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Dan Gabriel Cacuci
cacuci@cec.sc.edu

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Illustrative Application of the nth-Order Comprehensive Adjoint Sensitivity Analysis Methodology for Nonlinear Systems to the Nordheim–Fuchs Reactor Dynamics/Safety Model

Dan Gabriel Cacuci

Center for Nuclear Science and Energy, University of South Carolina, Columbia, SC 29208, USA; cacuci@cec.sc.edu

Abstract: The application of the recently developed "nth-order comprehensive sensitivity analysis methodology for nonlinear systems" (abbreviated as "nth-CASAM-N") has been previously illustrated on paradigm nonlinear space-dependent problems. To complement these illustrative applications, this work illustrates the application of the nth-CASAM-N to a paradigm nonlinear time-dependent model chosen from the field of reactor dynamics/safety, namely the well-known Nordheim–Fuchs model. This phenomenological model describes a short-time self-limiting power transient in a nuclear reactor system having a negative temperature coefficient in which a large amount of reactivity is suddenly inserted, either intentionally or by accident. This model is sufficiently complex to demonstrate all the important features of applying the nth-CASAM-N methodology yet admits exact closed-form solutions for the energy released in the transient, which is the most important system response. All of the expressions of the first- and second-level adjoint functions and, subsequently, the first- and second-order sensitivities of the released energy to the model's parameters are obtained analytically in closed form. The principles underlying the application of the 3rd-CASAM-N methodology for the computation of the third-order sensitivities are demonstrated for both mixed and unmixed second-order sensitivities. For the Nordheim–Fuchs model, a single adjoint computation suffices to obtain the six 1st-order sensitivities, while two adjoint computations suffice to obtain all of the 36 second-order sensitivities (of which 21 are distinct). This illustrative example demonstrates that the number of (large-scale) adjoint computations increases at most linearly within the nth-CASAM-N methodology, as opposed to the exponential increase in the parameter-dimensional space which occurs when applying conventional statistical and/or finite difference schemes to compute higher-order sensitivities. For very large and complex models, the nth-CASAM-N is the only practical methodology for computing response sensitivities comprehensively and accurately, overcoming the curse of dimensionality in sensitivity analysis of nonlinear systems.

Keywords: large-scale nonlinear models; high-order sensitivities; adjoint operators; curse of dimensionality

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1. Introduction

The *nth-Order Comprehensive Adjoint Sensitivity Analysis Methodology for Nonlinear Systems* (nth-CASAM-N) has been presented in [1]. The nth-CASAM-N methodology enables the most efficient computation of exactly-determined expressions of arbitrarily high-order sensitivities of results of interest (called "responses") produced by models that are nonlinear in their underlying state functions, with respect to the model's parameters, uncertain boundaries, and internal interfaces in the model's phase-space. The nth-CASAM-N is formulated in linearly increasing higher-dimensional Hilbert spaces (as opposed to exponentially increasing parameter-dimensional spaces), thus overcoming the curse of dimensionality in sensitivity analysis of nonlinear systems. In previous works [2–5], the principles underlying the application of the nth-CASAM-N have been illustrated on paradigm time-independent (i.e., stationary) nonlinear problems, including a nonlinear heat conduction model and a Bernoulli model. These paradigm models were chosen because they admitted closed-form expressions for all of the high-order sensitivities of responses with respect to the models' uncertain parameters. Noteworthy, the results obtained in these illustrative applications included response sensitivities to imprecisely-known domain boundaries in space, such as would arise from manufacturing tolerances outside of the user's control.

This work aims to illustrate the principles underlying the application of the nth-CASAM-N to dynamical (i.e., time-dependent) models. Dynamical models deserve particular attention because, contrary to static models, dynamic models can display not only steady-state asymptotic behavior but also periodic (i.e., limit-cycle) and aperiodic (i.e., chaotic) behavior. The sensitivity analysis of such models is particularly challenging, as has been demonstrated by Cacuci and DiRocco [6], who applied the 1st-CASAM-N to the reduced-order phenomenological model of boiling water reactor (BWR) dynamics originally developed by March-Leuba, Cacuci, and Perez [7]. Cacuci and DiRocco [6] have shown that in the stable region, the sensitivities of the model's state functions/variables (i.e., the neutron density; the delayed neutron precursors; the fuel temperature; the coolant density; the reactivity) with respect to the model's uncertain parameters attain asymptotically time-independent values. In the "limit-cycle" regions, however, the sensitivities of the state functions oscillate among two, four, and eight unstable equilibrium points, respectively. The 1st-CASAM-N also accurately predicts the response sensitivities in these regions. In the chaotic region, the sensitivities of the state function with respect to the initial conditions and the model parameters oscillate aperiodically among infinitely many unstable equilibrium points, while the amplitudes of the oscillations of the sensitivities increase exponentially in time, reaching very large values (10^{23}), thus confirming that the model is extremely sensitive to any perturbation in the chaotic region. These novel results demonstrated that the 1st-CASAM-N reliably produces the exact 1st-order sensitivities of state functions with respect to the model parameters not only in the stable region in phase-space but also in the "limit-cycle" regions and in the "chaotic" region, in contradistinction with the unreliable results produced by "brute-force" methods using finite-differences [6,8]. The first-order uncertainty analysis presented by DiRocco and Cacuci [8] used the sensitivity analysis results produced in [6] to show that in the stable region, the standard deviations induced by the imprecisely known model parameters and initial conditions in each of the BWR-model's state functions are very large immediately after perturbing the initially critical reactor, reaching values that are about ten times larger than the respective state functions themselves. Although these standard deviations decay to small values after a while, the amplitudes of the oscillations of these standard deviations at the start of the transient are so large as to possibly cause the BWR-system to transit from the stable region into an oscillatory region in phase-space.

As the reduced-order reactor dynamics model of March-Leuba, Cacuci, and Perez [7] has been able to predict in advance reactor transients such as those undergone by the LaSalle reactor [9], it has been used in BWR simulators. Furthermore, since this reduced-order model was shown in [6] to possess large sensitivities of its state functions to its model parameters, it would be prudent to quantify the effects of higher-order sensitivities on the responses of such dynamical models to establish the actual importance of higher-order sensitivities quantitatively. The development of the nth-CASAM-N [1] makes it now possible to quantify the effects of arbitrarily-high order of response sensitivities for nonlinear models. The application of the nth-CASAM-N to a nonlinear dynamical model will be illustrated in this work by considering a well-known paradigm model that describes a short-time self-limiting power excursion in a nuclear reactor system having a negative temperature coefficient in which a large amount of reactivity is suddenly inserted, either intentionally or by accident. In his textbook, Lamarsh [10] refers to this model as the "Fuchs model", while in the textbook of Hetrick [11], this model is called the "Nordheim–

Fuchs model". The Nordheim–Fuchs model (as it will be called in this work) provides a benchmark for all reactor safety/dynamics models. In particular, the reduced-order model of March-Leuba et al. [7] also reduces to the Nordheim–Fuchs model when all neutrons are considered to be prompt. The Nordheim–Fuchs paradigm model is evidently incapable of simulating the oscillatory regions in which a BWR may enter under high-power/low flow conditions, created either intentionally during start-up or accidentally, such as undergone by the LaSalle reactor [9]. However, on the other hand, the Nordheim–Fuchs model is sufficiently complex to model realistically self-limiting power excursions for short times while admitting closed-form exact expressions for the time-dependence of the neutron flux, temperature distribution, and energy released during the transient power burst.

This work is structured as follows: Section 2 presents the balance equations under the Nordheim–Fuchs phenomenological model. Section 3 illustrates the application of the 1st-CASAM-N to obtain the exact expressions of the sensitivities of a generic response of this phenomenological model with respect to the model's imprecisely known (i.e., uncertain) parameters. In particular, Section 3 also presents the closed-form analytical expressions of the first-order sensitivities of the total energy released during the modeled power burst with respect to the parameters that describe a prompt-critical reactor transient. Section 4 illustrates the application of the 2nd-CASAM-N to obtain the exact expressions of all of the second-order sensitivities of the total energy released during the modeled power-burst with respect to the model's imprecisely known parameters. Section 5 illustrates the application of the 3rd-CASAM-N to obtain the exact expressions of selected third-order sensitivities of the total energy released during the modeled power-burst with respect to typical uncertain parameters. Section 6 concludes this work by discussing the didactic significance of this illustrative paradigm application of the nth-CASAM-N for efficiently determining the exact expressions of user-selected high order response sensitivities to model parameters, which provide analytical benchmark solutions for verifying production software codes.

2. The Nordheim–Fuchs Phenomenological Reactor Dynamics/Safety Model

The Nordheim–Fuchs [10,11] phenomenological model describes a short-time self-limiting power transient in a nuclear reactor system having a negative temperature coefficient in which a large amount of reactivity is suddenly inserted, either intentionally or by accident. The response of such a reactor system can be estimated by considering that the reactivity insertion is sufficiently large and the time-span of the transient phenomena under consideration is sufficiently small (i.e., of the order of the lifetime of prompt-neutrons) to consider that all neutrons in the system are prompt neutrons and that the heat generated in the transient remains within the reactor. For such short times, the local spatial variations of the neutron distribution in the reactor are negligible. Using the notation provided by Lamarsh [10], the Nordheim–Fuchs paradigm model describing the aforementioned self-limiting power transient comprises the following balance equations:

1. The time-dependent neutron balance (point kinetics) equation for the neutron flux $\varphi(t)$:

$$\frac{d\varphi(t)}{dt} = \frac{k(t)-1}{l_p}\varphi(t), \quad t>0 \tag{1}$$

$$\varphi(0) = \varphi_0, \quad t=0 \tag{2}$$

where l_p denotes the prompt-neutron lifetime, $k(t)$ denotes the reactor's multiplication factor, and φ_0 denotes the initial (i.e., extant flux) prior to initiating the transient at time $t=0$.

2. The reactivity-temperature feedback equation:

$$k(t) = k_0 - \alpha_T k_0 [T(t) - T_0] \tag{3}$$

where $k_0 \triangleq k(0) \geq 1$ denotes the changed multiplication factor following the reactivity insertion at $t=0$, α_T denotes the magnitude of the negative temperature coefficient,

$T(t)$ denotes the reactor's temperature, and T_0 denotes the reactor's initial temperature at time $t = 0$.

3. The energy conservation equation:

$$c_p[T(t) - T_0] = W(t), \;\; W(t) = \gamma \Sigma_f \int_0^t \varphi(x)\, dx \tag{4}$$

where $W(t)$ denotes the total energy released (per cm^3) at time t in the reactor since the onset of reactivity change, c_p denotes the specific heat (per cm^3) of the reactor, γ denotes the recoverable energy per fission, and Σ_f denotes the reactor's effective macroscopic fission cross-section.

The model parameters involved in Equations (1)–(4) are considered to be the components of a "vector of model parameters" denoted as $\boldsymbol{\alpha}$ and defined as follows:

$$\boldsymbol{\alpha} \triangleq (\alpha_1, \ldots, \alpha_8)^\dagger \triangleq \left(\gamma, \Sigma_f, \varphi_0, l_p, \alpha_T, c_p, T_0, k_0\right)^\dagger \tag{5}$$

In this work, all vectors are considered column vectors and the dagger symbol $(\dagger)$ will be used to denote "transposition". The model parameters are considered to be uncertain (i.e., imprecisely known) but have known nominal values, which will be denoted using a superscript "zero", as follows:

$$\boldsymbol{\alpha}^0 \triangleq \left(\alpha_1^0, \ldots, \alpha_8^0\right)^\dagger \triangleq \left(\gamma^0, \Sigma_f^0, \varphi_0^0, l_p^0, \alpha_T^0, c_p^0, T_0^0, k_0^0\right)^\dagger \tag{6}$$

Using Equations (3) and (4) in Equation (1) yields the following relation:

$$\frac{d\varphi(t)}{dt} = \frac{k_0 - 1}{l_p \gamma \Sigma_f} \frac{dW(t)}{dt} - \frac{\alpha_T k_0}{l_p c_p \gamma \Sigma_f} W(t) \frac{dW(t)}{dt} \tag{7}$$

Integrating Equation (7) while using the initial condition provided in Equation (2) yields the following relation:

$$\varphi(t) = \varphi_0 + \frac{k_0 - 1}{l_p \gamma \Sigma_f} W(t) - \frac{\alpha_T k_0}{2 l_p c_p \gamma \Sigma_f} W^2(t) \tag{8}$$

Multiplying Equation (8) by $\gamma \Sigma_f$ and using the relation provided in Equation (4) yields the following Riccati-type equation $W(t)$:

$$\frac{dW(t)}{dt} = b(\boldsymbol{\alpha}) W^2(t) + \omega_0(\boldsymbol{\alpha}) W(t) + P_0(\boldsymbol{\alpha}), \;\; W(0) = 0, \tag{9}$$

where:

$$b(\boldsymbol{\alpha}) \triangleq -\frac{\alpha_T k_0}{2 l_p c_p}; \;\; \omega_0(\boldsymbol{\alpha}) \triangleq \frac{k_0 - 1}{l_p}; \;\; P_0(\boldsymbol{\alpha}) \triangleq \varphi_0 \gamma \Sigma_f \tag{10}$$

The initial condition $W(0) = 0$ results from Equation (4), the quantity $P_0(\boldsymbol{\alpha})$ is the initial power density of the reactor, and the quantity $\omega_0(\boldsymbol{\alpha})$ is the inverse initial reactor period.

The Riccati equation represented by Equation (9) can be readily integrated to obtain the following closed-form expression for the released total energy $W(t)$:

$$W(t) = 2P_0(\boldsymbol{\alpha}) \frac{\exp[t\omega(\boldsymbol{\alpha})] - 1}{[\omega(\boldsymbol{\alpha}) - \omega_0(\boldsymbol{\alpha})] \exp[t\omega(\boldsymbol{\alpha})] + [\omega(\boldsymbol{\alpha}) + \omega_0(\boldsymbol{\alpha})]} \tag{11}$$

where the "inverse reactor period" $\omega(\boldsymbol{\alpha})$ is defined as follows:

$$\omega(\boldsymbol{\alpha}) \triangleq \left[\omega_0{}^2(\boldsymbol{\alpha}) - 4b(\boldsymbol{\alpha}) P_0(\boldsymbol{\alpha})\right]^{1/2} > 0 \tag{12}$$

Using the expression obtained in Equation (11) in Equation (8) or, alternately, differentiating Equation (11) and dividing the resulting expression by $\gamma\Sigma_f$ yields the following closed-form expression for the neutron flux $\varphi(t)$:

$$\varphi(t) = \frac{4\varphi_0\omega^2(\boldsymbol{\alpha})\exp[t\omega(\boldsymbol{\alpha})]}{\{[\omega(\boldsymbol{\alpha}) - \omega_0(\boldsymbol{\alpha})]\exp[t\omega(\boldsymbol{\alpha})] + \omega(\boldsymbol{\alpha}) + \omega_0(\boldsymbol{\alpha})\}^2} \tag{13}$$

It is apparent from Equation (13) that the neutron flux $\varphi(t)$ increases up a maximum value which is attained at a time $t = t_m$, at which its time-derivative vanishes; after having reached its maximum values, the neutron flux steadily decreases in time. Setting the left side of Equation (7) to zero or, alternatively, setting the time-derivative of Equation (13) to zero and resolving the resulting algebraic equation yields the following expression for t_m:

$$t_m = \frac{1}{\omega(\boldsymbol{\alpha})}\ln\frac{\omega(\boldsymbol{\alpha}) + \omega_0(\boldsymbol{\alpha})}{\omega(\boldsymbol{\alpha}) - \omega_0(\boldsymbol{\alpha})} \tag{14}$$

The maximum value of the flux, denoted as $\varphi_m \triangleq \varphi(t_m)$, has the following expression:

$$\varphi_m = \frac{\varphi_0}{1 - [\omega_0(\boldsymbol{\alpha})/\omega(\boldsymbol{\alpha})]^2} \tag{15}$$

At $t = t_m$, when the neutron flux $\varphi(t)$ attains its maximum value, the released total energy attains the following value:

$$W(t_m) = \frac{2P_0(\boldsymbol{\alpha})\omega_0(\boldsymbol{\alpha})}{\omega^2(\boldsymbol{\alpha}) - \omega_0^2(\boldsymbol{\alpha})} \tag{16}$$

It is apparent from Equations (4) and (11) that released total energy $W(t)$ is a continuously increasing function of time, which remains finite at all times. If the phenomenological model were valid for an unlimited amount of time (which it is not), the released total energy would reach the following limiting value:

$$W(\infty) = \frac{2P_0(\boldsymbol{\alpha})}{\omega(\boldsymbol{\alpha}) - \omega_0(\boldsymbol{\alpha})} \tag{17}$$

It is observed from the results provided in Equations (16) and (17) that, after the flux attains its maximum value at $t = t_m$, the released total energy continues to increase. If the model were valid for an infinitely long amount of time, the maximum theoretical increase of the released total energy after the time instance $t = t_m$ would be as follows:

$$W(\infty) - W(t_m) = \frac{2P_0(\boldsymbol{\alpha})\omega(\boldsymbol{\alpha})}{\omega^2(\boldsymbol{\alpha}) - \omega_0^2(\boldsymbol{\alpha})} = \omega(\boldsymbol{\alpha})\frac{l_p c_p}{\alpha_T k_0} > 0 \tag{18}$$

The most important response for the model comprising Equations (1)–(4) is the released total energy $W(\tau)$ from the initiation of the power transient until some *user-chosen* (final) time $0 \le t = t_f \le \infty$, when this model ceases to represent the long-time evolution of the reactor system. The evolution of the reactor beyond $t = t_f$ would necessarily need to include the effects of delayed neutrons and other physical phenomena, which are unimportant during the short time span modeled by Equations (1)–(4). From a phenomenological point of view, the released total energy $W(t)$ increases monotonically in time up to the limiting value shown in Equation (17) regardless of whether the reactor becomes instantly prompt critical or prompt supercritical when undergoing self-limiting power transients as described by Equations (1)–(4). Therefore, the application of the nth-CASAM-N for performing sensitivity analysis (with respect to the model parameters) of the total released energy can be illustrated by considering the "prompt-critical reactor" ($k_0 = 1$) case, thereby reducing the complexity of the mathematical manipulations without loss of conceptual generality. The same mathematically simplifying effect can also be achieved, as done by Hetrick [11], by modeling the transient phenomena that occur just after the neutron flux has peaked by shifting the origin of time to $t = t_m$.

