of time steps	Nominal value V_{fj} (j103) (m/s)	Adjoint Method V_{fj} perturbed (m/s)	Exact Recalculation V_{fj} recalc. (m/s)
$3.048*10^{-2}$ m/s (0.1 ft/s) at t = 0	0.05 sec. / 5 t.s.	1.3319	1.3331	1.3331
	0.1 sec. / 10 t.s.	2.2565	2.2573	2.2573
	0.2 sec. / 20 t.s.	2.8760	2.8761	2.8761
	0.5 sec. /50 t.s.	2.9662	2.9662	2.9662
	1.0 sec. /100 t.s.	2.9664	2.9664	2.9664
$3.048*10^{-1}$ m/s (1 ft/s) at t = 0	0.05 sec. / 5 t.s.	1.3319	1.3447	1.3442
	0.1 sec. / 10 t.s.	2.2565	2.2647	2.2643
	0.2 sec. / 20 t.s.	2.8760	2.8774	2.8770
	0.5 sec. /50 t.s.	2.9662	2.9662	2.9662
	1.0 sec. /100 t.s.	2.9664	2.9664	2.9664
.9144 m/s (3 ft/s) at t = 0	0.05 sec. / 5 t.s.	1.3319	1.3703	1.3687
	0.1 sec. / 10 t.s.	2.2565	2.2812	2.2799
	0.2 sec. / 20 t.s.	2.8760	2.8804	2.8790
	0.5 sec. /50 t.s.	2.9662	2.9662	2.9662
	1.0 sec. /100 t.s.	2.9664	2.9664	2.9664

TABLE V "Two-Loops With Pumps" – liquid-phase: influence of pump head perturbations on pressure.

Perturbation	Transient Duration / No. of time steps	Nominal Value (N/m^2)	$P_{pred}-P^o$	$P_{recal}-P^o$
1% of the initial pump head	0.01 sec	1.57426E+7	1165.3	1100
	0.05 sec	1.57372E+7	1032.9	900
	0.1 sec	1.57238E+7	829.68	700
	0.5 sec	1.57058E+7	253.37	100
	1 sec (100 t.s.)	1.57319E+7	256.37	100
10% of the initial pump head	0.01 sec	1.57426E+7	11653	11600
	0.05 sec	1.57372E+7	10329	8700
	0.1 sec	1.57238E+7	8296.8	4300
	0.5 sec	1.57058E+7	2533.7	1200
	1 sec (100 t.s.)	1.57319E+7	2563.7	600

4.2 Validation of the ASM-REL/TF for Gas-Phase Using Modified "Two-Loops With Pumps" and "Edward's Pipe" RELAP5/MOD3.2 Problems

To validate the solution of the ASM-REL/TF for the gas-phase, the "Two-Loops With Pumps Problem" described above in Sec. 4.1 has been modified by replacing the water (liquid) by steam (gas). This modification was effected by using the following initial conditions: P_{init}=7.0E+6 Pa and $T_{g,init}$=620K. Otherwise, the geometry was kept unchanged.

TABLE VI "Two-Loops With Pumps" – gas-phase: influence of perturbations in the initial pressure in volume 103 (3 volumes away from pump) on the pressure in same volume.

Perturbation	Transient Duration / No. of time steps	Nominal Value (N/m^2)	P_{pred}-P^o	P_{recal}-P^o
0.1% of the initial pressure	0.1 sec. / 10 t.s.	7.00433E+6	331.48	320
	0.5 sec. / 50 t.s.	7.00627E+6	331.47	320
	1 sec. / 100 t.s.	7.00984E+6	331.48	330
	5. sec. / 142 t.s.	7.03846E+6	331.27	330
	20. sec./ 292 t.s.	7.14594E+6	330.82	320
1% of the initial pressure	0.1 sec. / 10 t.s.	7.00433E+6	3314.8	3320
	0.5 sec. / 50 t.s.	7.00627E+6	3314.7	3320
	1 sec./ 100 t.s.	7.00984E+6	3314.8	3330
	5. sec. / 142 t.s.	7.03846E+6	3312.7	3330
	20. sec./ 292 t.s.	7.14594E+6	3308.2	3320
10% of the initial pressure	0.1 sec. / 10 t.s.	7.00433E+6	33148	32590
	0.5 sec. / 50 t.s.	7.00627E+6	33147	32560
	1 sec. / 100 t.s.	7.00984E+6	33148	32560
	5. sec. / 142 t.s.	7.03846E+6	33127	32540
	20. sec./ 292 t.s.	7.14594E+6	33082	32530

The influence of perturbations in the initial pressure in volume 103, which is located three volumes away from pump, on the pressure in same volume is illustrated by the results presented in TABLE VI. Just as has been noted for the liquid-phase problem analyzed in Sec. 4.1, these perturbations are introduced numerically, and do not correspond to actual physical processes; they are used as mathematical means to verify the accuracy and stability of the numerical solution of the ASM-REL/TF. The results in TABLE VI show that the solution of the ASM-REL/TF, which is used to obtain P_{pred}, is very accurate and stable, practically coinciding with the exact recalculations for the entire duration of the transient (292 time steps), for all the perturbations (0.1%; 1%; 10%) effected in the initial pressure.

TABLE VII "Two-Loops With Pumps" – gas-phase: influence of pump head perturbations on the pressure in volume 103.

Perturbation	Transient Duration / No. of time steps	Nominal Value (N/m^2)	P_{pred}-P^o	P_{recal}-P^o
1% of the initial pump head	0.1 sec (10 t.s.)	7.00433E+6	27.335	20
	0.5 sec (50 t.s.)	7.00627E+6	9.8272	9
	1 sec (100 t.s.)	7.00984E+6	9.8588	10

10% of the initial pump head	0.1 sec (10 t.s.)	7.00433E+6	273.35	160
	0.5 sec (50 t.s.)	7.00627E+6	98.272	50
	1 sec (100 t.s.)	7.00984E+6	98.588	50

TABLE VIII "Two-Loops With Pumps" – gas-phase: influence of pump head perturbations on the pressure in volume 101 (adjacent to the pump).

Perturbation	Transient Duration / No. of time steps	Nominal Value (N/m^2)	$P_{pred}-P^o$	$P_{recal}-P^o$
1% of the initial pump head	0.1 sec (10 t.s.)	7.00487E+6	31.278	30
	0.5 sec (50 t.s.)	7.00630E+6	9.8284	10
	1 sec (100 t.s.)	7.00988E+6	9.9438	9
10% of the initial pump head	0.1 sec (10 t.s.)	7.00487E+6	312.78	180
	0.5 sec (50 t.s.)	7.00630E+6	98.284	50
	1 sec (100 t.s.)	7.00988E+6	99.438	40

The influence of varying the pump head on the time-dependent behavior of the pressure in various volumes has also been investigated. Typical examples of the sensitivities of the volume-averaged pressures to variations in the pump-head are presented below in TABLE VII, for volume 103, and TABLE VIII, for volume 101, respectively. Although the results presented in these tables are reproduced with all the digits printed by the RELAP code (in order to emphasize the respective differences), these results indicate that the pressure variations predicted by using the ASM-REL/TF are practically indistinguishable from the exact recalculations.

To verify further the accuracy and stability of the numerical solution of the ASM-REL/TF for the gas-phase, the well-known "Edwards Pipe" problem, supplied with the RELAP5/MOD3.2 code, has been modified by filling it initially with pure steam, rather than water, as in the original setting of this problem. The modified "Edwards Pipe" problem thus contains steam (i.e., gas-phase) only, initially at rest in the pipe, with initial pressure and internal energy of 7 MPa and 0.27E+7 J/kg, respectively. The pipe is then depressurized by opening an end into a large reservoir at atmospheric pressure and an internal energy of 0.25E+7 J/kg. To maintain pure gas (steam)-conditions throughout the depressurization, the transient calculation was restricted to the first 57 time steps after initiation of the transient depressurization, since condensation begins to appear beyond this point in time.

TABLE IX "Edwards Pipe" – gas-phase: influence of perturbations in the initial pressure in volume 301 (near to the pipe's closed end) on the pressure in the same volume

Perturbation	Transient duration / No. Of time steps	Nominal value (N/m^2)	P_{pred}-P^o	P_{recal}-P^o
0.1% of the initial pressure 7.0E+6 (N/m^2)	0.001 sec./19 t.s.	7.0E+6	-322.86	-320
	0.005 sec./38 t.s.	6.8909E+6	16.078	20
	0.01 sec / 57 t.s.	3.4896E+6	116.69	120
5% of the initial pressure 7.0E+6 (N/m^2)	0.001 sec./19 t.s.	7.0E+6	-16143	-14300
	0.005 sec./38 t.s.	6.8909E+6	803.90	710
	0.01 sec / 57 t.s.	3.4896E+6	5834.3	7910
10% of the initial pressure 7.0E+6 (N/m^2)	0.001 sec./19 t.s.	7.0E+6	-32286	-25060
	0.005 sec./38 t.s.	6.8909E+6	1607.8	1370
	0.01 sec / 57 t.s.	3.4896E+6	11669	13970

The ASM-REL/TF results and the respective comparisons with exact recalculations are presented in Fig. 7 and TABLE IX. These results indicate that the pressure response variations predicted by using the sensitivities calculated with the ASM-REL/TF agree well with the exactly recalculated variations. For the larger (10%) variations, the effect of nonlinearities becomes more evident, particularly as the condensation point is approached in time. All in all, the results shown in TABLE IX and Fig. 7 indicate that the numerical method used for solving the ASM-REL/TF is also quite accurate for the gas phase segment of the two-fluid model.

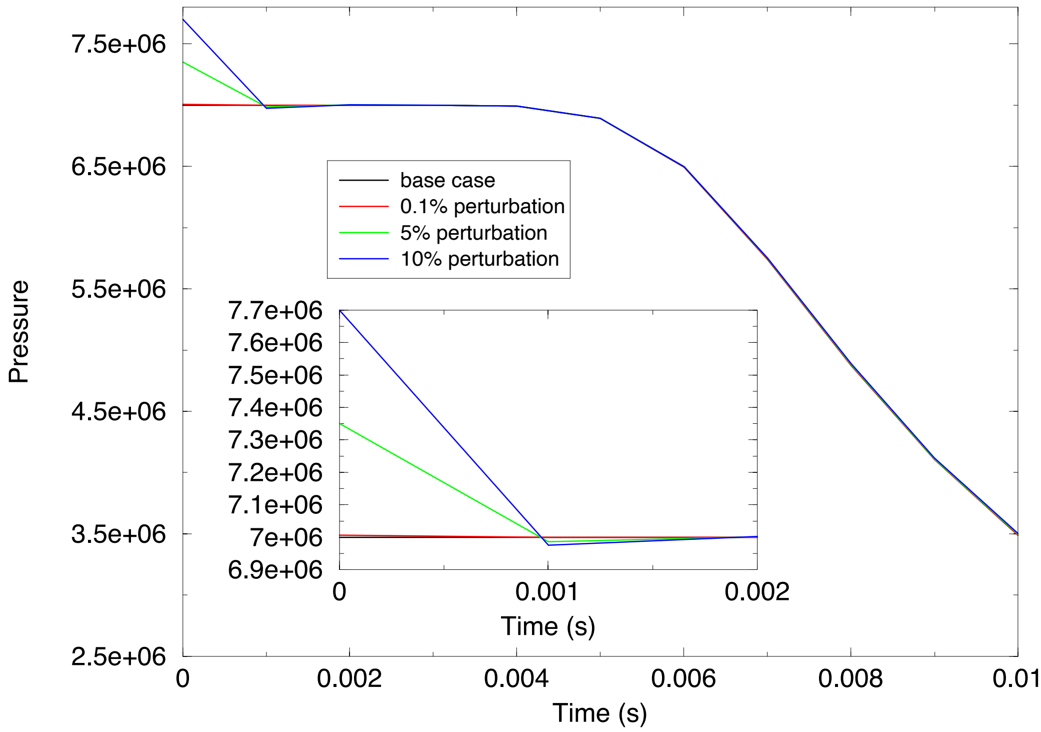

Fig. 7. "Edwards Pipe" – gas-phase: influence of perturbations in the initial pressure in volume 301 on the pressure in the same volume

4.3 Validation of the ASM-REL/TF for Two-Phase Using the “Edwards Pipe” RELAP5/MOD3.2 Sample Problem

In addition to having verified the numerical solution of the ASM-REL/TF by using sample problems involving single-phase fluids as described in the foregoing in Sec. 2.1 and 2.2, the solution of the ASM-REL/TF has been also verified by using the original “Edwards Pipe” sample problem supplied with the RELAP5/MOD3.2 code. In this (original) setting, “Edwards Pipe” models the depressurization of a pipe, filled initially with single-phase water at a pressure of 7 MPa and temperature of 502 K. The transient depressurization of the single-phase water is initiated by releasing one end of the pipe. The time-dependent behavior of the liquid, namely water turning into a two-phase mixture during the pipe depressurization, simulates the basic features of a loss of coolant accident in a pressurized water reactor. It is important to mention that the calculation of the transient behavior of the pressure, temperature, and fluid- and gas-velocities that describe “Edwards Pipe” problem requires the complete hydrodynamics of the RELAP5/MOD3.2 two-fluid model, including several flow regimes.

Illustrative results for validating the numerical solution of the ASM-REL/TF for the first 0.1s (109 time steps) of the “Edwards Pipe” problem are presented in TABLE X. The two-phase flow regimes involved during these 109 time-steps are bubbly, slug, and mist flows, respectively; the transitions between regimes occur very rapidly. The results presented in TABLE X illustrate the effects of perturbations in the initial pressure in volume 305 on the subsequent time-evolution of the pressure in the same volume. The good agreement between the results for the predicted responses obtained using the ASM-REL/TF and the exactly recalculated responses indicates that the solution of the ASM-REL/TF is calculated robustly and accurately for the respective two-phase flow regimes. Beyond the first 109 time-steps, horizontal stratification begins to occur in some volumes. Validation of the solution of the ASM-REL/TF for this regime is currently in progress.

TABLE X "Edwards Pipe" – two-phase: influence of perturbations in the initial pressure in volume 305 on the pressure in the same volume.

Perturbation	Transient duration / no. of time steps	Nominal value (N/m^2)	P_{pred}	P_{recal}
0.1% of the initial pressure 7.0E+6 (N/m^2)	0.01 sec. / 19 t.s.	2.66073E+6	2.66070E+6	2.66071E+6
	0.06. sec / 69 t.s.	2.57470E+6	2.57471E+6	2.57473E+6
	0.1 sec / 109 t.s.	2.58221E+6	2.58238E+6	2.58241E+6
10% of the initial pressure 7.0E+6 (N/m^2)	0.01 sec. / 19 t.s.	2.66073E+6	2.66218E+6	2.66222E+6
	0.06. sec / 69 t.s.	2.57470E+6	2.57609E+6	2.57613E+6
	0.1 sec / 109 t.s.	2.58221E+6	2.57538E+6	2.57548E+6

5 SENSITIVITIES OF WATER MATERIAL PROPERTIES: ILLUSTRATIVE EXAMPLES

The material properties of water play an essential role in all calculations with RELAP5/MOD3.2. The standard reference for the mathematical formulae of the thermodynamic properties of ordinary water substance is the well-known monograph[12] entitled "ASME Steam Tables" (1993). In particular, this reference contains expressions for the specific fluid volume, V_f, the specific gas volume, V_g, the specific isobaric fluid heat capacity, C_{pf}, the specific isobaric gas heat capacity, C_{pg}, the volumetric expansion coefficient for fluid, $ß_f$, the volumetric expansion coefficient for gas, $ß_g$, the specific fluid enthalpy, h_f, the specific gas enthalpy, h_g, the isothermal coefficient of compressibility for fluid, k_f, and the isothermal coefficient for gas, k_g. The mathematical expressions for these thermodynamic properties comprise highly nonlinear functions of pressure, P, and temperature, T, and each expression involves many tens of experimentally determined numerical parameters.

The influence of such parameters, as well as of T and P, on results involving water as the working fluid can be quantitatively assessed by calculating the *sensitivities* of the various material properties; as already discussed in the foregoing, these sensitivities are actually the partial G-derivatives of the various material properties with respect to T, P, and the respective parameters. Exact explicit mathematical formulae have been obtained for the sensitivities of *all* of the material properties with respect to T, P, and numerical parameters by using the symbolic computer language MAPLE V[13]. Illustrative examples of sensitivities calculated with MAPLE V are presented in Appendix B.

The *relative sensitivity* of a material property, symbolically denoted below by $[\mathrm{Mat.\,Prop.}]$, to a parameter β, which can, in particular, represent T, P, or any other numerical coefficient, is defined as

$$\text{Relative Sensitivity with respect to } \beta \equiv \left[\left(\frac{\partial[\text{Mat. Prop.}]}{\partial\beta}\right)\left(\frac{\beta}{[\text{Mat. Prop.}]}\right)\right]^{o}.$$

In the above definition, the superscript zero signifies that all quantities enclosed within the outside brackets are to be evaluated at known base-case (nominal) values. On the other hand, the *recalculated relative changes* is defined as

$$\text{Recalculated Relative Change} \equiv \left[\text{Mat. Prop.}\left(\beta^{o} + \Delta\beta\right) - \text{Mat. Prop.}\left(\beta^{o}\right)\right]\frac{1}{\Delta\beta}\frac{\beta^{o}}{\text{Mat. Prop.}\left(\beta^{o}\right)},$$

where $\left[\text{Mat. Prop.}\left(\beta^{o} + \Delta\beta\right)\right]$ denotes the exactly recalculated (perturbed) value of the respective material property, using the perturbed parameter value $\left(\beta^{o} + \Delta\beta\right)$. In view of Eq. (3.6), the difference between the relative sensitivity and the recalculated relative change provides a quantitative measure of the nonlinear dependence of the respective material property on the parameter in question.

The sensitivities of all thermodynamic properties of water to the temperature, T, and pressure, P, are presented in TABLE XI. The nominal values T_f^o, T_g^o, and P^o for the temperatures and pressure, respectively, were selected to be in ranges of interest to reactor calculations. As can be seen from TABLE XI, the absolute values of the relative sensitivities of the material properties to temperature are quite large, with C_{pg} showing the largest relative sensitivity to variations in T. On the other hand, the quantity most sensitive to (and nonlinear in) pressure is the specific volume of gas, V_g. Least sensitive to pressure is the specific fluid enthalpy h_f, even though h_f is quite sensitive to temperature changes. The influence of nonlinearities becomes evident by comparing the relative sensitivities with the respective recalculated relative changes. Thus, the good agreement between the respective values in Table XI for small parameter variations indicates that the numerical value of the respective sensitivity has been calculated correctly. The nonlinear effects become markedly evident when the respective parameter variations are increased.

TABLE XI Relative sensitivities of water material properties to temperatures and pressures typically encountered in reactor safety analysis ($T_f^o = 564.7K, T_g^o = 620.6K, P^o = 159.2bar$)

Water Prop.	Relative sensitivity with respect to T	Rel. var.	Recalculated relative change	Relative sensitivity with respect to P	Rel. var.	Recalculated relative change
1. V_f	1.447	10^{-5}	1.447	-.0358	10^{-5}	-.0358
		10^{-4}	1.448		10^{-4}	-.0358
		10^{-3}	1.453		10^{-3}	-.0358
		10^{-2}	1.507		10^{-2}	-.0357
2. V_g	12.671	10^{-5}	12.667	-3.327	10^{-5}	-3.327
		10^{-4}	12.626		10^{-4}	-3.328
		10^{-3}	12.253		10^{-3}	-3.335
		10^{-2}	10.146		10^{-2}	-3.420
3. C_{pf}	2.112	10^{-5}	2.112	-.082	10^{-5}	-.0816
		10^{-4}	2.114		10^{-4}	-.0816
		10^{-3}	2.127		10^{-3}	-.0816
		10^{-2}	2.271		10^{-2}	-.0813
4. C_{pg}	-87.002	10^{-5}	-86.885	14.205	10^{-5}	14.208
		10^{-4}	-85.844		10^{-4}	14.232
		10^{-3}	-76.565		10^{-3}	14.479
		10^{-2}	-36.224		10^{-2}	17.440
5. β_f	6.390	10^{-5}	6.390	-.240	10^{-5}	-.240
		10^{-4}	6.394		10^{-4}	-.240
		10^{-3}	6.434		10^{-3}	-.240
		10^{-2}	6.870		10^{-2}	-.239
6. β_g	-84.259	10^{-5}	-84.152	14.089	10^{-5}	14.091
		10^{-4}	-83.208		10^{-4}	14.114
		10^{-3}	-74.803		10^{-3}	14.345
		10^{-2}	-37.918		10^{-2}	17.115
7. h_f	3.526	10^{-5}	3.526	-.077	10^{-5}	-.0762
		10^{-4}	3.530		10^{-4}	-.0762
		10^{-3}	3.568		10^{-3}	-.0761
		10^{-2}	4.211		10^{-2}	-.0752
8. h_g	3.688	10^{-4}	3.672	-.674	10^{-4}	-.674
		10^{-3}	3.541		10^{-3}	-.678
		10^{-2}	2.829		10^{-2}	-.720
9. κ_f	9.703	10^{-5}	9.703	-.337	10^{-5}	-.336
		10^{-4}	9.711		10^{-4}	-.336
		10^{-3}	9.786		10^{-3}	-.336
		10^{-2}	10.600		10^{-2}	-.335
10. κ_g	-53.661	10^{-5}	-53.597	8.107	10^{-5}	8.108
		10^{-4}	-53.037		10^{-4}	8.121
		10^{-3}	-48.034		10^{-3}	8.250
		10^{-2}	-25.596		10^{-2}	9.796

The sensitivities of the thermodynamic properties of water to the numerical parameters that enter in their respective mathematical formulae are presented in TABLE XII through TABLE XXI and have been grouped according to their relative importance to the fluid and gas phases, respectively. The base-case values for evaluating the sensitivities of the thermodynamic properties of fluid water have been chosen to be $T_f^o = 523.15K,\ P^o = 150.0bar$, which are conditions typically used in RELAP5/MOD3.2 for simulating reactor operational transients. On the other hand, the thermodynamic properties of gaseous water have been evaluated at the base-case values $T_g^o = 613.15K,\ P^o = 146.0bar$, where the gas is at saturation. Finally, the specific fluid enthalpy, h_f, and the specific gas enthalpy, h_g, have been evaluated at $T_f^o = T_g^o = 523.15K,\ P^o = 39.7bar$, since these base-case conditions correspond to non-saturated fluid/gas at the typical temperatures used in RELAP5/MOD3.2. These base-case values also close to values provided in the Steam Tables[5], which facilitates their direct verification.

The sensitivities of the specific isobaric fluid heat capacity, C_{pf}, and the specific isobaric gas heat capacity, C_{pg}, are presented in TABLE XII and, TABLE XIII respectively. These results show that C_{pf} and C_{pg} are extremely sensitive to variations in the first 30% (of the order of ten parameters); they are moderately or negligibly sensitive to the remaining parameters. It is important to note, though, that the dependence of C_{pf} and C_{pg} on the most sensitive parameters is *linear*, so the respective sensitivities predict *exactly* (not just to first order!) the effects of variations in the respective parameters. Nevertheless, as will be discussed in the sequel, such large sensitivities could propagate large uncertainties into the RELAP5/MOD3.2 results from the respective material properties.

