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SENSITIVITY ANALYSIS FOR MATHEMATICAL MODELING OF FIRES IN RESIDENTIAL BUILDINGS

Kostreva, M. M.

Clemson University
Clemson, SC 29631

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FINAL TECHNICAL REPORT

"SENSITIVITY ANALYSIS FOR MATHEMATICAL MODELING OF FIRES IN RESIDENTIAL BUILDINGS"

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Report Prepared by:Dr. Michael M. Kostreva

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The Building and Fire Research Laboratory engages in research and development of mathematical models of fires in residential buildings together with human egress of the building occupants. HAZARD I, the first implementation of a systems model for such phenomena has been made available to the fire safety community. Continued research into fires and human fire interactions wi likely result in a more sophisticated HAZARD methodology. HAZARD II is nearing completion ar testing is under way. The research here analyzes the existing approach of HAZARD I, together with the likely modifications incorporated into HAZARD II (CONRAD2)and establishes a prototyı sensitivity analysis equipped fire model computer program, thereby evaluating and demonstrating recently obtained results on the mathematical foundations of fire models.

The mathematical model of the spread of fire, smoke and toxic gases (FAST) which is part of HAZARD I [1] is an initial value problem for a system of ordinary and partial differential equations. Depending on the requested analyses of the user, this system may contain upwards of twenty equations per room of the residence. The solution of these differential equations is obtained by numerical integration, forward in time, from a set of initial conditions on each of the state variables. To set up the equations HAZARD I requires input parameters. User inputs include information about the geometry of the building, the construction materials, data about the type of fire and its location, etc. Collecting the input data to construct a model of a fire within HAZARD I, verifying data correctness and entering it into the computer comprise a major component of the user's time and cost to apply HAZARD I. In almost all cases, the user is not interested in a single fire scenario, but a collection of related scenarios which will be run together, compared and analyzed. After the runs are completed, it is likely that the user will be presenting the results and conclusions to managers or clients. Inevitably, these presentation interfaces include questions about the sensitivity of response of the model to the input parameters. If the answers to such questions are not given, the credibility of the model is decreased. However, to expect a user of a model as complicated as HAZARD I to understand the response of the model to the input (or all possible nearby input parameters) is not realistic. Thus it will be in the interest of fire hazard researchers to have a capability for sensitivity analysis which could be requested by users, managers and clients. This may be a selective function, available to isolate certain input variables for a detailed sensitivity analysis.

The differential equations which model the temperature in the rooms and model the accumulation of smoke and toxic chemicals (as well as other phenomena) are of the form:

$$x'(t) = f(x(t),u(t), a(t), t) \text{ and } x(t_0) = x_0.$$

Consider the case where (parameter vector) $a(t) = \text{constant} \in R^n$ and where u is a control function, not yet determined. See [1] for a more detailed version. Assume that the functions u are square integrable and that the functions x are absolutely continuous with square integrable derivatives. Assume that for given (u,a) a solution of the differential equation of the model exists. Define the mapping P by the integral relation:

$$P(x,u,a) = x(t) - x_0 - \int_{t_0}^{t} f(x(s),u(s),a(s),s)\, ds$$

Notice that a solution of the model makes $P(x,u,a) = 0$. Suppose that the function f is continuously differentiable with respect to x and a. It is of interest to find the variations which are denoted by
$\bar{x}$ and $\bar{a}$.
Then the Gateaux differentials of the mapping P exist , namely

$$(P_x(x,u,a)\bar{x})\ (t) = \bar{x}(t) - \int_{t_0}^{t} f_x(x(s),u(s),a(s),s)\bar{x}(s)ds \quad \text{and}$$

$$(P_a(x,u,a)\bar{a})(t) = -\int_{t_0}^{t} f_a(x(s),u(s),a(s),s)\bar{a}(s)ds \ .$$