3. Illustrative Application of the 1st-CASAM-N to Compute First-Order Response Sensitivities

The state functions (i.e., dependent variables) for the model represented by Equations (1)–(4) are the neutron flux distribution $\varphi(t)$, the reactor's temperature $T(t)$, and the total energy released $W(t)$, per cm^3 at time t. To keep the subsequent notation as simple as possible, these state functions are considered to be components of a "vector of state functions" denoted as $\mathbf{u}(t) \triangleq [\varphi(t), T(t), W(t)]^\dagger$. A generic response for this model can be represented mathematically by the following function of the model's dependent variables $\mathbf{u}(t)$ and parameters $\boldsymbol{\alpha}$:

$$R(\mathbf{u};\boldsymbol{\alpha}) = \int_0^{t_f} F(\mathbf{u};\boldsymbol{\alpha})dt \tag{19}$$

where $F(\mathbf{u};\boldsymbol{\alpha})$ denotes a suitably differentiable function of its arguments. The application of the 1st-CASAM-N to obtain the generic expressions of the first-order sensitivities with respect to the model parameters when the initial reactivity insertion renders the reactor prompt supercritical (i.e., $k_0 > 1$) is presented in the next Subsection.

3.1. First-Order Sensitivity Analysis of the Prompt Supercritical Power Transient

The first-order sensitivities of $R(\mathbf{u};\boldsymbol{\alpha})$ with respect to the model parameters are provided by the first-order total Gateaux (G-) differential, $\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0\delta\mathbf{u};\delta\boldsymbol{\alpha}\right)$, of this response computed at the nominal parameter values for arbitrary variations $\delta\boldsymbol{\alpha} \triangleq \boldsymbol{\alpha} - \boldsymbol{\alpha}^0$ in the model parameters around the respective nominal values and corresponding variations $\mathbf{v}^{(1)}(t) \triangleq [\delta\varphi(t), \delta T(t), \delta W(t)]^\dagger$, $\delta\varphi(t) \triangleq \varphi(t) - \varphi^0(t)$, $\delta T(t) \triangleq T(t) - T^0(t)$, $\delta W(t) \triangleq W(t) - W^0(t)$, in the state functions. The first-order G-differential $\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0\delta\mathbf{u};\delta\boldsymbol{\alpha}\right)$ is defined as follows:

$$\begin{aligned}\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0;\delta\mathbf{v}^{(1)};\delta\boldsymbol{\alpha}\right) &\triangleq \frac{d}{d\varepsilon}\left\{\int_0^{t_f} F\left(\mathbf{u}^0 + \varepsilon\mathbf{v}^{(1)};\boldsymbol{\alpha}^0 + \varepsilon\delta\boldsymbol{\alpha}\right)dt\right\}_{\varepsilon=0} \\ &\triangleq \left\{\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0;\delta\boldsymbol{\alpha}\right)\right\}_{dir} + \left\{\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0;\delta\mathbf{v}^{(1)}\right)\right\}_{ind},\end{aligned} \tag{20}$$

where the "direct-effect term" and, respectively, the "indirect-effect term" are defined as follows:

$$\left\{\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0;\delta\boldsymbol{\alpha}\right)\right\}_{dir} \triangleq \int_0^{t_f} \left\{\frac{\partial F(\mathbf{u};\boldsymbol{\alpha})}{\partial\boldsymbol{\alpha}}\right\}_{\boldsymbol{\alpha}^0=0} dt \tag{21}$$

$$\begin{aligned}\left\{\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0;\delta\mathbf{v}^{(1)}\right)\right\}_{ind} &\triangleq \int_0^{t_f} \left\{\frac{\partial F(\mathbf{u};\boldsymbol{\alpha})}{\partial\mathbf{u}}\mathbf{v}^{(1)}(t)\right\}_{\boldsymbol{\alpha}^0=0} dt \\ &= \left\{\int_0^{t_f}\left[\frac{\partial F}{\partial\varphi}\delta\varphi(t) + \frac{\partial F}{\partial T}\delta T(t) + \frac{\partial F}{\partial W}\delta W(t)\right]dt\right\}_{\boldsymbol{\alpha}^0=0}.\end{aligned} \tag{22}$$

The direct-effect term can be evaluated immediately, but the indirect-effect term can be evaluated only after having obtained the variations $\mathbf{v}^{(1)}(t) \triangleq [\delta\varphi(t), \delta T(t), \delta W(t)]^\dagger$. For given variations $\delta\boldsymbol{\alpha} \triangleq \boldsymbol{\alpha} - \boldsymbol{\alpha}^0$, the variations $\mathbf{v}^{(1)}(t) \triangleq [\delta\varphi(t), \delta T(t), \delta W(t)]^\dagger$ are the solutions of the 1st-Level Variational Sensitivity System (1st-LVSS), which is obtained by determining the first-order G-differentials of the equations underlying the model, in which it is convenient to use Equation (9) instead of Equation (1). Applying the definition of the G-differential to these equations yields the following relations:

$$\begin{aligned}&\frac{d}{d\varepsilon}\left\{\frac{d\left[W^0(t)+\varepsilon\delta W(t)\right]}{dt} - b^0(\boldsymbol{\alpha})\left[W^0(t)+\varepsilon\delta W(t)\right]^2 - \omega_0^0(\boldsymbol{\alpha})\left[W^0(t)+\varepsilon\delta W(t)\right]\right\}_{\varepsilon=0} \\ &= \frac{d}{d\varepsilon}\left\{\left[b^0(\boldsymbol{\alpha})+\varepsilon\delta b(\boldsymbol{\alpha})\right]W^2(t) + \left[\omega_0^0(\boldsymbol{\alpha})+\varepsilon\delta\omega_0(\boldsymbol{\alpha})\right]W(t) + P_0^0(\boldsymbol{\alpha}) + \varepsilon\delta P_0(\boldsymbol{\alpha})\right\}_{\varepsilon=0},\end{aligned} \tag{23}$$

$$\frac{d}{d\varepsilon}\left\{W^0(0) + \varepsilon\delta W(0)\right\}_{\varepsilon=0} = 0 \tag{24}$$

$$\frac{d}{d\varepsilon}\left\{T^0(t)+\varepsilon\delta T(t)\right\}_{\varepsilon=0}=\frac{d}{d\varepsilon}\left\{\frac{W^0(t)+\varepsilon\delta W(t)}{c_p^0+\varepsilon\delta c_p}+T_0^0+\varepsilon\delta T_0\right\}_{\varepsilon=0} \tag{25}$$

$$\frac{d}{d\varepsilon}\left\{\varphi^0(t)+\varepsilon\delta\varphi(t)\right\}_{\varepsilon=0}=\frac{1}{(\gamma^0+\varepsilon\delta\gamma)\left(\Sigma_f^0+\varepsilon\delta\Sigma_f\right)}\frac{d\left[W^0(t)+\varepsilon\delta W(t)\right]}{dt} \tag{26}$$

Carrying out the operations indicated in Equations (23)–(26) yields the following matrix form for the 1st-LVSS:

$$\left\{\mathbf{N}^{(1)}(\mathbf{u};\boldsymbol{\alpha})\mathbf{v}^{(1)}(t)\right\}_{\boldsymbol{\alpha}^0}=\left\{\mathbf{q}_V^{(1)}(\mathbf{u};\boldsymbol{\alpha};\delta\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0},\ t>0, \tag{27}$$

$$\delta W(0)=0,\ \ t=0. \tag{28}$$

where

$$\mathbf{N}^{(1)}(\mathbf{u};\boldsymbol{\alpha})\triangleq\begin{pmatrix}\frac{d}{dt}-2b(\boldsymbol{\alpha})W(t)-\omega_0(\boldsymbol{\alpha}) & 0 & 0\\ -1/c_p & 1 & 0\\ \left(1/\gamma\Sigma_f\right)d/dt & 0 & 1\end{pmatrix}; \tag{29}$$

$$\mathbf{v}^{(1)}(t)\triangleq\begin{pmatrix}\delta W(t)\\ \delta T(t)\\ \delta\varphi(t)\end{pmatrix};\ \ \mathbf{q}_V^{(1)}(\mathbf{u};\boldsymbol{\alpha};\delta\boldsymbol{\alpha})\triangleq\begin{pmatrix}\delta b(\boldsymbol{\alpha})W^2(t)+\delta\omega_0(\boldsymbol{\alpha})W(t)+P_0(\boldsymbol{\alpha})\\ -\left[W(t)/c_p^2\right]\delta c_p+\delta T_0\\ -\left(\delta\gamma/\gamma^2\Sigma_f+\delta\Sigma_f/\gamma\Sigma_f^2\right)dW(t)/dt\end{pmatrix}; \tag{30}$$

$$\delta b(\boldsymbol{\alpha})\triangleq\left\{-\frac{\delta\alpha_T}{2l_pc_p}+\frac{\alpha_T}{2l_p\left(c_p\right)^2}\delta c_p+\frac{\alpha_T}{2\left(l_p\right)^2c_p}\delta l_p\right\}_{\boldsymbol{\alpha}^0} \tag{31}$$

$$\delta P_0(\boldsymbol{\alpha})\triangleq\left\{\gamma\Sigma_f(\delta\varphi_0)+\varphi_0\Sigma_f(\delta\gamma)+\varphi_0\gamma\left(\delta\Sigma_f\right)\right\}_{\boldsymbol{\alpha}^0};\ \ \delta\omega_0(\boldsymbol{\alpha})\triangleq\left\{\frac{\delta k_0}{l_p}+\frac{\delta l_p}{l_p^2}\right\}_{\boldsymbol{\alpha}^0} \tag{32}$$

The notation $\{\}_{\boldsymbol{\alpha}^0}$, which appears in Equations (27), (31), and (32), is −and will henceforth be− used to signify that the quantity within the braces is to be evaluated at the nominal values of the respective parameters and state functions (i.e., dependent variables).

Evidently, the 1st-LVSS would need to be solved anew for every parameter variation to determine the corresponding the variations $\mathbf{v}^{(1)}(t)\triangleq[\delta\varphi(t),\delta T(t),\delta W(t)]^\dagger$, which is impractical for the large-scale systems encountered in practice. Such repeated computations can be avoided by expressing the indirect-effect term defined in Equation (22) by applying the principles of the 1st-CASAM-N to derive an alternative expression for the indirect-effect term $\left\{\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0;\delta\mathbf{v}^{(1)}\right)\right\}_{ind}$, involving a 1st-level adjoint sensitivity function, which will be denoted as $\mathbf{a}^{(1)}(t)\triangleq\left[a_1^{(1)}(t);a_2^{(1)}(t);a_3^{(1)}(t)\right]^\dagger$, which will be independent of parameter variations and will be the solution of a 1st-Level Adjoint Sensitivity System (1st-LASS) constructed as follows:

(i) Consider that the vector $\mathbf{u}(t)$ and, hence, $\mathbf{v}^{(1)}(t)$ are elements of a Hilbert space denoted as H_1, which is endowed with an inner product of two vectors $\mathbf{u}^{(a)}(\mathbf{x})\in H_1$ and $\mathbf{u}^{(b)}(\mathbf{x})\in H_1$ denoted as $\left\langle\mathbf{u}^{(a)},\mathbf{u}^{(b)}\right\rangle_1$ and defined as follows:

$$\left\langle\mathbf{u}^{(a)},\mathbf{u}^{(b)}\right\rangle_1\triangleq\left\{\int_0^{t_f}\sum_{i=1}^{3}u_i^{(a)}(t)u_i^{(b)}(t)dt\right\}_{\boldsymbol{\alpha}^0} \tag{33}$$

(ii) Using the definition of the adjoint operator in $H_1(\Omega_x)$, the left side of Equation (27) is transformed as follows:

$$\begin{aligned}\left\{\left\langle\mathbf{a}^{(1)},\mathbf{N}^{(1)}(\mathbf{u};\boldsymbol{\alpha})\mathbf{v}^{(1)}\right\rangle_1\right\}_{\boldsymbol{\alpha}^0}&=\left\{\left\langle\left[\mathbf{N}^{(1)}(\mathbf{u};\boldsymbol{\alpha})\right]^*\mathbf{a}^{(1)},\mathbf{v}^{(1)}\right\rangle_1\right\}_{\boldsymbol{\alpha}^0}\\&+\left[a_1^{(1)}\left(t_f\right)+a_3^{(1)}\left(t_f\right)/\gamma\Sigma_f\right]\delta W\left(t_f\right).\end{aligned} \tag{34}$$

where the symbol $[]^*$ indicates "formal adjoint" operator, which implies that the operator $\left[N^{(1)}(E;\boldsymbol{\alpha})\right]^*$ has the following expression:

$$\left[N^{(1)}(E;\boldsymbol{\alpha})\right]^* \triangleq \begin{pmatrix} -\frac{d}{dt} - 2b(\boldsymbol{\alpha})W(t) - \omega_0(\boldsymbol{\alpha}) & -1/c_p & \left(-1/\gamma\Sigma_f\right)d/dt \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{35}$$

(iii) Require the first term on the right side of Equation (34) to represent the indirect-effect term represented by Equation (22) by imposing the following relationship:

$$\begin{gathered}\left\{\left[\mathbf{N}^{(1)}(\mathbf{u};\boldsymbol{\alpha})\right]^* \mathbf{a}^{(1)}(\mathbf{x})\right\}_{\boldsymbol{\alpha}^0} = \left\{\mathbf{q}_A^{(1)}[\mathbf{u}(\mathbf{x});\boldsymbol{\alpha}]\right\}_{\boldsymbol{\alpha}^0},\ t>0, \\ \mathbf{q}_A^{(1)}[\mathbf{u}(\mathbf{x});\boldsymbol{\alpha}] \triangleq [\partial F/\partial W, \partial F/\partial T, \partial F/\partial \varphi]^\dagger. \end{gathered} \tag{36}$$

In component form, Equation (36) reads as follows:

$$-\left[\frac{d}{dt} + 2b(\boldsymbol{\alpha})W(t) + \omega_0(\boldsymbol{\alpha})\right]a_1^{(1)}(t) - \frac{a_2^{(1)}(t)}{c_p} - \frac{1}{\gamma\Sigma_f}\frac{da_3^{(1)}(t)}{dt} = \frac{\partial F}{\partial W} \tag{37}$$

$$a_2^{(1)}(t) = \frac{\partial F}{\partial T} \tag{38}$$

$$\frac{1}{\gamma\Sigma_f}\frac{da_3^{(1)}(t)}{dt} = \frac{\partial F}{\partial \varphi} \tag{39}$$

(iv) The boundary terms on the right side of Equation (34) will vanish by imposing the following "final-time" condition on the 1st-level adjoint function $\mathbf{a}^{(1)}(t)$:

$$\mathbf{a}^{(1)}\left(t_f\right) = 0,\ t = t_f \tag{40}$$

Equations (36) and (40) constitute the 1st-Level Adjoint Sensitivity System (1st-LASS) for the 1st-level adjoint sensitivity function $\mathbf{a}^{(1)}(t)$.

(v) In view of Equations (27), (34)−(40), it follows that the indirect-effect term $\left\{\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0;\delta\mathbf{v}^{(1)}\right)\right\}_{ind}$ is now given by the following expression:

$$\left\{\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0;\delta\mathbf{v}^{(1)}\right)\right\}_{ind} = \left\{\int_0^{t_f} \mathbf{a}^{(1)}(t)\mathbf{q}_V^{(1)}(\mathbf{u};\boldsymbol{\alpha};\delta\boldsymbol{\alpha})dt\right\}_{\boldsymbol{\alpha}^0} \tag{41}$$

The total sensitivity (total G-differential) $\delta R\left(\mathbf{u}^0;\boldsymbol{\alpha}^0\delta\mathbf{u};\delta\boldsymbol{\alpha}\right)$ is obtained by adding the expression for the indirect-effect term provided in Equation (41) with the expression for the direct-effect term provided in Equation (21). Notably, the 1st-LASS is independent of parameter variations, so it needs to be solved just once to obtain the 1st-level adjoint sensitivity function $\mathbf{a}^{(1)}(t)$. The partial sensitivities $\partial R(\mathbf{u};\boldsymbol{\alpha})/\delta\alpha_i$ are subsequently obtained exactly and efficiently by using quadrature formulas, rather than having to solve the 1st-LVSS repeatedly. This will be demonstrated explicitly in the next subsection by considering a specific (rather than a general) response, namely the total energy released after the initiation of a prompt-critical power transient.

3.2. Closed-Form Expressions for the First-Order Sensitivities of the Energy Released during a Prompt Critical Power Transient

In the particular case when the reactivity insertion is $k_0 = 1$, the reactor system becomes "prompt critical", in which case $\omega_0(\boldsymbol{\alpha}) = 0$. In this case, the balance equation satisfied by the energy released within the prompt-critical reactor takes on the following particular form of Equation (9):

$$\frac{dE(t)}{dt} = b(\boldsymbol{\alpha})E^2(t) + P_0(\boldsymbol{\alpha}), \ \ E(0) = 0, \tag{42}$$

where $E(t) \triangleq W(t; k_0 = 1)$ denotes the energy released within the prompt-critical reactor. Furthermore, the expressions provided in Equations (11)−(13) for the inverse reactor period $\omega(\boldsymbol{\alpha})$, the neutron flux and the released total energy, respectively, take on the following particular expressions:

$$\tau(\boldsymbol{\alpha}) \triangleq \omega(\boldsymbol{\alpha}; k_0 = 1) = [-4b(\boldsymbol{\alpha})P_0(\boldsymbol{\alpha})]^{1/2} = \left[2\frac{\alpha_T \varphi_0 \gamma \Sigma_f}{l_p c_p}\right]^{1/2} \tag{43}$$

$$E(t) \triangleq W(t; k_0 = 1) = \frac{2P_0(\boldsymbol{\alpha})}{\tau(\boldsymbol{\alpha})} \tanh\left[t\frac{\tau(\boldsymbol{\alpha})}{2}\right] \tag{44}$$

$$\varphi_p(t) \triangleq \varphi(t; k_0 = 1) = \varphi_0 \left\{ \operatorname{sech}\left[\frac{t\tau(\boldsymbol{\alpha})}{2}\right]\right\}^2 \tag{45}$$

When the initial reactivity insertion renders the reactor prompt critical, the results provided in Equations (14)–(17) take on the following particular forms:

$$\begin{array}{l} t_m(k_0 = 1) = 0; \ \varphi_m(t_m; k_0 = 1) = \varphi_0; \\ W(t_m; k_0 = 1) = 0; \ E(\infty) \triangleq W(\infty; k_0 = 1) = \frac{2P_0(\boldsymbol{\alpha})}{\tau(\boldsymbol{\alpha})} \end{array} \tag{46}$$

The response considered for the sensitivity analysis presented in this Subsection is the total energy, $E\left(t_f\right)$, released after the initiation at $t = 0$ of a prompt-critical ($k_0 = 1$) power transient up to a user-chosen final-time $t = t_f$. This response can be defined mathematically in several equivalent ways, the simplest of which is as follows:

$$E\left(t_f\right) = \int_0^{t_f} E(t)\delta\left(t - t_f\right)dt \tag{47}$$

where $\delta(t - \tau)$ denotes the Dirac-delta functional.