TABLE XIV presents numerical results for the sensitivities of the specific fluid enthalpy h_f to all of the 33 empirical parameters that enter in its mathematical formula. These sensitivities are again ordered according to their absolute values, from high to low, and display features that are similar to those for C_{pf} and C_{pg} in the previous two tables. Thus, the sensitivities of h_f to the first ten parameters are extremely large, the sensitivities to the next five are moderately large, while the sensitivities to the last eighteen or so are negligible regarding their respective effects on h_f. It is important to note that h_f depends *linearly* on the parameters associated with the largest sensitivities; this fact is also reflected by the numerical results presented in the columns labeled $\left(h_f^{pred} - h_f^o\right)$ and $\left(h_f^{recal} - h_f^o\right)$, respectively. The respective values agree exactly, as would be expected in case of a linear dependence. Nevertheless, such high sensitivities would lead to potentially large contributions to the overall uncertainty in h_f.

The sensitivities of h_g shown in TABLE XV are quite small; note that the base-case conditions for calculating the sensitivities of h_g are *not* at saturation. This is in contrast to the calculation of the sensitivities of the other material properties of gaseous water, namely: (i) the specific gas volume, V_g, presented in TABLE XVI; (ii) the volumetric expansion coefficient for gas, $ß_g$, presented in TABLE XVII, and (iii) the isothermal coefficient for gas, k_g, presented in TABLE XVIII. The base-case conditions for calculating these sensitivities have been chosen to be $T_g^o = 613.15\text{K}, \quad P^o = 146.0\text{bar}$, where the gas is at saturation. The results in these tables show trends that are similar to those shown in TABLE XII through TABLE XIV for C_{pf}, C_{pg}, and h_f, respectively. Although the dependence of V_g on the most sensitive parameters is *linear* (so the respective sensitivities predict *exactly* the effects of variations in the respective parameters), the dependencies of $ß_g$, and k_g on the most sensitive parameters are *non-linear.*

Finally, TABLE XIX through TABLE XXI display the sensitivities of the remaining fluid thermodynamic properties, namely: (i) the specific fluid volume, V_f, shown in TABLE XIX; (ii) the volumetric expansion coefficient for fluid, $ß_f$, shown in TABLE XX; and (iii) the isothermal coefficient of compressibility for fluid, k_f, shown in TABLE XXI, respectively. All of these sensitivities are quite small, and would be important to consider in an uncertainty analysis only if the corresponding uncertainties were extremely large.

In closing, it is also important to discuss the essential role played by sensitivities for performing uncertainty analysis. The use of sensitivities for uncertainty analysis can be readily illustrated by recalling (see., e.g., Ronen[15]) that *the linear approximation of the variance of a response R* is given by $\text{var}\langle R\rangle = \sum_{i,j=1}^{J} S_i S_j \text{cov}(g_i, g_j)$, where S_i is the sensitivity of R to the parameter g_i and $\text{cov}(g_i, g_j)$ is the covariance matrix for the parameters g_i and g_j. If all of the parameters are uncorrelated, then this formula reduces to $\text{var}\langle R\rangle = \sum_{j=1}^{J} S_j^2 \sigma_j^2$, where σ_j^2 is the variance (uncertainty) of the distribution of the parameter g_j. These formulae highlight the interplay between the parameter sensitivities and uncertainties in contributing to the overall response uncertainty - as expressed by $\text{var}\langle R\rangle$. Thus, the largest contributions to the response uncertainty, $\mathrm{var}\langle R \rangle$, come from those parameters g_j that display not only a large uncertainty σ_j^2 but also a high sensitivity S_j. If either one (e.g., the sensitivity S_j) or the other (e.g., the uncertainty σ_j^2) of these two components is small, then their respective product will obviously contribute less to $\mathrm{var}\langle R \rangle$ than if both components were simultaneously large.

TABLE XII Sensitivities of the isobaric fluid heat capacity, C_{pf}, to the numerical parameters that enter its ASME mathematical formulation ($P^o = 150.0\text{bar}, \quad T_f^o = 523.15\text{K}$)

Param g_j	Rel. sens. $\frac{\partial C_{pf}}{\partial g_j}\frac{g_j^o}{C_{pf}^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$C_{pf}^{pred} - C_{pf}^o$	$C_{pf}^{recal} - C_{pf}^o$	Param g_j	Rel. sens. $\frac{\partial C_{pf}}{\partial g_j}\frac{g_j^o}{C_{pf}^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$C_{pf}^{pred} - C_{pf}^o$	$C_{pf}^{recal} - C_{pf}^o$
1.A_6	21356.05	0.1	10111.91	10111.91			10^{-2}	-.6605E-3	-.6486E-3
	linear dep.	0.5	50559.59	50559.59			10^{-1}	-.6605E-2	-.5561E-2
2.A_7	-20340	0.1	-9627.17	-9627.17	16.A_{20}	.557E-2	0.1	.2637E-2	.2637E-2
	linear dep.	0.5	-48135.87	-48135.87		linear dep.	0.5	.1318E-1	.1318E-1
3.A_5	-14357.93	0.1	-6795.50	-6795.50	17.a_6	.300E-2	10^{-4}	.1421E-5	.1419E-5
	linear dep.	0.5	-33977.50	-33977.50			10^{-3}	.1421E-4	.1400E-4
4.A_8	12085.68	0.1	5720.06	5720.06			10^{-2}	.1421E-3	.1227E-3
	linear dep.	0.5	28600.31	28600.31			10^{-1}	.1421E-2	.4146E-3
5.A_4	6039.87	0.1	2858.62	2858.62	18.a_2	-.266E-2	10^{-4}	-.1263E-5	-.1263E-5
	linear dep.	0.5	14293.14	14293.14			10^{-3}	-.1263E-4	-.1263E-4
6.A_9	-4094.11	0.1	-1937.71	-1937.71			10^{-2}	-.1263E-3	-.1263E-3
	linear dep.	0.5	-9688.57	-9688.57			10^{-1}	-.1263E-2	-.1262E-2
7.A_3	-1458.13	0.1	-690.12	-690.12	19.a_9	.829E-3	0.1	.3926E-3	.3926E-3
	linear dep.	0.5	-3450.62	-3450.62		linear dep.	0.5	.1963E-2	.1963E-2
8.A_{10}	605.16	0.1	286.41	286.41	20.A_{14}	-.573E-3	0.1	-.2712E-3	-.2712E-3
	linear dep.	0.5	1432.09	1432.09		linear dep.	0.5	-.1356E-2	-.1356E-2
9. A_0	156.20	0.1	73.93	73.93	21.a_{11}	.469E-3	0.1	.2222E-3	.2222E-3
	linear dep.	0.5	369.65	369.65		linear dep.	0.5	.1111E-2	.1111E-2
10.a_1	.25957	10^{-4}	.1228E-3	.1228E-3	22.A_{15}	-.887E-4	0.1	-.4198E-4	-.4198E-4
		10^{-3}	.1228E-2	.1230E-2		linear dep.	0.5	-.2099E-3	-.2099E-3
		10^{-2}	.1228E-1	.1251E-1	23.A_{17}	.546E-5	0.1	.2588E-5	.2588E-5
		10^{-1}	.1228	.1502		linear dep.	0.5	.1294E-4	.1294E-4
11.a_3	-.10989	10^{-4}	-.5201E-4	-.5201E-4	24.A_{18}	.388E-6	0.1	.1839E-6	.1839E-6
		10^{-3}	-.5201E-3	-.5200E-3		linear dep.	0.5	.9197E-6	.9197E-6
		10^{-2}	-.5201E-2	-.5196E-2	25.A_{16}	-.529E-7	0.1	-.2506E-7	-.2506E-7
		10^{-1}	-.5201E-1	-.5155E-1		linear dep.	0.5	-.1253E-6	-.1253E-6
12.a_4	.786E-1	10^{-4}	.3720E-4	.3720E-4	26.A_{19}	.134E-7	0.1	.6344E-8	.6344E-8
		10^{-3}	.3720E-3	.3721E-3		linear dep.	0.5	.3172E-7	.3172E-7
		10^{-2}	.3720E-2	.3731E-2	27.a_8	-.353E-8	10^{-4}	-.167E-11	-.167E-11
		10^{-1}	.3720E-1	.3832E-1			10^{-3}	-.167E-10	-.167E-10
13.A_{11}	.581E-1	0.1	.2750E-1	.2750E-1			10^{-2}	-.167E-9	-.167E-9
		0.5	.1375	.1375			10^{-1}	-.167E-8	-.167E-8
14.a_5	-.321E-1	10^{-4}	-.1521E-4	-.1521E-4	28.a_7	.135E-10	10^{-4}	.642E-14	.642E-14
		10^{-3}	-.1521E-3	-.1521E-3			10^{-3}	.642E-13	.642E-13
		10^{-2}	-.1521E-2	-.1519E-2			10^{-2}	.642E-12	.642E-12
		10^{-1}	-.1521E-1	-.1497E-1			10^{-1}	.642E-11	.642E-11
15.a_{10}	-.139E-1	10^{-4}	-.6605E-5	-.6604E-5	29.A_{22}	-.10E-10	0.1	-.509E-11	-.509E-11
		10^{-3}	-.6605E-4	-.6593E-4		linear dep.	0.5	-.254E-10	-.254E-10

TABLE XIII Sensitivities of the specific isobaric gas heat capacity, C_{pg}, to the numerical parameters that enter its ASME mathematical formulation ($P^o = 146.0\text{bar}, \quad T_g^o = 613.15\text{K}$)

Param g_j	Rel. Sens. $\frac{\partial C_{pg}}{\partial g_j}\frac{g_j^o}{C_{pg}^o}$	$\frac{\Delta g_j}{g_j^o}$	$C_{pg}^{pred} - C_{pg}^o$	$C_{pg}^{recal} - C_{pg}^o$	Param g_j	Rel. Sens. $\frac{\partial C_{pg}}{\partial g_j}\frac{g_j^o}{C_{pg}^o}$	$\frac{\Delta g_j}{g_j^o}$	$C_{pg}^{pred} - C_{pg}^o$	$C_{pg}^{recal} - C_{pg}^o$
1.B_{93}	19063.26	0.1	23277.92	23277.92		linear dep.	0.5	1.178	1.178
	linear dep.	0.5	116389.6	116389.6	19.b_{82}	-.1501	10^{-4}	-.1833E-3	-.1833E-3
2.B_{94}	-18611.13	0.1	-22725.84	-22725.84			10^{-3}	-.1833E-2	-.1833E-2
	linear dep.	0.5	-113629.2	-113629.2			10^{-2}	-.1833E-1	-.1827E-1
3.B_{92}	-10903.58	0.1	-13314.24	-13314.24			10^{-1}	-.1833	-.1767
	linear dep.	0.5	-66571.2	-66571.2	20.B_0	.1493	0.1	.1823	.1823
4.B_{95}	9623.61	0.1	11751.28	11751.28		linear dep.	0.5	.9119	.9119
	linear dep.	0.5	58756.42	58756.42	21.B_{71}	.1455	0.1	.1776	.1776
5.B_{91}	3300.47	0.1	4030.17	4030.17		linear dep.	0.5	.8883	.8883
	linear dep.	0.5	20150.85	20150.85	22.B_{21}	.1197	0.1	.1462	.1462
6.B_{96}	-2059.82	0.1	-2515.22	-2515.22		linear dep.	0.5	.7314	.7314
	linear dep.	0.5	-12576.14	-12576.14	23.B_{11}	.615E-1	0.1	.7511E-1	.7511E-1
7.B_{90}	-412.84	0.1	-504.12	-504.12		linear dep.	0.5	.3755	.3755
	linear dep.	0.5	-2520.61	-2520.61	24.B_{12}	.456E-1	0.1	.5568E-1	.5568E-1
8.L_1	-20.52	10^{-4}	-.2506E-1	-.2573E-1		linear dep.	0.5	.2784	.2784
		10^{-3}	-.2506	-.3319	25.B_{04}	.312E-1	0.1	.3818E-1	.3818E-1
		10^{-2}	-2.506	-351.46		linear dep.	0.5	.1909	.1909
		10^{-1}	-25.06	.5204	26.B_{42}	-.283E-1	0.1	-.3463E-1	-.3463E-1
9.L_2	10.73	10^{-4}	.1311E-1	.1293E-1		linear dep.	0.5	-.1731	-.1731
		10^{-3}	.1311	.1146	27.B_{32}	.225E-1	0.1	.2752E-1	.2752E-1
		10^{-2}	1.311	.4654		linear dep.	0.5	.1376	.1376
		10^{-1}	13.11	.5204	28.B_{72}	-.216E-1	0.1	-.2643E-1	-.2643E-1
10.L_0	10.21	10^{-4}	.1247E-1	.1230E-1		linear dep.	0.5	-.1321	-.1321
		10^{-3}	.1247	.1097	29.B_{61}	.137E-1	0.1	.1676E-1	.1676E-1
		10^{-2}	1.247	.4601		linear dep.	0.5	.8384E-1	.8384E-1
		10^{-1}	12.47	.5204	30.B_{82}	.132E-1	0.1	.1612E-1	.1612E-1
11.b	5.246	10^{-4}	.6406E-2	.6410E-2		linear dep.	0.5	.8060E-1	.8060E-1
		10^{-3}	.6406E-1	.6444E-1	31.b_{71}	-.853E-2	10^{-4}	-.1041E-4	-.1041E-4
		10^{-2}	.6406	.6805			10^{-3}	-.1041E-3	-.1041E-3
		10^{-1}	6.406	15.13			10^{-2}	-.1041E-2	-.1041E-2
12.B_{51}	1.360	0.1	1.6607	1.6607			10^{-1}	-.1041E-1	-.1036E-1
	linear dep.	0.5	8.3039	8.3039	32.B_{62}	-.844E-2	0.1	-.1031E-1	-.1031E-1
13.b_{81}	1.329	10^{-4}	.1623E-2	.1623E-2		linear dep.	0.5	-.5158E-1	-.5158E-1
		10^{-3}	.1623E-1	.1628E-1	33.B_{05}	-.774E-2	0.1	-.9463E-2	-.9463E-2
		10^{-2}	.1623	.1672		linear dep.	0.5	-.4731E-1	-.4731E-1
		10^{-1}	1.623	2.248	34.B_{03}	-.727E-2	0.1	-.8887E-2	-.8887E-2
14.B_{41}	-.9511	0.1	-1.161	-1.161		linear dep.	0.5	-.4443E-1	-.4443E-1
	linear dep.	0.5	-5.807	-5.807	35.b_{61}	-.246E-2	10^{-4}	-.3015E-5	-.3015E-5
15.B_{52}	-.7675	0.1	-.9372	-.9372			10^{-3}	-.3015E-4	-.3014E-4
	linear dep.	0.5	-4.686	-4.686			10^{-2}	-.3015E-3	-.3007E-3
16.B_{31}	.4262	0.1	.5204	.5204			10^{-1}	-.3015E-2	-.2938E-2
	linear dep.	0.5	2.602	2.602	36.B_{22}	-.241E-3	0.1	.2954E-3	.2954E-3
17.B_{81}	.2527	0.1	.3086	.3086		linear dep.	0.5	.1477E-2	.1477E-2
	linear dep.	0.5	1.543	1.543	37.B_{23}	-.749E-4	0.1	-.9154E-4	-.9154E-4
18.B_{53}	.1930	0.1	.2357	.2357		linear dep.	0.5	-.4577E-3	-.4577E-3

TABLE XIV Sensitivities of the specific fluid enthalpy, h_f, to parameters in its mathematical formulation($P^o = 39.7\text{bar}, \quad T_f^o = 523.15\text{K}$)

Param g_j	Rel. Sens. $\frac{\partial h_f}{\partial g_j}\frac{g_j^o}{h_f^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$h_f^{pred} - h_f^o$	$h_f^{recal} - h_f^o$	Param g_j	Rel. Sens. $\frac{\partial h_f}{\partial g_j}\frac{g_j^o}{h_f^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$h_f^{pred} - h_f^o$	$h_f^{recal} - h_f^o$
1. A_6	9744.20	0.1	.105E7	.105E7	17.A_{20}	.737E-3	0.1	.8009E-1	.8009E-1
	Linear dep.	0.5	.529E7	.529E7		linear dep.	0.5	.4004	.4004
2. A_5	-8185.48	0.1	-.888E6	-.888E6	18. a_5	.413E-3	10^{-4}	.4491E-4	.4491E-4
	Linear dep.	0.5	-.444E7	-.444E7			10^{-3}	.4491E-3	.4492E-3
3. A_7	-7730.90	0.1	-.839E6	-.839E6			10^{-2}	.4491E-2	.4500E-2
	Linear dep.	0.5	-.419E7	-.419E7			10^{-1}	.4491E-1	.4588E-1
4. A_4	4591.12	0.1	.498E6	.498E6	19. A_{12}	-.303E-3	0.1	-.329E-1	-.329E-1
	Linear dep.	0.5	.249E7	.249E7		linear dep.	0.5	-.1649	-.1649
5. A_8	3937.18	0.1	.427E6	.427E6	20. A_{14}	-.173E-3	0.1	-.188E-1	-.188E-1
	Linear dep.	0.5	.213E7	.213E7		linear dep.	0.5	-.940E-1	-.940E-1
6. A_3	-1662.57	0.1	-.180E6	-.180E6	21. a_9	.120E-3	0.1	.1303E-1	.1303E-1
	Linear dep.	0.5	-.902E6	-.902E6		linear dep.	0.5	.6516E-1	.6516E-1
7. A_9	-1167.03	0.1	-.126E6	-.126E6	22. a_6	.424E-4	10^{-4}	.4610E-5	.4603E-5
	Linear dep.	0.5	-.633E6	-.633E6			10^{-3}	.4610E-4	.4533E-4
8. A_0	356.208	0.1	.386E5	.386E5			10^{-2}	.4610E-3	.3904E-3
	Linear dep.	0.5	.193E6	.193E6			10^{-1}	.4610E-2	.1204E-2
9. A_{10}	153.33	0.1	.166E5	.166E5	23. a_{11}	.144E-4	0.1	.1567E-2	.1567E-2
	Linear dep.	0.5	.832E5	.832E5		linear dep.	0.5	.7836E-2	.7836E-2
10. A_1	-35.015	0.1	-3801.97	-3801.97	24. A_{15}	-.111E-5	0.1	-.121E-3	-.121E-3
	Linear dep.	0.5	-.190E5	-.190E5		linear dep.	0.5	-.606E-3	-.606E-3
11. a_3	.44819	10^{-4}	.4866E-1	.4866E-1	25. A_{17}	-.300E-6	0.1	-.326E-4	-.326E-4
		10^{-3}	.4866	.4866		linear dep.	0.5	-.163E-3	-.163E-3
		10^{-2}	4.866	4.864	26. A_{18}	-.566E-8	0.1	-.615E-6	-.615E-6
		10^{-1}	48.66	48.50		linear dep.	0.5	-.307E-5	-.307E-5
12. a_1	.854E-1	10^{-4}	.9274E-2	.9276E-2	27. A_{16}	.168E-8	0.1	.183E-6	.183E-6
		10^{-3}	.9274E-1	.9292E-1		linear dep.	0.5	.915E-6	.915E-6
		10^{-2}	.9274	.9457	28. a_{12}	.100E-8	0.1	.108E-6	.108E-6
		10^{-1}	9.274	11.38		linear dep.	0.5	.544E-6	.544E-6
13.A_{11}	-.493E-1	0.1	-5.362	-5.362	29. A_{21}	.100E-8	0.1	.108E-6	.108E-6
	Linear dep.	0.5	-26.81	-26.81		linear dep.	0.5	.544E-6	.544E-6
14. a_4	.284E-1	10^{-4}	.3085E-2	.3085E-2	30. a_8	.923E-10	10^{-4}	.100E-10	.100E-10
		10^{-3}	.3085E-1	.3085E-1			10^{-3}	.100E-9	.100E-9
		10^{-2}	.3085	.3090			10^{-2}	.100E-8	.100E-8
		10^{-1}	3.085	3.142			10^{-1}	.100E-7	.100E-7
15. a_{10}	-.211E-2	10^{-4}	-.229E-3	-.229E-3	31. A_{19}	-.51E-10	0.1	-.562E-8	-.562E-8
		10^{-3}	-.229E-2	-.229E-2		linear dep.	0.5	-.281E-7	-.281E-7
		10^{-2}	-.229E-1	-.225E-1	32. a_7	-.21E-12	10^{-4}	-.234E-13	-.234E-13
		10^{-1}	-.2296	-.1912			10^{-3}	-.234E-12	-.234E-12
16. a_2	.861E-3	10^{-4}	.9355E-4	.9355E-4			10^{-2}	-.234E-11	-.234E-11
		10^{-3}	.9355E-3	.9355E-3			10^{-1}	-.234E-10	-.234E-10
		10^{-2}	.9355E-2	.9355E-2	33. A_{22}	.606E-14	0.1	.658E-12	.658E-12
		10^{-1}	.9355E-1	.9352E-1		linear dep.	0.5	.329E-11	.329E-11

TABLE XV Sensitivities of the specific fluid enthalpy h_g, to parameters in its mathematical formulation ($P^o = 39.7\text{bar}, \quad T_g^o = 523.15\text{K}$)