Under appropriate assumptions these also define the Frechet derivatives since the mappings P_x and P_a are continuous in variables x and a. The operator $P_x^{-1}(x,u,a)$ is defined by

$$(P_x^{-1}(x,u,a)\bar{\bar{x}})\ (t) = \Phi(t,t_0)\bar{\bar{x}}(t_0) - \int_{t_0}^{t} \Phi(t,s)\bar{\bar{x}}'(s)ds \quad \text{where}$$

$$\bar{\bar{x}}'(t) = \bar{x}'(t) - f_x(x(t),u(t),a(t),t)\bar{x}(t), \quad \bar{x}(t_0) = \bar{\bar{x}}(t_0)$$

and

$\Phi(t,s)$ is the solution of the equation

$$\frac{d}{dt}\Phi(t,t_0) = f_x\ (x(t),u(t),a(t),t)\quad \Phi(t,t_0)$$

with the initial conditions

$$\Phi(t_0,t_0) = I$$

All of this machinery is designed to allow the application of the implicit function theorem. Now we may conclude that the variation
$\bar{x}$ of the state variables x caused by the variation of the parameter vector $\bar{a}$ is a solution to

$$\bar{x}\,'(t) = f_x\ (x(t),\ u(t),\ a(t),\ t)\ \bar{x} + f_a(x(t),\ u(t),\ a(t),\ t)\ \bar{a}$$

$$\bar{x}\ (t_0)= 0.$$

Thus *to calculate the sensitivity or variation of the state variables to any variation in the input parameters a and to consider the variation as function of time*, one appends these differential equations to the original model. Of course, the above theory supposes that the partial derivatives contained in these equations are available explicitly. This assumption may not be valid in certain models, especially if the model is complex, and contains several numerical submodels.

It is a practical matter that dictates how the above analysis may be applied. That is, it may not be possible, or desirable, to integrate all of the differential equations at the same time for all possible sensitivities to all of the input parameters. Therefore, it will be necessary to be selective about which of these additional equations are to be appended. It is suggested that, the selection be made by the model builders at NIST, will be convenient for the user and not diminish much from the totality of sensitivity analysis, if it is provided.

Sensitivity analysis capabilities for sophisticated dynamical systems such as FAST and CFAST have not yet been developed at NIST. Certain issues were explored in [6] by C. L. Forney, but only in the context of the simpler ASET [7] models. Now it is time to make use of those analyses, as well as additional ones described above, and to bring them to the newer codes of Forney and Moss [8] and Moss and Forney [9]. Since these models involve more complex configurations, which lead to algebraic-differential systems of equations, some additional research is needed to derive the mathematical theory corresponding to CONRAD2 models. According to our investigation, derivation and programming of this theory is underway at University of Minnesota [10] and is planned as the computer code DASSLSO. We obtained a version of the computer code DASSLSO, and combined it with CONRAD2 to attempt the desired sensitivity analysis runs. Our finding is that the code is not yet debugged and DASSLSO would not perform the CONRAD2 sensitivity computations. We verified the status (still not debugged) of the code DASSLSO by implementing some other methods of sensitivity analysis, and comparing the results.

Some other approaches which suggest themselves quite naturally were considered and found to be quite practical in this context. For example, finite differences, though somewhat unwieldy, especially with the number of state variables and input parameters in FAST/CFAST models, have now been applied to CONRAD2 models. These computations were done by means of individual runs for each chosen parameter to remove any question of interpretation of the finite differences.

We now consider finite difference sensitivity analyses for CONRAD2. All relevant details will be given and then a discussion and graphical presentation of the sensitivity functions will be made.

Two models will be considered: a one room building and a four room building. Four state variables will be analyzed: relative pressure, gas level, lower mass and upper mass. (Upper and lower refer to the two zones assumed in the CONRAD2 model.) These variables are directly from the output of CONRAD2, which are the variables accessible to the user. For the model with four rooms, the state variables corresponding to the first room only are considered.

Three parameters were selected: the power of the fire, the height of the room (a common height for the four room case), and Γ, the gas constant. Thus for each model, and for each state variable, we consider three sensitivity functions. We compute the sensitivity functions through a time horizon of 600 seconds, and hence report twelve functions of time, on the interval [0,600]. It is important to reason about the sensitivity functions across the entire time interval, rather than at one particular point. The sensitivity functions represent the ratio of the relative change in the state variable to the relative change in the parameter which caused the change in the state variable.

To establish all twelve sensitivity functions, the code was run thirteen times. First with default values, and the twelve more times, once for each parameter/state variable combination. For these twelve, the parameter was perturbed by 1%, and the rest of the parameters on default values. Hence the sensitivities represent the % change in the state variable caused by a 1% perturbation of the parameter.

The results are presented graphically on Figures 0.1-0.8. (See Appendix). Figures 0.1-0.4 correspond to the one room model while 0.5-0.8 correspond to the four room model. Each of the figures contains two subplots, with the upper containing the relevant state variable, and the lower containing the three sensitivity functions corresponding to it.