The first-order G-differential $\delta E\left(t_f\right)$ of $E\left(t_f\right)$ for known parameter variations $\delta\boldsymbol{\alpha} \triangleq \boldsymbol{\alpha} - \boldsymbol{\alpha}^0$ around the nominal values $\left(E^0; \boldsymbol{\alpha}^0\right)$ is obtained, by definition, as follows:

$$\delta E\left(t_f\right) = \int_0^{t_f} \delta E(t)\delta(t - \tau)\, dt \tag{48}$$

Taking the G-differential of Equation (42), the 1st-LVSS for the variational function $\delta E(t)$ is obtained as follows:

$$\left\{\left[\frac{d}{dt} - 2b(\boldsymbol{\alpha})E(t)\right]\delta E(t)\right\}_{\boldsymbol{\alpha}^0} = \left\{\delta b(\boldsymbol{\alpha})E^2(t) + \delta P_0(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0}, \ t > 0, \tag{49}$$

$$\delta E(0) = 0, \ \ t = 0. \tag{50}$$

In view of Equation (48), the solution $\mathbf{a}^{(1)}(t)$ of the 1st-LASS, cf. Equations (36) and (40), takes on the particular form $\mathbf{a}^{(1)}(t) = \left[a_1^{(1)}(t); 0; 0\right]^{\dagger}$, where the non-zero component $a_1^{(1)}(t)$ satisfies the following simplified form of the 1st-LASS:

$$\left\{\left[-\frac{d}{dt} - 2b(\boldsymbol{\alpha})E(t)\right]a^{(1)}(t)\right\}_{\boldsymbol{\alpha}^0} = \delta\left(t - t_f\right), \ \ t > 0 \tag{51}$$

$$a^{(1)}\left(t_f\right) = 0,\ t = t_f \tag{52}$$

Furthermore, the first-order total G-differential $\delta E\left(t_f\right)$ of the response $E\left(t_f\right)$ takes on the following expression in terms of the 1st-level adjoint function $a^{(1)}(t)$:

$$\delta E\left(t_f\right) = \left\{\delta b(\boldsymbol{\alpha})\int_0^{t_f} a^{(1)}(t)E^2(t)dt + \delta P_0(\boldsymbol{\alpha})\int_0^{t_f} a^{(1)}(t)dt\right\}_{\boldsymbol{\alpha}^0} \tag{53}$$

The integrating factor for the left side of Equation (51) has the following expression:

$$\begin{aligned} I(t) &= \exp\left[2b(\boldsymbol{\alpha})\int^t E(x)dx\right] = \exp\left[\tfrac{4b(\boldsymbol{\alpha})P_0(\boldsymbol{\alpha})}{\tau(\boldsymbol{\alpha})}\int_0^t \tanh\left[\tfrac{x\tau(\boldsymbol{\alpha})}{2}\right]dx\right] \\ &= \exp\{-2\ln[\cosh t\tau(\boldsymbol{\alpha})/2]\} = \cosh^{-2}[t\tau(\boldsymbol{\alpha})/2]. \end{aligned} \tag{54}$$

Solving the 1st-LASS yields the following expression for the 1st-level adjoint function $a^{(1)}(t)$:

$$a^{(1)}(t) = \mathrm{H}\left(t_f - t\right)\left\{\frac{\cosh[t\tau(\boldsymbol{\alpha})/2]}{\cosh\left[t_f\tau(\boldsymbol{\alpha})/2\right]}\right\}^2 \tag{55}$$

where $\mathrm{H}\left(t - t_f\right)$ denotes the Heaviside functional. Using the expression obtained in Equation (55) in Equation (53) yields the following results:

$$\begin{aligned} &\frac{\partial E\left(t_f\right)}{\partial b(\boldsymbol{\alpha})}\delta b(\boldsymbol{\alpha}) = \delta b(\boldsymbol{\alpha})\int_0^{t_f} a^{(1)}(t)E^2(t)\,dt \\ &= \frac{P_0(\boldsymbol{\alpha})}{b(\boldsymbol{\alpha})}\left\{\frac{t_f}{2\cosh^2\left[t_f\tau(\boldsymbol{\alpha})/2\right]} - \frac{\tanh\left[t_f\tau(\boldsymbol{\alpha})/2\right]}{\tau(\boldsymbol{\alpha})}\right\}\delta b(\boldsymbol{\alpha}); \end{aligned} \tag{56}$$

$$\begin{aligned} &\frac{\partial E\left(t_f\right)}{\partial P_0(\boldsymbol{\alpha})}\delta P_0(\boldsymbol{\alpha}) = \delta P_0(\boldsymbol{\alpha})\int_0^{t_f} a^{(1)}(t)dt \\ &= \left\{\frac{1}{\tau(\boldsymbol{\alpha})}\tanh\left[t_f\tau(\boldsymbol{\alpha})/2\right] + \frac{t_f}{\cosh^2\left[t_f\tau(\boldsymbol{\alpha})/2\right]}\right\}\delta P_0(\boldsymbol{\alpha}). \end{aligned} \tag{57}$$

The above expressions are to be evaluated at the nominal parameter and state functions, but the notation $\{\}_{\boldsymbol{\alpha}^0}$ has been omitted for simplicity.

Using the expressions obtained in Equation (31) and, respectively, Equation (32) in Equation (56) and, respectively, Equation (57) yields the following expressions for the respective partial first-order sensitivities:

$$\begin{aligned} &\frac{\partial E\left(t_f\right)}{\partial \alpha_1} \triangleq \frac{\partial E\left(t_f\right)}{\partial \gamma} = \varphi_0\Sigma_f\int_0^{t_f} a^{(1)}(t)dt \\ &= \varphi_0\Sigma_f\left\{\frac{1}{\tau(\boldsymbol{\alpha})}\tanh\left[t_f\tau(\boldsymbol{\alpha})/2\right] + \frac{t_f}{\cosh^2\left[t_f\tau(\boldsymbol{\alpha})/2\right]}\right\}; \end{aligned} \tag{58}$$

$$\begin{aligned} &\frac{\partial E\left(t_f\right)}{\partial \alpha_2} \triangleq \frac{\partial E\left(t_f\right)}{\partial \Sigma_f} = \varphi_0\gamma\int_0^{t_f} a^{(1)}(t)dt \\ &= \varphi_0\gamma\left\{\frac{1}{\tau(\boldsymbol{\alpha})}\tanh\left[t_f\tau(\boldsymbol{\alpha})/2\right] + \frac{t_f}{\cosh^2\left[t_f\tau(\boldsymbol{\alpha})/2\right]}\right\}; \end{aligned} \tag{59}$$

$$\begin{aligned} &\frac{\partial E\left(t_f\right)}{\partial \alpha_3} \triangleq \frac{\partial E\left(t_f\right)}{\partial \varphi_0} = \gamma\Sigma_f\int_0^{t_f} a^{(1)}(t)dt \\ &= \gamma\Sigma_f\left\{\frac{1}{\tau(\boldsymbol{\alpha})}\tanh\left[t_f\tau(\boldsymbol{\alpha})/2\right] + \frac{t_f}{\cosh^2\left[t_f\tau(\boldsymbol{\alpha})/2\right]}\right\}; \end{aligned} \tag{60}$$

$$\begin{aligned} &\frac{\partial E\left(t_f\right)}{\partial \alpha_4} \triangleq \frac{\partial E\left(t_f\right)}{\partial l_p(\boldsymbol{\alpha})} = \frac{\alpha_T}{2\left(l_p\right)^2 c_p}\int_0^{t_f} a^{(1)}(t)E^2(t)dt \\ &= \frac{\alpha_T}{2\left(l_p\right)^2 c_p}\frac{P_0(\boldsymbol{\alpha})}{b(\boldsymbol{\alpha})}\left\{\frac{t_f}{2\cosh^2\left[t_f\tau(\boldsymbol{\alpha})/2\right]} - \frac{\tanh\left[t_f\tau(\boldsymbol{\alpha})/2\right]}{\tau(\boldsymbol{\alpha})}\right\}; \end{aligned} \tag{61}$$

$$\frac{\partial E(t_f)}{\partial \alpha_5} \triangleq \frac{\partial E(t_f)}{\partial \alpha_T} = -\frac{1}{2l_p c_p}\int_0^{t_f} a^{(1)}(t)E^2(t)dt$$
$$= -\frac{1}{2l_p c_p}\frac{P_0(\boldsymbol{\alpha})}{b(\boldsymbol{\alpha})}\left\{\frac{t_f}{2\cosh^2[t_f\tau(\boldsymbol{\alpha})/2]} - \frac{\tanh[t_f\tau(\boldsymbol{\alpha})/2]}{\tau(\boldsymbol{\alpha})}\right\}; \tag{62}$$

$$\frac{\partial E(t_f)}{\partial \alpha_6} \triangleq \frac{\partial E(t_f)}{\partial c_p} = \frac{\alpha_T}{2l_p (c_p)^2}\int_0^{t_f} a^{(1)}(t)E^2(t)dt$$
$$= \frac{\alpha_T}{2l_p (c_p)^2}\frac{P_0(\boldsymbol{\alpha})}{b(\boldsymbol{\alpha})}\left\{\frac{t_f}{2\cosh^2[t_f\tau(\boldsymbol{\alpha})/2]} - \frac{\tanh[t_f\tau(\boldsymbol{\alpha})/2]}{\tau(\boldsymbol{\alpha})}\right\}. \tag{63}$$

As $E(t_f)$ does not depend on the temperature $T(t)$, it follows that $\partial E(t_f)/\partial T_0 \equiv 0$. The expressions obtained in Equations (58)–(63) can be verified by differentiating the expression provided in Equation (44), evaluated at a user-chosen time $t = t_f$. Since this user-chosen time instance is arbitrary within the interval $0 < t_f < \infty$, it follows that the expressions of the sensitivities obtained in Equations (58)–(63) are also valid at any instance $t = t_f$.

In summary, the application of the 1st-CASAM-N necessitates a *single large-scale computation* (for solving the 1st-LASS) to obtain all of the six first-order sensitivities for the Nordheim–Fuchs reactor safety model. Using any other methods (e.g., statistical or finite-differences) would require at least 2 × 6 large-scale computations for solving the original model with altered parameter values if a simple two-point finite-difference scheme is used.

4. Illustrative Application of the 2nd-CASAM-N to Compute Second-Order Response Sensitivities

The fundamental principle of the 2nd-CASAM-N is to compute the second-order sensitivities by treating each first-order sensitivity as a "model response" and subsequently determining the G-differential of the respective "model response". These concepts will be illustrated in this Section by considering the first-order sensitivities of the response $E(t_f)$ obtained in Section 2 above.

The response $E(t_f)$ admits six non-zero sensitivities, as obtained in Equations (58)–(63). In principle, each of these non-zero sensitivities would be considered a response. Each of these responses would give rise to a 2nd-level adjoint sensitivity system (2nd-LASS), which means that, in principle, there would be six such systems to be solved to obtain the 2nd-level adjoint sensitivity function that would correspond to the respective response. However, writing Equation (53) in the following form:

$$\delta E(t_f) = \left[-\frac{\delta\alpha_T}{2l_p c_p} + \frac{\alpha_T}{2l_p (c_p)^2}\delta c_p + \frac{\alpha_T}{2(l_p)^2 c_p}\delta l_p\right]\int_0^{t_f} a^{(1)}(t)E^2(t)dt$$
$$+\left[\varphi_0\Sigma_f(\delta\gamma) + \varphi_0\gamma(\delta\Sigma_f) + \gamma\Sigma_f(\delta\varphi_0)\right]\int_0^{t_f} a^{(1)}(t)dt. \tag{64}$$

reveals that the indirect-effect terms for all of the 2nd-order sensitivities will arise from only two functionals that depend on the state functions, namely $\int_0^{t_f} a^{(1)}(t)dt$, which underlies the three non-zero first-order sensitivities with respect to the parameters comprising the initial power $P_0(\boldsymbol{\alpha})$, and $\int_0^{t_f} a^{(1)}(t)E^2(t)dt$, which underlies the remaining three non-zero first-order sensitivities. As the number of large-scale computations arises from solving the 2nd-LASS and as each indirect-effect term gives rise to a 2nd-LASS, it follows from Equation (64) that the number of 2nd-LASS that would need to be solved can be reduced to just two (from the possible total of six), thereby reducing the computational work by a factor of three.

4.1. Second-Order Sensitivities Stemming from the First-Order Sensitivities $\partial E\left(t_f\right)/\partial\alpha_{j_1}$, $j_1 = 1,2,3$

In this work, the index j_1 will be used to enumerate the 1st-order sensitivities of $E\left(t_f\right)$ with respect to the six model parameters. Recalling the definitions of the first three model parameters, i.e., $\alpha_1 \triangleq \gamma$, $\alpha_2 \triangleq \Sigma_f$, and $\alpha_3 \triangleq \varphi_0$, it follows from Equation (64) that the 1st-order sensitivities of the released energy $E\left(t_f\right)$ to the parameters underlying the reactor's initial power $P_0(\boldsymbol{\alpha}) = \gamma\Sigma_f\varphi_0$ can be written in the following form:

$$\begin{aligned}&\frac{\partial E(t_f)}{\partial\alpha_{j_1}} = C_{j_1}(\boldsymbol{\alpha})\int_0^{t_f} a^{(1)}(t)\,dt;\;\; j_1 = 1,2,3;\\ &C_1(\boldsymbol{\alpha}) \triangleq \varphi_0\Sigma_f;\;\; C_2(\boldsymbol{\alpha}) \triangleq \varphi_0\gamma;\;\; C_3(\boldsymbol{\alpha}) \triangleq \gamma\Sigma_f.\end{aligned} \tag{65}$$

The 2nd-order sensitivities which stem from the 1st-order ones defined in Equation (65) are obtained from the first-order G-differential $\delta\left\{\partial E\left(t_f\right)/\partial\alpha_i\right\}$, which is obtained, by definition, as follows:

$$\begin{aligned}&\delta\left\{\frac{\partial E(t_f)}{\partial\alpha_{j_1}}\right\} \triangleq \left\{\frac{d}{d\varepsilon}\left[C_{j_1}\left(\boldsymbol{\alpha}^0+\varepsilon\delta\boldsymbol{\alpha}\right)\int_0^{t_f}\left(a^{(1)}+\varepsilon\delta a^{(1)}\right)dt\right]\right\}_{\varepsilon=0}\\ &\triangleq \left\{\delta\left[\partial E\left(t_f\right)/\partial\alpha_{j_1}\right]\right\}_{dir} + \left\{\delta\left[\partial E\left(t_f\right)/\partial\alpha_{j_1}\right]\right\}_{ind},\;\; j_1 = 1,2,3;\end{aligned} \tag{66}$$

where

$$\left\{\delta\left[\partial E\left(t_f\right)/\partial\alpha_{j_1}\right]\right\}_{dir} \triangleq \left\{\left[\frac{\partial C_{j_1}(\boldsymbol{\alpha})}{\partial\boldsymbol{\alpha}}\delta\boldsymbol{\alpha}\right]\int_0^{t_f} a^{(1)}(t)dt\right\}_{\boldsymbol{\alpha}^0},\;\; j_1 = 1,2,3; \tag{67}$$

$$\left\{\delta\left[\partial E\left(t_f\right)/\partial\alpha_{j_1}\right]\right\}_{ind} \triangleq \left\{C_{j_1}(\boldsymbol{\alpha})J(E)\right\}_{\boldsymbol{\alpha}^0};\;\; J(E) \triangleq \int_0^{t_f}\delta a^{(1)}(t)dt;\;\; j_1 = 1,2,3. \tag{68}$$

The direct-effect term defined in Equation (67) can be computed immediately. The functional $J(E)$ defined in Equation (68) can be determined only after having computed the variational function $\delta a^{(1)}(t)$, which is the solution of the system of equations obtained by G-differentiating the 1st-LASS defined by Equations (51) and (52). Performing the G-differentiation of the 1st-LASS yields the following equations:

$$\left\{\left[-\frac{d}{dt} - 2b(\boldsymbol{\alpha})E(t)\right]\delta a^{(1)}(t) - 2b(\boldsymbol{\alpha})\delta E(t)\right\}_{\boldsymbol{\alpha}^0} = 2\{\delta b(\boldsymbol{\alpha})E(t)\}_{\boldsymbol{\alpha}^0},\;\; t>0, \tag{69}$$

$$\delta a^{(1)}\left(t_f\right) = 0,\;\; t = t_f \tag{70}$$

Concatenating Equations (69) and (70) with the 1st-LVSS for $\delta E(t)$ defined in Equations (49) and (50) yields the following 2nd-Level Variational Sensitivity System (2nd-LVSS) for the 2nd-level variational function $\mathbf{V}^{(2)}(2;t) \triangleq \left[v^{(2)}(1;t), v^{(2)}(2;t)\right]^{\dagger} \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^{\dagger}$:

$$\left\{\mathbf{VM}^{(2)}[2\times 2;\boldsymbol{\alpha}]\mathbf{V}^{(2)}(2;t)\right\}_{\boldsymbol{\alpha}^0} = \left\{\mathbf{Q}_V^{(2)}[2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\right\}_{\boldsymbol{\alpha}^0},\;\; t>0, \tag{71}$$

$$\left\{\mathbf{B}_V^{(2)}\left[2;\mathbf{V}^{(2)}(2;t);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0} = 0[2],\;\; 0[2] \triangleq [0,0]^{\dagger},\;\; t=0 \tag{72}$$

where

$$\mathbf{VM}^{(2)}[2\times 2;\boldsymbol{\alpha}] \triangleq \begin{pmatrix}\frac{d}{dt} - 2b(\boldsymbol{\alpha})E(t) & 0\\ -2b(\boldsymbol{\alpha}) & -\frac{d}{dt} - 2b(\boldsymbol{\alpha})E(t)\end{pmatrix} \tag{73}$$

$$\mathbf{Q}_V^{(2)}[2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}] \triangleq \begin{pmatrix}\delta b(\boldsymbol{\alpha})E^2(t) + \delta P_0(\boldsymbol{\alpha})\\ 2\delta b(\boldsymbol{\alpha})E(t)\end{pmatrix} \tag{74}$$

$$\mathbf{B}_V^{(2)}\left[2;\mathbf{V}^{(2)}(2;t);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right] \triangleq \begin{pmatrix} \delta E(0) \\ \delta a^{(1)}\left(t_f\right) \end{pmatrix} \tag{75}$$