Param g_j	Rel. Sens. $\frac{\partial h_g}{\partial g_j}\frac{g_j^o}{h_g^o}$	$\frac{\Delta g_j}{g_j^o}$	$h_g^{pred} - h_g^o$	$h_g^{recal} - h_g^o$	Param g_j	Rel. Sens. $\frac{\partial h_g}{\partial g_j}\frac{g_j^o}{h_g^o}$	$\frac{\Delta g_j}{g_j^o}$	$h_g^{pred} - h_g^o$	$h_g^{recal} - h_g^o$
1. B_{01}	.71513	0.1	200.26	200.26	23.B_{61}	-.1507E-3	0.1	-.4222E-1	-.4222E-1
	linear dep.	0.5	1001.34	1001.34		linear dep.	0.5	-.2111	-.2111
2. B_0	.34070	0.1	95.41	95.41	24.B_{96}	-.1079E-3	0.1	-.3022E-1	-.3022E-1
	linear dep.	0.5	477.06	477.06		linear dep.	0.5	-.1511	-.1511
3. b	-.14198	10^{-4}	-.3976E-1	-.3976E-1	25.B_{62}	.9998E-4	0.1	.2799E-1	.2799E-1
		10^{-3}	-.3976	-.3981		linear dep.	0.5	.1399	.1399
		10^{-2}	-3.976	-4.027	26.B_{22}	-.6337E-4	0.1	-.1774E-1	-.1774E-1
		10^{-1}	-39.76	-45.36		linear dep.	0.5	-.8874E-1	-.8874E-1
4. B_{12}	-.2766E-1	0.1	-7.746	-7.746	27.B_{23}	.5112E-4	0.1	.1431E-1	.1431E-1
	linear dep.	0.5	-38.731	-38.731		linear dep.	0.5	.7158E-1	.7158E-1
5. B_{11}	-.1817E-1	0.1	-5.088	-5.088	28.B_{72}	.4614E-4	0.1	.1292E-1	.1292E-1
	linear dep.	0.5	-25.444	-25.444		linear dep.	0.5	.6461E-1	.6461E-1
6. B_{04}	.1731E-1	0.1	4.847	4.847	29.B_{90}	-.1882E-4	0.1	-.5270E-2	-.5270E-2
	linear dep.	0.5	24.237	24.237		linear dep.	0.5	-.2635E-1	-.2635E-1
7. B_{21}	-.1146E-1	0.1	-3.211	-3.211	30. L_1	-.4299E-5	10^{-4}	-.1203E-5	-.1235E-5
	linear dep.	0.5	-16.058	-16.058			10^{-3}	-.1203E-4	-.1571E-4
8. B_{31}	-.1111E-1	0.1	-3.111	-3.111			10^{-2}	-.1203E-3	-.7334E-2
	linear dep.	0.5	-15.559	-15.559			10^{-1}	-.1203E-2	.2466E-4
9. B_{41}	.9985E-2	0.1	2.796	2.796	31.B_{81}	-.3759E-5	0.1	-.1052E-2	-.1052E-2
	linear dep.	0.5	13.981	13.981		linear dep.	0.5	-.5264E-2	-.5264E-2
10.B_{03}	-.7082E-2	0.1	-1.983	-1.983	32. L_0	.2312E-5	10^{-4}	.6475E-6	.6386E-6
	linear dep.	0.5	-9.917	-9.917			10^{-3}	.6475E-5	.5657E-5
11.B_{51}	-.6300E-2	0.1	-1.764	-1.764			10^{-2}	.6475E-4	.2256E-4
	linear dep.	0.5	-8.822	-8.822			10^{-1}	.6475E-3	.2466E-4
12.B_{05}	-.2745E-2	0.1	-.7687	-.7687	33. L_2	.2074E-5	10^{-4}	.5810E-6	.5741E-6
	linear dep.	0.5	-3.843	-3.843			10^{-3}	.5810E-5	.5170E-5
13.B_{52}	.2676E-2	0.1	-7494	-7494			10^{-2}	.5810E-4	.2241E-4
	linear dep.	0.5	3.747	3.747			10^{-1}	.5810E-3	.2466E-4
14.B_{94}	-.9234E-3	0.1	-.2586	-.2586	34.b_{81}	-.9547E-6	10^{-4}	-.2673E-6	-.2673E-6
	linear dep.	0.5	-1.293	-1.293			10^{-3}	-.2673E-5	-.2674E-5
15.B_{93}	.9229E-3	0.1	.2584	.2584			10^{-2}	-.2673E-4	-.2677E-4
	linear dep.	0.5	1.292	1.292			10^{-1}	-.2673E-3	-.2711E-3
16.B_{53}	-.5183E-3	0.1	-.1451	-.1451	35.b_{61}	.3074E-6	10^{-4}	.8608E-7	.8608E-7
	linear dep.	0.5	-.7258	-.7258			10^{-3}	.8608E-6	.8608E-6
17.B_{92}	-.5161E-3	0.1	-.1445	-.1445			10^{-2}	.8608E-5	.8608E-5
	linear dep.	0.5	-.7227	-.7227			10^{-1}	.8608E-4	.8604E-4
18.B_{95}	.4902E-3	0.1	.1373	.1373	36.b_{71}	.1681E-6	10^{-4}	.4708E-7	.4708E-7
	linear dep.	0.5	.6865	.6865			10^{-3}	.4708E-6	.4708E-6
19.B_{32}	-.4824E-3	0.1	-.1350	-.1350			10^{-2}	.4708E-5	.4708E-5
	linear dep.	0.5	-.6754	-.6754			10^{-1}	.4708E-4	.4708E-4
20.B_{71}	-.4204E-3	0.1	-.1177	-.1177	37.B_{82}	-.5067E-7	0.1	-.1419E-4	-.1419E-4
	linear dep.	0.5	-.5887	-.5887		linear dep.	0.5	-.7095E-4	-.7095E-4
21.B_{42}	.1733E-3	0.1	.4854E-1	.4854E-1	38.b_{82}	.5166E-8	10^{-4}	.1446E-8	.1446E-8
	linear dep.	0.5	.2427	.2427			10^{-3}	.1446E-7	.1446E-7
22.B_{91}	.1531E-3	0.1	.4288E-1	.4288E-1			10^{-2}	.1446E-6	.1446E-6
	linear dep.	0.5	.2144	.2144			10^{-1}	.1446E-5	.1446E-5

TABLE XVI Sensitivities of the specific gas volume, V_g, to the numerical parameters that enter its ASME mathematical formulation ($P^o = 146.0\text{bar}, \quad T_g^o = 613.15\text{K}$)

Param g_j	Rel. sens. $\frac{\partial V_g}{\partial g_j}\frac{g_j^o}{V_g^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$V_g^{pred} - V_g^o$	$V_g^{recal} - V_g^o$	Param g_j	Rel. Sens. $\frac{\partial V_g}{\partial g_j}\frac{g_j^o}{V_g^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$V_g^{pred} - V_g^o$	$V_g^{recal} - V_g^o$
1. B_{93}	-12239.7	0.1	-13194.87	-13194.87	18.B_{53}	-.15242	0.1	-.16432	-.16432
	linear dep.	0.5	-65974.36	-65974.36		linear dep.	0.5	-.82160	-.82160
2. B_{94}	11250.28	0.1	12128.23	12128.23	19.B_{71}	-.11813	0.1	-.12735	-.12735
	linear dep.	0.5	60641.19	60641.19		linear dep.	0.5	-.63677	-.63677
3. B_{92}	7454.4	0.1	8036.13	8036.13	20.B_{21}	-.6726E-1	0.1	-.725E-1	-.725E-1
	linear dep.	0.5	40180.65	40180.65		linear dep.	0.5	-.3625	-.3625
4. B_{95}	-5489.58	0.1	-5917.98	-5917.98	21.B_{32}	-.6150E-1	0.1	-.6630E-1	-.6630E-1
	linear dep.	0.5	-29589.91	-29589.91		linear dep.	0.5	-.3315	-.3315
5. B_{91}	-2409.25	0.1	-2597.26	-2597.26	22.B_{42}	-.5264E-1	0.1	-5674E-1	-5674E-1
	linear dep.	0.5	-12986.34	-12986.34		linear dep.	0.5	.2837	.2837
6. B_{96}	1111.1	0.1	1197.81	1197.81	23.B_{61}	-.5084E-1	0.1	.5480E-1	.5480E-1
	linear dep.	0.5	5989.06	5989.06		linear dep.	0.5	-.27404	-.27404
7. B_{90}	322.75	0.1	347.94	347.94	24.b_{81}	-.5060E-1	10^{-4}	-.5455E-4	-.5456E-4
	linear dep.	0.5	1739.72	1739.72			10^{-3}	-.5455E-3	-.5466E-3
8. l_1	1.79724	0.1	1.9374	1.9374			10^{-2}	-.5455E-2	-.5567E-2
	linear dep.	0.5	9.6874	9.6874			10^{-1}	-.5455E-1	-.6790E-1
9. L_1	.94649	10^{-4}	.1020E-2	.1046E-2	25.B_{62}	.4047E-1	0.1	.4363E-1	.4363E-1
		10^{-3}	.1020E-1	.1333E-1		linear dep.	0.5	.2181	.2181
		10^{-2}	.1020	10.2894	26.B_{11}	-.3310E-1	0.1	-.3569E-1	-.3569E-1
		10^{-1}	1.020	-.2224E-1		linear dep.	0.5	-.17846	-.17846
10.B_{51}	-.60403	0.1	-.6511	-.6511	27.B_{72}	-3200E-1	0.1	-3450E-1	-3450E-1
	linear dep.	0.5	-3.255	-3.255		linear dep.	0.5	.17251	.17251
11.B_{41}	.55367	0.1	.59688	.59688	28.B_{81}	-.1779E-1	0.1	-.1918E-1	-.1918E-1
	linear dep.	0.5	2.9844	2.9844		linear dep.	0.5	-.9590E-1	-.9590E-1
12. L_2	-.50675	10^{-4}	-.54629E-3	-.53899E-3	29.B_{23}	.1363E-1	0.1	.1470E-1	.1470E-1
		10^{-3}	-.54629E-2	-.47920E-2		linear dep.	0.5	.7350E-1	.7350E-1
		10^{-2}	-.54629E-1	-.19767E-1	30.B_{22}	-.1100E-1	0.1	-.1186E-1	-.1186E-1
		10^{-1}	-.54629	-.22241E-1		linear dep.	0.5	-.5931E-1	-.5931E-1
13.B_{12}	-.46088	0.1	-.49685	-.49685	31.b_{82}	.6918E-2	10^{-4}	.7457E-5	.7457E-5
	linear dep.	0.5	-2.4842	-2.4842			10^{-3}	.7457E-4	.7455E-4
14. L_0	-.46037	10^{-4}	-.4963E-3	-.4902E-3			10^{-2}	.7457E-3	.7437E-3
		10^{-3}	-.4963E-2	-.4404E-2			10^{-1}	.7457E-2	.7257E-2
		10^{-2}	-.4963E-1	-.1927E-1	32.b_{71}	.3921E-2	10^{-4}	.4227E-5	.4227E-5
		10^{-1}	-.4963	-.2224E-1			10^{-3}	.4227E-4	.4227E-4
15. b	-.44629	10^{-4}	-.4811E-3	-.4812E-3			10^{-2}	.4227E-3	.4225E-3
		10^{-3}	-.4811E-2	-4819E-2			10^{-1}	.4227E-2	.4212E-2
		10^{-2}	-.4811E-1	-.4900E-1	33.b_{61}	.2447E-2	10^{-4}	.2638E-5	.2638E-5
		10^{-1}	-.4811	-.6283			10^{-3}	.2638E-4	.2638E-4
16.B_{52}	.44523	0.1	.47997	.47997			10^{-2}	.2638E-3	.2633E-3
	linear dep.	0.5	2.3998	2.3998			10^{-1}	.2638E-2	.2592E-2
17.B_{31}	-.35894	0.1	-.38696	-.38696	34.B_{82}	-.1036E-2	0.1	-.1117E-2	-.1117E-2
	linear dep.	0.5	-1.9348	-1.9348		linear dep.	0.5	-.5587E-2	-.5587E-2

TABLE XVII Sensitivities of the volumetric expansion coefficient for gas, ß$_g$, to parameters in its mathematical formulation ($P^o = 146\text{bar}, T_g^o = 613.15\text{K}$)

Param g_j	Rel. sens. $\frac{\partial \beta_g}{\partial g_j} \frac{g_j^o}{\beta_g^o}$	$\frac{\Delta g_j}{g_j^o}$	$\beta_g^{pred} - \beta_g^o$	$\beta_g^{recal} - \beta_g^o$	Param g_j	Rel. Sens. $\frac{\partial \beta_g}{\partial g_j} \frac{g_j^o}{\beta_g^o}$	$\frac{\Delta g_j}{g_j^o}$	$\beta_g^{pred} - \beta_g^o$	$\beta_g^{recal} - \beta_g^o$
1.B_{93}	55764.89	10^{-4}	.8861E-1	-.3956	13. I_1	-1.612	10^{-4}	-.2562E-5	-.2562E-5
		10^{-3}	.8861	-.7883E-1			10^{-3}	-.2562E-4	-.2558E-4
		10^{-2}	8.861	-.7299E-1			10^{-2}	-.2562E-3	-.2517E-3
		10^{-1}	88.61	-.7245E-1			10^{-1}	-.2562E-2	-.2172E-2
2.B_{94}	-52091.92	10^{-4}	-.8277E-1	-.3895E-1	14.B_{41}	-1.580	10^{-4}	-.2512E-5	-.2512E-5
		10^{-3}	-.8277	-.6757E-1			10^{-3}	-.2512E-4	-.2510E-4
		10^{-2}	-8.277	-.7292E-1			10^{-2}	-.2512E-3	-.2498E-3
		10^{-1}	-82.77	-.7351E-1			10^{-1}	-.2512E-2	-.2380E-2
3.B_{92}	-33409.52	10^{-4}	-.5308E-1	-.3041E-1	15.B_{52}	-1.370	10^{-4}	-.2177E-5	-.2177E-5
		10^{-3}	-.5308	-.6279E-1			10^{-3}	-.2177E-4	-.2176E-4
		10^{-2}	-5.308	-.7027E-1			10^{-2}	-.2177E-3	-.2167E-3
		10^{-1}	-53.08	-.7112E-1			10^{-1}	-.2177E-2	-.2084E-2
4.B_{95}	25825.68	10^{-4}	.4103E-1	.9098E-1	16.b_{81}	1.103	10^{-4}	.1752E-5	.1753E-5
		10^{-3}	.4103	-.9140E-1			10^{-3}	.1752E-4	.1757E-4
		10^{-2}	4.103	-.7614E-1			10^{-2}	.1752E-3	.1804E-3
		10^{-1}	41.03	-.7489E-1			10^{-1}	.1752E-2	.2412E-2
5.B_{91}	10619.12	10^{-4}	.1687E-1	.2223E-1	17.B_{31}	.8384	10^{-4}	.1332E-5	.1332E-5
		10^{-3}	.1687	-.1197			10^{-3}	.1332E-4	.1332E-4
		10^{-2}	1.687	-.7307E-1			10^{-2}	.1332E-3	.1337E-3
		10^{-1}	16.87	-.7033E-1			10^{-1}	.1332E-2	.1381E-2
6.B_{96}	-5309.63	10^{-4}	-.8437E-2	-.7593E-2	18.B_{12}	.5634	10^{-4}	.8954E-6	.8954E-6
		10^{-3}	-.8437E-1	-.3996E-1			10^{-3}	.8954E-5	.8958E-5
		10^{-2}	-.8437	-.6966E-1			10^{-2}	.8954E-4	.8995E-4
		10^{-1}	-8.437	-.7525E-1			10^{-1}	.8954E-3	.9386E-3
7.B_{90}	-1398.64	10^{-4}	-.2222E-2	-.2153E-2	19.B_{53}	.4239	10^{-4}	.6736E-6	.6736E-6
		10^{-3}	-.2222E-1	-.1680E-1			10^{-3}	.6736E-5	.6737E-5
		10^{-2}	-.2222	-.5257E-1			10^{-2}	.6736E-4	.6746E-4
		10^{-1}	-2.222	-.6679E-1			10^{-1}	.6736E-3	.6840E-3
8. L_1	-13.53	10^{-4}	-.2150E-4	-.2205E-4	20.B_{71}	.3209	10^{-4}	.5100E-6	.5100E-6
		10^{-3}	-.2150E-3	-.2818E-3			10^{-3}	.5100E-5	.5100E-5
		10^{-2}	-.2150E-2	-.1243			10^{-2}	.5100E-4	.5106E-4
		10^{-1}	-.2150E-1	.4620E-3			10^{-1}	.5100E-3	.5161E-3
9. L_2	7.192	10^{-4}	.1142E-4	.1127E-4	21.B_{81}	.2280	10^{-4}	.3623E-6	.3623E-6
		10^{-3}	.1142E-3	.1001E-3			10^{-3}	.3623E-5	.3623E-5
		10^{-2}	.1142E-2	.4114E-3			10^{-2}	.3623E-4	.3623E-4
		10^{-1}	.1142E-1	.4620E-3			10^{-1}	.3623E-3	.3629E-3
10. L_0	6.628	10^{-4}	-.1053E-4	.1040E-4	22.B_{21}	.1571	10^{-4}	.2496E-6	.2496E-6
		10^{-3}	-.1053E-3	.9326E-4			10^{-3}	.2496E-5	.2496E-5
		10^{-2}	-.1053E-2	.4029E-3			10^{-2}	.2496E-4	.2498E-4
		10^{-1}	-.1053E-1	.4620E-3			10^{-1}	.2496E-3	.2513E-3
11. b	4.165	10^{-4}	.6618E-5	.6622E-5	23.b_{82}	-.1369	10^{-4}	-.2175E-6	-.2175E-6
		10^{-3}	.6618E-4	.6655E-4			10^{-3}	-.2175E-5	-.2175E-5
		10^{-2}	.6618E-3	.7009E-3			10^{-2}	-.2175E-4	-.2167E-4
		10^{-1}	.6618E-2	.1511E-1			10^{-1}	-.2175E-3	-.2095E-3
12.B_{51}	2.038	10^{-4}	.3239E-5	.3239E-5	24.B_{42}	-.1073	10^{-4}	-.1705E-6	-.1705E-6
		10^{-3}	.3239E-4	.3241E-4			10^{-3}	-.1705E-5	-.1705E-5
		10^{-2}	.3239E-3	.3258E-3			10^{-2}	-.1705E-4	-.1704E-4
		10^{-1}	.3239E-2	.3447E-2			10^{-1}	-.1705E-3	-.1696E-3

Param g_j	Rel. sens. $\frac{\partial \beta_g}{\partial g_j}\frac{g_j^o}{\beta_g^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$\beta_g^{pred} - \beta_g^o$	$\beta_g^{recal} - \beta_g^o$	Param g_j	Rel. Sens. $\frac{\partial \beta_g}{\partial g_j}\frac{g_j^o}{\beta_g^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$\beta_g^{pred} - \beta_g^o$	$\beta_g^{recal} - \beta_g^o$
25.B_{32}	.1071	10^{-4}	.1702E-6	.1702E-6	29.B_{62}	-.6358E-1	10^{-4}	-.1010E-6	-.1010E-6
		10^{-3}	.1702E-5	.1702E-5			10^{-3}	-.1010E-5	-.1010E-5
		10^{-2}	.1702E-4	.1703E-4			10^{-2}	-.1010E-4	-.1010E-4
		10^{-1}	.1702E-3	.1713E-3			10^{-1}	-.1010E-3	-.1006E-3
26.B_{61}	.8365E-1	10^{-4}	.1329E-6	.1329E-6	30.b_{71}	-.1670E-1	10^{-4}	-.2654E-7	-.2654E-7
		10^{-3}	.1329E-5	.1329E-5			10^{-3}	-.2654E-6	-.2654E-6
		10^{-2}	.1329E-4	.1329E-4			10^{-2}	-.2654E-5	-.2653E-5
		10^{-1}	.1329E-3	.1336E-3			10^{-1}	-.2654E-4	-.2641E-4
27.B_{72}	-.7270E-1	10^{-4}	-.1155E-6	-.1155E-6	31.B_{23}	-.1464E-1	10^{-4}	-.2327E-7	-.2327E-7
		10^{-3}	-.1155E-5	-.1155E-5			10^{-3}	-.2327E-6	-.2327E-6
		10^{-2}	-.1155E-4	-.1154E-4			10^{-2}	-.2327E-5	-.2327E-5
		10^{-1}	-.1155E-3	-.1151E-3			10^{-1}	-.2327E-4	-.2324E-4
28.B_{11}	.6505E-1	10^{-4}	.1033E-6	.1033E-6	32.B_{22}	.1263E-1	10^{-4}	.2008E-7	.2008E-7
		10^{-3}	.1033E-5	.1033E-5			10^{-3}	.2008E-6	.2008E-6
		10^{-2}	.1033E-4	.1034E-4			10^{-2}	.2008E-5	.2008E-5
		10^{-1}	.1033E-3	.1037E-3			10^{-1}	.2008E-4	.2010E-4

TABLE XVIII Sensitivities of the isothermal coefficient of compressibility for gas, k_g, to parameters in its mathematical formulation ($P^o = 146\text{bar}, T_g^o = 613.15\text{K}$)

Param g_j	Rel. sens. $\frac{\partial \kappa_g}{\partial g_j}\frac{g_j^o}{\kappa_g^o}$	$\frac{\Delta g_j}{g_j^o}$	$\kappa_g^{pred} - \kappa_g^o$	$\kappa_g^{recal} - \kappa_g^o$	Param g_j	Rel. Sens. $\frac{\partial \kappa_g}{\partial g_j}\frac{g_j^o}{\kappa_g^o}$	$\frac{\Delta g_j}{g_j^o}$	$\kappa_g^{pred} - \kappa_g^o$	$\kappa_g^{recal} - \kappa_g^o$
1.B_{93}	55788.72	10^{-4}	.1073E-5	-.4793E-5	13. l_1	-1.157	10^{-4}	-.2227E-10	-.2227E-10
		10^{-3}	.1073E-4	-.9551E-6			10^{-3}	-.2227E-9	-.2223E-9
		10^{-2}	.1073E-3	-.8843E-6			10^{-2}	-.2227E-8	-.2188E-8
		10^{-1}	.1073E-2	-.8778E-6			10^{-1}	-.2227E-7	-.1888E-7
2.B_{94}	-51278.92	10^{-4}	-.9867E-6	-.4643E-6	14.B_{41}	-1.144	10^{-4}	-.2202E-10	-.2202E-10
		10^{-3}	-.9867E-5	-.8055E-6			10^{-3}	-.2202E-9	-.2201E-9
		10^{-2}	-.9867E-4	-.8693E-6			10^{-2}	-.2202E-8	-.2190E-8
		10^{-1}	-.9867E-3	-.8763E-6			10^{-1}	-.2202E-7	-.2087E-7
3.B_{92}	-33977.24	10^{-4}	-.6538E-6	-.3746E-6	15.B_{52}	-1.078	10^{-4}	-.2076E-10	-.2076E-10
		10^{-3}	-.6538E-5	-.7733E-6			10^{-3}	-.2076E-9	-.2075E-9
		10^{-2}	-.6538E-4	-.8655E-6			10^{-2}	-.2076E-8	-.2066E-8
		10^{-1}	-.6538E-3	-.8759E-6			10^{-1}	-.2076E-7	-.1987E-7
4.B_{95}	25021.58	10^{-4}	.4815E-6	.1067E-5	16.b_{81}	.6245	10^{-4}	.1201E-10	.1202E-10
		10^{-3}	.4815E-5	-.1072E-5			10^{-3}	.1201E-9	.1205E-9
		10^{-2}	.4815E-4	-.8933E-6			10^{-2}	.1201E-8	.1236E-8
		10^{-1}	.4815E-3	-.8787E-6			10^{-1}	.1201E-7	.1639E-7
5.B_{91}	10981.41	10^{-4}	.2113E-6	.2783E-6	17.B_{31}	.6143	10^{-4}	.1182E-10	.1182E-10
		10^{-3}	.2113E-5	-.1499E-5			10^{-3}	.1182E-9	.1182E-9
		10^{-2}	.2113E-4	-.9151E-6			10^{-2}	.1182E-8	.1186E-8
		10^{-1}	.2113E-3	-.8807E-6			10^{-1}	.1182E-7	.1226E-7
6.B_{96}	-5064.42	10^{-4}	-.9745E-7	-.8771E-7	18.B_{12}	.4608	10^{-4}	.8869E-11	.8869E-11
		10^{-3}	-.9745E-6	-.4616E-6			10^{-3}	.8869E-10	.8873E-10
		10^{-2}	-.9745E-5	-.8046E-6			10^{-2}	.8869E-9	.8910E-9
		10^{-1}	-.9745E-4	-.8692E-6			10^{-1}	.8869E-8	.9297E-8
7.B_{90}	-1471.13	10^{-4}	-.2830E-7	-.2742E-7	19.B_{53}	.3693	10^{-4}	.7107E-11	.7107E-11
		10^{-3}	-.2830E-6	-.2140E-6			10^{-3}	.7107E-10	.7108E-10
		10^{-2}	-.2830E-5	-.6696E-6			10^{-2}	.7107E-9	.7118E-9
		10^{-1}	-.2830E-4	-.8507E-6			10^{-1}	.7107E-8	.7217E-8
8. L_1	-4.314	10^{-4}	-.8301E-10	-.8514E-10	20.B_{71}	.2766	10^{-4}	.5324E-11	.5324E-11
		10^{-3}	-.8301E-9	-.1083E-8			10^{-3}	.5324E-10	.5325E-10
		10^{-2}	-.8301E-8	-.4283E-6			10^{-2}	.5324E-9	.5330E-9
		10^{-1}	-.8301E-7	.1813E-8			10^{-1}	.5324E-8	.5388E-8
9. L_2	2.309	10^{-4}	.4444E-10	.4385E-10	21.B_{81}	.1375	10^{-4}	.2647E-11	.2647E-11
		10^{-3}	.4444E-9	.3900E-9			10^{-3}	.2647E-10	.2647E-10
		10^{-2}	.4444E-8	.1611E-8			10^{-2}	.2647E-9	.2647E-9
		10^{-1}	.4444E-7	.1813E-8			10^{-1}	.2647E-8	.2652E-8
10. L_0	2.098	10^{-4}	.4038E-10	.3989E-10	22.B_{42}	-.1088	10^{-4}	-.2094E-11	-.2094E-11
		10^{-3}	.4038E-9	.3585E-9			10^{-3}	-.2094E-10	-.2094E-10
		10^{-2}	.4038E-8	.1570E-8			10^{-2}	-.2094E-9	-.2093E-9
		10^{-1}	.4038E-7	.1813E-8			10^{-1}	-.2094E-8	-.2083E-8
11. b	2.001	10^{-4}	.3851E-10	.3854E-10	23.B_{32}	.1052	10^{-4}	.2025E-11	.2025E-11
		10^{-3}	.3851E-9	.3873E-9			10^{-3}	.2025E-10	.2025E-10
		10^{-2}	.3851E-8	.4077E-8			10^{-2}	.2025E-9	.2026E-9
		10^{-1}	.3851E-7	.8649E-7			10^{-1}	.2025E-8	.2038E-8
12.B_{51}	1.463	10^{-4}	.2816E-10	.2816E-10	24.B_{21}	.9119E-1	10^{-4}	.1754E-11	.1754E-11
		10^{-3}	.2816E-9	.2818E-9			10^{-3}	.1754E-10	.1754E-10
		10^{-2}	.2816E-8	.2833E-8			10^{-2}	.1754E-9	.1756E-9
		10^{-1}	.2816E-7	.2997E-7			10^{-1}	.1754E-8	.1766E-8