For the one room model, the state variable pressure attains a steady level rather quickly, after an initial drop. Sensitivities also level out quickly, taking the magnitude of unity. On the other hand gas level, has sensitivities which are much smaller in magnitude, even though everything settles down at about 100 seconds. Lower mass is apparently the most sensitive, achieving magnitudes about twice as large as those of pressure. Upper mass, settling down quickly, takes on small magnitude sensitivities as above with gas level.

In summary, the one room model is rather insensitive to the selected parameters. The sensitivity to room height is the smallest and generally tends to zero with time. The sensitivity to the gas constant is the greatest one, but still within a reasonable range. All functions considered display definite transient character at the beginning of the time horizon, and generally achieve their steady level after about 100 seconds.

Considering now the larger model, with four rooms, we notice a different behavior. The state variable pressure does not achieve a steady level within the time of 600 seconds. This is likely due to transfer of pressure to the other rooms. The sensitivities are close to zero initially, but they achieve some high values near the end of the simulation. In particular, sensitivity to room height reaches a value of 100. Since the integration is so lengthy, namely 600 seconds, one may question whether numerical integration is the cause of this big change in sensitivity. (Spurious solutions to the difference equations may be present.) Physically, it seems highly unlikely that a 1% change in room height could cause a 100% change in pressure at a time 600 seconds in the future. For gas level, the state variable and the sensitivities display oscillatory character. The magnitude does not exceed 1.5, which seems to be quite reasonable. Lower mass and upper mass behave about the same in the larger four room model. The state variable in each case decreases without reaching a steady value. The sensitivities behave monotonically and near the end of the horizon they achieve some values near five in magnitude. This case is harder to understand although the slow monotonic growth is not ruled out with spurious solutions. That is, the high sensitivity may not be real, but simply a feature of computing with numerical integrations over long intervals.