The need for solving the 2nd-LVSS is circumvented by deriving an alternative expression for the functional $J(E)$ defined in Equation (68), in which the variational function $\delta a^{(1)}(t)$ is replaced by a 2nd-level adjoint function which will be denoted as $\mathbf{A}^{(2)}(2;t) \triangleq \left[a^{(2)}(1;t), a^{(2)}(2;t)\right]^{\dagger} \in \mathrm{H}_2$ and which will be the solution of a 2nd-Level Adjoint Sensitivity System (2nd-LASS) to be constructed by applying the 2nd-CASAM-N. The 2nd-LASS is constructed in a Hilbert space, denoted as H_2, which comprises as elements vectors of the same form as $\mathbf{V}^{(2)}(2;t)$, and is endowed with the following inner product of two vectors $\boldsymbol{\Psi}^{(2)}(2;t) \triangleq \left[\psi^{(2)}(1;t), \psi^{(2)}(2;t)\right]^{\dagger} \in \mathrm{H}_2$ and $\boldsymbol{\Phi}^{(2)}(t) \triangleq \left[\varphi^{(2)}(1;t), \varphi^{(2)}(2;t)\right]^{\dagger} \in \mathrm{H}_2$:

$$\left\langle \boldsymbol{\Psi}^{(2)}(2;t), \boldsymbol{\Phi}^{(2)}(2;t) \right\rangle_2 \triangleq \sum_{i=1}^{2} \int_0^{t_f} \psi^{(2)}(i;t)\varphi^{(2)}(i;t)dt \tag{76}$$

The inner product defined in Equation (76) is used to construct the 2nd-Level Adjoint Sensitivity System (2nd-LASS) for the 2nd-level adjoint function $\mathbf{A}^{(2)}(2;j_1 = 1,2,3;t) \triangleq \left[a^{(2)}(1;j_1 = 1,2,3;t), a^{(2)}(2;j_1 = 1,2,3;t)\right]^{\dagger} \in \mathrm{H}_2$, as follows:

(i) Using Equation (76), form the inner product of $\mathbf{A}^{(2)}(2;j_1 = 1,2,3;t) \triangleq \left[a^{(2)}(1;j_1 = 1,2,3;t), a^{(2)}(2;j_1 = 1,2,3;t)\right]^{\dagger}$ with Equation (71) to obtain the following relation:

$$\begin{array}{l} \left\{ \left\langle \mathbf{A}^{(2)}(2;t), \mathbf{VM}^{(2)}[2\times 2;\boldsymbol{\alpha}]\mathbf{V}^{(2)}(2;t) \right\rangle_2 \right\}_{\boldsymbol{\alpha}^0} = \left\{ a^{(2)}(1;t)\delta E(t) - a^{(2)}(2;t)\delta a^{(1)}(t) \right\}_{t=0}^{t=t_f} \\ +\left\{ \left\langle \mathbf{V}^{(2)}(2;t), \mathbf{AM}^{(2)}[2\times 2;\boldsymbol{\alpha}]\mathbf{A}^{(2)}(2;t) \right\rangle_2 \right\}_{\boldsymbol{\alpha}^0} = \left\{ \left\langle \mathbf{A}^{(2)}(2;t), \mathbf{Q}_V^{(2)}(2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}) \right\rangle_2 \right\}_{\boldsymbol{\alpha}^0}. \end{array} \tag{77}$$

The notation for $\mathbf{A}^{(2)}(2;j_1 = 1,2,3;t) \triangleq \left[a^{(2)}(1;j_1 = 1,2,3;t), a^{(2)}(2;j_1 = 1,2,3;t)\right]^{\dagger}$ has the following significance: (i) the letter "A" indicates "adjoint"; (ii) the superscript "(2)" indicates "second-level"; (iii) the first argument, i.e., "2", indicates that this vector has 2 components; (iv) the second argument, i.e., "$j_1 = 1,2,3$", indicates that this adjoint vector will correspond to the first three 1st-order sensitivities under consideration, in this case $\partial E\left(t_f\right)/\partial\alpha_{j_1}$, $j_1 = 1,2,3$. In the most general case, when all sensitivities have distinct "indirect-effect terms", there will be a distinct 2nd-level adjoint sensitivity vector of the same type as $\mathbf{A}^{(2)}(2;j_1 = 1,2,3;t)$, corresponding for each 1st-order sensitivity. Each of the components $a^{(2)}(i;j_1 = 1,2,3;t)$, $i = 1,2$, of $\mathbf{A}^{(2)}(2;j_1 = 1,2,3;t)$ are scalar-valued functions of time. The index $j_1 = 1,2,3$ will be omitted, for simplicity, in the derivations to follow below, but will be reinstated after obtaining the final closed-form expressions for the components $a^{(2)}(i;j_1 = 1,2,3;t)$.

(ii) Eliminate the boundary terms on the right side of Equation (77) and require the term on the right side of the second equality in Equation (77) to represent the functional $J\left(E_f\right)$, by imposing the following relations:

$$\left\{ \mathbf{AM}^{(2)}[2\times 2;\boldsymbol{\alpha}]\mathbf{A}^{(2)}(2;t) \right\}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{78}$$

$$\left\{ \mathbf{B}_A^{(2)}\left[2;\mathbf{A}^{(2)}(2;t);\boldsymbol{\alpha}\right] \right\}_{\boldsymbol{\alpha}^0} \triangleq \left\{ \begin{pmatrix} a^{(2)}\left(1;t_f\right) \\ a^{(2)}(2;0) \end{pmatrix} \right\}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{79}$$

where:

$$\mathbf{AM}^{(2)}[2\times 2;\boldsymbol{\alpha}] \triangleq \left[\mathbf{VM}^{(2)}(2\times 2;\boldsymbol{\alpha})\right]^{*} \triangleq \begin{pmatrix} -\frac{d}{dt} - 2b(\boldsymbol{\alpha})E(t) & -2b(\boldsymbol{\alpha}) \\ 0 & \frac{d}{dt} - 2b(\boldsymbol{\alpha})E(t) \end{pmatrix} \tag{80}$$

The relations represented by Equations (78) and (79) constitute the 2nd-LASS for the 2nd-level adjoint function $\mathbf{A}^{(2)}(2;t) \triangleq \left[a^{(2)}(1;t), a^{(2)}(2;t)\right]^{\dagger}$.

(iii) Use the relations provided in Equations (68) and (77) together with the 2nd-LASS to obtain the following expression for the functional $J(E)$ in terms of the 2nd-level adjoint function $\mathbf{A}^{(2)}(2;t)$:

$$J(E) = \{\delta P_0(\boldsymbol{\alpha}) J_1(\boldsymbol{\alpha}) + \delta b(\boldsymbol{\alpha}) J_2(\boldsymbol{\alpha})\}_{\boldsymbol{\alpha}^0} \tag{81}$$

where

$$\begin{aligned} &J_1(\boldsymbol{\alpha}) \triangleq \int_0^{t_f} a^{(2)}(1; j_1 = 1,2,3; t) dt; \\ &J_2(\boldsymbol{\alpha}) \triangleq \int_0^{t_f} \left[a^{(2)}(1; j_1 = 1,2,3; t) E^2(t) + 2a^{(2)}(2; j_1 = 1,2,3; t) E(t)\right] dt. \end{aligned} \tag{82}$$

In Equation (81), the 1st-level adjoint sensitivity function $a^{(1)}(t)$ is the solution of the 1st-LASS comprising Equations (51) and (52), while the 2nd-level adjoint sensitivity function $\mathbf{A}^{(2)}(2; j_1 = 1,2,3; t) \triangleq \left[a^{(2)}(1; j_1 = 1,2,3; t), a^{(2)}(2; j_1 = 1,2,3; t)\right]^{\dagger}$ is the solution of the 2nd-LVSS comprising Equations (78) and (79). Notably, the 2nd-LASS comprises Equations (78) and (79) is independent of parameter variations, so it needs to be solved just once to obtain the 2nd-level adjoint sensitivity function $\mathbf{A}^{(2)}(2; j_1 = 1,2,3; t)$. Furthermore, the 2nd-LASS is an upper-triangular system, so the equations need not solved simultaneously, but can be solved sequentially, first for the component $a^{(2)}(2;t)$ and subsequently for the component $a^{(2)}(1;t)$. This procedure yields the following closed-form expressions for the components of the 2nd-level adjoint sensitivity function:

$$a^{(2)}(1; j_1 = 1,2,3; t) = \frac{2b(\boldsymbol{\alpha})}{\tau^2(\boldsymbol{\alpha})} \left\{ -\cosh^2[t\tau(\boldsymbol{\alpha})/2] + \frac{\cosh^4\left[t_f \tau(\boldsymbol{\alpha})/2\right]}{\cosh^2[t\tau(\boldsymbol{\alpha})/2]} \right\} \tag{83}$$

$$a^{(2)}(2; j_1 = 1,2,3; t) = -\frac{1}{\tau(\boldsymbol{\alpha})} \sinh[\tau(\boldsymbol{\alpha}) t] \tag{84}$$

The components of $\mathbf{A}^{(2)}(2; j_1 = 1,2,3; t) \triangleq \left[a^{(2)}(1; j_1 = 1,2,3; t), a^{(2)}(2; j_1 = 1,2,3; t)\right]^{\dagger}$ are to be evaluated at the nominal parameter values, but the notation $\{\}_{\boldsymbol{\alpha}^0}$ has been omitted for simplicity.

Collecting the results obtained in Equations (67), (68) and (81) yields the expressions for the 2nd-order sensitivities, which stem from the first-order sensitivities $\partial E\left(t_f\right)/\partial \alpha_i$, $i = 1,2,3$, as presented below.

4.1.1. Second-Order Sensitivities Stemming from $\partial E\left(t_f\right)/\partial \alpha_1 \triangleq \partial E\left(t_f\right)/\partial \gamma$

Collecting the results for $j_1 = 1$ in Equations (67), (68), (81) and using the expressions provided in Equations (31) and (32) yields the following expression for the 2nd-order partial differential stemming from $\partial E\left(t_f\right)/\partial \alpha_1 \triangleq \partial E\left(t_f\right)/\partial \gamma$:

$$\begin{aligned} &\frac{\partial^2 E(t_f)}{\partial \boldsymbol{\alpha} \partial \gamma} \delta \boldsymbol{\alpha} = \left(\varphi_0 \partial \Sigma_f + \Sigma_f \partial \varphi_0\right) \int_0^{t_f} a^{(1)}(t) dt \\ &+\varphi_0 \Sigma_f \left\{ \gamma \Sigma_f (\delta \varphi_0) + \varphi_0 \Sigma_f (\delta \gamma) + \varphi_0 \gamma \left(\delta \Sigma_f\right) \right\} J_1(\boldsymbol{\alpha}) \\ &+\varphi_0 \Sigma_f \left[-\frac{\delta \alpha_T}{2 l_p c_p} + \frac{\alpha_T}{2 l_p \left(c_p\right)^2} \delta c_p + \frac{\alpha_T}{2 \left(l_p\right)^2 c_p} \delta l_p \right] J_2(\boldsymbol{\alpha}), \end{aligned} \tag{85}$$

Collecting the terms that multiply the same parameter variations on the left side and, respectively, right side of Equation (85) yields the following expressions for the respective 2nd-order partial sensitivities:

$$\frac{\partial^2 E\left(t_f\right)}{\partial\gamma\partial\gamma} = \left(\varphi_0\Sigma_f\right)^2 J_1(\boldsymbol{\alpha}) \quad (86)$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\Sigma_f\partial\gamma} = \varphi_0\int_0^{t_f} a^{(1)}(t)dt + (\varphi_0)^2\gamma\Sigma_f J_1(\boldsymbol{\alpha}) \quad (87)$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\varphi_0\partial\gamma} = \Sigma_f\int_0^{t_f} a^{(1)}(t)dt + \varphi_0\gamma\left(\Sigma_f\right)^2 J_1(\boldsymbol{\alpha}) \quad (88)$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial l_p\partial\gamma} = \frac{\varphi_0\Sigma_f\alpha_T}{2(l_p)^2 c_p} J_2(\boldsymbol{\alpha}) \quad (89)$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\alpha_T\partial\gamma} = -\frac{\varphi_0\Sigma_f}{2l_p c_p} J_2(\boldsymbol{\alpha}) \quad (90)$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial c_p\partial\gamma} = \frac{\varphi_0\Sigma_f\alpha_T}{2l_p(c_p)^2} J_2(\boldsymbol{\alpha}) \quad (91)$$

4.1.2. Second-Order Sensitivities Stemming from $\partial E\left(t_f\right)/\partial\alpha_2 \triangleq \partial E\left(t_f\right)/\partial\Sigma_f$

Collecting the results for $j_1 = 2$ in Equations (67), (68), (81) and using the expressions provided in Equations (31) and (32) yields the following expressions for the 2nd-order partial differential stemming from $\partial E\left(t_f\right)/\partial\alpha_2 \triangleq \partial E\left(t_f\right)/\partial\Sigma_f$:

$$\begin{aligned}\frac{\partial^2 E(t_f)}{\partial\boldsymbol{\alpha}\partial\Sigma_f}\delta\boldsymbol{\alpha} &= (\varphi_0\delta\gamma + \gamma\delta\varphi_0)\int_0^{t_f} a^{(1)}(t)dt \\ &+\varphi_0\gamma\left[\gamma\Sigma_f(\delta\varphi_0) + \varphi_0\Sigma_f(\delta\gamma) + \varphi_0\gamma\left(\delta\Sigma_f\right)\right]J_1(\boldsymbol{\alpha}) \\ &+\varphi_0\gamma\left[-\frac{\delta\alpha_T}{2l_p c_p} + \frac{\alpha_T}{2l_p(c_p)^2}\delta c_p + \frac{\alpha_T}{2(l_p)^2 c_p}\delta l_p\right]J_2(\boldsymbol{\alpha}).\end{aligned} \quad (92)$$

Collecting the terms that multiply the same parameter variations on the left side and, respectively, right side of Equation (92) yields the following expressions for the respective 2nd-order partial sensitivities:

$$\frac{\partial^2 E\left(t_f\right)}{\partial\gamma\partial\Sigma_f} = \varphi_0\int_0^{t_f} a^{(1)}(t)dt + (\varphi_0)^2\gamma\Sigma_f J_1(\boldsymbol{\alpha}) \quad (93)$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\Sigma_f\partial\Sigma_f} = (\varphi_0\gamma)^2 J_1(\boldsymbol{\alpha}) \quad (94)$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\varphi_0\partial\Sigma_f} = \gamma\int_0^{t_f} a^{(1)}(t)dt + \gamma^2\varphi_0\Sigma_f J_1(\boldsymbol{\alpha}) \quad (95)$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial l_p\partial\Sigma_f} = \frac{\varphi_0\gamma\alpha_T}{2(l_p)^2 c_p} J_2(\boldsymbol{\alpha}) \quad (96)$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial \alpha_T \partial \Sigma_f} = -\frac{\varphi_0 \gamma}{2 l_p c_p} J_2(\boldsymbol{\alpha}) \tag{97}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial c_p \partial \Sigma_f} = \frac{\varphi_0 \gamma \alpha_T}{2 l_p \left(c_p\right)^2} J_2(\boldsymbol{\alpha}) \tag{98}$$

4.1.3. Second-Order Sensitivities Stemming from $\partial E\left(t_f\right)/\partial \alpha_3 \triangleq \partial E\left(t_f\right)/\partial \varphi_0$

Collecting the results for $j_1 = 3$ in Equations (67), (68), (81), and using the expressions provided in Equations (31) and (32) yields the following expressions for the 2nd-order partial differential stemming from $\partial E\left(t_f\right)/\partial \alpha_3 \triangleq \partial E\left(t_f\right)/\partial \varphi_0$:

$$\begin{aligned} &\frac{\partial^2 E(t_f)}{\partial \boldsymbol{\alpha} \partial \varphi_0} \delta \boldsymbol{\alpha} \triangleq \left(\gamma \delta \Sigma_f + \Sigma_f \delta \gamma\right) \int_0^{t_f} a^{(1)}(t) dt \\ &+ \gamma \Sigma_f \left[\gamma \Sigma_f (\delta \varphi_0) + \varphi_0 \Sigma_f (\delta \gamma) + \varphi_0 \gamma \left(\delta \Sigma_f\right)\right] J_1(\boldsymbol{\alpha}) \\ &+ \gamma \Sigma_f \left[-\frac{\delta \alpha_T}{2 l_p c_p} + \frac{\alpha_T}{2 l_p \left(c_p\right)^2} \delta c_p + \frac{\alpha_T}{2 \left(l_p\right)^2 c_p} \delta l_p\right] J_2(\boldsymbol{\alpha}). \end{aligned} \tag{99}$$

Collecting the terms that multiply the same parameter variations on the left side and, respectively, right side of Equation (99) yields the following expressions for the respective 2nd-order partial sensitivities:

$$\frac{\partial^2 E\left(t_f\right)}{\partial \gamma \partial \varphi_0} = \Sigma_f \int_0^{t_f} a^{(1)}(t) dt + \left(\Sigma_f\right)^2 \varphi_0 \gamma J_1(\boldsymbol{\alpha}) \tag{100}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial \Sigma_f \partial \varphi_0} = \gamma \int_0^{t_f} a^{(1)}(t) dt + \gamma^2 \Sigma_f \varphi_0 J_1(\boldsymbol{\alpha}) \tag{101}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial \varphi_0 \partial \varphi_0} = \left(\gamma \Sigma_f\right)^2 J_1(\boldsymbol{\alpha}) \tag{102}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial l_p \partial \varphi_0} = \frac{\gamma \Sigma_f \alpha_T}{2 \left(l_p\right)^2 c_p} J_2(\boldsymbol{\alpha}) \tag{103}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial \alpha_T \partial \varphi_0} = -\frac{\gamma \Sigma_f}{2 l_p c_p} J_2(\boldsymbol{\alpha}) \tag{104}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial c_p \partial \varphi_0} = \frac{\gamma \Sigma_f \alpha_T}{2 l_p \left(c_p\right)^2} J_2(\boldsymbol{\alpha}) \tag{105}$$