Param g_j	Rel. sens. $\frac{\partial \kappa_g}{\partial g_j} \frac{g_j^o}{\kappa_g^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$\kappa_g^{pred} - \kappa_g^o$	$\kappa_g^{recal} - \kappa_g^o$	Param g_j	Rel. Sens. $\frac{\partial \kappa_g}{\partial g_j} \frac{g_j^o}{\kappa_g^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$\kappa_g^{pred} - \kappa_g^o$	$\kappa_g^{recal} - \kappa_g^o$
25.B_{61}	.8803E-1	10^{-4}	.1694E-11	.1694E-11	29.B_{11}	.3310E-1	10^{-4}	.6371E-12	.6371E-12
		10^{-3}	.1694E-10	.1694E-10			10^{-3}	.6371E-11	.6371E-11
		10^{-2}	.1694E-9	.1694E-9			10^{-2}	.6371E-10	.6373E-10
		10^{-1}	.1694E-8	.1702E-8			10^{-1}	.6371E-9	.6392E-9
26.b_{82}	-.8538E-1	10^{-4}	-.1643E-11	-.1643E-11	30.B_{23}	-.1848E-1	10^{-4}	-.3558E-12	-.3558E-12
		10^{-3}	-.1643E-10	-.1642E-10			10^{-3}	-.3558E-11	-.3558E-11
		10^{-2}	-.1643E-9	-.1636E-9			10^{-2}	-.3558E-10	-.3557E-10
		10^{-1}	-.1643E-8	-.1581E-8			10^{-1}	-.3558E-9	-.3553E-9
27.B_{72}	-.7496E-1	10^{-4}	-.1442E-11	-.1442E-11	31.b_{71}	-.1600E-1	10^{-4}	-.3079E-12	-.3079E-12
		10^{-3}	-.1442E-10	-.1442E-10			10^{-3}	-.3079E-11	-.3079E-11
		10^{-2}	-.1442E-9	-.1442E-9			10^{-2}	-.3079E-10	-.3077E-10
		10^{-1}	-.1442E-8	-.1437E-8			10^{-1}	-.3079E-9	-.3063E-9
28.B_{62}	-.7007E-1	10^{-4}	-.1348E-11	-.1348E-11	32.B_{22}	.1492E-1	10^{-4}	.2871E-12	.2871E-12
		10^{-3}	-.1348E-10	-.1348E-10			10^{-3}	.2871E-11	.2871E-11
		10^{-2}	-.1348E-9	-.1347E-9			10^{-2}	.2871E-10	.2871E-10
		10^{-1}	-.1348E-8	-.1343E-8			10^{-1}	.2871E-9	.2874E-9

TABLE XIX Sensitivities of the specific fluid volume, V_f, to the numerical parameters that enter its ASME mathematical formulation ($P^o = 150.0\text{bar}$, $T_f^o = 523.15\text{K}$)

Param g_j	Rel. sens. $\frac{\partial V_f}{\partial g_j}\frac{g_j^o}{V_f^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$V_f^{pred} - V_f^o$	$V_f^{recal} - V_f^o$	Param g_j	Rel. Sens. $\frac{\partial V_f}{\partial g_j}\frac{g_j^o}{V_f^o}$	Rel. Par. Var. $\frac{\Delta g_j}{g_j^o}$	$V_f^{pred} - V_f^o$	$V_f^{recal} - V_f^o$
1. A_{11}	1.0254	0.1	.1263	.1263	11.A_{20}	.322E-3	0.1	.3968E-4	.3968E-4
	linear dep.	0.5	.6319	.6319		linear dep.	0.5	.1984E-3	.1984E-3
2. a_5	1.0064	10^{-4}	.124E-3	.124E-3	12. a_6	-.2041E-3	10^{-4}	-.2515E-7	-.2510E-7
		10^{-3}	.124E-2	.124E-2			10^{-3}	-.2515E-6	-.2468E-6
		10^{-2}	.124E-1	.124E-1			10^{-2}	-.2515E-5	-.2086E-5
		10^{-1}	.124	.123			10^{-1}	-.2515E-4	-.5920E-5
3. a_1	.4076	10^{-4}	.5024E-4	.5024E-4	13. a_{11}	-.1715E-3	0.1	-.2113E-4	-.2113E-4
		10^{-3}	.5024E-3	.5028E-3		linear dep.	0.5	-.1056E-3	-.1056E-3
		10^{-2}	.5024E-2	.5071E-2	14. a_9	.5746E-4	0.1	.7081E-5	.7081E-5
		10^{-1}	.5024E-1	.5559E-1		linear dep.	0.5	.3540E-4	.3540E-4
4. a_3	-.9702E-1	10^{-4}	-.1195E-4	-.1195E-4	15.A_{21}	-.2804E-4	0.1	-.3456E-5	-.3456E-5
		10^{-3}	-.1195E-3	-.1195E-3		linear dep.	0.5	-.1728E-4	-.1728E-4
		10^{-2}	-.1195E-2	-.1189E-2	16. a_{12}	.9469E-5	0.1	.1166E-5	.1166E-5
		10^{-1}	-.1195E-1	-.1139E-1		linear dep.	0.5	.5834E-5	.5834E-5
5. A_{12}	-.6730E-1	0.1	-.8294E-2	-.8294E-2	17.A_{17}	-.5552E-5	0.1	-.6843E-6	-.6843E-6
	linear dep.	0.5	-.4147E-1	-.4147E-1		linear dep.	0.5	-.3421E-5	-.3421E-5
6. A_{14}	.3837E-1	0.1	.4729E-2	.4729E-2	18.A_{15}	.4823E-5	0.1	.5944E-6	.5944E-6
	linear dep.	0.5	.2364E-1	.2364E-1		linear dep.	0.5	.2972E-5	.2972E-5
7. a_4	.3352E-1	10^{-4}	.4131E-5	.4131E-5	19.A_{18}	-.789E-6	0.1	-.9724E-7	-.9724E-7
		10^{-3}	.4131E-4	.4131E-4		linear dep.	0.5	-.4862E-6	-.4862E-6
		10^{-2}	.4131E-3	.4138E-3	20.A_{19}	-.4082E-7	0.1	-.5030E-8	-.5030E-8
		10^{-1}	.4131E-2	.4204E-2		linear dep.	0.5	-.2515E-7	-.2515E-7
8. A_{13}	.3164E-2	0.1	.390E-3	.390E-3	21.A_{16}	.1866E-7	0.1	.2300E-8	.2300E-8
	linear dep.	0.5	.195E-2	.195E-2		linear dep.	0.5	.1150E-7	.1150E-7
9. a_{10}	-.1799E-2	10^{-4}	-.2218E-6	-.2217E-6	22. a_8	.1003E-8	10^{-3}	.1236E-11	.1236E-11
		10^{-3}	-.2218E-5	-.2213E-5			10^{-2}	.1236E-10	.1236E-10
		10^{-2}	-.2218E-4	-.2168E-4			10^{-1}	.1236E-19	.1236E-19
		10^{-1}	-.2218E-3	-.1791E-3	23.A_{22}	.3430E-11	0.1	.4228E-12	.4228E-12
10. a_2	.1423E-2	10^{-4}	.1753E-6	.1753E-6		linear dep.	0.5	.2114E-11	.2114E-11
		10^{-3}	.1753E-5	.1753E-5	24. a_7	-.122E-11	10^{-3}	-.1512E-14	-.1512E-14
		10^{-2}	.1753E-4	.1753E-4			10^{-2}	-.1512E-13	-.1512E-13
		10^{-1}	.1753E-3	.1754E-3			10^{-1}	-.1512E-12	-.1512E-12

TABLE XX Sensitivities of the volumetric expansion coefficient for fluid, ß$_f$, to parameters in its mathematical formulation ($P^o = 150\text{bar}, T_f^o = 523.15\text{K}$)

Param g_j	Rel. sens. $\frac{\partial \beta_f}{\partial g_j}\frac{g_j^o}{\beta_f^o}$	$\frac{\Delta g_j}{g_j^o}$	$\beta_f^{pred} - \beta_f^o$	$\beta_f^{recal} - \beta_f^o$	Param g_j	Rel. Sens. $\frac{\partial \beta_f}{\partial g_j}\frac{g_j^o}{\beta_f^o}$	$\frac{\Delta g_j}{g_j^o}$	$\beta_f^{pred} - \beta_f^o$	$\beta_f^{recal} - \beta_f^o$
1. a_1	2.2207	10^{-4}	.3934E-6	.3935E-6	13. a_9	.1058E-2	10^{-4}	.1875E-9	.1875E-9
		10^{-3}	.3934E-5	.3940E-5			10^{-3}	.1875E-8	.1875E-8
		10^{-2}	.3934E-4	.3998E-4			10^{-2}	.1875E-7	.1875E-7
		10^{-1}	.3934E-3	.4687E-3			10^{-1}	.1875E-6	.1875E-6
2. a_4	.2441	10^{-4}	.4325E-7	.4325E-7	14.A_{15}	.2674E-3	10^{-4}	.4737E-10	.4737E-10
		10^{-3}	.4325E-6	.4326E-6			10^{-3}	.4737E-9	.4737E-9
		10^{-2}	.4325E-5	.4339E-5			10^{-2}	.4737E-8	.4737E-8
		10^{-1}	.4325E-4	.4468E-4			10^{-1}	.4737E-7	.4737E-7
3. a_5	-.2370	10^{-4}	-.4200E-7	-.4200E-7	15.A_{13}	.2497E-3	10^{-4}	.4424E-10	.4424E-10
		10^{-3}	-.4200E-6	-.4197E-6			10^{-3}	.4424E-9	.4424E-9
		10^{-2}	-.4200E-5	-.4175E-5			10^{-2}	.4424E-8	.4424E-8
		10^{-1}	-.4200E-4	-.3965E-4			10^{-1}	.4424E-7	.4423E-7
4. A_{11}	-.1188	10^{-4}	-.2105E-7	-.2105E-7	16.A_{17}	.7143E-4	10^{-4}	.1265E-10	.1265E-10
		10^{-3}	-.2105E-6	-.2103E-6			10^{-3}	.1265E-9	.1265E-9
		10^{-2}	-.2105E-5	-.2083E-5			10^{-2}	.1265E-8	.1265E-8
		10^{-1}	-.2105E-4	-.1909E-4			10^{-1}	.1265E-7	.1265E-7
5. a_3	-.9089E-1	10^{-4}	-.1610E-7	-.1610E-7	17.A_{21}	-.1242E-4	10^{-4}	-.2202E-11	-.2202E-11
		10^{-3}	-.1610E-6	-.1608E-6			10^{-3}	-.2202E-10	-.2202E-10
		10^{-2}	-.1610E-5	-.1593E-5			10^{-2}	-.2202E-9	-.2202E-9
		10^{-1}	-.1610E-4	-.1455E-4			10^{-1}	-.2202E-8	-.2202E-8
6. A_{12}	.6730E-1	10^{-4}	.1192E-7	.1192E-7	18.A_{18}	.1015E-4	10^{-4}	.1798E-11	.1798E-11
		10^{-3}	.1192E-6	.1192E-6			10^{-3}	.1798E-10	.1798E-10
		10^{-2}	.1192E-5	.1193E-5			10^{-2}	.1798E-9	.1798E-9
		10^{-1}	.1192E-4	.1200E-4			10^{-1}	.1798E-8	.1798E-8
7. A_{14}	.4443E-1	10^{-4}	.7872E-8	.7872E-8	19. a_{12}	-.9469E-5	10^{-4}	-.1677E-11	-.1677E-11
		10^{-3}	.7872E-7	.7872E-7			10^{-3}	-.1677E-10	-.1677E-10
		10^{-2}	.7872E-6	.7869E-6			10^{-2}	-.1677E-9	-.1677E-9
		10^{-1}	.7872E-5	.7842E-5			10^{-1}	-.1677E-8	-.1677E-8
8. a_{10}	-.3634E-1	10^{-4}	-.6438E-8	-.6437E-8	20.A_{19}	.5252E-6	10^{-4}	.9305E-13	.9305E-13
		10^{-3}	-.6438E-7	-.6424E-7			10^{-3}	.9305E-12	.9305E-12
		10^{-2}	-.6438E-6	-.6294E-6			10^{-2}	.9305E-11	.9305E-11
		10^{-1}	-.6438E-5	-.5202E-5			10^{-1}	.9305E-10	.9305E-10
9. a_6	-.1016E-1	10^{-4}	-.1800E-8	-.1797E-8	21.A_{16}	-.4013E-6	10^{-4}	-.7110E-13	-.7110E-13
		10^{-3}	-.1800E-7	-.1770E-7			10^{-3}	-.7110E-12	-.7110E-12
		10^{-2}	-.1800E-6	-.1524E-6			10^{-2}	-.7110E-11	-.7110E-11
		10^{-1}	-.1800E-5	-.4704E-6			10^{-1}	-.7110E-10	-.7110E-10
10.A_{20}	.6502E-2	10^{-4}	.1152E-8	.1152E-8	22. a_8	-.2481E-7	10^{-4}	-.4395E-14	-.4395E-14
		10^{-3}	.1152E-7	.1152E-7			10^{-3}	-.4395E-13	-.4395E-13
		10^{-2}	.1152E-6	.1152E-6			10^{-2}	-.4395E-12	-.4395E-12
		10^{-1}	.1152E-5	.1152E-5			10^{-1}	-.4395E-11	-.4395E-11
11. a_2	-.4530E-2	10^{-4}	-.8027E-9	-.8027E-9	23.A_{22}	-.774E-10	10^{-4}	-.1372E-16	-.1372E-16
		10^{-3}	-.8027E-8	-.8027E-8			10^{-3}	-.1372E-15	-.1372E-15
		10^{-2}	-.8027E-7	-.8027E-7			10^{-2}	-.1372E-14	-.1372E-14
		10^{-1}	-.8027E-6	-.8031E-6			10^{-1}	-.1372E-13	-.1372E-13
12. a_{11}	-.3463E-2	10^{-4}	-.6135E-9	-.6135E-9	24. a_7	.5153E-10	10^{-4}	.9129E-17	.9129E-17
		10^{-3}	-.6135E-8	-.6135E-8			10^{-3}	.9129E-16	.9129E-16
		10^{-2}	-.6135E-7	-.6135E-7			10^{-2}	.9129E-15	.9129E-15
		10^{-1}	-.6135E-6	-.6135E-6			10^{-1}	.9129E-14	.9129E-14

TABLE XXI Sensitivities of the isothermal coefficient of compressibility for fluid, k_f, to parameters in its mathematical formulation ($P^o = 150\text{bar}, T_f^o = 523.15\text{K}$)

Param g_j	Rel. sens. $\frac{\partial \kappa_f}{\partial g_j}\frac{g_j^o}{\kappa_f^o}$	$\frac{\Delta g_j}{g_j^o}$	$\kappa_f^{pred} - \kappa_f^o$	$\kappa_f^{recal} - \kappa_f^o$	Param g_j	Rel. Sens. $\frac{\partial \kappa_f}{\partial g_j}\frac{g_j^o}{\kappa_f^o}$	$\frac{\Delta g_j}{g_j^o}$	$\kappa_f^{pred} - \kappa_f^o$	$\kappa_f^{recal} - \kappa_f^o$
1. a_1	2.752	10^{-4}	.3540E-12	.3541E-12	11.A_{13}	-.3164E-2	10^{-4}	-.4070E-15	-.4070E-15
		10^{-3}	.3540E-11	.3548E-11			10^{-3}	-.4070E-14	-.4070E-14
		10^{-2}	.3540E-10	.3619E-10			10^{-2}	-.4070E-13	-.4070E-13
		10^{-1}	.3540E-9	.4508E-9			10^{-1}	-.4070E-12	-.4069E-12
2. a_3	-.8948	10^{-4}	-.1150E-12	-.1150E-12	12.A_{21}	.2935E-2	10^{-4}	.3775E-15	.3775E-15
		10^{-3}	-.1150E-11	-.1149E-11			10^{-3}	.3775E-14	.3775E-14
		10^{-2}	-.1150E-10	-.1139E-10			10^{-2}	.3775E-13	.3775E-13
		10^{-1}	-.1150E-9	-.1047E-9			10^{-1}	.3775E-12	.3775E-12
3. a_5	.7747	10^{-4}	.9964E-13	.9964E-13	13. a_9	.1554E-2	10^{-4}	.1999E-15	.1999E-15
		10^{-3}	.9964E-12	.9963E-12			10^{-3}	.1999E-14	.1999E-14
		10^{-2}	.9964E-11	.9948E-11			10^{-2}	.1999E-13	.1999E-13
		10^{-1}	.9964E-10	.9806E-10			10^{-1}	.1999E-12	.1999E-12
4. a_4	.3091	10^{-4}	.3976E-13	.3976E-13	14. a_{12}	-.9911E-3	10^{-4}	-.1274E-15	-.1274E-15
		10^{-3}	.3976E-12	.3977E-12			10^{-3}	-.1274E-14	-.1274E-14
		10^{-2}	.3976E-11	.3990E-11			10^{-2}	-.1274E-13	-.1274E-13
		10^{-1}	.3976E-10	.4118E-10			10^{-1}	-.1274E-12	-.1274E-12
5.A_{12}	.6730E-1	10^{-4}	.8656E-14	.8656E-14	15. a_6	.2041E-3	10^{-4}	.2625E-16	.2620E-16
		10^{-3}	.8656E-13	.8656E-13			10^{-3}	.2625E-15	.2575E-15
		10^{-2}	.8656E-12	.8662E-12			10^{-2}	.2625E-14	.2177E-14
		10^{-1}	.8656E-11	.8714E-11			10^{-1}	.2625E-13	.6178E-14
6. a_{10}	-.3938E-1	10^{-4}	-.5065E-14	-.5063E-14	16. a_{11}	.1715E-3	10^{-4}	.2205E-16	.2205E-16
		10^{-3}	-.5065E-13	-.5051E-13			10^{-3}	.2205E-15	.2205E-15
		10^{-2}	-.5065E-12	-.4928E-12			10^{-2}	.2205E-14	.2205E-14
		10^{-1}	-.5065E-11	-.3921E-11			10^{-1}	.2205E-13	.2205E-13
7.A_{14}	-.3837E-1	10^{-4}	-.4936E-14	-.4936E-14	17.A_{18}	.4168E-4	10^{-4}	.5361E-17	.5361E-17
		10^{-3}	-.4936E-13	-.4935E-13			10^{-3}	.5361E-16	.5361E-16
		10^{-2}	-.4936E-12	-.4934E-12			10^{-2}	.5361E-15	.5361E-15
		10^{-1}	-.4936E-11	-.4917E-11			10^{-1}	.5361E-14	.5361E-14
8.A_{11}	-.3745E-1	10^{-4}	-.4817E-14	-.4816E-14	18.A_{17}	.5552E-5	10^{-4}	.7141E-18	.7141E-18
		10^{-3}	-.4817E-13	-.4812E-13			10^{-3}	.7141E-17	.7141E-17
		10^{-2}	-.4817E-12	-.4768E-12			10^{-2}	.7141E-16	.7141E-16
		10^{-1}	-.4817E-11	-.4369E-11			10^{-1}	.7141E-15	.7141E-15
9. a_2	.9608E-2	10^{-4}	.1235E-14	.1235E-14	19.A_{15}	-.4823E-5	10^{-4}	-.6203E-18	-.6203E-18
		10^{-3}	.1235E-13	.1235E-13			10^{-3}	-.6203E-17	-.6203E-17
		10^{-2}	.1235E-12	.1235E-12			10^{-2}	-.6203E-16	-.6203E-16
		10^{-1}	.1235E-11	.1236E-11			10^{-1}	-.6203E-15	-.6203E-15
10.A_{20}	.8711E-2	10^{-4}	.1120E-14	.1120E-14	20.A_{19}	.4272E-5	10^{-4}	.5495E-18	.5495E-18
		10^{-3}	.1120E-13	.1120E-13			10^{-3}	.5495E-17	.5495E-17
		10^{-2}	.1120E-12	.1120E-12			10^{-2}	.5495E-16	.5495E-16
		10^{-1}	.1120E-11	.1120E-11			10^{-1}	.5495E-15	.5495E-15

Param g_j	Rel. sens. $\frac{\partial \kappa_f}{\partial g_j}\frac{g_j^o}{\kappa_f^o}$	$\frac{\Delta g_j}{g_j^o}$	$\kappa_f^{pred} - \kappa_f^o$	$\kappa_f^{recal} - \kappa_f^o$	Param g_j	Rel. Sens. $\frac{\partial \kappa_f}{\partial g_j}\frac{g_j^o}{\kappa_f^o}$	$\frac{\Delta g_j}{g_j^o}$	$\kappa_f^{pred} - \kappa_f^o$	$\kappa_f^{recal} - \kappa_f^o$
21.A_{16}	-.1866E-7	10^{-4}	-.2400E-20	-.2400E-20	23.A_{22}	-.5369E-9	10^{-4}	-.6905E-22	-.6905E-22
		10^{-3}	-.2400E-19	-.2400E-19			10^{-3}	-.6905E-21	-.6905E-21
		10^{-2}	-.2400E-18	-.2400E-18			10^{-2}	-.6905E-20	-.6905E-20
		10^{-1}	-.2400E-17	-.2400E-17			10^{-1}	-.6905E-19	-.6905E-19
22. a_8	-.8097E-8	10^{-4}	-.1041E-20	-.1041E-20	24. a_7	.1227E-11	10^{-4}	.1578E-24	.1578E-24
		10^{-3}	-.1041E-19	-.1041E-19			10^{-3}	.1578E-23	.1578E-23
		10^{-2}	-.1041E-18	-.1041E-18			10^{-2}	.1578E-22	.1578E-22
		10^{-1}	-.1041E-17	-.1041E-17			10^{-1}	.1578E-21	.1578E-21

6 CONCLUSIONS

This work has highlighted the implementation of the deterministic, *local* sensitivity analysis theory originally developed by Cacuci[3-5] for the non-homogeneous, non-equilibrium, one-dimensional two-fluid model in RELAP5/MOD3.2. Particular emphasis has been given to the implementation of the *Adjoint Sensitivity Analysis Procedure (ASAP),* since this procedure is practically the only way to perform a *complete* and *systematic sensitivity analysis* of the reactor plant transients calculated with RELAP5/MOD3.2. Underlying the ASAP are the Differential ASM-REL/TF, which comprises nine coupled differential equations that are *linear in the adjoint function,* and its discrete counterpart, the Discrete ASM-REL/TF, which comprises thirteen *linear coupled algebraic equations* that result from the use of the RELAP5/MOD3.2 time discretization(s) and staggered-mesh spatial discretization procedures. The following fundamental characteristics of the ASAP have been highlighted during its implementation in the RELAP5/MOD3.2 two-fluid model: (a) the adjoint functions are independent of parameter variations; (b) the adjoint functions must be calculated anew for every response; (c) the ASM-REL/TF is linear in the adjoint function and may be solved by methods that are, in principle, independent of those used to solve the original, nonlinear equations; and (d) the adjoint functions depend (nonlinearly, in general) on the base-case solution, which must therefore be available prior to solving the ASM-REL/TF.