Appendix

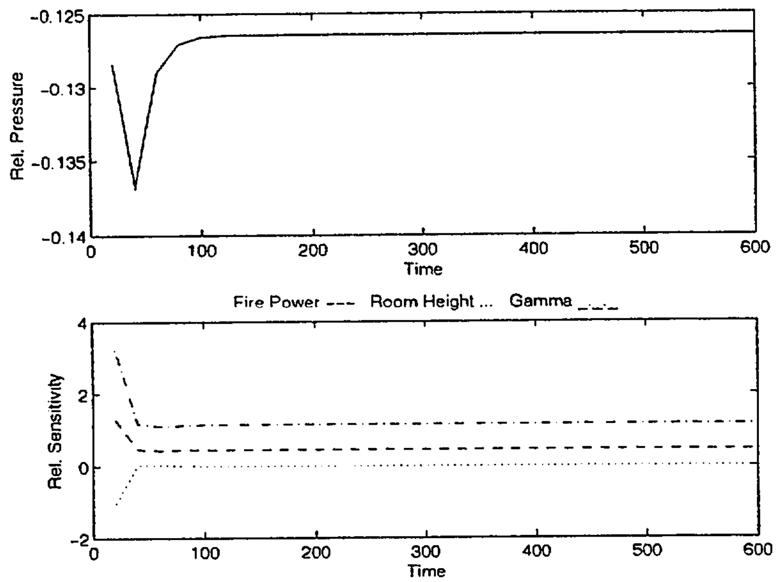


Figure 0.1: Pressure in the 1 room problem

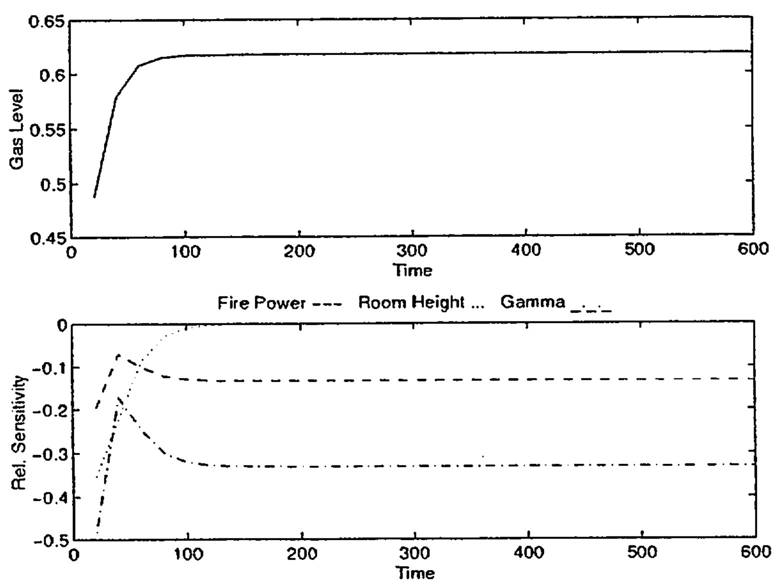
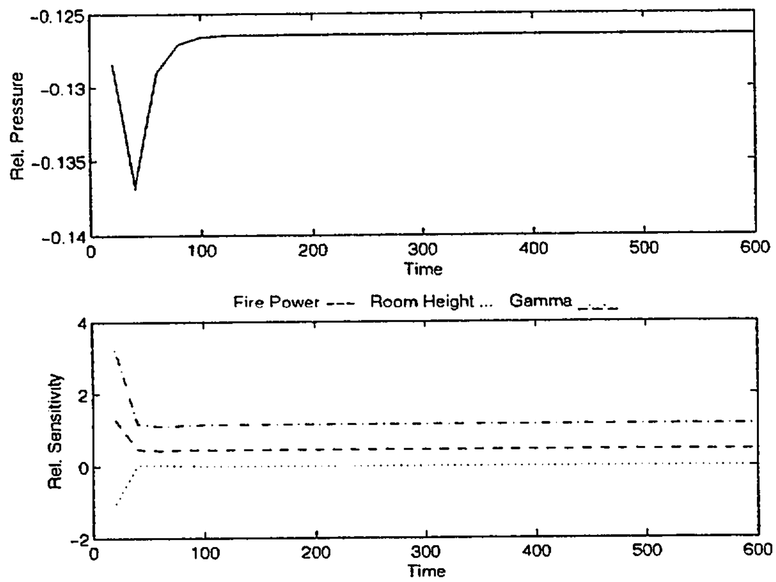


Figure 0.2: Gas level in the 1 room problem

Appendix



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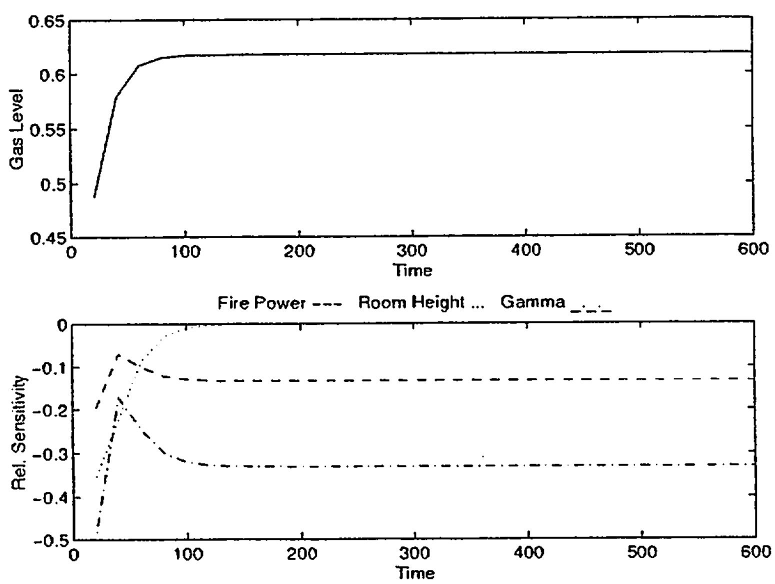