4.2. Second-Order Sensitivities Stemming from the First-Order Sensitivities $\partial E\left(t_f\right)/\partial \alpha_{j_1}$, $j_1 = 4, 5, 6$

Recalling the definitions of the first three model parameters, i.e., $\alpha_4 \triangleq l_p$, $\alpha_5 \triangleq \alpha_T$, and $\alpha_6 \triangleq c_p$, it follows from Equation (64) that the 1st-order sensitivities $\partial E\left(t_f\right)/\partial l_p$, $\partial E\left(t_f\right)/\partial \alpha_T$ and $\partial E\left(t_f\right)/\partial c_p$ can be written in the following form:

$$\begin{aligned} &\frac{\partial E(t_f)}{\partial \alpha_{j_1}} = C_{j_1}(\boldsymbol{\alpha}) \int_0^{t_f} a^{(1)}(t) E^2(t) dt; \;\; j_1 = 4, 5, 6; \\ &C_4(\boldsymbol{\alpha}) \triangleq \frac{\alpha_T}{2\left(l_p\right)^2 c_p}; \;\; C_5(\boldsymbol{\alpha}) \triangleq -\frac{1}{2 l_p c_p}; \;\; C_6(\boldsymbol{\alpha}) \triangleq \frac{\alpha_T}{2 l_p \left(c_p\right)^2}. \end{aligned} \tag{106}$$

The 2nd-order sensitivities which stem from the 1st-order ones defined in Equation (106) are obtained by applying the definition of the first-order G-differential to Equation (106), which yields the following relations:

$$\begin{aligned}&\delta\left\{\frac{\partial E(t_f)}{\partial\alpha_{j_1}}\right\} \triangleq \left\{\frac{d}{d\varepsilon}\left[C_{j_1}\left(\boldsymbol{\alpha}^0+\varepsilon\delta\boldsymbol{\alpha}\right)\int_0^{t_f}\left(a^{(1)}+\varepsilon\delta a^{(1)}\right)[E(t)+\varepsilon\delta E(t)]^2 dt\right]\right\}_{\varepsilon=0}\\ &\triangleq \left\{\delta\left[\partial E\left(t_f\right)/\partial\alpha_{j_1}\right]\right\}_{dir}+\left\{\delta\left[\partial E\left(t_f\right)/\partial\alpha_{j_1}\right]\right\}_{ind},\quad j_1=4,5,6,\end{aligned} \tag{107}$$

where

$$\left\{\delta\left[\partial E\left(t_f\right)/\partial\alpha_{j_1}\right]\right\}_{dir} \triangleq \left\{\left[\frac{\partial C_{j_1}(\boldsymbol{\alpha})}{\partial\boldsymbol{\alpha}}\delta\boldsymbol{\alpha}\right]\int_0^{t_f} a^{(1)}(t)E^2(t)dt\right\}_{\boldsymbol{\alpha}^0},\quad j_1=4,5,6; \tag{108}$$

$$\begin{aligned}&\left\{\delta\left[\partial E\left(t_f\right)/\partial\alpha_{j_1}\right]\right\}_{ind} \triangleq \left\{C_{j_1}(\boldsymbol{\alpha})K(E)\right\}_{\boldsymbol{\alpha}^0};\ j_1=4,5,6;\\ &K(E)\triangleq\int_0^{t_f}\left[\delta a^{(1)}(t)E^2(t)+2a^{(1)}(t)E(t)\delta E(t)\right]dt.\end{aligned} \tag{109}$$

The direct-effect term defined in Equation (108) can be computed immediately. The functional $K(E)$ defined in Equation (109) can be determined only after solving the 2nd-Level Variational Sensitivity System (2nd-LVSS) defined by Equations (71) and (72) to obtain the 2nd-level variational function $\mathbf{V}^{(2)}(2;t) \triangleq \left[v^{(2)}(1;t), v^{(2)}(2;t)\right]^\dagger \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^\dagger$.

As before, the need for solving the 2nd-LVSS is circumvented by deriving an alternative expression for the functional $K(E)$, in which the variational function $\mathbf{V}^{(2)}(2;t)$ is replaced by a 2nd-level adjoint function denoted as $\mathbf{A}^{(2)}(2;j_1=4,5,6;t) \triangleq \left[a^{(2)}(1;j_1=4,5,6;t), a^{(2)}(2;j_1=4,5,6;t)\right]^\dagger \in \mathrm{H}_2$, which will be the solution of a 2nd-Level Adjoint Sensitivity System (2nd-LASS) to be constructed by applying the 2nd-CASAM-N. The 2nd-LASS is constructed in the same Hilbert space, which was denoted as H_2 in the previous subsection, and which is endowed with the inner product defined in Equation (76). This inner product is used to construct the 2nd-Level Adjoint Sensitivity System (2nd-LASS) for the 2nd-level adjoint function $\mathbf{A}^{(2)}(2;j_1=4,5,6;t)$, as follows:

(i) Using Equation (76), form the inner product of $\mathbf{A}^{(2)}(2;j_1=4,5,6;t)$ with Equation (71) to obtain the following relation, which has the same form as shown in Equation (77), namely:

$$\begin{aligned}&\left\{\left\langle\mathbf{A}^{(2)}(2;j_1=4,5,6;t),\mathbf{VM}^{(2)}[2\times2;\boldsymbol{\alpha}]\mathbf{V}^{(2)}(2;t)\right\rangle_2\right\}_{\boldsymbol{\alpha}^0}\\ &=\left\{a^{(2)}(1;j_1=4,5,6;t)\delta E(t)-a^{(2)}(2;j_1=4,5,6;t)\delta a^{(1)}(t)\right\}_{t=0}^{t=t_f}\\ &+\left\{\left\langle\mathbf{V}^{(2)}(2;t),\mathbf{AM}^{(2)}[2\times2;\boldsymbol{\alpha}]\mathbf{A}^{(2)}(2;j_1=4,5,6;t)\right\rangle_2\right\}_{\boldsymbol{\alpha}^0}\\ &=\left\{\left\langle\mathbf{A}^{(2)}(2;j_1=4,5,6;t),\mathbf{Q}_V^{(2)}(2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha})\right\rangle_2\right\}_{\boldsymbol{\alpha}^0},\end{aligned} \tag{110}$$

where the operator $\mathbf{AM}^{(2)}[2\times2;\boldsymbol{\alpha}]$ has the same expression as defined in Equation (80).

(ii) Eliminate the boundary terms on the right side of Equation (110) and require the term on the right side of the second equality in Equation (110) to represent the functional $K(E)$, by imposing the following relations:

$$\left\{\mathbf{AM}^{(2)}[2\times2;\boldsymbol{\alpha}]\mathbf{A}^{(2)}(2;j_1=4,5,6;t)\right\}_{\boldsymbol{\alpha}^0}=\left\{\begin{pmatrix}2a^{(1)}(t)E(t)\\ E^2(t)\end{pmatrix}\right\}_{\boldsymbol{\alpha}^0} \tag{111}$$

$$\left\{\mathbf{B}_A^{(2)}\left[2;\mathbf{A}^{(2)}(2;j_1=4,5,6;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0}\triangleq\left\{\begin{pmatrix}a^{(2)}\left(1;j_1=4,5,6;t_f\right)\\ a^{(2)}(2;j_1=4,5,6;0)\end{pmatrix}\right\}_{\boldsymbol{\alpha}^0}=\begin{pmatrix}0\\0\end{pmatrix} \tag{112}$$

The relations represented by Equations (111) and (112) constitute the 2nd-LASS for the function, the 2nd-level adjoint function $\mathbf{A}^{(2)}(2;j_1=4,5,6;t)$. Notably, the 2nd-LASS is independent of parameter variations, so it needs to be solved just once to obtain

$\mathbf{A}^{(2)}(2; j_1 = 4,5,6; t)$. Furthermore, the 2nd-LASS is an upper-triangular system, so the equations need not be solved simultaneously but can be solved sequentially, first for the component $\psi^{(2)}(2;t)$ and subsequently for the component $\psi^{(2)}(1;t)$.

(iii) Use the relations provided in Equations (110) and (109) together with Equations (111) and (112) to obtain the following expression for the functional $K(E)$ in terms of the 2nd-level adjoint function $\mathbf{A}^{(2)}(2; j_1 = 4,5,6; t)$:

$$K(E) = \{\delta P_0(\boldsymbol{\alpha})K_1(\boldsymbol{\alpha}) + \delta b(\boldsymbol{\alpha})K_2(\boldsymbol{\alpha})\}_{\boldsymbol{\alpha}^0} \tag{113}$$

where

$$\begin{aligned} &K_1(\boldsymbol{\alpha}) \triangleq \int_0^{t_f} a^{(2)}(1; j_1 = 4,5,6; t)dt; \\ &K_2(\boldsymbol{\alpha}) \triangleq \int_0^{t_f} \left[a^{(2)}(1; j_1 = 4,5,6; t)E^2(t) + 2a^{(2)}(2; j_1 = 4,5,6; t)E(t)\right]dt. \end{aligned} \tag{114}$$

Solving Equations (111) and (112) yields the following closed-form expressions for the components of the 2nd-level adjoint sensitivity function $\mathbf{A}^{(2)}(2; j_1 = 4,5,6; t)$:

$$\begin{aligned} &a^{(2)}(1; j_1 = 4,5,6; t) = \cosh^{-2}\left[\tfrac{\tau(\boldsymbol{\alpha})t}{2}\right] \\ &\times \int_t^{t_f} \left[2a^{(1)}(x)E(x) + 2b(\boldsymbol{\alpha})\psi^{(2)}(2;x)\right]\cosh^2\left[\tfrac{\tau(\boldsymbol{\alpha})x}{2}\right]dx \\ &= \cosh^{-2}(\tau t/2)\left\{\tfrac{8P_0}{\tau^2}\left[1 - \tfrac{\cosh(\tau t/2)}{\cosh\left(\tau t_f/2\right)}\right] + \tfrac{8b}{3\tau^2}\left(\tfrac{2P_0}{\tau}\right)^2\left[\tfrac{1}{2}\cosh^2\left(\tau t_f/2\right)\right.\right. \\ &\quad \left.\left. - \tfrac{1}{2}\cosh^2(\tau t/2) - \ln\tfrac{\cosh\left(\tau t_f/2\right)}{\cosh(\tau t/2)}\right]\right\}; \end{aligned} \tag{115}$$

$$\begin{aligned} &a^{(2)}(2; j_1 = 4,5,6; t) = \cosh^2[\tau(\boldsymbol{\alpha})t/2]\int_0^t E^2(x)\cosh^{-2}[\tau(\boldsymbol{\alpha})x/2]dx \\ &= \tfrac{2}{3\tau(\boldsymbol{\alpha})}\left[\tfrac{2P_0(\boldsymbol{\alpha})}{\tau(\boldsymbol{\alpha})}\right]^2 \tanh[\tau(\boldsymbol{\alpha})t/2]\sinh^2[\tau(\boldsymbol{\alpha})t/2]. \end{aligned} \tag{116}$$

Collecting the results obtained in Equations (108), (109), and (113) yields the expressions for the 2nd-order sensitivities, which stem from the first-order sensitivities $\partial E\left(t_f\right)/\partial\alpha_{j_1}$, $j_1 = 4,5,6$, as presented below.

4.2.1. Second-Order Sensitivities Stemming from $\partial E\left(t_f\right)/\partial\alpha_4 \triangleq \partial E\left(t_f\right)/\partial l_p$

Collecting the results for $j_1 = 4$ in Equations (107)−(109), (113), and using the expressions provided in Equations (31) and (32) yields the following expressions for the 2nd-order partial differential stemming from $\partial E\left(t_f\right)/\partial\alpha_4 \triangleq \partial E\left(t_f\right)/\partial l_p$:

$$\begin{aligned} \frac{\partial^2 E\left(t_f\right)}{\partial\boldsymbol{\alpha}\partial l_p}\delta\boldsymbol{\alpha} \triangleq &\left[\frac{\delta\alpha_T}{2\left(l_p\right)^2 c_p} - \frac{\alpha_T\delta c_p}{2\left(l_p c_p\right)^2} - \frac{\alpha_T\delta l_p}{\left(l_p\right)^3 c_p}\right]\int_0^{t_f} a^{(1)}(t)E^2(t)dt \\ &+ C_4(\boldsymbol{\alpha})\left[\gamma\Sigma_f(\delta\varphi_0) + \varphi_0\Sigma_f(\delta\gamma) + \varphi_0\gamma\left(\delta\Sigma_f\right)\right]K_1(\boldsymbol{\alpha}) \\ &+ C_4(\boldsymbol{\alpha})\left[-\frac{\delta\alpha_T}{2l_p c_p} + \frac{\alpha_T}{2l_p\left(c_p\right)^2}\delta c_p + \frac{\alpha_T}{2\left(l_p\right)^2 c_p}\delta l_p\right]K_2(\boldsymbol{\alpha}). \end{aligned} \tag{117}$$

Collecting the terms that multiply the same parameter variations on the left side and, respectively, right side of Equation (117) yields the following expressions for the respective 2nd-order partial sensitivities:

$$\frac{\partial^2 E\left(t_f\right)}{\partial\gamma\partial l_p} = \Sigma_f\varphi_0 C_4(\boldsymbol{\alpha})K_1(\boldsymbol{\alpha}) \tag{118}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\Sigma_f\partial l_p} = \gamma\varphi_0 C_4(\boldsymbol{\alpha})K_1(\boldsymbol{\alpha}) \tag{119}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial \varphi_0 \partial l_p} = \gamma \Sigma_f C_4(\boldsymbol{\alpha}) K_1(\boldsymbol{\alpha}) \tag{120}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial l_p \partial l_p} = -\frac{\alpha_T}{\left(l_p\right)^3 c_p} \int_0^{t_f} a^{(1)}(t) E^2(t) dt + \frac{\alpha_T C_4(\boldsymbol{\alpha})}{2\left(l_p\right)^2 c_p} K_2(\boldsymbol{\alpha}) \tag{121}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial \alpha_T \partial l_p} = \frac{1}{2\left(l_p\right)^2 c_p} \int_0^{t_f} a^{(1)}(t) E^2(t) dt - \frac{C_4(\boldsymbol{\alpha})}{2 l_p c_p} K_2(\boldsymbol{\alpha}) \tag{122}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial c_p \partial l_p} = -\frac{\alpha_T}{2\left(l_p c_p\right)^2} \int_0^{t_f} a^{(1)}(t) E^2(t) dt + \frac{\alpha_T C_4(\boldsymbol{\alpha})}{2 l_p \left(c_p\right)^2} K_2(\boldsymbol{\alpha}) \tag{123}$$

4.2.2. Second-Order Sensitivities Stemming from $\partial E\left(t_f\right) / \partial \alpha_5 \triangleq \partial E\left(t_f\right) / \partial \alpha_T$

Collecting the results for $j_1 = 5$ in Equations (107)–(109), (113), and using the expressions provided in Equations (31) and (32) yields the following expressions for the 2nd-order partial differential stemming from $\partial E\left(t_f\right) / \partial \alpha_5 \triangleq \partial E\left(t_f\right) / \partial \alpha_T$:

$$\begin{aligned} \frac{\partial^2 E\left(t_f\right)}{\partial \boldsymbol{\alpha} \partial \alpha_T} \delta \boldsymbol{\alpha} \triangleq & \left[\frac{\delta l_p}{2\left(l_p\right)^2 c_p} + \frac{\delta c_p}{2 l_p \left(c_p\right)^2}\right] \int_0^{t_f} a^{(1)}(t) E^2(t) dt \\ & + C_5(\boldsymbol{\alpha}) \left[\gamma \Sigma_f (\delta \varphi_0) + \varphi_0 \Sigma_f (\delta \gamma) + \varphi_0 \gamma \left(\delta \Sigma_f\right)\right] K_1(\boldsymbol{\alpha}) \\ & + C_5(\boldsymbol{\alpha}) \left[-\frac{\delta \alpha_T}{2 l_p c_p} + \frac{\alpha_T}{2 l_p \left(c_p\right)^2} \delta c_p + \frac{\alpha_T}{2\left(l_p\right)^2 c_p} \delta l_p\right] K_2(\boldsymbol{\alpha}). \end{aligned} \tag{124}$$

Collecting the terms that multiply the same parameter variations on the left side and, respectively, right side of Equation (124) yields the following expressions for the respective 2nd-order partial sensitivities:

$$\frac{\partial^2 E\left(t_f\right)}{\partial \gamma \partial \alpha_T} = \Sigma_f \varphi_0 C_5(\boldsymbol{\alpha}) K_1(\boldsymbol{\alpha}) \tag{125}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial \Sigma_f \partial \alpha_T} = \gamma \varphi_0 C_5(\boldsymbol{\alpha}) K_1(\boldsymbol{\alpha}) \tag{126}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial \varphi_0 \partial \alpha_T} = \gamma \Sigma_f C_5(\boldsymbol{\alpha}) K_1(\boldsymbol{\alpha}) \tag{127}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial l_p \partial \alpha_T} = \frac{1}{2\left(l_p\right)^2 c_p} \int_0^{t_f} a^{(1)}(t) E^2(t) dt + \frac{\alpha_T C_5(\boldsymbol{\alpha})}{2\left(l_p\right)^2 c_p} K_2(\boldsymbol{\alpha}) \tag{128}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial \alpha_T \partial \alpha_T} = \frac{1}{2\left(l_p\right)^2 c_p} \int_0^{t_f} a^{(1)}(t) E^2(t) dt - \frac{C_5(\boldsymbol{\alpha})}{2 l_p c_p} K_2(\boldsymbol{\alpha}) \tag{129}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial c_p \partial \alpha_T} = \frac{1}{2 l_p \left(c_p\right)^2} \int_0^{t_f} a^{(1)}(t) E^2(t) dt + \frac{\alpha_T C_5(\boldsymbol{\alpha})}{2 l_p \left(c_p\right)^2} K_2(\boldsymbol{\alpha}) \tag{130}$$

4.2.3. Second-Order Sensitivities Stemming from $\partial E\left(t_f\right)/\partial\alpha_6 \triangleq \partial E\left(t_f\right)/\partial c_p$