This work has also underscored the fundamentally important aspect of *consistency between the differential and the corresponding discretized equations used for sensitivity analysis*. In this context, consistency means that the discretized representation converges to the corresponding differential and/or integral representation in the limit of vanishing spatial mesh- and time-step sizes. Assuming a priori that the original systems of differential equations (in this case, the REL/CDE) had been discretized consistently, the following consistency correspondences must be assured: (i) if the FSAP is used, then the Discretized FSM must be consistent with the Differential FSM; (ii) if the ASAP is used, then the Discretized ASM-REL/TF must be consistent with the Differential ASM-REL/TF; and (iii) the Discretized Response Sensitivity and the Integral Response Sensitivity must be consistent with each other in both the FSAP and the ASAP formulations. If these consistency requirements cannot be naturally fulfilled when deriving the Discretized ASM-REL/TF, then *the differential and/or integral forms* *(i.e., the Differential FSM, ASM-REL/TF, and Integral-Response-representation)* must be used and discretized independently in a consistent manner since it is *the differential/integral forms* that *contain/model physical reality.*

The accuracy and robustness of the solution of the Adjoint Sensitivity Model (ASM-REL/TF) corresponding to the RELAP5/MOD3.2 two-fluid model with non-condensable(s) has been verified by using sample problems involving: (i) liquid-phase only, (ii) gas-phase only, and (iii) two-phase mixture (of water and steam). Thus, the "Two-Loops with Pumps" sample problem supplied with RELAP5/MOD3.2 has been used to verify the accuracy and stability of the numerical solution of the ASM-REL/TF when only the liquid-phase is present. Furthermore, the "Edwards Pipe" sample problem, also supplied with RELAP5/MOD3.2, has been used to verify the accuracy and stability of the numerical solution of the ASM-REL/TF when both (i.e., liquid and gas) phases are present: the particular regimes considered were bubbly, slug, and mist flows. In addition, the accuracy and stability of the numerical solution of the ASM-REL/TF have been verified when only the gas-phase is present by using modified "Two-Loops with Pumps" and the "Edwards Pipe" sample problems, in which the liquid and two-phase fluids, respectively, were replaced by pure steam. The results obtained for all of these sample problems represent typical sensitivities of junction velocities and volume-averaged pressures to perturbations in initial conditions, and indicate that the numerical solution of the ASM-REL/TF is as robust, stable, and accurate as the original RELAP5/MOD3.2 calculations.

The sensitivities of the thermodynamic properties of water to temperature, pressure, and the experimentally-determined parameters that enter in their respective mathematical formulations play an essential role for sensitivity analyses of results calculated by thermal-hydraulic codes, such as RELAP5/MOD3.2, which use water as the working fluid (e.g.,). Such sensitivities are of interest to many applications including, but not limited to, the analysis of light water reactors. Therefore, this work has also presented typical analytical and numerical results for sensitivities of water material properties based on the mathematical formulations listed in the ASME 1993 Steam Tables[12]. Such sensitivities can be used to rank the respective parameters according to their importance, and to assess the effects of nonlinearities on results calculated by the respective code. Furthermore, the sensitivities for the ASME 1993 Steam Tables[12] are expected to indicate priority areas for investigating the new, IAPWS-IF97 formulations[16] for the material properties of water, since these formulations will eventually form the basis for all calculations involving water. More generally, once these sensitivities are available, they can be used for: (a) ranking the importance of parameters as they affect the calculated response; (b) analyzing the effects of parameter variations on the response; (c) performing extensive uncertainty analysis; (d) prioritizing the introduction of improvements in the respective computer code; and (e) eliminating unimportant phenomena for later considerations in a *global* analysis.

Future research could encompass both the analysis of international benchmarks with the RELAP5/PANBOX/COBRA (R/P/C) code system, and the continuing validation of the ASM-REL/TF for the two-fluid model in RELAP5/MOD3.2. Furthermore the coupling of the ASM-REL/TF of RELAP5/MOD3.2 to the corresponding three-dimensional ASM for the neutron kinetics model in PANBOX, when it becomes available within the R/P/C multipurpose code system, would provide an efficient way to perform comprehensive deterministic and statistical sensitivity/uncertainty analyses for reactor transient analysis.

REFERENCES

1. C.J. Jackson, D.G. Cacuci, and H.B. Finnemann, "Dimensionally Adaptive Neutron Kinetics for Multidimensional Reactor Safety Transients. I. New Features of RELAP5/PANBOX", *Nucl. Sci. Eng.*, **131**, 143-163 (1999).

2. C.J. Jackson, D.G. Cacuci, and H.B. Finnemann, "Dimensionally Adaptive Neutron Kinetics for Multidimensional Reactor Safety Transients. II. Dimensionally Adaptive Switching Algorithms", *Nucl. Sci. Eng.*, **131**, 164-186 (1999).

3. D.G. Cacuci, C.F. Weber, E.M. Oblow, and J.H. Marable, "Sensitivity Theory for General Systems of Nonlinear Equations", *Nucl. Sci. Eng.*, **75**, 88-110 (1980).

4. D.G. Cacuci, "Sensitivity Theory for Nonlinear Systems: I. Nonlinear Functional Analysis Approach", *J. Math. Phys.*, **22**, 2794-2802 (1981).

5. D.G. Cacuci, "Sensitivity Theory for Nonlinear Systems: II. Extensions to Additional Classes of Responses", *J. Math. Phys.*, **22**, 2803-2812 (1981).

6. D. G. Cacuci, "Global Optimization and Sensitivity Analysis", *Nucl. Sci. Eng.*, **104**, 78-88 (1990).

7. RELAP5/MOD3 Code Manual, Volume 1: Code Structure, Systems Models, and Solution Methods", NUREG/CR-5535, EGG-2596, Idaho National Engineering Laboratory, Idaho Falls (1995).

8. D.G. Cacuci and E. Wacholder, "Adjoint Sensitivity Analysis for Transient Two-Phase Flow", *Nucl. Sci. Eng.,* **82**, 461-468 (1982).

9. D.G. Cacuci, E. Wacholder, S. Kaizerman, and N. Toomarian, "Adjoint Sensitivity Analysis of a Thermal-Hydraulic System Undergoing Phase Change Due to Boiling Transition", *Trans. Am. Nucl. Soc.,* **46**, 870 (1984).

10. E. Wacholder, S. Kaizerman, N. Toomarian, and D.G. Cacuci, "An Exact Sensitivity Analysis of a Simplified Transient Two-Phase Flow Problem", *Nucl. Sci. Eng.,* **89**, 1-35 (1985).

11. A. Ounsy, B. Brun and F. de Crecy, “The Adjoint Sensitivity Method, a Contribution to the Code Uncertainty Evaluation”, *Nucl. Eng. and Des.*, 149, 357-364 (1994).

12. ASME Steam Tables, 1993. Thermodynamic and Transport Properties of Steam. 6th Edition, The American Society of Mechanical Engineers, New York, 1993.

13. M. B. Monagan et al., *MAPLE V Programming Guide*, Springer Verlag, New York (1996).

14. P. N. Brown, A. C. Hindmarsh, “Reduced Storage Matrix Methods in Stiff ODE Systems”, Lawrence Livermore National Laboratory Report UCRL-95088, Rev. 1, Livermore, California, June 1987.

15. Y. Ronen, “Uncertainty Analysis”, in *Uncertainty Analysis*, Y. RONEN (Ed.), CRC Press, Boca Raton, Florida, 41-69 (1988).

16. W. Wagner and A. Kruze, *Properties of Water and Steam: The Industrial Standard IAPWS-IF97 for the Thermodynamic Properties and Supplementary Equations for Other Properties*, Springer-Verlag, Berlin (1998).

17. I. S. Duff, “Permutation for a zero-free diagonal”, ACM Transactions on Mathematical Software 7, 387-390 (1981).

18. B. N. Parlett and C. Reinsch, “Balancing a Matrix for Calculation of Eigenvalues and Eigenvectors”, *Handbook for Automatic Computation*, F. L. Bauer (Ed.), Springer Verlag, Berlin, 315-326 (1971).

APPENDIX A: THE RELAP5/MOD3.2 DISCRETIZED SET OF "NUMERICALLY CONVENIENT DIFFEREN-TIAL EQUATIONS"

The components of the matrix $\underline{\underline{A}}$ introduced in Eq. (2.13) are defined as follows:

$$A_{11} = \alpha_g \left(X_n \frac{\partial \rho_g}{\partial X_n} + \rho_g \right), \quad A_{12} = \alpha_g X_n \frac{\partial \rho_g}{\partial U_g}, \quad A_{14} = \rho_g X_n, \quad A_{15} = \alpha_g X_n \frac{\partial \rho_g}{\partial P},$$

$$A_{21} = \alpha_g U_g \frac{\partial \rho_g}{\partial X_n} + \left(\frac{h_f^*}{h_g^* - h_f^*} \right) \Delta t \frac{P_s}{P} H_{ig} \left(\frac{\partial T^s}{\partial X_n} - \frac{\partial T_g}{\partial X_n} \right) + \left(\frac{h_g^*}{h_g^* - h_f^*} \right) \Delta t H_{if} \frac{\partial T^s}{\partial X_n} + \Delta t \frac{P - P_s}{P} H_{gf} \frac{\partial T_g}{\partial X_n},$$

$$A_{22} = \alpha_g U_g \frac{\partial \rho_g}{\partial U_g} + \left(\frac{h_f^*}{h_g^* - h_f^*} \right) \Delta t \frac{P_s}{P} H_{ig} \left(\frac{\partial T^s}{\partial U_g} - \frac{\partial T_g}{\partial U_g} \right) + \left(\frac{h_g^*}{h_g^* - h_f^*} \right) \Delta t H_{if} \frac{\partial T^s}{\partial U_g} + \Delta t \frac{P - P_s}{P} H_{gf} \frac{\partial T_g}{\partial U_g},$$

$$A_{23} = -\left(\frac{h_g^*}{h_g^* - h_f^*} \right) \Delta t H_{if} \frac{\partial T_f}{\partial U_f} - \Delta t \frac{P - P_s}{P} H_{gf} \frac{\partial T_f}{\partial U_f}, \quad A_{24} = \rho_g U_g + P,$$

$$A_{25} = \alpha_g U_g \frac{\partial \rho_g}{\partial P} + \left(\frac{h_f^*}{h_g^* - h_f^*} \right) \Delta t \frac{P_s}{P} H_{ig} \left(\frac{\partial T^s}{\partial P} - \frac{\partial T_g}{\partial P} \right) + \left(\frac{h_g^*}{h_g^* - h_f^*} \right) \Delta t H_{if} \frac{\partial T^s}{\partial P} + \Delta t \frac{P - P_s}{P} H_{gf} \left(\frac{\partial T_g}{\partial P} - \frac{\partial T_f}{\partial P} \right),$$

$$A_{31} = -\left(\frac{h_f^*}{h_g^* - h_f^*} \right) \Delta t \frac{P_s}{P} H_{ig} \left(\frac{\partial T^s}{\partial X_n} - \frac{\partial T_g}{\partial X_n} \right) - \left(\frac{h_g^*}{h_g^* - h_f^*} \right) \Delta t H_{if} \frac{\partial T^s}{\partial X_n} - \Delta t \frac{P - P_s}{P} H_{gf} \frac{\partial T_g}{\partial X_n},$$

$$A_{32} = -\left(\frac{h_f^*}{h_g^* - h_f^*} \right) \Delta t \frac{P_s}{P} H_{ig} \left(\frac{\partial T^s}{\partial U_g} - \frac{\partial T_g}{\partial U_g} \right) - \left(\frac{h_g^*}{h_g^* - h_f^*} \right) \Delta t H_{if} \frac{\partial T^s}{\partial U_g} - \Delta t \frac{P - P_s}{P} H_{gf} \frac{\partial T_g}{\partial U_g},$$

$$A_{33} = \alpha_f \left(U_f \frac{\partial \rho_f}{\partial U_f} + \rho_f \right) + \left(\frac{h_g^*}{h_g^* - h_f^*} \right) \Delta t H_{if} \frac{\partial T_f}{\partial U_f} + \Delta t \frac{P - P_s}{P} H_{gf} \frac{\partial T_f}{\partial U_f}, \quad A_{34} = -\rho_f U_f - P,$$

$$A_{35} = \alpha_f U_f \frac{\partial \rho_f}{\partial P} - \left(\frac{h_f^*}{h_g^* - h_f^*} \right) \Delta t \frac{P_s}{P} H_{ig} \left(\frac{\partial T^s}{\partial P} - \frac{\partial T_g}{\partial P} \right) - \left(\frac{h_g^*}{h_g^* - h_f^*} \right) \Delta t H_{if} \frac{\partial T^s}{\partial P} - \Delta t \frac{P - P_s}{P} H_{gf} \left(\frac{\partial T_g}{\partial P} - \frac{\partial T_f}{\partial P} \right),$$

$$A_{41} = \alpha_g \frac{\partial \rho_g}{\partial X_n} + \left(\frac{2}{h_g^* - h_f^*} \right) \Delta t \frac{P_s}{P} H_{ig} \left(\frac{\partial T^s}{\partial X_n} - \frac{\partial T_g}{\partial X_n} \right) + \left(\frac{2}{h_g^* - h_f^*} \right) \Delta t H_{if} \frac{\partial T^s}{\partial X_n},$$

$$A_{42} = \alpha_g \frac{\partial \rho_g}{\partial U_g} + \left(\frac{2}{h_g^* - h_f^*}\right)\Delta t \frac{P_s}{P} H_{ig}\left(\frac{\partial T^s}{\partial U_g} - \frac{\partial T_g}{\partial U_g}\right) + \left(\frac{2}{h_g^* - h_f^*}\right)\Delta t H_{if} \frac{\partial T^s}{\partial U_g},$$

$$A_{43} = -\alpha_f \frac{\partial \rho_f}{\partial U_f} - \left(\frac{2}{h_g^* - h_f^*}\right)\Delta t H_{if} \frac{\partial T_f}{\partial U_f}, \quad A_{44} = \rho_g + \rho_f,$$

$$A_{45} = \alpha_g \frac{\partial \rho_g}{\partial P} - \alpha_f \frac{\partial \rho_f}{\partial P} + \left(\frac{2}{h_g^* - h_f^*}\right)\Delta t \frac{P_s}{P} H_{ig}\left(\frac{\partial T^s}{\partial P} - \frac{\partial T_g}{\partial P}\right) + \left(\frac{2}{h_g^* - h_f^*}\right)\Delta t H_{if} \frac{\partial T^s}{\partial P},$$

$$A_{51} = \alpha_g \frac{\partial \rho_g}{\partial X_n}, \quad A_{52} = \alpha_g \frac{\partial \rho_g}{\partial U_g}, \quad A_{53} = \alpha_f \frac{\partial \rho_f}{\partial U_f}, \quad A_{54} = \rho_g - \rho_f, \quad A_{55} = \alpha_g \frac{\partial \rho_g}{\partial P} + \alpha_f \frac{\partial \rho_f}{\partial P},$$

The components of the vector $\underline{b}$ introduced in Eq. (2.13) are defined as follows:

$$b_2 = -\left(\frac{h_f^*}{h_g^* - h_f^*}\right)\Delta t \frac{P_s}{P} H_{ig}\left(T^s - T_g\right) - \left(\frac{h_g^*}{h_g^* - h_f^*}\right)\Delta t H_{if}\left(T^s - T_f\right) - \Delta t \frac{P - P_s}{P} H_{gf}\left(T_g - T_f\right)$$
$$+ \Delta t \Gamma_w \left[\left(\frac{1-\varepsilon}{2}\right)h_f' + \left(\frac{1+\varepsilon}{2}\right)h_g'\right] + Q_{wg}\Delta t + DISS_g \Delta t,$$

$$b_3 = \left(\frac{h_f^*}{h_g^* - h_f^*}\right)\Delta t \frac{P_s}{P} H_{ig}\left(T^s - T_g\right) + \left(\frac{h_g^*}{h_g^* - h_f^*}\right)\Delta t H_{if}\left(T^s - T_f\right) + \Delta t \frac{P - P_s}{P} H_{gf}\left(T_g - T_f\right)$$
$$- \Delta t \Gamma_w \left[\left(\frac{1-\varepsilon}{2}\right)h_f' + \left(\frac{1+\varepsilon}{2}\right)h_g'\right] + Q_{wf}\Delta t + DISS_f \Delta t,$$

$$b_4 = -\left(\frac{2}{h_g^* - h_f^*}\right)\Delta t \frac{P_s}{P} H_{ig}\left(T^s - T_g\right) - \left(\frac{2}{h_g^* - h_f^*}\right)\Delta t H_{if}\left(T^s - T_f\right) + 2\Delta t \Gamma_w .$$

The components of the vectors $\underline{f}^1, \underline{f}^2, \underline{g}^1, \underline{g}^2$ introduced in Eq. (2.13) are defined below:

$$f_3^1 = -\left[\dot{\alpha}_{f,j+1}\left(\dot{\rho}_{f,j+1}\dot{U}_{f,j+1} + P_L\right)A_{j+1}\right]\Delta t / V, \quad f_4^1 = \left(\dot{\alpha}_f \dot{\rho}_f A\right)_{j+1}\Delta t / V, \quad f_5^1 = -\left(\dot{\alpha}_f \dot{\rho}_f A\right)_{j+1}\Delta t / V;$$

$$f_3^2 = \left[\dot{\alpha}_{f,j}\left(\dot{\rho}_{f,j}\dot{U}_{f,j} + P_L\right)A_j\right]\Delta t/V, \quad f_4^2 = -\left(\dot{\alpha}_f\dot{\rho}_f A\right)_j \Delta t/V, \quad f_5^2 = \left(\dot{\alpha}_f\dot{\rho}_f A\right)_j \Delta t/V;$$

$$g_1^1 = -\left(\dot{\alpha}_g\dot{\rho}_g\dot{X}_n A\right)_{j+1}\Delta t/V, \quad g_2^1 = -\left[\dot{\alpha}_{g,j+1}\left(\dot{\rho}_{g,j+1}\dot{U}_{g,j+1} + P_L\right)A_{j+1}\right]\Delta t/V, \quad g_4^1 = g_5^1 = -\left(\dot{\alpha}_g\dot{\rho}_g A\right)_{j+1}\Delta t/V;$$

$$g_1^2 = \left(\dot{\alpha}_g\dot{\rho}_g\dot{X}_n A\right)_j \Delta t/V, \quad g_2^2 = \left[\dot{\alpha}_{g,j}\left(\dot{\rho}_{g,j}\dot{U}_{g,j} + P_L\right)A_j\right]\Delta t/V, \quad g_4^2 = g_5^2 = \left(\dot{\alpha}_g\dot{\rho}_g A\right)_j \Delta t/V.$$

The fluid specific internal energy, $\left(U_f\right)_L^{n+1}$, is calculated for a volume L at time-step (n+1) by using the following sequence of three operations: (i) The non-expanded liquid energy equation, which reads

$$\begin{aligned}
&V_L\left[\left(\alpha_f\rho_f U_f\right)_L^{n+1} - \left(\alpha_f\rho_f U_f\right)_L^n\right] + \left[\dot{\alpha}_{f,j+1}\left(\dot{\rho}_{f,j+1}\dot{U}_{f,j+1} + P_L\right)v_{f,j+1}^{n+1}A_{j+1} - \dot{\alpha}_{f,j}\left(\dot{\rho}_{f,j}\dot{U}_{f,j} + P_L\right)v_{f,j}^{n+1}A_j\right]\Delta t \\
&= V_L P_L^n\left(\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n\right) + \left\{\left(\frac{h_f^*}{h_g^* - h_f^*}\right)_L^n \frac{P_{s,L}^n}{P_L^n} H_{ig,L}^n\left(\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}\right) + \left(\frac{h_g^*}{h_g^* - h_f^*}\right)_L^n H_{if,L}^n\left(\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1}\right)\right. \\
&\left. + \frac{P_L^n - P_{s,L}^n}{P_L^n} H_{gf,L}^n\left(\tilde{T}_{g,L}^{n+1} - \tilde{T}_{f,L}^{n+1}\right) - \Gamma_{w,L}^n\left[\left(\frac{1-\varepsilon}{2}\right)\left(h'_{f,L}\right)^n + \left(\frac{1+\varepsilon}{2}\right)\left(h'_{g,L}\right)^n\right] + Q_{wf,L}^n + DISS_{f,L}^n\right\} V_L\Delta t,
\end{aligned}$$

is solved to obtain $\left(\alpha_f\rho_f U_f\right)_L^{n+1}$; (ii) the non-expanded liquid density equation, which reads

$$\begin{aligned}
&V_L\left[\left(\alpha_f\rho_f\right)_L^{n+1} - \left(\alpha_f\rho_f\right)_L^n\right] + \left(\dot{\alpha}_{f,j+1}\dot{\rho}_{f,j+1}v_{f,j+1}^{n+1}A_{j+1} - \dot{\alpha}_{f,j}\dot{\rho}_{f,j}v_{f,j}^{n+1}A_j\right)\Delta t \\
&= \left(\frac{\dfrac{P_{s,L}^n}{P_L^n} H_{ig,L}^n\left(\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}\right) + H_{if,L}^n\left(\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1}\right)}{\left(h'_{g,L}\right)^n - \left(h'_{f,L}\right)^n} - \Gamma_{w,L}^n\right) V_L\Delta t,
\end{aligned}$$

is solved to obtain $\left(\alpha_f\rho_f\right)_k^{n+1}$; and (iii) the ratio of the results obtained in steps (i) and (ii), respectively, is calculated to obtain $\left(U_f\right)_L^{n+1} = \left(\alpha_f\rho_f U_f\right)_L^{n+1}/\left(\alpha_f\rho_f\right)_L^{n+1}$.

The total non-condensable mass fraction, $(X_n)_L^{n+1}$ for volume L at time-step (n+1) is calculated by first solving the non-expanded total non-condensable density equation

$$V_L\left[(\alpha_g\rho_g X_n)_L^{n+1} - (\alpha_g\rho_g X_n)_L^{n}\right] + \left(\dot{\alpha}_{g,j+1}\dot{\rho}_{g,j+1}\dot{X}_{n,j+1}^{n} v_{g,j+1}^{n+1} A_{j+1} - \dot{\alpha}_{g,j}\dot{\rho}_{g,j}\dot{X}_{n,j}^{n} v_{g,j}^{n+1} A_j\right)\Delta t = 0,$$

to obtain $(\alpha_g\rho_g X_n)_L^{n+1}$, and then calculating directly $(X_n)_L^{n+1} = (\alpha_g\rho_g X_n)_L^{n+1} / (\alpha_g\rho_g)_L^{n+1}$ by using the previously calculated value of $(\alpha_g\rho_g)_L^{n+1}$.