Figure 0.2: Gas level in the 1 room problem

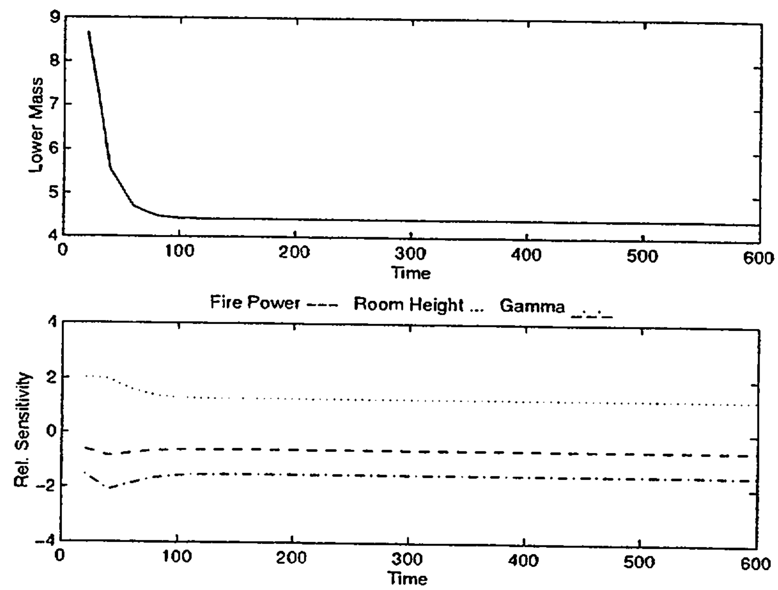

Figure 0.3: Lower mass in the 1 room problem

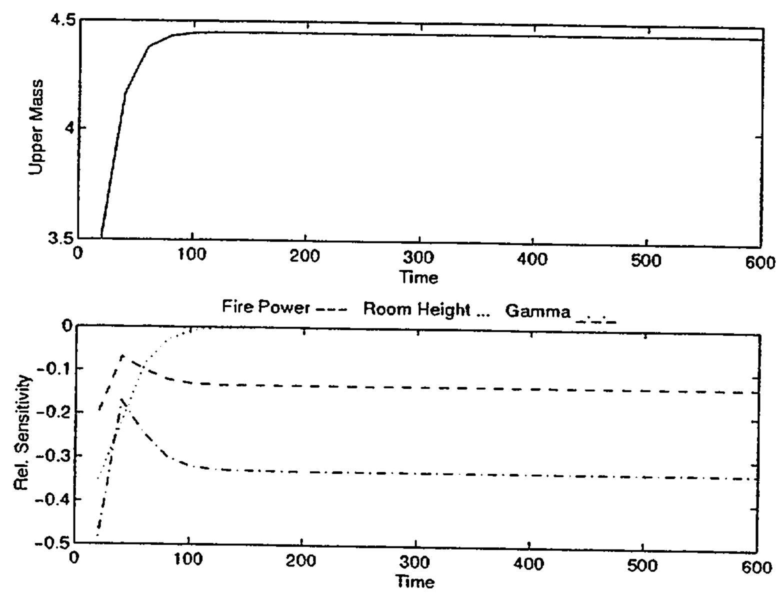

Figure 0.4: Upper mass in the 1 room problem

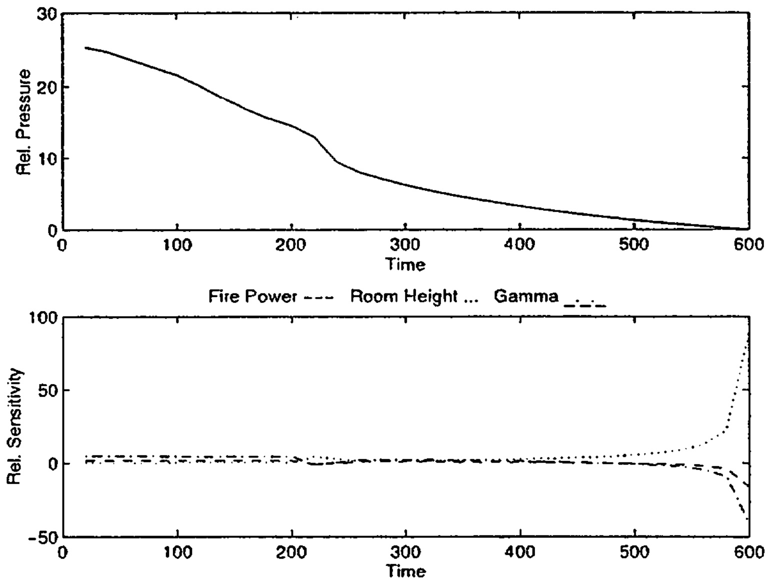

Figure 0.5: Pressure in the 4 room problem

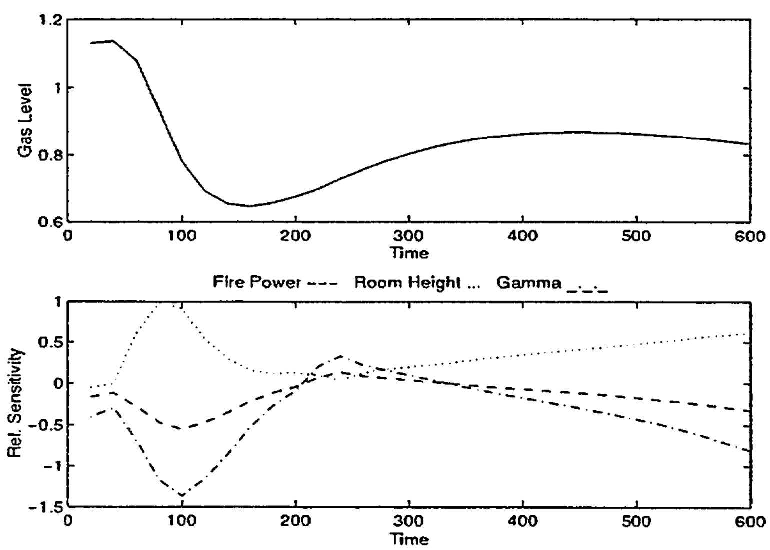

Figure 0.6: Gas level in the 4 room problem