Collecting the results for $j_1 = 6$ in Equations (107)–(109), (113), and using the expressions provided in Equations (31) and (32) yields the following expressions for the 2nd-order partial differential stemming from $\partial E\left(t_f\right)/\partial\alpha_6 \triangleq \partial E\left(t_f\right)/\partial c_p$:

$$\begin{aligned} \frac{\partial^2 E(t_f)}{\partial\boldsymbol{\alpha}\partial c_p}\delta\boldsymbol{\alpha} \triangleq & \left[\frac{\delta\alpha_T}{2l_p(c_p)^2} - \frac{\alpha_T\delta l_p}{2(l_p c_p)^2} - \frac{\alpha_T\delta c_p}{l_p(c_p)^3}\right]\int_0^{t_f} a^{(1)}(t)E^2(t)dt \\ & + C_6(\boldsymbol{\alpha})\left[\gamma\Sigma_f(\delta\varphi_0) + \varphi_0\Sigma_f(\delta\gamma) + \varphi_0\gamma\left(\delta\Sigma_f\right)\right]K_1(\boldsymbol{\alpha}) \\ & + C_6(\boldsymbol{\alpha})\left[-\frac{\delta\alpha_T}{2l_p c_p} + \frac{\alpha_T}{2l_p(c_p)^2}\delta c_p + \frac{\alpha_T}{2(l_p)^2 c_p}\delta l_p\right]K_2(\boldsymbol{\alpha}). \end{aligned} \tag{131}$$

Collecting the terms that multiply the same parameter variations on the left side and, respectively, right side of Equation (131) yields the following expressions for the respective 2nd-order partial sensitivities:

$$\frac{\partial^2 E\left(t_f\right)}{\partial\gamma\partial c_p} = \Sigma_f\varphi_0 C_6(\boldsymbol{\alpha})K_1(\boldsymbol{\alpha}) \tag{132}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\Sigma_f\partial c_p} = \gamma\varphi_0 C_6(\boldsymbol{\alpha})K_1(\boldsymbol{\alpha}) \tag{133}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\varphi_0\partial c_p} = \gamma\Sigma_f C_6(\boldsymbol{\alpha})K_1(\boldsymbol{\alpha}) \tag{134}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial l_p\partial c_p} = -\frac{\alpha_T}{2(l_p c_p)^2}\int_0^{t_f} a^{(1)}(t)E^2(t)dt + \frac{\alpha_T C_6(\boldsymbol{\alpha})}{2(l_p)^2 c_p}K_2(\boldsymbol{\alpha}) \tag{135}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\alpha_T\partial c_p} = \frac{1}{2l_p(c_p)^2}\int_0^{t_f} a^{(1)}(t)E^2(t)dt - \frac{C_6(\boldsymbol{\alpha})}{2l_p c_p}K_2(\boldsymbol{\alpha}) \tag{136}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial c_p\partial c_p} = -\frac{\alpha_T}{l_p(c_p)^3}\int_0^{t_f} a^{(1)}(t)E^2(t)dt + \frac{\alpha_T C_6(\boldsymbol{\alpha})}{2l_p(c_p)^2}K_2(\boldsymbol{\alpha}) \tag{137}$$

4.3. Computational Advantages of Using the 2nd-CASAM-N

"Large-scale" computations are those needed to solve differential and/or integral equations, such as those underlying the original model and the 1st-LASS. By comparison, the computational effort involved in evaluating integrals by means of quadrature formulas are "small-scale". The application of the 1st-CASAM-N has shown that a single large-scale computation needed to solve the 1st-LASS to obtain the 1st-level adjoint sensitivity function suffices to obtain all of the 1st-order sensitivities of a model response with respect to the underlying model parameters, which are computed using quadrature formulas to evaluate integrals involving the 1st-level adjoint sensitivity function. Using any other methods (e.g., statistical methods or finite-difference methods) would require at least as many large-scale computations—for solving the original model with altered parameter values—as there are model parameters.

Each of the first-order sensitivities becomes the "model response" for the application of the 2nd-CASAM-N. If all of the first-order sensitivities have differing (among each other) functional dependencies on the original state functions and 1st-level adjoint sensitivity functions, then there will be as many 2nd-Level Adjoint Systems to be solved as there are 1st-order sensitivities. Notably, all of these 2nd-LASS have the same left side; only the sources on the right sides of these 2nd-LASS would differ from each other, each source stemming from one of the distinct 1st-level sensitivities. Thus, the same software package would be used to invert the (matrix-valued) operator on the left side of the 2nd-LASS.

In most practical situations, however, the 1st-order sensitivities do share common expressions involving the original state functions and 1st-level adjoint sensitivity functions. For the paradigm Nordheim–Fuchs model, the sensitivities $\partial E\left(t_f\right)/\partial\alpha_{j_1}$, $j_1 = 1,2,3$, have in common the functional $J(E)$, while the sensitivities $\partial E\left(t_f\right)/\partial\alpha_{j_1}$, $j_1 = 4,5,6$, have in common the functional $K(E)$. In such cases, the number of 2nd-level adjoint sensitivity functions (and corresponding large-scale computations) is reduced considerably; in the case of the Nordheim–Fuchs model, the number of large-scale computations is reduced by a factor of 3 (from 6 to 2), as illustrated in Section 4.2.

As has been illustrated in Section 4.2, one adjoint computation for solving the 2nd-LASS for a selected 1st-order sensitivity provides the 2nd-level adjoint needed for computing all of the partial 2nd-order sensitivities stemming from the selected 1st-order sensitivities. The order of priority of computing the 2nd-order sensitivities should be established in the ranking order of the magnitude of the 1st-order sensitivities: thus, the 2nd-order sensitivities stemming from the largest (in absolute value) 1st-order sensitivity should be computed with the highest priority, the 2nd-order sensitivities stemming from the next-largest (in absolute value) 1st-order sensitivity should be computed next, and so on. The user may decide if any of the 1st-order sensitivities would be sufficiently insignificant to be neglected in this process.

As there are 6 first-order sensitivities, there will be 36 second-order sensitivities, of which 21 are distinct from one another. As illustrated by the results obtained in Section 4.2, the unmixed 2ndorder sensitivities of the form $\partial^2 E\left(t_f\right)/\partial\alpha_{j_1}\partial\alpha_{j_1}$, $j_1 = 1,\ldots,6$, have individually distinct expressions, each involving the 2nd-level adjoint sensitivity function corresponding to the originating 1st-order sensitivities. In contradistinction, the mixed 2nd-order sensitivities $\partial^2 E\left(t_f\right)/\partial\alpha_{j_2}\partial\alpha_{j_1}$, $j_2 \neq j_1 = 1,\ldots,6$, are obtained twice, using distinct (in general) 2nd-level adjoint systems. Occasionally, although obtained following two different computational paths, some of these mixed sensitivities have the same expression, as exemplified by the 2nd-order sensitivities, which involve the functionals $J_1(\boldsymbol{\alpha})$ and $K_2(\boldsymbol{\alpha})$, respectively, as shown below:

$$\frac{\partial^2 E\left(t_f\right)}{\partial\Sigma_f\partial\gamma} = \varphi_0\int_0^{t_f} a^{(1)}(t)dt + (\varphi_0)^2\gamma\Sigma_f J_1(\boldsymbol{\alpha}) = \frac{\partial^2 E\left(t_f\right)}{\partial\gamma\partial\Sigma_f} \tag{138}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\varphi_0\partial\gamma} = \Sigma_f\int_0^{t_f} a^{(1)}(t)dt + \varphi_0\gamma\left(\Sigma_f\right)^2 J_1(\boldsymbol{\alpha}) = \frac{\partial^2 E\left(t_f\right)}{\partial\gamma\partial\varphi_0} \tag{139}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\varphi_0\partial\Sigma_f} = \gamma\int_0^{t_f} a^{(1)}(t)dt + \gamma^2\varphi_0\Sigma_f J_1(\boldsymbol{\alpha}) = \frac{\partial^2 E\left(t_f\right)}{\partial\Sigma_f\partial\varphi_0} \tag{140}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial\alpha_T\partial l_p} = \frac{1}{2\left(l_p\right)^2 c_p}\int_0^{t_f} a^{(1)}(t)E^2(t)dt - \frac{C_4(\boldsymbol{\alpha})}{2l_p c_p}K_2(\boldsymbol{\alpha}) = \frac{\partial^2 E\left(t_f\right)}{\partial l_p\partial\alpha_T} \tag{141}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial c_p\partial l_p} = -\frac{\alpha_T}{2\left(l_p c_p\right)^2}\int_0^{t_f} a^{(1)}(t)E^2(t)dt + \frac{\alpha_T C_4(\boldsymbol{\alpha})}{2l_p\left(c_p\right)^2}K_2(\boldsymbol{\alpha}) = \frac{\partial^2 E\left(t_f\right)}{\partial l_p\partial c_p} \tag{142}$$

$$\frac{\partial^2 E\left(t_f\right)}{\partial c_p\partial\alpha_T} = \frac{1}{2l_p\left(c_p\right)^2}\int_0^{t_f} a^{(1)}(t)E^2(t)dt + \frac{\alpha_T C_5(\boldsymbol{\alpha})}{2l_p\left(c_p\right)^2}K_2(\boldsymbol{\alpha}) = \frac{\partial^2 E\left(t_f\right)}{\partial\alpha_T\partial c_p} \tag{143}$$

In most cases, however, the mixed sensitivities have distinct expressions involving distinct adjoint functions, as is apparent from the results obtained in Section 4.2. In all cases, though, the symmetry property $\partial^2 E\left(t_f\right)/\partial\alpha_{j_1}\partial\alpha_{j_2} = \partial^2 E\left(t_f\right)/\partial\alpha_{j_2}\partial\alpha_{j_1}$ provides an intrinsic verification procedure for assessing the accuracy of computing the respective 2nd-level adjoint sensitivity functions. Furthermore, the user can select which of the alternative −but equivalent− expressions of the 2nd-order mixed sensitivity under consideration is computationally more advantageous to use. For example, the expressions in Equations (118) and (89) must be equivalent, i.e.,

$$\begin{aligned}
&\frac{\partial^2 E(t_f)}{\partial\gamma\partial l_p} = \frac{\Sigma_f \varphi_0 \alpha_T}{2\left(l_p\right)^2 c_p}\int_0^{t_f} a^{(2)}(1; j_1 = 4,5,6; t)dt = \frac{\partial^2 E(t_f)}{\partial l_p \partial\gamma} \\
&= \frac{\varphi_0 \Sigma_f \alpha_T}{2\left(l_p\right)^2 c_p}\int_0^{t_f}\left[a^{(2)}(1; j_1 = 1,2,3; t)E^2(t) + 2a^{(2)}(2; j_1 = 1,2,3; t)E(t)\right]dt.
\end{aligned} \tag{144}$$

Consequently, either of the two equivalent expressions above can be used to evaluate $\partial^2 E\left(t_f\right)/\partial l_p \partial\gamma$ but the expression involving the integral over $a^{(2)}(1; j_1 = 4,5,6; t)$ appears to be simpler to compute. Similar considerations apply to the remaining mixed 2nd-order sensitivities.

In summary, the application of the 2nd-CASAM-N has necessitated *2 large-scale computations* (for solving the two 2nd-LASS) to obtain all of the 36 second-order sensitivities for the Nordheim–Fuchs reactor safety model. Using any other methods (e.g., statistical or finite-differences) would have required ca. 5×36 large-scale computations for solving the original model with altered parameter values, as needed for the respective finite-difference or statistical schemes.

5. Illustrative Application of the 3rd-CASAM-N to Compute Third-Order Response Sensitivities

The fundamental principle of the 3rd-CASAM-N is to compute the second-order sensitivities by treating each second-order sensitivity as a "model response" and subsequently determining the G-differential of the respective "model response". Roughly speaking, the third-order sensitivities are obtained from their recursive definition of being the "first-order sensitivities of the second-order sensitivities". These concepts will be illustrated in this Section by determining the 3rd-order sensitivities stemming from an unmixed 2nd-order sensitivity of the response $E\left(t_f\right)$, since the unmixed sensitivities have unique expressions, as shown in Section 3, above. In practice, the order of priority for computing the 3rd-order sensitivities should be established by following the ranking order of the magnitudes of the 2nd-order sensitivities: the largest (in absolute value) 2nd-order sensitivity should be considered with the highest priority. The user may decide if any of the 2nd-order sensitivities would be sufficiently insignificant to be neglected in this process.

Two paradigm examples illustrating the application of the 3rd-CASAM-N for computing 3rd-order sensitivities will be presented in this Section. The first example will illustrate the determination of the 3rd-order sensitivities stemming from a representative unmixed 2nd-order sensitivity, while the second example will illustrate the determination of the 3rd-order sensitivities stemming from a representative mixed 2nd-order sensitivity.

5.1. *Computation of the Third-Order Sensitivities Stemming from* $\partial^2 E\left(t_f\right)/\partial c_p \partial c_p$

As indicated in Equation (137), the expression of the unmixed 2nd-order sensitivity $\partial^2 E\left(t_f\right)/\partial c_p \partial c_p$ of the response $E\left(t_f\right)$ with respect to the sixth parameter ($j_1 = 6$) $\alpha_6 \triangleq c_p$, involves all of the key elements (i.e., model parameters, original state function, 1st-level adjoint sensitivity function, 2nd-level adjoint sensitivity function) that could be comprised in the expression of a 2nd-order sensitivity and is, therefore, representative of the operations involved in determining the (six) 3rd-order sensitivities that arise from a 2nd-order sensitivity. For subsequent mathematical considerations, it is convenient to recast the expression of $\partial^2 E\left(t_f\right)/\partial c_p \partial c_p$ in the following form:

$$\begin{aligned}&\frac{\partial^2 E(t_f)}{\partial c_p \partial c_p} = D_1(\boldsymbol{\alpha})\int_0^{t_f} a^{(1)}(t)E^2(t)dt \\ &+D_2(\boldsymbol{\alpha})\int_0^{t_f}\left[a^{(2)}(1;6;t)E^2(t) + 2a^{(2)}(2;6;t)E(t)\right]t;\end{aligned} \tag{145}$$

$$D_1(\boldsymbol{\alpha}) \triangleq -\frac{\alpha_T}{l_p\left(c_p\right)^3};\;\; D_2(\boldsymbol{\alpha}) \triangleq \frac{\alpha_T C_6(\boldsymbol{\alpha})}{2l_p\left(c_p\right)^2} \tag{146}$$

The 3rd-order sensitivities which stem from $\partial^2 E\left(t_f\right)/\partial c_p \partial c_p$ are obtained by applying the definition of the first-order G-differential to Equation (145), which yields the following relations:

$$\begin{aligned}&\delta\left\{\frac{\partial^2 E(t_f)}{\partial c_p \partial c_p}\right\} \triangleq \left\{\frac{d}{d\varepsilon}D_1\left(\boldsymbol{\alpha}^0 + \varepsilon\delta\boldsymbol{\alpha}\right)\int_0^{t_f}\left(a^{(1)} + \varepsilon\delta a^{(1)}\right)[E(t) + \varepsilon\delta E(t)]^2 dt\right. \\ &+D_2\left(\boldsymbol{\alpha}^0 + \varepsilon\delta\boldsymbol{\alpha}\right)\int_0^{t_f}\left[a^{(2)}(1;6;t) + \varepsilon\delta a^{(2)}(1;6;t)\right][E(t) + \varepsilon\delta E(t)]^2 dt \\ &\left.+2D_2\left(\boldsymbol{\alpha}^0 + \varepsilon\delta\boldsymbol{\alpha}\right)\int_0^{t_f}\left[a^{(2)}(2;6;t) + \varepsilon\delta a^{(2)}(2;6;t)\right][E(t) + \varepsilon\delta E(t)]dt\right\}_{\varepsilon=0} \\ &\triangleq \left\{\delta\left[\partial^2 E\left(t_f\right)/\partial c_p \partial c_p\right]\right\}_{dir} + \left\{\delta\left[\partial^2 E\left(t_f\right)/\partial c_p \partial c_p\right]\right\}_{ind},\end{aligned} \tag{147}$$

where

$$\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial c_p \partial c_p\right]\right\}_{dir} \triangleq \left\{\left[\frac{\partial D_1(\boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}}\delta\boldsymbol{\alpha}\right]F_1(\boldsymbol{\alpha}) + \left[\frac{\partial D_2(\boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}}\delta\boldsymbol{\alpha}\right]F_2(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} \tag{148}$$

with

$$F_1(\boldsymbol{\alpha}) \triangleq \left\{\int_0^{t_f} a^{(1)}(t)E^2(t)dt\right\}_{\boldsymbol{\alpha}^0} \tag{149}$$

$$F_2(\boldsymbol{\alpha}) \triangleq \int_0^{t_f}\left[a^{(2)}(1;6;t)E^2(t) + 2a^{(2)}(2;6;t)E(t)\right]dt \tag{150}$$

and

$$\begin{aligned}&\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial c_p \partial c_p\right]\right\}_{ind} \triangleq \left\{D_1(\boldsymbol{\alpha})\int_0^{t_f}\left[\delta a^{(1)}E^2(t) + 2a^{(1)}(t)E(t)\delta E(t)\right]dt\right. \\ &+D_2(\boldsymbol{\alpha})\int_0^{t_f}\left[\delta a^{(2)}(1;6;t)E^2(t) + 2E(t)a^{(2)}(1;6;t)\delta E(t)\right]dt \\ &\left.+2D_2(\boldsymbol{\alpha})\int_0^{t_f}\left[\delta a^{(2)}(2;6;t)E(t) + a^{(2)}(2;6;t)\delta E(t)\right]dt\right\}_{\boldsymbol{\alpha}^0}.\end{aligned} \tag{151}$$