The gas void fraction, $(\alpha_g)_L^{n+1}$, for a volume L at time-step (n+1), is calculated as follows:

$$(\alpha_g)_L^{n+1} = 1 - \alpha_{f,L}^{n+1} = 1 - \frac{(\alpha_f\rho_f)_L^{n+1}}{\hat{\rho}_{f,L}^{n+1}}, \quad \text{where}$$

$$\hat{\rho}_{f,L}^{n+1} \equiv \rho_{f,L}^{n} + \left(\frac{\partial\rho_f}{\partial P}\right)_L^n \left(P_L^{n+1} - P_L^n\right) + \left(\frac{\partial\rho_f}{\partial U_f}\right)_L^n \left(U_{f,L}^{n+1} - U_{f,L}^n\right).$$

The non-condensable mass fraction for the i-th non-condensable species, $(X_{ni})_L^{n+1}$, for volume L at time-step (n+1) is calculated by first solving the non-expanded equation for the individual non-condensable density

$$\begin{aligned} &V_L\left[(\alpha_g\rho_g X_n X_{ni})_L^{n+1} - (\alpha_g\rho_g X_n X_{ni})_L^{n}\right] \\ &+ \left(\dot{\alpha}_{g,j+1}\dot{\rho}_{g,j+1}\dot{X}_{n,j+1}^{n}\dot{X}_{ni,j+1}^{n} v_{g,j+1}^{n+1} A_{j+1} - \dot{\alpha}_{g,j}\dot{\rho}_{g,j}\dot{X}_{n,j}^{n}\dot{X}_{ni,j}^{n} v_{g,j}^{n+1} A_j\right)\Delta t = 0, \end{aligned}$$

to obtain $(\alpha_g\rho_g X_n X_{ni})_L^{n+1}$, and then by using the previously calculated quantity $(\alpha_g\rho_g X_n)_L^{n+1}$ to obtain $(X_{ni})_L^{n+1} = (\alpha_g\rho_g X_n X_{ni})_L^{n+1} / (\alpha_g\rho_g X_n)_L^{n+1}$.

APPENDIX B: COEFFICIENTS IN THE EQUATIONS COMPRISING THE FSM

Taking the G-derivative of the vapor energy equation yields the following expressions for the components $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$:

$$S_{11}(x,t) \equiv \alpha_g^o \rho_g^o + \alpha_g^o U_g^o \left(\frac{\partial \rho_g}{\partial U_g} \right)_o, \quad T_{11}(x,t) \equiv \alpha_g^o U_g^o v_g^o \left(\frac{\partial \rho_g}{\partial U_g} \right)_o + \alpha_g^o \rho_g^o v_g^o, \quad U_{11}(x,t) \equiv -\left(\frac{\partial E_1}{\partial U_g} \right)_o,$$

$$S_{12}(x,t) \equiv 0, \quad T_{12}(x,t) \equiv 0, \quad U_{12}(x,t) \equiv -\left(\frac{\partial E_1}{\partial U_f} \right)_o,$$

$$S_{13}(x,t) \equiv \alpha_g^o U_g^o \left(\frac{\partial \rho_g}{\partial P} \right)_o, \quad T_{13}(x,t) \equiv \alpha_g^o U_g^o v_g^o \left(\frac{\partial \rho_g}{\partial P} \right)_o, \quad U_{13}(x,t) \equiv \frac{\partial \rho_g^o}{\partial t} + \frac{1}{A^o} \frac{\partial}{\partial x} \left(\alpha_g^o v_g^o A^o \right) - \left(\frac{\partial E_1}{\partial P} \right)_o,$$

$$S_{14}(x,t) \equiv \rho_g^o U_g^o + P^o, \quad T_{14}(x,t) \equiv \rho_g^o v_g^o U_g^o + P^o v_g^o, \quad U_{14}(x,t) \equiv -\frac{\partial P^o}{\partial t} - \left(\frac{\partial E_1}{\partial \alpha_g} \right)_o - v_g^o \frac{\partial P^o}{\partial x},$$

$$S_{15}(x,t) \equiv \alpha_g^o U_g^o \left(\frac{\partial \rho_g}{\partial X_n} \right)_o, \quad T_{15}(x,t) \equiv \alpha_g^o U_g^o v_g^o \left(\frac{\partial \rho_g}{\partial X_n} \right)_o, \quad U_{15}(x,t) \equiv -\left(\frac{\partial E_1}{\partial X_n} \right)_o,$$

$$S_{18}(x,t) \equiv 0, \quad T_{18}(x,t) \equiv \alpha_g^o \left(\rho_g^o U_g^o + P^o \right), \quad U_{18}(x,t) \equiv -\alpha_g^o \frac{\partial P^o}{\partial x} - \left(\frac{\partial E_1}{\partial v_g} \right)_o,$$

$$S_{19}(x,t) \equiv 0, \quad T_{19}(x,t) \equiv 0, \quad U_{19}(x,t) \equiv -\left(\frac{\partial E_1}{\partial v_f} \right)_o,$$

and where the quantity $E_1(\underline{\chi},\underline{G})$ is defined as

$$E_1(\underline{\chi},\underline{G}) \equiv -\left(\frac{h'_f}{h'_g - h'_f}\right) H_{ig}\left(T^s - T_g\right) - \left(\frac{h'_g}{h'_g - h'_f}\right) H_{if}\left(T^s - T_f\right)$$

$$-\frac{P - P_s}{P} H_{gf}\left(T_g - T_f\right) + \left[\left(\frac{1+\varepsilon}{2}\right) h_g^s + \left(\frac{1-\varepsilon}{2}\right) h_f^s\right]\Gamma_w + Q_{wg} + DISS_g .$$

Taking the G-derivative of the liquid energy equation yields the following expressions for the components $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$:

$$S_{21}(x,t) \equiv 0, \quad T_{21}(x,t) \equiv 0, \quad U_{21}(x,t) \equiv -\left(\frac{\partial E_2}{\partial U_g}\right)_o ,$$

$$S_{22}(x,t) \equiv \alpha_f^o\left(\rho_f^o + U_f^o\left(\frac{\partial \rho_f}{\partial U_f}\right)_o\right), \quad T_{22}(x,t) \equiv \alpha_f^o v_f^o\left(\rho_f^o + U_f^o\left(\frac{\partial \rho_f}{\partial U_f}\right)_o\right), \quad U_{22}(x,t) \equiv -\left(\frac{\partial E_2}{\partial U_f}\right)_o ,$$

$$S_{23}(x,t) \equiv \alpha_f^o U_f^o\left(\frac{\partial \rho_f}{\partial P}\right)_o , \quad T_{23}(x,t) \equiv \alpha_f^o v_f^o U_f^o\left(\frac{\partial \rho_f}{\partial P}\right)_o , \quad U_{23}(x,t) \equiv \frac{\partial \alpha_f}{\partial t} + \frac{1}{A^o}\frac{\partial}{\partial x}\left(\alpha_f^o v_f^o A^o\right) - \left(\frac{\partial E_2}{\partial P}\right)_o ,$$

$$S_{24}(x,t) \equiv -\left(\rho_f^o U_f^o + P^o\right), \quad T_{24}(x,t) \equiv -v_f^o\left(\rho_f^o U_f^o + P^o\right), \quad U_{24}(x,t) \equiv -\left(\frac{\partial E_2}{\partial \alpha_g}\right)_o + \frac{\partial P^o}{\partial t} + v_f^o \frac{\partial P^o}{\partial x},$$

$$S_{25}(x,t) \equiv 0, \quad T_{25}(x,t) \equiv 0, \quad U_{25}(x,t) \equiv -\left(\frac{\partial E_2}{\partial X_n}\right)_o ,$$

$$S_{28}(x,t) \equiv 0, \quad T_{28}(x,t) \equiv 0, \quad U_{28}(x,t) \equiv -\left(\frac{\partial E_2}{\partial v_g}\right)_o ,$$

$$S_{29}(x,t) \equiv 0, \quad T_{29}(x,t) \equiv \alpha_f^o\left(\rho_f^o U_f^o + P^o\right), \quad U_{29}(x,t) \equiv -\alpha_f^o \frac{\partial P^o}{\partial x} - \left(\frac{\partial E_2}{\partial v_f}\right)_o ,$$

and where the quantity $E_2(\underline{\chi},\underline{G})$ is defined as

$$E_2(\underline{\chi},\underline{G}) \equiv \left(\frac{h'_f}{h'_g - h'_f}\right) H_{ig}\left(T^s - T_g\right) + \left(\frac{h'_g}{h'_g - h'_f}\right) H_{if}\left(T^s - T_f\right)$$
$$+ \frac{P - P_s}{P} H_{gf}\left(T_g - T_f\right) - \left[\left(\frac{1+\varepsilon}{2}\right) h_g^s + \left(\frac{1-\varepsilon}{2}\right) h_f^s\right]\Gamma_w + Q_{wf} + DISS_f .$$

Taking the G-derivative of the sum density equation yields the following expressions for the components $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$:

$$S_{31}(x,t) \equiv \alpha_g^o \left(\frac{\partial \rho_g}{\partial U_g}\right)_o , \quad T_{31}(x,t) \equiv \alpha_g^o v_g^o \left(\frac{\partial \rho_g}{\partial U_g}\right)_o , \quad U_{31}(x,t) \equiv 0,$$

$$S_{32}(x,t) \equiv \alpha_f^o \left(\frac{\partial \rho_f}{\partial U_f}\right)_o , \quad T_{32}(x,t) \equiv \alpha_f^o v_f^o \left(\frac{\partial \rho_f}{\partial U_f}\right)_o , \quad U_{32}(x,t) \equiv 0,$$

$$S_{33}(x,t) \equiv \alpha_g^o \left(\frac{\partial \rho_g}{\partial P}\right)_o + \alpha_f^o \left(\frac{\partial \rho_f}{\partial P}\right)_o , \quad T_{33}(x,t) \equiv \alpha_g^o v_g^o \left(\frac{\partial \rho_g}{\partial P}\right)_o + \alpha_f^o v_f^o \left(\frac{\partial \rho_f}{\partial P}\right)_o , \quad U_{33}(x,t) \equiv 0,$$

$$S_{34}(x,t) \equiv \rho_g^o - \rho_f^o , \quad T_{34}(x,t) \equiv \rho_g^o v_g^o - \rho_f^o v_f^o , \quad U_{34}(x,t) \equiv 0,$$

$$S_{35}(x,t) \equiv \alpha_g^o \left(\frac{\partial \rho_g}{\partial X_n}\right)_o , \quad T_{35}(x,t) \equiv \alpha_g^o v_g^o \left(\frac{\partial \rho_g}{\partial X_n}\right)_o , \quad U_{35}(x,t) \equiv 0,$$

$$S_{38}(x,t) \equiv 0, \quad T_{38}(x,t) \equiv \alpha_g^o \rho_g^o , \quad U_{38}(x,t) \equiv 0,$$

$$S_{39}(x,t) \equiv 0, \quad T_{39}(x,t) \equiv \alpha_f^o \rho_f^o, \quad U_{39}(x,t) \equiv 0,$$

Taking the G-derivative of the difference density equation gives the following expressions for the components $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$:

$$S_{41}(x,t) \equiv \alpha_g^o \left(\frac{\partial \rho_g}{\partial U_g} \right)_o, \quad T_{41}(x,t) \equiv \alpha_g^o v_g^o \left(\frac{\partial \rho_g}{\partial U_g} \right)_o, \quad U_{41}(x,t) \equiv -\left(\frac{\partial E_4}{\partial U_g} \right)_o,$$

$$S_{42}(x,t) \equiv -\alpha_f^o \left(\frac{\partial \rho_f}{\partial U_f} \right)_o, \quad T_{42}(x,t) \equiv -\alpha_f^o v_f^o \left(\frac{\partial \rho_f}{\partial U_f} \right)_o, \quad U_{42}(x,t) \equiv -\left(\frac{\partial E_4}{\partial U_f} \right)_o,$$

$$S_{43}(x,t) \equiv \alpha_g^o \left(\frac{\partial \rho_g}{\partial P} \right)_o - \alpha_f^o \left(\frac{\partial \rho_f}{\partial P} \right)_o, \quad T_{43}(x,t) \equiv \alpha_g^o v_g^o \left(\frac{\partial \rho_g}{\partial P} \right)_o - \alpha_f^o v_f^o \left(\frac{\partial \rho_f}{\partial P} \right)_o, \quad U_{43}(x,t) \equiv -\left(\frac{\partial E_4}{\partial P} \right)_o,$$

$$S_{44}(x,t) \equiv \rho_f^o + \rho_g^o, \quad T_{44}(x,t) \equiv \rho_g^o v_g^o + \rho_f^o v_f^o, \quad U_{44}(x,t) \equiv -\left(\frac{\partial E_4}{\partial \alpha_g} \right)_o,$$

$$S_{45}(x,t) \equiv \alpha_g^o \left(\frac{\partial \rho_g}{\partial X_n} \right)_o, \quad T_{45}(x,t) \equiv \alpha_g^o v_g^o \left(\frac{\partial \rho_g}{\partial X_n} \right)_o, \quad U_{45}(x,t) \equiv -\left(\frac{\partial E_4}{\partial X_n} \right)_o,$$

$$S_{48}(x,t) \equiv 0, \quad T_{48}(x,t) \equiv \alpha_g^o \rho_g^o, \quad U_{48}(x,t) \equiv -\left(\frac{\partial E_4}{\partial v_g} \right)_o,$$

$$S_{49}(x,t) \equiv 0, \quad T_{49}(x,t) \equiv -\alpha_f^o \rho_f^o, \quad U_{49}(x,t) \equiv -\left(\frac{\partial E_4}{\partial v_f} \right)_o,$$

and where the quantity $E_4(\underline{\chi}, \underline{G})$ is defined as

$$E_4(\underline{\chi},\underline{G}) \equiv -\frac{2\left[H_{ig}\left(T^s - T_g\right) + H_{if}\left(T^s - T_f\right)\right]}{h'_g - h'_f} + 2\Gamma_w .$$

Taking the G-derivative of the non-condensable density equation gives the following expressions for the components $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$:

$$S_{51}(x,t) \equiv \alpha_g^o X_n^o \left(\frac{\partial \rho_g}{\partial U_g}\right)_o , \quad T_{51}(x,t) \equiv \alpha_g^o X_n^o v_g^o \left(\frac{\partial \rho_g}{\partial U_g}\right)_o , \quad U_{51}(x,t) \equiv 0,$$

$$S_{52}(x,t) \equiv 0, \quad T_{52}(x,t) \equiv 0, \quad U_{52}(x,t) \equiv 0,$$

$$S_{53}(x,t) \equiv \alpha_g^o X_n^o \left(\frac{\partial \rho_g}{\partial P}\right)_o , \quad T_{53}(x,t) \equiv \alpha_g^o v_g^o X_n^o \left(\frac{\partial \rho_g}{\partial P}\right)_o , \quad U_{53}(x,t) \equiv 0,$$

$$S_{54}(x,t) \equiv \rho_g^o X_n^o, \quad T_{54}(x,t) \equiv \rho_g^o X_n^o v_g^o, \quad U_{54}(x,t) \equiv 0,$$

$$S_{55}(x,t) \equiv \alpha_g^o \rho_g^o + \alpha_g^o X_n^o \left(\frac{\partial \rho_g}{\partial X_n}\right)_o , \quad T_{55}(x,t) \equiv \alpha_g^o v_g^o \left(\rho_g^o + X_n^o \left(\frac{\partial \rho_g}{\partial X_n}\right)_o\right), \quad U_{55}(x,t) \equiv 0,$$

$$S_{58}(x,t) \equiv 0, \quad T_{58}(x,t) \equiv \alpha_g^o \rho_g^o X_n^o, \quad U_{58}(x,t) \equiv 0,$$

$$S_{59}(x,t) \equiv 0, \quad T_{59}(x,t) \equiv 0, \quad U_{59}(x,t) \equiv 0.$$

Taking the G-derivative of the mass conservation equation for each non-condensable component gives the following expressions for the components $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$:

$$S_{61}(x,t) \equiv \alpha_g^o X_n^o X_{ni}^o \left(\frac{\partial \rho_g}{\partial U_g} \right)_o, \quad T_{61}(x,t) \equiv \alpha_g^o X_n^o X_{ni}^o v_g^o \left(\frac{\partial \rho_g}{\partial U_g} \right)_o, \quad U_{61}(x,t) \equiv 0,$$

$$S_{62}(x,t) \equiv 0, \quad T_{62}(x,t) \equiv 0, \quad U_{62}(x,t) \equiv 0,$$

$$S_{63}(x,t) \equiv \alpha_g^o X_n^o X_{ni}^o \left(\frac{\partial \rho_g}{\partial P} \right)_o, \quad T_{63}(x,t) \equiv \alpha_g^o v_g^o X_n^o X_{ni}^o \left(\frac{\partial \rho_g}{\partial P} \right)_o, \quad U_{63}(x,t) \equiv 0,$$

$$S_{64}(x,t) \equiv \rho_g^o X_n^o X_{ni}^o, \quad T_{64}(x,t) \equiv \rho_g^o X_n^o X_{ni}^o v_g^o, \quad U_{64}(x,t) \equiv 0,$$

$$S_{65}(x,t) \equiv \alpha_g^o X_{ni}^o \left(\rho_g^o + X_n^o \left(\frac{\partial \rho_g}{\partial X_n} \right)_o \right), \quad T_{65}(x,t) \equiv \alpha_g^o v_g^o X_{ni}^o \left(\rho_g^o + X_n^o \left(\frac{\partial \rho_g}{\partial X_n} \right)_o \right), \quad U_{65}(x,t) \equiv 0,$$

$$S_{66}(x,t) \equiv \alpha_g^o \rho_g^o X_n^o, \quad T_{66}(x,t) \equiv \alpha_g^o \rho_g^o v_g^o X_n^o, \quad U_{66}(x,t) \equiv 0,$$

$$S_{68}(x,t) \equiv 0, \quad T_{68}(x,t) \equiv \alpha_g^o \rho_g^o X_n^o X_{ni}^o, \quad U_{68}(x,t) \equiv 0,$$

$$S_{69}(x,t) \equiv 0, \quad T_{69}(x,t) \equiv 0, \quad U_{69}(x,t) \equiv 0.$$

Taking the G-derivative of the boron density equation yields the following expressions for the components $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$:

$$S_{71}(x,t) \equiv 0, \quad T_{71}(x,t) \equiv 0, \quad U_{71}(x,t) \equiv 0,$$

$$S_{72}(x,t) \equiv 0, \quad T_{72}(x,t) \equiv 0, \quad U_{72}(x,t) \equiv 0,$$

$$S_{73}(x,t) \equiv 0, \quad T_{73}(x,t) \equiv 0, \quad U_{73}(x,t) \equiv 0,$$

$$S_{74}(x,t) \equiv 0, \quad T_{74}(x,t) \equiv 0, \quad U_{74}(x,t) \equiv 0,$$

$$S_{75}(x,t) \equiv 0, \quad T_{75}(x,t) \equiv 0, \quad U_{75}(x,t) \equiv 0,$$

$$S_{76}(x,t) \equiv 0, \quad T_{76}(x,t) \equiv 0, \quad U_{76}(x,t) \equiv 0,$$

$$S_{77}(x,t) \equiv 1, \quad T_{77}(x,t) \equiv v_f^o, \quad U_{77}(x,t) \equiv 0,$$

$$S_{78}(x,t) \equiv 0, \quad T_{78}(x,t) \equiv 0, \quad U_{78}(x,t) \equiv 0,$$

$$S_{79}(x,t) \equiv 0, \quad T_{79}(x,t) \equiv \rho_b^o, \quad U_{79}(x,t) \equiv 0.$$

Taking the G-derivative of the sum momentum equation gives the following expressions for the components $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$:

$$S_{81}(x,t) \equiv 0, \quad T_{81}(x,t) \equiv 0, \quad U_{81}(x,t) \equiv \alpha_g^o \left(\frac{\partial v_g^o}{\partial t} + \frac{1}{2} \frac{\partial \left(v_g^o\right)^2}{\partial x} \right) \left(\frac{\partial \rho_g}{\partial U_g} \right)_o - \left(\frac{\partial E_8}{\partial U_g} \right)_o,$$

$$S_{85}(x,t) \equiv 0, \quad T_{85}(x,t) \equiv 0, \quad U_{85}(x,t) \equiv \alpha_g^o \left(\frac{\partial v_g^o}{\partial t} + \frac{1}{2} \frac{\partial \left(v_g^o\right)^2}{\partial x} \right) \left(\frac{\partial \rho_g}{\partial X_n} \right)_o - \left(\frac{\partial E_8}{\partial X_n} \right)_o,$$

$$S_{83}(x,t) \equiv 0, \quad T_{83}(x,t) \equiv 1,$$

$$U_{83}(x,t) \equiv -\frac{1}{A^o}\frac{dA^o}{dx} + \alpha_g^o\left(\frac{\partial v_g^o}{\partial t} + \frac{1}{2}\frac{\partial (v_g^o)^2}{\partial x}\right)\left(\frac{\partial \rho_g}{\partial P}\right)_o + \alpha_f^o\left(\frac{\partial v_f^o}{\partial t} + \frac{1}{2}\frac{\partial (v_f^o)^2}{\partial x}\right)\left(\frac{\partial \rho_f}{\partial P}\right)_o - \left(\frac{\partial E_8}{\partial P}\right)_o,$$

$$S_{84}(x,t) \equiv 0, \quad T_{84}(x,t) \equiv 0, \quad U_{84}(x,t) \equiv \rho_g^o\left(\frac{\partial v_g^o}{\partial t} + \frac{1}{2}\frac{\partial (v_g^o)^2}{\partial x}\right) - -\rho_f^o\left(\frac{\partial v_f^o}{\partial t} + \frac{1}{2}\frac{\partial (v_f^o)^2}{\partial x}\right) - \left(\frac{\partial E_8}{\partial \alpha_g}\right)_o,$$

$$S_{85}(x,t) \equiv 0, \quad T_{85}(x,t) \equiv 0, \quad U_{85}(x,t) \equiv \alpha_g^o\left(\frac{\partial v_g^o}{\partial t} + \frac{1}{2}\frac{\partial (v_g^o)^2}{\partial x}\right)\left(\frac{\partial \rho_g}{\partial X_n}\right)_o - \left(\frac{\partial E_8}{\partial X_n}\right)_o,$$

$$S_{88}(x,t) \equiv \alpha_g^o\rho_g^o, \quad T_{88}(x,t) \equiv \alpha_g^o\rho_g^o v_g^o, \quad U_{88}(x,t) \equiv -\frac{\partial}{\partial t}(\alpha_g^o\rho_g^o) - \frac{1}{A^o}v_g^o\frac{\partial}{\partial x}(A^o\alpha_g^o\rho_g^o) - \left(\frac{\partial E_8}{\partial v_g}\right)_o,$$

$$S_{89}(x,t) \equiv \alpha_f^o\rho_f^o, \quad T_{89}(x,t) \equiv \alpha_f^o\rho_f^o v_f^o, \quad U_{89}(x,t) \equiv -\frac{\partial}{\partial t}(\alpha_f^o\rho_f^o) - \frac{1}{A^o}v_f^o\frac{\partial}{\partial x}(A^o\alpha_f^o\rho_f^o) - \left(\frac{\partial E_8}{\partial v_f}\right)_o,$$

where the quantity $E_8(\underline{\chi},\underline{G})$ is defined as

$$E_8(\underline{\chi},\underline{G}) \equiv \rho B_x - \alpha_g\rho_g v_g FWG - \alpha_f\rho_f v_f FWF - \Gamma_g(v_g - v_f).$$