The direct-effect term defined in Equation (148) can be computed already at this stage. However, the indirect-effect term defined in Equation (151) can be computed only after having determined the vectors of variational functions $\delta\mathbf{A}^{(2)}(2;6;t) \triangleq \left[\delta a^{(2)}(1;6;t), \delta a^{(2)}(2;6;t)\right]^{\dagger}$ and $\mathbf{V}^{(2)}(2;t) \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^{\dagger}$. Recall that $\mathbf{V}^{(2)}(2;t) \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^{\dagger}$ is the solution of the 2nd-Level Variational Sensitivity System (2nd-LVSS) defined by Equations (71) and (72). On the other hand, the vector $\delta\mathbf{A}^{(2)}(2;6;t) \triangleq \left[\delta a^{(2)}(1;6;t), \delta a^{(2)}(2;6;t)\right]^{\dagger}$ is the solution of the G-differentiated 2nd-LASS, which is obtained by applying the definition of the G-differential to Equations (111) and (112), to obtain the following system:

$$\begin{aligned}&\left\{\frac{d}{d\varepsilon}\left[-\frac{d}{dt} - 2b\left(\boldsymbol{\alpha}^0 + \varepsilon\delta\boldsymbol{\alpha}\right)\left(E^0 + \varepsilon\delta E\right)\right]\left[a^{(2,0)}(1;6;t) + \varepsilon\delta a^{(2)}(1;6;t)\right]\right. \\ &\left.-2b\left(\boldsymbol{\alpha}^0 + \varepsilon\delta\boldsymbol{\alpha}\right)\left[a^{(2,0)}(2;6;t) + \varepsilon\delta a^{(2)}(2;6;t)\right] - 2\left(a^{(1,0)} + \varepsilon\delta a^{(1)}\right)\left(E^0 + \varepsilon\delta E\right)\right\}_{\varepsilon=0} = 0,\end{aligned} \tag{152}$$

$$\left\{ \frac{d}{d\varepsilon} \left[\frac{d}{dt} - 2b\left(\boldsymbol{\alpha}^0 + \varepsilon\delta\boldsymbol{\alpha}\right)\left(E^0 + \varepsilon\delta E\right) \right] \left[a^{(2,0)}(2;6;t) + \varepsilon\delta a^{(2)}(2;6;t) \right] - \left(E^0 + \varepsilon\delta E\right)^2 \right\}_{\varepsilon=0} = 0, \tag{153}$$

$$\left\{ \delta\mathbf{B}_A^{(2)}\left[2;\mathbf{A}^{(2)}(2;6;t);\boldsymbol{\alpha}\right] \right\}_{\boldsymbol{\alpha}^0} \triangleq \left\{ \begin{pmatrix} \delta a^{(2)}\left(1;6;t_f\right) \\ \delta a^{(2)}(2;6;0) \end{pmatrix} \right\}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{154}$$

Carrying out the operations indicated in Equations (152)–(154) and concatenating the resulting equations with the equations underlying the 2nd-LVSS yields the following 3rd-Level Variational Sensitivity System (3rd-LVSS) for the 3rd-level variational function $\mathbf{V}^{(3)}(4;6;t) \triangleq \left[\mathbf{V}^{(2)}(2;t), \delta\mathbf{A}^{(2)}(2;6;t)\right]^{\dagger} \triangleq \left[\delta E(t), \delta a^{(1)}(t), \delta a^{(2)}(1;6;t), \delta a^{(2)}(2;6;t)\right]^{\dagger}$:

$$\left\{ \mathbf{VM}^{(3)}[4\times 4]\mathbf{V}^{(3)}(4;6;t) \right\}_{\boldsymbol{\alpha}^0} = \left\{ \mathbf{Q}_V^{(3)}[4;6;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}] \right\}_{\boldsymbol{\alpha}^0},\ t > 0, \tag{155}$$

where

$$\mathbf{VM}^{(3)}[4\times 4;\boldsymbol{\alpha}] \triangleq \begin{pmatrix} \mathbf{VM}^{(2)}[2\times 2;\boldsymbol{\alpha}] & 0[2\times 2] \\ \mathbf{VM}_{21}^{(3)}[2\times 2;\boldsymbol{\alpha}] & \mathbf{VM}_{22}^{(3)}[2\times 2;\boldsymbol{\alpha}] \end{pmatrix}; \tag{156}$$

$$\mathbf{VM}_{21}^{(3)}[2\times 2;\boldsymbol{\alpha}] \triangleq \begin{pmatrix} -2b(\boldsymbol{\alpha}) - 2a^{(1)}(t) & -2E(t) \\ -2b(\boldsymbol{\alpha}) - 2E(t) & 0 \end{pmatrix};\quad 0[2\times 2] \triangleq \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}; \tag{157}$$

$$\mathbf{VM}_{22}^{(3)}[2\times 2;\boldsymbol{\alpha}] \triangleq \mathbf{AM}^{(2)}[2\times 2;\boldsymbol{\alpha}] \triangleq \begin{pmatrix} -\frac{d}{dt} - 2b(\boldsymbol{\alpha})E(t) & -2b(\boldsymbol{\alpha}) \\ 0 & \frac{d}{dt} - 2b(\boldsymbol{\alpha})E(t) \end{pmatrix} \tag{158}$$

$$\mathbf{Q}_V^{(3)}[4;6;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}] \triangleq \begin{pmatrix} \mathbf{Q}_V^{(2)}[2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}] \\ \mathbf{Q}_2^{(3)}[2;6;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}] \end{pmatrix}; \quad \mathbf{Q}_2^{(3)}[2;6;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}] \triangleq \begin{pmatrix} 2\delta b(\boldsymbol{\alpha})E(t)a^{(2)}(1;6;t) + 2\delta b(\boldsymbol{\alpha})a^{(2)}(2;6;t) \\ 2\delta b(\boldsymbol{\alpha})E(t)a^{(2)}(2;6;t) \end{pmatrix}. \tag{159}$$

The first argument (i.e., "4") of the 3rd-level variational vector $\mathbf{V}^{(3)}(4;6;t)$ indicates that this vector has four components. The second argument (i.e., "6") indicates that this vector's components stem from a 2nd-level adjoint function related to the 2nd-order sensitivity involving the sixth parameter ($j_1 = 6$), i.e., $\alpha_6 \triangleq c_p$. For the block-matrix $\mathbf{VM}^{(3)}[4\times 4;\boldsymbol{\alpha}]$, the argument "$4\times 4$" indicates the dimensions of this matrix.

The boundary conditions for the components of $\mathbf{V}^{(3)}(4;6;t)$, which are included within the 3rd-LVSS, are as follows:

$$\left[\delta E(0), \delta a^{(1)}\left(t_f\right), \delta a^{(2)}\left(1;6;t_f\right), \delta a^{(2)}(2;6;0)\right]^{\dagger} = [0,0,0,0]^{\dagger} \tag{160}$$

The need for solving the 3rd-LVSS for all parameter variations is circumvented by applying the 3rd-CASAM-N to eliminate the appearance of the variational function $\mathbf{V}^{(3)}(4;6;t)$ in the expression of the indirect-effect term defined in Equation (151) by expressing this indirect-effect term in terms of a 3rd-level adjoint sensitivity function which would be independent of parameter variations. This 3rd-level adjoint function is the solution of a 3rd-Level Adjoint Sensitivity System (3rd-LASS) which is constructed in a Hilbert space denoted as H_3, and which comprises as elements block-vectors of the same form as $\mathbf{V}^{(3)}(4;6;t)$. The inner product, denoted as $\left\langle \boldsymbol{\Psi}^{(3)}(4;t), \boldsymbol{\Phi}^{(3)}(4;t) \right\rangle_3$, of two generic vectors $\boldsymbol{\Psi}^{(3)}(4;t) \triangleq \left[\psi^{(3)}(1;t), \ldots, \psi^{(3)}(4;t)\right]^{\dagger} \in H_3$ and $\boldsymbol{\Phi}^{(3)}(4;t) \triangleq \left[\varphi^{(3)}(1;t), \ldots, \varphi^{(3)}(4;t)\right]^{\dagger} \in H_3$ in the Hilbert space H_3 is defined as follows:

$$\left\langle \boldsymbol{\Psi}^{(3)}(4;t), \boldsymbol{\Phi}^{(3)}(4;t) \right\rangle_3 \triangleq \sum_{i=1}^{4} \int_0^{t_f} \psi^{(3)}(i;t)\varphi^{(3)}(i;t)dt \tag{161}$$

The 3rd-Level Adjoint Sensitivity System (3rd-LASS) for the 3rd-level adjoint function $\mathbf{A}^{(3)}(4;6;t) \triangleq \left[a^{(3)}(1;6;t), a^{(3)}(2;6;t), a^{(3)}(3;6;t), a^{(3)}(4;6;t)\right]^{\dagger} \in \mathrm{H}_3$ is constructed as follows:

(i) Using Equation (161), form the inner product of the vector $\mathbf{A}^{(3)}(4;6;t)$ with Equation (155) to obtain the following relation:

$$\begin{aligned}
&\left\{\left\langle \mathbf{A}^{(3)}(4;6;t), \mathbf{VM}^{(3)}[4\times 4]\mathbf{V}^{(3)}(4;6;t)\right\rangle_3\right\}_{\boldsymbol{\alpha}^0} = \left\{a^{(3)}(1;6;t)\delta E(t)\right.\\
&\left.-a^{(3)}(2;6;t)\delta a^{(1)}(t) - a^{(3)}(3;6;t)\delta a^{(2)}(1;6;t) + a^{(3)}(4;6;t)\delta a^{(2)}(2;6;t)\right\}_{t=0}^{t=t_f}\\
&+\left\{\left\langle \mathbf{V}^{(3)}(4;6;t), \mathbf{AM}^{(3)}[4\times 4]\mathbf{A}^{(3)}(4;6;t)\right\rangle_3\right\}_{\boldsymbol{\alpha}^0}\\
&= \left\{\left\langle \mathbf{A}^{(3)}(4;6;t), \mathbf{Q}_V^{(3)}[4;6;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\right\rangle_3\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned} \tag{162}$$

(ii) Eliminate the boundary terms on the right side of Equation (162) and require the second term on the right side of the first equality in Equation (162) to represent the indirect-effect term $\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial c_p \partial c_p\right]\right\}_{ind}$ defined in Equation (151) by imposing the following relations:

$$\left\{\mathbf{AM}^{(3)}[4\times 4]\mathbf{A}^{(3)}(4;6;t)\right\}_{\boldsymbol{\alpha}^0} = \left\{\mathbf{Q}_A^{(3)}[4;j_2;6;\boldsymbol{\alpha}]\right\}_{\boldsymbol{\alpha}^0} \tag{163}$$

$$\left\{\mathbf{B}_A^{(3)}\left[4;\mathbf{A}^{(3)}(4;6;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0} \triangleq \begin{pmatrix} a^{(3)}\left(1;6;t_f\right) \\ a^{(3)}(2;6;0) \\ a^{(3)}(3;6;0) \\ a^{(3)}\left(4;6;t_f\right) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}; \tag{164}$$

where the block-matrix $\mathbf{AM}^{(3)}[4\times 4] \triangleq \left[\mathbf{VM}^{(3)}[4\times 4]\right]^*$ is the formal adjoint of the block-matrix $\mathbf{VM}^{(3)}[4\times 4]$ and is obtained by transposing the adjoints of the elements of $\mathbf{VM}^{(3)}[4\times 4]$, namely:

$$\mathbf{AM}^{(3)}[4\times 4] \triangleq \left[\mathbf{VM}^{(3)}[4\times 4]\right]^* = \begin{pmatrix} \left\{\left[\mathbf{VM}^{(2)}\right]^*\right\}^{\dagger} & \left\{\left[\mathbf{VM}_{21}^{(3)}\right]^*\right\}^{\dagger} \\ 0[2\times 2] & \left\{\left[\mathbf{VM}_{22}^{(3)}\right]^*\right\}^{\dagger} \end{pmatrix}; \tag{165}$$

and where:

$$\mathbf{Q}_A^{(3)}[4;6;\boldsymbol{\alpha}] \triangleq \left[\mathbf{q}_A^{(3)}(1;6;\boldsymbol{\alpha}), \ldots, \mathbf{q}_A^{(3)}(4;6;\boldsymbol{\alpha})\right]^{\dagger}; \tag{166}$$

$$\mathbf{q}_A^{(3)}(1;6;\boldsymbol{\alpha}) \triangleq 2D_1(\boldsymbol{\alpha})a^{(1)}(t)E(t) + 2D_2(\boldsymbol{\alpha})E(t)a^{(2)}(1;6;t) + 2D_2(\boldsymbol{\alpha})a^{(2)}(2;6;t); \tag{167}$$

$$\mathbf{q}_A^{(3)}(2;6;\boldsymbol{\alpha}) \triangleq D_1(\boldsymbol{\alpha})E^2(t) \tag{168}$$

$$\mathbf{q}_A^{(3)}\left(3;j_2;j_1;\mathbf{U}^{(3)};\boldsymbol{\alpha}\right) \triangleq D_2(\boldsymbol{\alpha})E^2(t) \tag{169}$$

$$\mathbf{q}_A^{(3)}\left(4;j_2;j_1;\mathbf{U}^{(3)};\boldsymbol{\alpha}\right) \triangleq 2D_2(\boldsymbol{\alpha})E(t) \tag{170}$$

The relations represented by Equations (163) and (164) constitute the 3rd-LASS for the 3rd-level adjoint function $\mathbf{A}^{(3)}(4;6;t) \triangleq \left[a^{(3)}(1;6;t), \ldots, a^{(3)}(4;6;t)\right]^{\dagger}$. Notably, the 3rd-LASS is independent of parameter variations; consequently, it needs to be solved just once to obtain the 3rd-level adjoint sensitivity function $\mathbf{A}^{(3)}(4;6;t)$. Furthermore, the 3rd-LASS is an upper-triangular system, so the equations need not be solved simultaneously by inverting the matrix-operator on the left side of Equation (163), but can be solved sequentially.

(iii) Use the relations provided in Equations (162) and (151) together with the 3rd-LASS to obtain the following expression for the indirect-effect term $\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial c_p \partial c_p\right]\right\}_{ind}$:

$$\begin{aligned}
&\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial c_p \partial c_p\right]\right\}_{ind} = \left\langle \mathbf{A}^{(3)}(4;6;t), \mathbf{Q}_V^{(3)}[4;6;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\right\rangle_3 \\
&= \{\delta P_0(\boldsymbol{\alpha}) G_1(\boldsymbol{\alpha}) + \delta b(\boldsymbol{\alpha}) G_2(\boldsymbol{\alpha})\}_{\boldsymbol{\alpha}^0} = \left\{\left[\gamma \Sigma_f(\delta\varphi_0) + \varphi_0 \Sigma_f(\delta\gamma) + \varphi_0 \gamma\left(\delta\Sigma_f\right)\right] G_1(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} \\
&+ \left\{\left[-\frac{\delta\alpha_T}{2 l_p c_p} + \frac{\alpha_T}{2 l_p \left(c_p\right)^2}\delta c_p + \frac{\alpha_T}{2\left(l_p\right)^2 c_p}\delta l_p\right] G_2(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned} \tag{171}$$

In addition to the definitions of $\delta b(\boldsymbol{\alpha})$ and $\delta P_0(\boldsymbol{\alpha})$ given in Equations (31) and (32), respectively, the following definitions have been used to obtain the expression in Equation (171):

$$G_1(\boldsymbol{\alpha}) \triangleq \int_0^{t_f} a^{(3)}(1;6;t)dt; \tag{172}$$

$$\begin{aligned}
G_2(\boldsymbol{\alpha}) \triangleq \int_0^{t_f} &\left\{E^2(t) a^{(3)}(1;6;t) + 2E(t) a^{(3)}(2;6;t) + 2a^{(3)}(3;6;t)\right. \\
&\times \left[E(t) a^{(2)}(1;6;t) + a^{(2)}(2;6;t)\right] + 2a^{(3)}(4;6;t) E(t) a^{(2)}(2;6;t)\left.\right\} dt.
\end{aligned} \tag{173}$$

The expression of the total first-order G-differential of the 2nd-order sensitivity $\partial^2 E\left(t_f\right)/\partial c_p \partial c_p$, which contains the partial 3rd-order sensitivities of the form $\partial^3 E\left(t_f\right)/\partial c_p \partial c_p \partial \alpha_{j_3}$, $j_3 = 1, \ldots, 6$, is obtained by adding the expression obtained in Equation (171) for the indirect-effect term with the expression obtained in Equation (148) for the direct-effect term. Using in Equation (148) the definitions of $D_1(\boldsymbol{\alpha})$ and $D_2(\boldsymbol{\alpha})$ provided in Equations (146) together with the definition of $C_6(\boldsymbol{\alpha})$ provided in Equation (106) yields the following explicit form of the direct-effect term:

$$\begin{aligned}
&\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial c_p \partial c_p\right]\right\}_{dir} \triangleq \left\{\left[-\frac{\delta\alpha_T}{l_p \left(c_p\right)^3} + \frac{\alpha_T \delta l_p}{\left(l_p\right)^2 \left(c_p\right)^3} + \frac{3\alpha_T \delta c_p}{l_p \left(c_p\right)^4}\right] F_1(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} \\
&+ \left\{\frac{\alpha_T}{l_p \left(c_p\right)^2}\left[\frac{\delta\alpha_T}{l_p \left(c_p\right)^2} - \frac{\alpha_T \delta l_p}{\left(l_p\right)^2 \left(c_p\right)^2} - \frac{2\alpha_T \delta c_p}{l_p \left(c_p\right)^3}\right] F_2(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned} \tag{174}$$

Adding Equation (171) with Equation (174) and collecting the coefficients that multiply the respective parameter variations yields the following expressions for the partial 3rd-order sensitivities stemming from the 2nd-order sensitivity $\partial^2 E\left(t_f\right)/\partial c_p \partial c_p$:

$$\frac{\partial^3 E\left(t_f\right)}{\partial\gamma \partial c_p \partial c_p} = \left\{\varphi_0 \Sigma_f G_1(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} \tag{175}$$

$$\frac{\partial^3 E\left(t_f\right)}{\partial\Sigma_f \partial c_p \partial c_p} = \{\varphi_0 \gamma G_1(\boldsymbol{\alpha})\}_{\boldsymbol{\alpha}^0} \tag{176}$$

$$\frac{\partial^3 E\left(t_f\right)}{\partial\varphi_0 \partial c_p \partial c_p} = \left\{\gamma \Sigma_f G_1(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} \tag{177}$$

$$\frac{\partial^3 E\left(t_f\right)}{\partial l_p \partial c_p \partial c_p} = \left\{\frac{\alpha_T G_2(\boldsymbol{\alpha})}{2\left(l_p\right)^2 c_p} + \frac{\alpha_T F_1(\boldsymbol{\alpha})}{\left(l_p\right)^2 \left(c_p\right)^3} - \left(\frac{\alpha_T}{l_p c_p}\right)^2 \frac{F_2(\boldsymbol{\alpha})}{l_p \left(c_p\right)^2}\right\}_{\boldsymbol{\alpha}^0} \tag{178}$$

$$\frac{\partial^3 E\left(t_f\right)}{\partial\alpha_T \partial c_p \partial c_p} = \left\{-\frac{G_2(\boldsymbol{\alpha})}{2 l_p c_p} - \frac{F_1(\boldsymbol{\alpha})}{l_p \left(c_p\right)^3} + \frac{\alpha_T F_2(\boldsymbol{\alpha})}{\left(l_p\right)^2 \left(c_p\right)^4}\right\}_{\boldsymbol{\alpha}^0} \tag{179}$$

$$\frac{\partial^3 E\left(t_f\right)}{\partial c_p \partial c_p \partial c_p} = \left\{\frac{\alpha_T G_2(\boldsymbol{\alpha})}{2 l_p \left(c_p\right)^2} + \frac{3\alpha_T F_1(\boldsymbol{\alpha})}{l_p \left(c_p\right)^4} - \frac{2(\alpha_T)^2 F_2(\boldsymbol{\alpha})}{\left(l_p\right)^2 \left(c_p\right)^5}\right\}_{\boldsymbol{\alpha}^0} \tag{180}$$