Taking the G-derivative of the difference momentum equation gives the following expressions for the components $S_{mn}(x,t)$, $T_{mn}(x,t)$, and $U_{mn}(x,t)$:

$$S_{91}(x,t) \equiv 0, \quad T_{91}(x,t) \equiv 0, \quad U_{91}(x,t) \equiv -\frac{1}{(\rho_g^o)^2}\frac{\partial P^o}{\partial x}\left(\frac{\partial \rho_g}{\partial U_g}\right)_o - \left(\frac{\partial E_9}{\partial U_g}\right)_o - \left(\frac{\partial E_{10}}{\partial U_g}\right)_o\frac{\partial (v_g^o - v_f^o)}{\partial t},$$

$$S_{92}(x,t) \equiv 0, \quad T_{92}(x,t) \equiv 0, \quad U_{92}(x,t) \equiv \frac{1}{\left(\rho_f^o\right)^2} \frac{\partial P^o}{\partial x} \left(\frac{\partial \rho_f}{\partial U_f} \right)_o - \left(\frac{\partial E_9}{\partial U_f} \right)_o - \left(\frac{\partial E_{10}}{\partial U_f} \right)_o \frac{\partial \left(v_g^o - v_f^o \right)}{\partial t},$$

$$S_{93}(x,t) \equiv 0, \quad T_{93}(x,t) \equiv \frac{1}{\rho_g^o} - \frac{1}{\rho_f^o}, \quad U_{93}(x,t) \equiv -\left(\frac{\partial E_9}{\partial P} \right)_o - \left(\frac{\partial E_{10}}{\partial P} \right)_o \frac{\partial \left(v_g^o - v_f^o \right)}{\partial t},$$

$$S_{94}(x,t) \equiv 0, \quad T_{94}(x,t) \equiv 0, \quad U_{94}(x,t) \equiv -\left(\frac{\partial E_9}{\partial \alpha_g} \right)_o - \left(\frac{\partial E_{10}}{\partial \alpha_g} \right)_o \frac{\partial \left(v_g^o - v_f^o \right)}{\partial t},$$

$$S_{95}(x,t) \equiv 0, \quad T_{95}(x,t) \equiv 0, \quad U_{95}(x,t) \equiv -\frac{1}{\left(\rho_g^o\right)^2} \frac{\partial P^o}{\partial x} \left(\frac{\partial \rho_g}{\partial X_n} \right)_o - \left(\frac{\partial E_9}{\partial X_n} \right)_o - \left(\frac{\partial E_{10}}{\partial X_n} \right)_o \frac{\partial \left(v_g^o - v_f^o \right)}{\partial t},$$

$$S_{98}(x,t) \equiv 1 - E_{10}^o, \quad T_{98}(x,t) \equiv v_g^o, \quad U_{98}(x,t) \equiv \frac{\partial E_{10}^o}{\partial t} - \frac{1}{A^o} v_g^o \frac{\partial A^o}{\partial x} - \left(\frac{\partial E_9}{\partial v_g} \right)_o,$$

$$S_{99}(x,t) \equiv E_{10}^o - 1, \quad T_{99}(x,t) \equiv -v_f^o, \quad U_{99}(x,t) \equiv \frac{1}{A^o} v_f^o \frac{\partial A^o}{\partial x} - \frac{\partial E_{10}^o}{\partial t} - \left(\frac{\partial E_9}{\partial v_f} \right)_o,$$

and where the quantities $E_9(\underline{\chi}, \underline{G})$ and $E_{10}(\underline{\chi}, \underline{G})$ are defined as

$$E_9(\underline{\chi}, \underline{G}) \equiv -v_g FWG + v_f FWF + \frac{\Gamma_g \left[\rho v_I - \left(\alpha_f \rho_f v_g + \alpha_g \rho_g v_f \right) \right]}{\alpha_g \rho_g \alpha_f \rho_f} - \rho FI \left(v_g - v_f \right),$$

and, respectively,

$$E_{10}(\underline{\chi}, \underline{G}) \equiv -C \frac{\rho^2}{\rho_g \rho_f}.$$

APPENDIX C: ELIMINATION OF THE INTERMEDIATE TIME-STEP VARIABLES IN THE DISCRETIZED FSM

The matrix $T_2^{(n)}$ is defined as $T_2^{(n)} \equiv \begin{bmatrix} (TI)_{11}^{(n)} & \cdots & (TI)_{1,M_2}^{(n)} \\ \vdots & & \vdots \\ (TI)_{M_2,1}^{(n)} & \cdots & (TI)_{M_2,M_2}^{(n)} \end{bmatrix}$, where M_2 is the number of intermediate time-step variables existing in the system. To simplify the notation for the derivations to follow in this Appendix, the time-step index n will be omitted, since all matrices involved in these derivations are evaluated at time-step n.

The matrix T_2 is partitioned in the form $T_2 \equiv \begin{bmatrix} T & U \\ L & V \end{bmatrix}$, where $T \equiv \begin{bmatrix} (TI)_{11} & (TI)_{12} \\ (TI)_{21} & (TI)_{22} \end{bmatrix}$, and where the matrices L, U, and V are defined below:

(a) if $M_2 = 3$, i.e., if only the quantities $\tilde{U}_g^k, \tilde{U}_f^k, \tilde{\alpha}_g^k$ appear as intermediate time-step variables in Eq. (III.12), then the matrices L, U, and V are defined as follows:

$$L \equiv \begin{bmatrix} (TI)_{31} & (TI)_{32} \end{bmatrix}; \quad U \equiv \begin{bmatrix} (TI)_{13} \\ (TI)_{23} \end{bmatrix}; \quad V \equiv (TI)_{33} \ .$$

(b) if $M_2 = 4$, i.e., all intermediate time-step variables exist in Eq. (III.12), then the matrices L, U, and V are defined as follows:

$$L \equiv \begin{bmatrix} (TI)_{31} & (TI)_{32} \\ (TI)_{41} & (TI)_{42} \end{bmatrix}; \quad U \equiv \begin{bmatrix} (TI)_{13} & (TI)_{14} \\ (TI)_{23} & (TI)_{24} \end{bmatrix}; \quad V \equiv \begin{bmatrix} (TI)_{33} & (TI)_{34} \\ (TI)_{43} & (TI)_{44} \end{bmatrix}.$$

The inverse $[T_2]^{-1}$ of T_2 can be calculated by partitioning; this yields

$\left[T_2\right]^{-1} = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix}$, where the matrices $P_{11}, P_{12}, P_{21}, P_{22}$ are defined as follows:

$$P_{22} \equiv \left[V - LT^{-1}U\right]^{-1},\ P_{21} \equiv -P_{22}LT^{-1},\ P_{12} \equiv -T^{-1}UP_{22},\ P_{11} \equiv T^{-1} + T^{-1}UP_{22}LT^{-1}.$$

To evaluate the matrices $P_{ij},\ i,j = 1,2$, it is necessary to evaluate T^{-1}. Using the same inversion-by-partitioning procedure as above for the matrix T_2 yields $T^{-1} \equiv \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix}$, where the matrices $t_{11}, t_{12}, t_{21}, t_{22}$ are defines as:

$$t_{22} \equiv \left[(TI)_{22} - (TI)_{21}(TI)_{11}^{-1}(TI)_{12}\right]^{-1}, \quad t_{21} \equiv -t_{22}(TI)_{21}(TI)_{11}^{-1},$$

$$t_{12} \equiv -(TI)_{11}^{-1}(TI)_{12}t_{22}, \quad t_{11} \equiv (TI)_{11}^{-1} + (TI)_{11}^{-1}(TI)_{12}t_{22}(TI)_{21}(TI)_{11}^{-1}.$$

Since the matrices $(TI)_{\mu\nu}^{n}$ are by definition diagonal matrices, it follows that

$$t_{22} = \mathrm{diag}\left\{\left[(ti)^{22} - (ti)^{21}(ti)^{12}/(ti)^{11}\right]^{-1}\right\}_k^n \equiv \mathrm{diag}\{\tau_{22}\}_k^n,$$

$$t_{21} = -\mathrm{diag}\left\{\tau_{22}(ti)^{21}/(ti)^{11}\right\}_k^n \equiv \mathrm{diag}\{\tau_{21}\}_k^n,$$

$$t_{12} = -\mathrm{diag}\left\{\tau_{22}(ti)^{12}/(ti)^{11}\right\}_k^n \equiv \mathrm{diag}\{\tau_{12}\}_k^n,$$

$$t_{11} = \mathrm{diag}\left\{\left[1 + (ti)^{12}(ti)^{21}\tau_{22}/(ti)^{11}\right]/(ti)^{11}\right\}_k^n \equiv \mathrm{diag}\{\tau_{11}\}_k^n, \text{ for } k=1, \ ,NV.$$

The matrices $P_{11}, P_{12}, P_{21}, P_{22}$ will now be calculated explicitly for the two cases (a) and (b) defined above:

Case (a): $M_2 = 3$:

In this case, P_{22} is obtained as follows:

$$P_{22} = \left\{ (TI)_{33} - \left[(TI)_{31} \quad (TI)_{32} \right] \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \begin{bmatrix} (TI)_{13} \\ (TI)_{23} \end{bmatrix} \right\}^{-1} = \mathrm{diag}\{p_{22}\}_k^n ,$$

where $p_{22} \equiv \left\{ (ti)^{33} - (ti)^{31} \left[\tau_{11}(ti)^{13} + \tau_{12}(ti)^{23} \right] - (ti)^{32} \left[\tau_{21}(ti)^{13} + \tau_{22}(ti)^{23} \right] \right\}^{-1}$.

Furthermore, the row-matrix P_{21} is obtained in the form

$P_{21} = \left[P_{21}^1 \quad P_{21}^2 \right]_{(1\times 2)}$, where $P_{21}^1 \equiv \mathrm{diag}\left\{ -p_{22}\left[(ti)^{31}\tau_{11} + (ti)^{32}\tau_{21} \right] \right\}_k^n \equiv \mathrm{diag}\{q_1\}_k^n$

$P_{21}^2 \equiv \mathrm{diag}\left\{ -p_{22}\left[(ti)^{31}\tau_{12} + (ti)^{32}\tau_{22} \right] \right\}_k^n \equiv \mathrm{diag}\{q_2\}_k^n$.

The column-matrix P_{12} is obtained as $P_{12} = \begin{bmatrix} P_{12}^1 \\ P_{12}^2 \end{bmatrix}_{(2\times 1)}$, where

$P_{12}^1 \equiv \mathrm{diag}\left\{ -p_{22}\left[\tau_{11}(ti)^{13} + \tau_{12}(ti)^{23} \right] \right\}_k^n \equiv \mathrm{diag}\{s_1\}_k^n$,

$P_{12}^2 \equiv \mathrm{diag}\left\{ -p_{22}\left[\tau_{21}(ti)^{13} + \tau_{22}(ti)^{23} \right] \right\}_k^n \equiv \mathrm{diag}\{s_2\}_k^n$.

Finally, the matrix P_{11}, defined as $P_{11} \equiv T^{-1}\left[I - UP_{21} \right]$ can be written in the form $P_{11} = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix}$, where, for all k=1,...,NV, the matrices $R_{11}, R_{12}, R_{21}, R_{22}$ are defined as follows:

$$\begin{aligned}
R_{11} &\equiv \mathrm{diag}\left\{ \tau_{11}\left[1 - (ti)^{13} q_1 \right] - \tau_{12}(ti)^{23} q_1 \right\}_k^n \\
R_{12} &\equiv \mathrm{diag}\left\{ -\tau_{11}(ti)^{13} q_2 + \tau_{12}\left[1 - (ti)^{23} q_2 \right] \right\}_k^n \\
R_{21} &\equiv \mathrm{diag}\left\{ \tau_{21}\left[1 - (ti)^{13} q_1 \right] - \tau_{22}(ti)^{23} q_1 \right\}_k^n \\
R_{22} &\equiv \mathrm{diag}\left\{ -\tau_{21}(ti)^{13} q_2 + \tau_{22}\left[1 - (ti)^{23} q_2 \right] \right\}_k^n
\end{aligned}$$

Case (b): $M_2 = 4$:

In this case, the matrix P_{22} is given by the expression

$$P_{22} = \left\{ \begin{bmatrix} (TI)_{33} & (TI)_{34} \\ (TI)_{43} & (TI)_{44} \end{bmatrix} - \begin{bmatrix} (TI)_{31} & (TI)_{32} \\ (TI)_{41} & (TI)_{42} \end{bmatrix} \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \begin{bmatrix} (TI)_{13} & (TI)_{14} \\ (TI)_{23} & (TI)_{24} \end{bmatrix} \right\}^{-1} \equiv \begin{bmatrix} P_{22}^{11} & P_{22}^{12} \\ P_{22}^{21} & P_{22}^{22} \end{bmatrix}^{-1},$$

where the following definitions have been used:

$$\begin{aligned}
P_{22}^{11} &\equiv (TI)_{33} - \left\{ (TI)_{31} \left[t_{11} (TI)_{13} + t_{12} (TI)_{23} \right] + (TI)_{32} \left[t_{21} (TI)_{13} + t_{22} (TI)_{23} \right] \right\} \equiv \mathrm{diag}\{p_{11}\}_k^n, \\
P_{22}^{12} &\equiv (TI)_{34} - \left\{ (TI)_{31} \left[t_{11} (TI)_{14} + t_{12} (TI)_{24} \right] + (TI)_{32} \left[t_{21} (TI)_{14} + t_{22} (TI)_{24} \right] \right\} \equiv \mathrm{diag}\{p_{12}\}_k^n, \\
P_{22}^{21} &\equiv (TI)_{43} - \left\{ (TI)_{41} \left[t_{11} (TI)_{13} + t_{12} (TI)_{23} \right] + (TI)_{42} \left[t_{21} (TI)_{13} + t_{22} (TI)_{23} \right] \right\} \equiv \mathrm{diag}\{p_{21}\}_k^n, \\
P_{22}^{22} &\equiv (TI)_{44} - \left\{ (TI)_{41} \left[t_{11} (TI)_{14} + t_{12} (TI)_{24} \right] + (TI)_{42} \left[t_{21} (TI)_{14} + t_{22} (TI)_{24} \right] \right\} \equiv \mathrm{diag}\{p_{22}\}_k^n.
\end{aligned}$$

Carrying out the above calculations leads to the following expression for P_{22}:

$P_{22} = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}$, where the components $W_{ij} \equiv \mathrm{diag}\{w_{ij}\}_k^n;\ i,j = 1,2$ are calculated from the formulae

$$W_{12} \equiv -\left(P_{22}^{11}\right)^{-1} P_{22}^{12} W_{22}; \qquad W_{11} \equiv \left(P_{22}^{11}\right)^{-1} - W_{12} P_{22}^{21} \left(P_{22}^{11}\right)^{-1};$$

$$W_{22} \equiv \left[P_{22}^{22} - P_{22}^{21} \left(P_{22}^{11}\right)^{-1} P_{22}^{12} \right]^{-1}; \qquad W_{21} \equiv -W_{22} P_{22}^{21} \left(P_{22}^{11}\right)^{-1}.$$

Carrying out the remaining calculations for the components $W_{ij} \equiv \mathrm{diag}\{w_{ij}\}_k^n;\ i,j = 1,2$ defined above gives:

$w_{11} = (1 - w_{12}p_{21})/\delta;\ w_{12} = -p_{12}/\delta;\ w_{21} = -p_{21}/\delta;\ \ w_{22} = p_{11}/\delta$, with $\delta \equiv p_{11}p_{22} - p_{12}p_{21}$.

Having calculated P_{22} and T^{-1}, the remaining matrices P_{21}, P_{12}, P_{11} are obtained as follows:

$$P_{21} = -\begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}\begin{bmatrix} (TI)_{31} & (TI)_{32} \\ (TI)_{41} & (TI)_{42} \end{bmatrix}\begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \equiv \begin{bmatrix} P_{21}^{11} & P_{21}^{12} \\ P_{21}^{21} & P_{21}^{22} \end{bmatrix},$$

where $P_{21}^{ij} \equiv \mathrm{diag}\{q_{ij}\}_k^n; \quad i, j = 1,2$, with

$$\begin{aligned}
q_{11} &\equiv -\left\{w_{11}\left[(ti)^{31}\tau_{11} + (ti)^{32}\tau_{21}\right] + w_{12}\left[(ti)^{41}\tau_{11} + (ti)^{42}\tau_{21}\right]\right\}, \\
q_{12} &\equiv -\left\{w_{11}\left[(ti)^{31}\tau_{12} + (ti)^{32}\tau_{22}\right] + w_{12}\left[(ti)^{41}\tau_{12} + (ti)^{42}\tau_{22}\right]\right\}, \\
q_{21} &\equiv -\left\{w_{21}\left[(ti)^{31}\tau_{11} + (ti)^{32}\tau_{21}\right] + w_{22}\left[(ti)^{41}\tau_{11} + (ti)^{42}\tau_{21}\right]\right\}, \\
q_{22} &\equiv -\left\{w_{21}\left[(ti)^{31}\tau_{12} + (ti)^{32}\tau_{22}\right] + w_{22}\left[(ti)^{41}\tau_{12} + (ti)^{42}\tau_{22}\right]\right\}.
\end{aligned}$$

Similarly, the matrix P_{12} is obtained as

$$P_{12} = -\begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix}\begin{bmatrix} (TI)_{13} & (TI)_{14} \\ (TI)_{23} & (TI)_{24} \end{bmatrix}\begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \equiv \begin{bmatrix} P_{12}^{11} & P_{12}^{12} \\ P_{12}^{21} & P_{12}^{22} \end{bmatrix},$$

where $P_{12}^{ij} \equiv \mathrm{diag}\{s_{ij}\}_k^n; \quad i, j = 1,2$, with

$$\begin{aligned}
s_{11} &\equiv -\left\{\tau_{11}\left[(ti)^{13}w_{11} + (ti)^{14}w_{21}\right] + \tau_{12}\left[(ti)^{23}w_{11} + (ti)^{24}w_{21}\right]\right\}, \\
s_{12} &\equiv -\left\{\tau_{11}\left[(ti)^{13}w_{12} + (ti)^{14}w_{22}\right] + \tau_{12}\left[(ti)^{23}w_{12} + (ti)^{24}w_{22}\right]\right\}, \\
s_{21} &\equiv -\left\{\tau_{21}\left[(ti)^{13}w_{11} + (ti)^{14}w_{21}\right] + \tau_{22}\left[(ti)^{23}w_{11} + (ti)^{24}w_{21}\right]\right\}, \\
s_{22} &\equiv -\left\{\tau_{21}\left[(ti)^{13}w_{12} + (ti)^{14}w_{22}\right] + \tau_{22}\left[(ti)^{23}w_{12} + (ti)^{24}w_{22}\right]\right\}.
\end{aligned}$$

Finally, the matrix P_{11} is obtained as follows:

$$P_{11} = T^{-1}\left[I - UP_{21}\right] = \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} (TI)_{13} & (TI)_{14} \\ (TI)_{23} & (TI)_{24} \end{bmatrix} \begin{bmatrix} P_{21}^{11} & P_{21}^{12} \\ P_{21}^{21} & P_{21}^{22} \end{bmatrix} \right\} \equiv \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix},$$

where the matrices $R_{11}, R_{12}, R_{21}, R_{22}$ are defined as follows: $R_{ij} = \mathrm{diag}\left\{ r_{ij} \right\}_k^n ; i, j = 1,2$, with

$$\begin{aligned} r_{11} &\equiv \tau_{11}\left\{1 - \left[(ti)^{13} q_{11} + (ti)^{14} q_{21}\right]\right\} - \tau_{12}\left[(ti)^{23} q_{11} + (ti)^{24} q_{21}\right] \\ r_{12} &\equiv -\tau_{11}\left[(ti)^{13} q_{12} + (ti)^{14} q_{22}\right] + \tau_{12}\left\{1 - \left[(ti)^{23} q_{12} + (ti)^{24} q_{22}\right]\right\} \\ r_{21} &\equiv \tau_{21}\left\{1 - \left[(ti)^{13} q_{11} + (ti)^{14} q_{21}\right]\right\} - \tau_{22}\left[(ti)^{23} q_{11} + (ti)^{24} q_{21}\right] \\ r_{22} &\equiv -\tau_{21}\left[(ti)^{13} q_{12} + (ti)^{14} q_{22}\right] + \tau_{22}\left\{1 - \left[(ti)^{23} q_{12} + (ti)^{24} q_{22}\right]\right\} \end{aligned}.$$

APPENDIX D: PROGRAMMING CONSIDERATIONS FOR IMPLEMENTING THE ADJOINT SENSITIVITY ANALYSIS PROCEDURE (ASAP)

Since the RELAP5/MOD3.2 code has a modular structure, each mathematical model is computed in a separate subroutine. This modular structure allows the implementation of the ASAP as a new “Option” in RELAP5/MOD3.2, without having to alter the functionality of the original code. If the ASAP Option is activated, the code calculates and stores at the end of each successful RELAP-time-step the information necessary to solve the ASM-REL/TF. As it has already been shown in Section III, the ASM-REL/TF must be computed backwards in time; therefore, the entire RELAP-calculation of the base-case problem must be stored for subsequent use in calculating the adjoint functions.

The flow-chart in Fig. 8, below, shows the modifications and additions effected in the RELAP5/MOD3.2 code in order to implement the ASAP Option. In this figure, the RELAP-subroutines that have been modified are listed with their original names, while the subroutines that have been added to RELAP are written in bold type. The modifications introduced in the original RELAP subroutines do not affect the base-case calculation; they are used solely to calculate derivative of various terms in the REL/CDE to state (i.e., dependent) variables and parameters.

The top-level of the transient/steady-state block in RELAP5, the TRNCTL subroutine, comprises the logic to call the lower-level subroutines; including: (i) the subroutine TRNSET, which controls the settings necessary to initiate the transient calculation, (ii) the subroutine TRAN, which controls the advancement of the solution, and (iii) the subroutine TRNFIN, which closes the transient. As an addition, the subroutine ADJSEN is called, at the end of the RELAP5-calculation, to solve the ASM-REL/TF; note that the various components that comprise the ASM-REL/TF would have already been calculated and stored in various files during the forward, RELAP-calculation of the base-case problem.

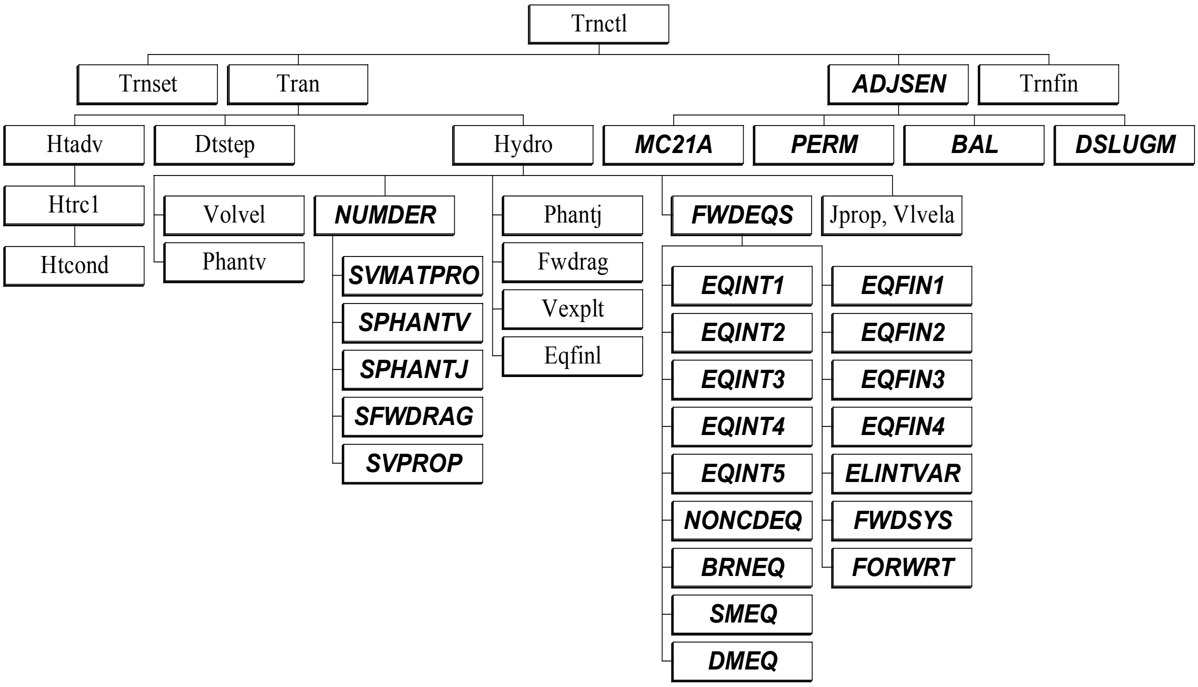

Fig. 8. Adjoint Sensitivity Model (ASM-REL/TF) Transient Block Diagram for the Two-Fluid Model in RELAP5/MOD3.2

There are two types of G-derivatives arising when implementing the ASAP, namely: G-derivatives with respect to the state variables, and G-derivatives with respect to the system parameters. In principle, such derivatives can be calculated either exactly by using the symbolic computer language MAPLE V[13] or by calculating them numerically. When MAPLE V is used, the respective derivatives are calculated in the original RELAP5-subroutines, as an addition to the original functions of that subroutine. For example, the RELAP5-subroutine VLVELA calculates the volume-averaged velocities. When the ASAP Option is activated, VLVELA calculates, in addition, all of the derivatives of the volume-averaged velocities with respect to the state variables.

On the other hand, if the analytical expression of the function is too complicated to calculate exactly via MAPLE V, then the respective derivatives are calculated numerically using difference schemes, by calling the subroutine NUMDER. Most often, the numerical derivatives are calculated using a centered-difference scheme; in this case, the numerical calculation of the derivative of a quantity F with respect to a state variable χ_d, for a volume or junction k, is implemented by calling twice the subroutine that calculates the quantity F, as follows:

$$
\begin{aligned}
&\left(\chi_d^1\right)_k = \left(\chi_d^o\right)_k \cdot (1-\varepsilon) \\
&\text{call F\_subroutine}\left(\left(\chi_d^1\right)_k\right) \Rightarrow F^{(1)} \\
&\left(\chi_d^2\right)_k = \left(\chi_d^o\right)_k \cdot (1+\varepsilon) \\
&\text{call F\_subroutine}\left(\left(\chi_d^2\right)_k\right) \Rightarrow F^{(2)} \\
&\frac{\partial F}{\partial \chi_d} = \frac{F^{(2)} - F^{(1)}}{\left(\chi_d^2\right)_k - \left(\chi_d^1\right)_k}
\end{aligned}
$$

where "$F\_subroutine$" denotes the RELAP5-subroutine that calculates the quantity F, and ε is a small scalar (usually 0.01-0.05). It is important to mention here that "$F\_subroutine$" does not represent an original RELAP-subroutine, but rather a new, specially written subroutine that calculates the quantity F as efficiently as practicable. For example, the RELAP-subroutine PHANTV calculates the gas and liquid interface heat transfer coefficients per unit volume H_{ig} and H_{if}, for *all* of the *volumes* in the system under consideration. However, to calculate the derivatives of H_{ig} and H_{if} with respect to *all of the state variables* but for *a single volume*, it is not necessary to calculate the values of H_{ig} and H_{if} for the unaffected volumes. Therefore, although the existing RELAP5-subroutine PHANTV could be called to calculate the derivatives of H_{ig} and H_{if} with respect to the state variables, this would be very inefficient; the new subroutine, SPHANTV, is called instead, since this subroutine has been written specifically to calculate the respective derivatives efficiently.

At the end of each successful time-step, the components of the ASM-REL/TF are calculated in the subroutine FWDEQS by taking the G-differential of each equation of the REL/CDE. The newly-written subroutines that calculate the respective G-differentiated equations are as follows:

EQINT1 calculates the G-differential of the vapor energy equation;

EQINT2 calculates the G-differential of the liquid energy equation;

EQINT3 calculates the G-differential of sum the density equation;

EQINT4 calculates the G-differential of the difference density equation;

EQINT5 calculates the G-differential of the non-condensable density equation;

NONCDEQ calculates the G-differential of the mass conservation equation for each non-condensable species;

BRNEQ calculates the G-differential of the boron density equation;

EQFIN1 calculates the G-differential of the equation for obtaining the final gas energy;

EQFIN2 calculates the G-differential of the equation for obtaining the final liquid energy;

EQFIN3 calculates the G-differential of the equation for obtaining the final gas void fraction;

EQFIN4 calculates the G-differential of the equation for obtaining the final total non-condensable mass fraction.

Prior to saving the components needed for solving the ASM-REL/TF, the subroutine ELINT-VAR is called to eliminate the various derivatives of the intermediate variables $\left(\widetilde{U}_g\right)_k^n, \left(\widetilde{U}_f\right)_k^n, \left(\widetilde{\alpha}_g\right)_k^n, \left(\widetilde{X}_n\right)_k^n$. After the elimination of these derivatives, the remaining ASM-REL/TF matrix has at each time-step the maximal order of $7 * NV + 2 * NJ$, where NV represents the total number of system volumes and NJ represents the total number of system junctions. Although this matrix is still large, it is sparse, so only the non-zero elements and their positions in the matrix need to be recorded. As will be discussed below, the sparse-matrix solver chosen for solving the ASM-REL/TF requires that the sparse-matrix be stored in the SLAP Triad Format[14]. This format is easy to generate and use; it requires storage of three arrays containing following quantities: (a) the array $A(i), \quad i = 1, \ldots, n$, containing the *non-zero* elements in the sparse matrix; here, n represents the total number of non-zero elements in the respective sparse matrix; (b) the arrays $(IA(i), JA(i))$, containing the indices that uniquely identify the position of the respective non-zero element in the original sparse matrix. An example of using the SLAP Triad Format is shown below:

5X5 Matrix

$$\begin{bmatrix} 11 & 12 & 0 & 0 & 15 \\ 21 & 22 & 0 & 0 & 0 \\ 0 & 0 & 33 & 0 & 35 \\ 0 & 0 & 0 & 44 & 0 \\ 51 & 0 & 53 & 0 & 55 \end{bmatrix}$$

SLAP Triad Format for the 5X5 matrix shown on the left

	1	2	3	4	5	6	7	8	9	10	11
A	51	12	11	33	15	53	55	22	35	44	21
IA	5	1	1	3	1	5	5	2	3	4	2
JA	1	2	1	3	5	3	5	2	5	4	1

At the end of each successful time-step, the subroutine FORWRT saves the elements of the ASM-REL/TF in a file called *forsen*. Optionally, the FSM can be solved in the subroutine FWDSYS to verify the accuracy of the information calculated at each successful time-step.

When the RELAP5 base-case calculation is completed, the subroutine ADJSEN is called to solve the ASM-REL/TF, backwards in time. For this purpose, the information stored in the file *forsen* is read backwards, starting with the last record. At each time step, the ASM-REL/TF is solved by using the sparse-matrix solver DSLUGM[14], which requires that all of the diagonal elements be non-zero. If this requirement is not fulfilled by the matrix read off the *forsen* file, the subroutine MC21A[17] is called to find a row permutation that yields a zero-free diagonal. The permutation of rows is then performed by calling the subroutine PERM. Optionally, the resulting matrix could be subsequently balanced by calling the subroutine BAL[18].

The subroutine DSLUGM[14] is an incomplete LU generalized minimum residual (GMRES) iterative sparse-matrix solver; the incomplete LU factorization is used for preconditioning non-symmetric linear systems. As input, DSLUGM requires the respective matrix in SLAP Triad Format[7] and the source of the system. Although the SLAP Triad format is easy to generate, it is not efficient to use on vector machines for computing iteratively the solution of a linear system. This drawback is circumvented by changing from the SLAP Triad Format to the SLAP Column Format[14] in DSLUGM. In the SLAP Column Format, the non-zeros are stored counting down columns (except for the diagonal entry, which must appear "first" in each column). These values are stored in the array A, for each column, starting with the diagonal element. The IA array holds the row index for each non-zero. The JA array holds the offsets into the IA and A arrays, for the beginning of each column. An example of the SLAP Column format is shown below:

5X5 Matrix

$$\begin{bmatrix} 11 & 12 & 0 & 0 & 15 \\ 21 & 22 & 0 & 0 & 0 \\ 0 & 0 & 33 & 0 & 35 \\ 0 & 0 & 0 & 44 & 0 \\ 51 & 0 & 53 & 0 & 55 \end{bmatrix}$$

SLAP Column format for the 5X5 Matrix on left

	1	2	3	4	5	6	7	8	9	10	11
A	11	21	51	22	12	33	53	44	55	15	35
IA	1	2	5	2	1	3	5	4	5	1	3
JA	1	4	6	8	9	12					

At the end of the calculation using the DSLUGM subroutine, the resulting matrix is returned in the SLAP Column Format.

APPENDIX E: SENSITIVITIES OF FLUID ISOTHERMAL COEFFICIENT OF COMPRESSIBILITY

To illustrate the use of the symbolic computer language MAPLE V[13] for computing exactly the sensitivities of the thermodynamic properties of water, this Appendix presents the expressions obtained using MAPLE V for the fluid isothermal coefficient of compressibility, κ_f. The mathematical formula given in the ASME Steam Tables[5] for κ_f reads:

$$\kappa_f = -\left(-\frac{5}{17}\frac{A_{11}a_5\left(\frac{\partial Z}{\partial P}\right)}{Z^{22/17}} - \frac{2\frac{A_{18}}{P_c} + 6\frac{A_{19}P}{P_c^2}}{a_8 + \theta^{11}} - 12\frac{A_{20}\theta^{18}\left(a_9 + \theta^2\right)}{\left(a_{10} + \beta\right)^5 P_c} + 6\frac{A_{21}\left(a_{12} - \theta\right)\beta}{P_c} + 3\frac{A_{22}\beta^2}{\theta^{20}P_c} \right)\frac{V_c}{V_f}$$

where $\beta \equiv \frac{P}{P_c}$, $\theta \equiv \frac{T_f}{T_c}$, and where

$$Y \equiv 1 - a_1\theta^2 - a_2\theta^6 , \quad Yp \equiv -2a_1\theta + 6a_2\theta^7 , \quad Z \equiv Y + \sqrt{a_3Y^2 - 2a_4\theta + 2a_5\beta} .$$

The derivative of κ_f with respect to the fluid temperature T_f has been obtained explicitly by using MAPLE V[6]; it reads:

$$\frac{\partial\kappa_f}{\partial T_f}=\left(\left(\left(-\frac{110}{289}\frac{A_{11}a_5\frac{\partial Z}{\partial P}}{Z^{39/17}}+\frac{5}{17}\frac{A_{11}a_5\kappa_f}{Z^{22/17}}\right)\frac{\partial Z}{\partial T_f}+24\frac{A_{20}\theta^{19}}{T_c(a_{10}+\beta)^5P_c}+\frac{5}{17}\frac{A_{11}a_5\left(\frac{\partial^2 Z}{\partial T_f\partial P}\right)}{Z^{22/17}}\right.\right.$$

$$-11\frac{\left(2\frac{A_{18}+6A_{19}\beta}{P_c}\right)\theta^{10}}{(a_8+\theta^{11})^2T_c}+216\frac{A_{20}\theta^{17}(a_9+\theta^2)}{T_c(a_{10}+\beta)^5P_c}+6\frac{A_{21}\beta}{T_cP_c}+60\frac{A_{22}\beta^2}{\beta^{20}T_fP_c}-\left(\frac{A_{13}}{T_c}-19\frac{A_{16}\theta^{18}}{(a_7+\theta^{19})^2T_c}\right.$$

$$+2\frac{A_{14}\theta}{T_c}-10\frac{A_{15}(a_6-\theta)^9}{T_c}-3\frac{A_{21}\beta^2}{T_c}+11\frac{(A_{17}+2A_{18}\beta+3A_{19}\beta^2)\theta^{10}}{(a_8+\theta^{11})^2T_c}-18\frac{A_{20}\theta^{17}(a_9+\theta^2)}{T_c}$$

$$\left.\left.\left(-\frac{3}{(a_{10}+\beta)^4}+a_{11}\right)-2\frac{A_{20}\theta^{19}}{T_c}\left(-\frac{3}{(a_{10}+\beta)^4}+a_{11}\right)-20\frac{A_{22}\beta^2}{\theta^{20}T_fP_c}\right)\kappa_f\right)\frac{V_c}{V_f},$$

Similarly, the derivative of κ_f with respect to the fluid pressure P has also been obtained explicitly by using MAPLE V, and it reads:

$$\frac{\partial\kappa_f}{\partial P}=\left(-\frac{110}{289}\frac{A_{11}a_5\left(\frac{\partial Z}{\partial P}\right)^2}{Z^{39/17}}+\frac{5}{17}\frac{A_{11}a_5\kappa_f\left(\frac{\partial Z}{\partial P}\right)}{Z^{22/17}}-6\frac{A_{21}(a_{12}-\theta)}{P_c^2}+\frac{5}{17}\frac{A_{11}a_5\left(\frac{\partial Z}{\partial P}\right)^2}{Z^{22/17}}+6\frac{A_{19}}{(a_8+\theta^{11})P_c^2}\right.$$

$$-60\frac{A_{20}\theta^{18}(a_9+\theta^2)}{(a_{10}+\beta)^6P_c^2}-6\frac{A_{22}\beta}{\theta^{20}P_c^2}-\left(3\frac{A_{22}\beta^2}{\theta^{20}P_c}-\frac{2\frac{A_{18}}{P_c}+6\frac{A_{19}\beta}{P_c}}{a_8+\theta^{11}}-12\frac{A_{20}\theta^{18}(a_9+\theta^2)}{(a_{10}+\beta)^5P_c}+6\frac{A_{21}(a_{12}-\theta)\beta}{P_c}\right)$$

$$\left.\kappa_f\right)\frac{V_c}{V_f}$$

The symbolic computer language MAPLE V has also been used to obtain explicitly the derivatives of κ_f with respect to all of the numerical parameters that enter in its mathematical formula. These derivatives are listed below:

$$\frac{\partial\kappa_f}{\partial A_{11}}=\frac{1}{17}\frac{a_5V_c\left(5\frac{\partial Z}{\partial P}-17\kappa_fZ\right)}{Z^{22/17}V_f},\quad \frac{\partial\kappa_f}{\partial A_{12}}=-\frac{V_c}{V_f}\kappa_f,\quad \frac{\partial\kappa_f}{\partial A_{13}}=-\theta\frac{V_c}{V_f}\kappa_f,\quad \frac{\partial\kappa_f}{\partial A_{14}}=-\theta^2\frac{V_c}{V_f}\kappa_f,$$

$$\frac{\partial\kappa_f}{\partial A_{15}} = -\frac{\left(-a_6 T_c + T_f\right)^{10}}{T_c^{10}} \frac{V_c}{V_f} \kappa_f, \quad \frac{\partial\kappa_f}{\partial A_{16}} = -\frac{T_c^{19}}{\left(a_7 T_c^{19} + T_f^{19}\right)} \frac{V_c}{V_f} \kappa_f, \quad \frac{\partial\kappa_f}{\partial A_{17}} = \frac{T_c^{11}}{\left(a_8 T_c^{11} + T_f^{11}\right)} \frac{V_c}{V_f} \kappa_f,$$

$$\frac{\partial\kappa_f}{\partial A_{18}} = 2\frac{T_c^{11}\left(1 + P\kappa_f\right)}{\left(a_8 T_c^{11} + T_f^{11}\right)} \frac{V_c}{P_c V_f} \kappa_f, \quad \frac{\partial\kappa_f}{\partial A_{19}} = 3\frac{T_c^{11}\left(2 + P\kappa_f\right)\beta}{\left(a_8 T_c^{11} + T_f^{11}\right)} \frac{V_c}{P_c V_f} \kappa_f,$$

$$\frac{\partial\kappa_f}{\partial A_{20}} = \theta^{18}\left(a_9 T_c^2 + T_f^2\right)V_c\left(12P_c^4 - 3\kappa_f P_c^5 a_{10} - 3\kappa_f P_c^4 P + \kappa_f a_{11} a_{10}^5 P_c^5 + 5\kappa_f a_{11} a_{10}^4 P_c^4 P\right.$$
$$\left. + 10\kappa_f a_{11} a_{10}^3 P_c^3 P^2 + 10\kappa_f a_{11} a_{10}^2 P_c^2 P^3 + 5\kappa_f a_{11} a_{10} P_c P^4 + \kappa_f a_{11} P^5\right) \Big/ \left(T_c^{20}\left(a_{10} P_c + P\right)^5 V_f\right),$$

$$\frac{\partial\kappa_f}{\partial A_{21}} = 3\frac{\left(-a_{12} T_c + T_f\right)V_c \beta\left(2 + P\kappa_f\right)}{T_c P_c V_f}, \quad \frac{\partial\kappa_f}{\partial A_{22}} = -\frac{\beta^2 V_c\left(3 + P\kappa_f\right)}{\theta^{20} P_c V_f},$$

$$\frac{\partial\kappa_f}{\partial a_1} = -\frac{5}{289} A_{11} a_5 V_c \left(22\left(\frac{\partial Z}{\partial P}\right)\left(\frac{\partial Z}{\partial a_1}\right) - 17\left(\frac{\partial^2 Z}{\partial P \partial a_1}\right)Z - 17\left(\frac{\partial Z}{\partial a_1}\right)\kappa_f Z\right) \Big/ \left(Z^{39/17} V_f\right),$$

$$\frac{\partial\kappa_f}{\partial a_2} = -\frac{5}{289} A_{11} a_5 V_c \left(22\left(\frac{\partial Z}{\partial P}\right)\left(\frac{\partial Z}{\partial a_2}\right) - 17\left(\frac{\partial^2 Z}{\partial P \partial a_2}\right)Z - 17\left(\frac{\partial Z}{\partial a_2}\right)\kappa_f Z\right) \Big/ \left(Z^{39/17} V_f\right),$$

$$\frac{\partial\kappa_f}{\partial a_3} = -\frac{5}{289} A_{11} a_5 V_c \left(22\left(\frac{\partial Z}{\partial P}\right)\left(\frac{\partial Z}{\partial a_3}\right) - 17\left(\frac{\partial^2 Z}{\partial P \partial a_3}\right)Z - 17\left(\frac{\partial Z}{\partial a_3}\right)\kappa_f Z\right) \Big/ \left(Z^{39/17} V_f\right),$$

$$\frac{\partial\kappa_f}{\partial a_4} = -\frac{5}{289} A_{11} a_5 V_c \left(22\left(\frac{\partial Z}{\partial P}\right)\left(\frac{\partial Z}{\partial a_4}\right) - 17\left(\frac{\partial^2 Z}{\partial P \partial a_4}\right)Z - 17\left(\frac{\partial Z}{\partial a_4}\right)\kappa_f Z\right) \Big/ \left(Z^{39/17} V_f\right),$$

$$\frac{\partial\kappa_f}{\partial a_5} = -\frac{A_{11} V_c}{289\left(Z^{39/17} V_f\right)}\left(-85\left(\frac{\partial Z}{\partial P}\right)Z + 110a_5\left(\frac{\partial Z}{\partial P}\right)\left(\frac{\partial Z}{\partial a_5}\right) - 85a_5\left(\frac{\partial^2 Z}{\partial P \partial a_5}\right)Z + 289\kappa_f Z a_5\left(\frac{\partial Z}{\partial a_5}\right)\right),$$

$$\frac{\partial \kappa_f}{\partial a_6} = 10\frac{A_{15}\left(-a_6 T_c + T_f\right)^9 V_c \kappa_f}{T_c^9 V_f}, \quad \frac{\partial \kappa_f}{\partial a_7} = \frac{A_{16} T_c^{38} V_c \kappa_f}{\left(a_7 T_c^{19} + T_f^{19}\right)^2 V_f},$$

$$\frac{\partial \kappa_f}{\partial a_8} = -\frac{T_c^{22} V_c \left(2A_{18} P_c + 6A_{19} P + \kappa_f A_{17} P_c^2 + 2\kappa_f A_{18} P P_c + 3\kappa_f A_{19} P^2\right)}{\left(a_8 T_c^{11} + T_f^{11}\right)^2 P_c^2 V_f},$$

$$\frac{\partial \kappa_f}{\partial a_9} = \frac{A_{20}\theta^{18} V_c}{\left(a_{10} P_c + P\right)^5 V_f}\left(12P_c^4 - 3\kappa_f P_c^5 a_{10} - 3\kappa_f P_c^4 P + \kappa_f a_{11} a_{10}^5 P_c^5 + 5\kappa_f a_{11} a_{10}^4 P_c^4 P + 10\kappa_f a_{11} a_{10}^3 P_c^3 P^2\right.$$
$$\left. + 10\kappa_f a_{11} a_{10}^2 P_c^2 P^3 + 5\kappa_f a_{11} a_{10} P_c P^4 + \kappa_f a_{11} P^5\right),$$

$$\frac{\partial \kappa_f}{\partial a_{10}} = 12\frac{A_{20}\theta^{18}\left(a_9 T_c^2 + T_f^2\right) P_c^5 V_c \left(-5 + \kappa_f a_{10} P_c + P\kappa_f\right)}{T_c^2 \left(a_{10} P_c + P\right)^6 V_f},$$

$$\frac{\partial \kappa_f}{\partial a_{11}} = \frac{A_{20}\theta^{18}\left(a_9 T_c^2 + T_f^2\right) V_c \kappa_f}{T_c^2 V_f}, \quad \frac{\partial \kappa_f}{\partial a_{12}} = -3\frac{A_{21}\beta V_c \left(-2 + P\kappa_f\right)}{P_c V_f}.$$

ACKNOWLEDGMENTS

First of all, I would like to thank my advisor, Prof. Dr. Dr. h.c. D.G. Cacuci for his constant support, advice and trust.

I would also like to thank the corporation Siemens KWU for its generous financial support. Special thanks go to Dr. H. Finnemann and Dr. F. Depisch of Siemens/KWU for many fruitful discussions, assistance, and continued support.

Most of this work was performed at the Forschungszentrum Karlsruhe (FZK), in the Institute for Reactor Safety (IRS). I wish to thank my colleagues in IRS, especially Dr. D. Struwe, for their friendly assistance and understanding.

I would also like to thank Prof. Dr. Dr. h.c. G. Keßler for agreeing to be the co-examiner on my dissertation committee.

Finally, I wish to thank the Dean of Mechanical Engineering, Prof. Dr. D. Löhe, as well as the faculty council, for allowing me to present my work in English.