5.2. Computation of the Third-Order Sensitivities Stemming from $\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p$

The 3rd-order sensitivities which stem from $\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p$ are obtained by applying the definition of the first-order G-differential to either one of the two equivalent expressions provided in Equation (144). Thus, applying the definition of the G-differential to the simpler expression of $\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p$ yields the following relation:

$$\begin{aligned}
&\delta\left\{\frac{\partial^2 E\left(t_f\right)}{\partial\gamma\partial l_p}\right\}=\left\{\frac{d}{d\varepsilon}\frac{\left(\Sigma_f^0+\varepsilon\delta\Sigma_f\right)\left(\varphi_0^0+\varepsilon\delta\varphi_0\right)\left(\alpha_T^0+\varepsilon\delta\alpha_T\right)}{2\left(l_p^0+\varepsilon\delta l_p\right)^2\left(c_p^0+\varepsilon\delta c_p\right)}\right.\\
&\left.\times\int_0^{t_f}\left[a^{(2,0)}(1;6;t)+\varepsilon\delta a^{(2)}(1;6;t)\right]dt\right\}_{\varepsilon=0}\\
&\triangleq\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial c_p\partial c_p\right]\right\}_{dir}+\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial c_p\partial c_p\right]\right\}_{ind},
\end{aligned} \tag{181}$$

where

$$\begin{aligned}
&\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p\right]\right\}_{dir}\triangleq\left\{\left[\frac{\varphi_0\alpha_T}{2\left(l_p\right)^2 c_p}\delta\Sigma_f+\frac{\Sigma_f\alpha_T}{2\left(l_p\right)^2 c_p}\delta\varphi_0+\frac{\Sigma_f\varphi_0}{2\left(l_p\right)^2 c_p}\delta\alpha_T\right.\right.\\
&\left.\left.-\frac{\Sigma_f\varphi_0\alpha_T}{\left(l_p\right)^3 c_p}\delta l_p-\frac{\Sigma_f\varphi_0\alpha_T}{2\left(l_p c_p\right)^2}\delta c_p\right]\int_0^{t_f}a^{(2)}(1;6;t)dt\right\}_{\boldsymbol{\alpha}^0};
\end{aligned} \tag{182}$$

$$\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p\right]\right\}_{ind}\triangleq\left\{\frac{\Sigma_f\varphi_0\alpha_T}{2\left(l_p\right)^2 c_p}\int_0^{t_f}\delta a^{(2)}(1;6;t)dt\right\}_{\boldsymbol{\alpha}^0} \tag{183}$$

The direct-effect term defined in Equation (182) can be computed already at this stage. The indirect-effect term can be computed after having solved the 3rd-LVSS to determine the variational function $\delta a^{(2)}(1;6;t)$ or, alternatively, by constructing a 3rd-LASS so as to replace the appearance of this variational function with a corresponding 3rd-level adjoint sensitivity function. This 3rd-LASS is constructed by applying the 3rd-CASAM-N, just as was done previously in Section 5.1. As the 3rd-LASS would correspond to the indirect-effect term $\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p\right]\right\}_{ind}$ stemming from a mixed (rather than unmixed) 2nd-order sensitivity, the corresponding 3rd-level adjoint sensitivity function would have an additional index, i.e., would have the form $\mathbf{A}^{(3)}(4;j_2;j_1;t)$, $j_2\neq j_1$, by comparison to the 3rd-level adjoint sensitivity function $\mathbf{A}^{(3)}(4;6;t)$, $j_2=j_1=6$, which was used in above in Section 5.1. Since 4th- and/or higher-order sensitivities will not be determined in this work, the proliferation of indices can be avoided in this particular case by designating as $\boldsymbol{\Psi}^{(3)}(4;t)\triangleq\left[\psi^{(3)}(1;t),\ldots,\psi^{(3)}(4;t)\right]^{\dagger}\in\mathrm{H}_3$ the 3rd-level adjoint sensitivity function to be determined for obtaining the alternative expression for $\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p\right]\right\}_{ind}$. Thus, the 3rd-Level Adjoint Sensitivity System (3rd-LASS) for the 3rd-level adjoint function $\boldsymbol{\Psi}^{(3)}(4;t)\triangleq\left[\psi^{(3)}(1;t),\ldots,\psi^{(3)}(4;t)\right]^{\dagger}$ is constructed as follows:

(i) Using Equation (161), form the inner product of the vector $\boldsymbol{\Psi}^{(3)}(4;t)$ with Equation (155) to obtain the following relation:

$$\begin{aligned}
&\left\{\left\langle\boldsymbol{\Psi}^{(3)}(4;t),\mathbf{VM}^{(3)}[4\times 4]\mathbf{V}^{(3)}(4;6;t)\right\rangle_3\right\}_{\boldsymbol{\alpha}^0}=\left\{\psi^{(3)}(1;t)\delta E(t)\right.\\
&\left.-\psi^{(2)}(2;t)\delta a^{(1)}(t)-\psi^{(3)}(3;t)\delta a^{(2)}(1;6;t)+\psi^{(3)}(4;t)\delta a^{(2)}(2;6;t)\right\}_{t=0}^{t=t_f}\\
&+\left\{\left\langle\mathbf{V}^{(3)}(4;6;t),\mathbf{AM}^{(3)}[4\times 4]\boldsymbol{\Psi}^{(3)}(4;t)\right\rangle_3\right\}_{\boldsymbol{\alpha}^0}\\
&=\left\{\left\langle\boldsymbol{\Psi}^{(3)}(4;t),\mathbf{Q}_V^{(3)}[4;6;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\right\rangle_3\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned} \tag{184}$$

(ii) Eliminate the boundary terms on the right side of Equation (184) and require the second term on the right side of the first equality in Equation (184) to represent the indirect-effect term $\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p\right]\right\}_{ind}$ by imposing the following relations:

$$\left\{\mathbf{AM}^{(3)}[4\times 4]\mathbf{\Psi}^{(3)}(4;t)\right\}_{\boldsymbol{\alpha}^0} = \left\{\left[0,0,\Sigma_f\varphi_0\alpha_T/2\left(l_p\right)^2 c_p,0\right]^{\dagger}\right\}_{\boldsymbol{\alpha}^0} \tag{185}$$

$$\psi^{(3)}\left(1;t_f\right) = \psi^{(3)}(2;0) = \psi^{(3)}(3;0) = \psi^{(3)}\left(4;t_f\right) = 0 \tag{186}$$

The relations represented by Equations (185) and (186) constitute the 3rd-LASS for the 3rd-level adjoint function $\mathbf{\Psi}^{(3)}(4;t)$. Notably, the left side of this 3rd-LASS is the same as the left side of Equation, so the system of equations in (185) and (186) is solved sequentially rather than simultaneously by inverting the matrix-operator on the left side of Equation (163) or (185). Only the sources on the right sides of these 3rd-LASS are different.

(iii) Use the relations provided in Equations (184)−(186) in Equation (183) to obtain the following expression for the indirect-effect term $\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p\right]\right\}_{ind}$:

$$\begin{aligned}
&\left\{\delta\left[\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p\right]\right\}_{ind} = \left\langle \mathbf{\Psi}^{(3)}(4;t), \mathbf{Q}_V^{(3)}[4;6;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\right\rangle_3 \\
&= \left\{\delta P_0(\boldsymbol{\alpha})H_1(\boldsymbol{\alpha}) + \delta b(\boldsymbol{\alpha})H_2(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} \\
&= \left\{\left[\gamma\Sigma_f(\delta\varphi_0) + \varphi_0\Sigma_f(\delta\gamma) + \varphi_0\gamma\left(\delta\Sigma_f\right)\right]H_1(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} \\
&+\left\{\left[-\tfrac{\delta\alpha_T}{2l_p c_p} + \tfrac{\alpha_T}{2l_p\left(c_p\right)^2}\delta c_p + \tfrac{\alpha_T}{2\left(l_p\right)^2 c_p}\delta l_p\right]H_2(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned} \tag{187}$$

In addition to the definitions of $\delta b(\boldsymbol{\alpha})$ and $\delta P_0(\boldsymbol{\alpha})$ given in Equations (31) and (32), respectively, the following definitions have been used to obtain the expression in Equation (187):

$$H_1(\boldsymbol{\alpha}) \triangleq \int_0^{t_f} \psi^{(3)}(1;t)dt; \tag{188}$$

$$\begin{aligned}
H_2(\boldsymbol{\alpha}) \triangleq \textstyle\int_0^{t_f}&\left\{E^2(t)\psi^{(3)}(1;t) + 2E(t)\psi^{(3)}(2;t) + 2\psi^{(3)}(3;t)\right.\\
&\times\left.\left[E(t)a^{(2)}(1;6;t) + a^{(2)}(2;6;t)\right] + 2\psi^{(3)}(4;t)E(t)a^{(2)}(2;6;t)\right\}dt.
\end{aligned} \tag{189}$$

The expression of the total first-order G-differential of the 2nd-order sensitivity $\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p$, which contains the partial 3rd-order sensitivities of the form $\partial^3 E\left(t_f\right)/\partial\gamma\partial l_p\partial\alpha_{j_3}$, $j_3 = 1,\ldots,6$, is obtained by adding the expression obtained in Equation (187) for the indirect-effect term with the expression obtained in Equation (182) for the direct-effect term. Collecting in the resulting expression the coefficients that multiply the respective parameter variations yields the following expressions for the partial 3rd-order sensitivities stemming from the 2nd-order sensitivity $\partial^2 E\left(t_f\right)/\partial\gamma\partial l_p$:

$$\frac{\partial^3 E\left(t_f\right)}{\partial\gamma\partial\gamma\partial l_p} = \left\{\varphi_0\Sigma_f H_1(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} \tag{190}$$

$$\frac{\partial^3 E\left(t_f\right)}{\partial\Sigma_f\partial\gamma\partial l_p} = \left\{\frac{\varphi_0\alpha_T}{2\left(l_p\right)^2 c_p}\int_0^{t_f} a^{(2)}(1;6;t)dt + \varphi_0\gamma H_1(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} \tag{191}$$

$$\frac{\partial^3 E\left(t_f\right)}{\partial\varphi_0\partial\gamma\partial l_p} = \left\{\frac{\Sigma_f\alpha_T}{2\left(l_p\right)^2 c_p}\int_0^{t_f} a^{(2)}(1;6;t)dt + \gamma\Sigma_f H_1(\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} \tag{192}$$

$$\frac{\partial^3 E\left(t_f\right)}{\partial l_p \partial \gamma \partial l_p} = \left\{ -\frac{\Sigma_f \varphi_0 \alpha_T}{\left(l_p\right)^3 c_p} \int_0^{t_f} a^{(2)}(1;6;t)dt + \frac{\alpha_T H_2(\boldsymbol{\alpha})}{2\left(l_p\right)^2 c_p} \right\}_{\boldsymbol{\alpha}^0} \tag{193}$$

$$\frac{\partial^3 E\left(t_f\right)}{\partial \alpha_T \partial \gamma \partial l_p} = \left\{ \frac{\Sigma_f \varphi_0}{2\left(l_p\right)^2 c_p} \int_0^{t_f} a^{(2)}(1;6;t)dt - \frac{H_2(\boldsymbol{\alpha})}{2 l_p c_p} \right\}_{\boldsymbol{\alpha}^0} \tag{194}$$

$$\frac{\partial^3 E\left(t_f\right)}{\partial c_p \partial \gamma \partial l_p} = \left\{ -\frac{\Sigma_f \varphi_0 \alpha_T}{2\left(l_p c_p\right)^2} \int_0^{t_f} a^{(2)}(1;6;t)dt + \frac{\alpha_T H_2(\boldsymbol{\alpha})}{2 l_p \left(c_p\right)^2} \right\}_{\boldsymbol{\alpha}^0} \tag{195}$$

6. Discussion

As has been shown in [1], the "nth-order comprehensive sensitivity analysis methodology for nonlinear systems" (abbreviated as "nth-CASAM-N") enables the determination of arbitrarily high-order sensitivities of model responses with respect to uncertain model parameters, interfaces, and external boundaries for computational models that are nonlinear in their underlying state functions. This work has illustrated the application of the nth-CASAM-N to the well-known Nordheim–Fuchs reactor dynamics/safety model [10,11]. This phenomenological model describes a short-time self-limiting power transient in a nuclear reactor system having a negative temperature coefficient in which a large amount of reactivity is suddenly inserted, either intentionally or by accident. This model has been chosen for demonstrating the application of the n-CASAM-N based on the following considerations:

(i) The demonstration model should be time-dependent (dynamic), nonlinear in its underlying state functions, and of practical relevance.

(ii) For didactical purposes, the model should admit exact closed-form expressions (in terms of elementary function) for the first- and higher-level adjoint functions, as well as for the first- and higher-order sensitivities of the chosen model response with respect to the model's uncertain parameters.

(iii) The expressions obtained for the first- and higher-level adjoint functions, as well as for the first- and higher-order sensitivities, should enable benchmarking of computational tools.

The Nordheim–Fuchs phenomenological model of a "severe accident" satisfies all of the above considerations, admitting exact closed-form transient solutions, expressible in terms of elementary functions, for the model's state functions (particularly for the energy released in the transient −which is the most important model response interest), adjoint functions and response sensitivities. Furthermore, the Nordheim–Fuchs model is independent of reactor type and is sufficiently complex to demonstrate all of the important features of applying the nth-CASAM-N methodology. The closed-form expressions obtained for the adjoint functions and sensitivities enable the benchmarking of computational tools for any, rather than for just a specific type of nuclear reactor. Numerical results have not been provided as numerical results cannot be universally valid (in contradistinction to mathematical expressions) but can be valid for only a specific type of reactor (e.g., results for a sodium fast reactor would be irrelevant for a boiling water reactor and/or for a molten salt reactor, etc.).

It is recommended that one should always compute the sensitivities of the next-higher order to demonstrate—rather than speculate—whether they are negligible or not. In other words, one should compute at least the second-order sensitivities to demonstrate whether they are negligible or not. If the second-order sensitivities are not negligible, then the 3rd-order sensitivities must be computed to ascertain whether they are important or not. It is for this reason that this work has outlined the application of the 3rd-CASAM-N methodology for the computation of the third-order sensitivities stemming from either mixed or unmixed second-order sensitivities for the Nordheim–Fuchs model. In general, the nth-CASAM-N methodology enables the user to select a priori the specific high-order sensitivities to be computed as well as the priority order in which the selected sensitivities are to be computed.

This work has also illustrated the linear increase of the dimension of the Hilbert space in which the various-order sensitivities are computed as the order of the respective sensitivities increases. This linear increase is in contradistinction to the exponential increase in the parameter-dimensional space, which occurs when using conventional statistical and/or finite difference schemes to compute higher-order sensitivities. For the Nordheim–Fuchs model, a single adjoint computation sufficed to obtain the six 1st-order sensitivities and two adjoint computations (to solve the 2nd-LASS with two distinct sets of source terms) sufficed to obtain all of the 36 second-order sensitivities (of which 21 are distinct).

As has been mentioned in the introductory Section 1 of this work, the 1st-CASAM-N has been implemented by Cacuci and DiRocco [6] to obtain first-order sensitivities for the reduced-order dynamic BWR model conceived by March-Leuba, Cacuci, and Perez [7], in both the stable and oscillatory (periodic and aperiodic) regions in phase-space. A higher-order sensitivity analysis of this model has not been performed yet. On the other hand, solvers for the computation of first-, second-, third- and fourth-order sensitivities for neutron transport models are available, as described in the works by Fang and Cacuci [12,13], where it was found that the microscopic total cross-sections of isotopes ^{1}H and ^{239}Pu of the reactor physics benchmark analyzed therein are the most important parameters affecting that benchmark's leakage response. In particular, it was shown that the largest unmixed 4th-order sensitivity is $S^{(4)}\left(\sigma_{t,6}^{g=30}, \sigma_{t,6}^{g=30}, \sigma_{t,6}^{g=30}, \sigma_{t,6}^{g=30}\right) = 2.720 \times 10^{6}$, which is with respect to the total cross-section $\sigma_{t,6}^{30}$ for the 30th energy group (which comprises thermalized neutrons in the energy interval from 1.39×10^{-4} eV to 0.152 eV) of isotope 6 (i.e., ^{1}H). This sensitivity is ca. 90 times larger than the corresponding largest 3rd-order relative sensitivity; ca. 6350 times larger than the corresponding largest 2nd-order one; and ca. 291,000 times larger than the corresponding largest 1st-order relative sensitivity. For example, considering that all of the microscopic total cross sections are uncorrelated, having a 5% relative standard deviation, a 5% relative standard deviation of $\sigma_{t,6}^{g=30}$ contributes around 99.8% to the leakage response's expected value, 99.97% to its variance, and 99.99% to its skewness.

The question of "when to stop computing progressively higher-order sensitivities ?" has been addressed by Cacuci [14] in conjunction with the question of convergence of the Taylor-series expansion of the response in terms of the uncertain model parameters as this Taylor-series expansion is the fundamental premise for the expressions provided by the "propagation of errors" methodology for the cumulants of the model response distribution in the phase-space of model parameters. The convergence of this Taylor series, which depends on both the response sensitivities to parameters and the uncertainties associated with the parameter distribution, must be ensured. This can be done by ensuring that the combination of parameter uncertainties and response sensitivities are sufficiently small to fall inside the radius of convergence of the Taylor-series expansion. If the Taylor-series fails to converge, targeted experiments must be performed to reduce the largest sensitivities as well as the largest uncertainties (particularly standard deviations) that affect the most important parameters by applying, e.g., the principles of the BERRU-PM [15] predictive-modeling methodology to obtain best-estimate parameter values with reduced uncertainties.

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