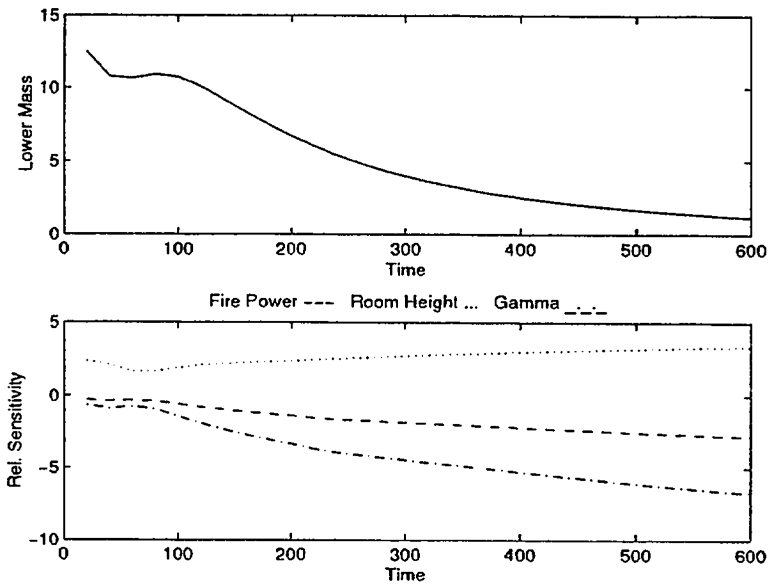

Figure 0.7: Lower mass in the 4 room problem

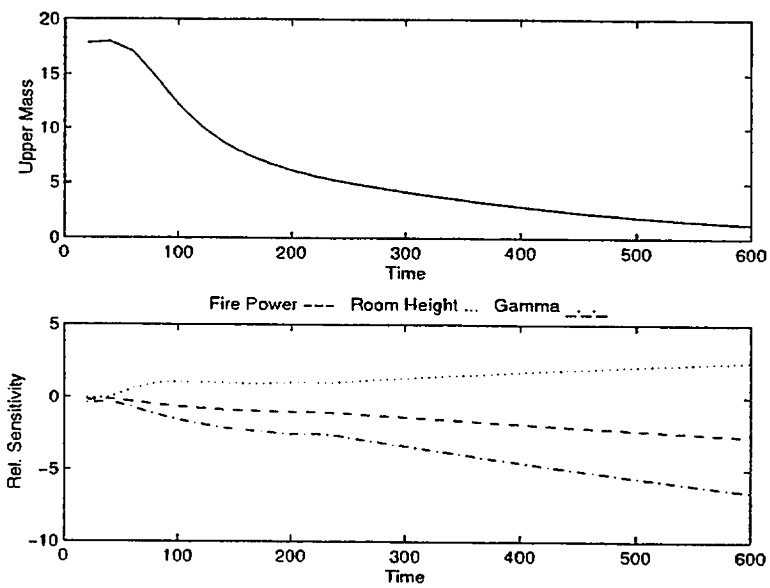

Figure 0.8: Upper mass in the 4 room problem

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Kostreva, M. M.
Clemson University, Clemson, SC

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SUPPLEMENTARY NOTES

ABSTRACT (A 2000-CHARACTER OR LESS FACTUAL SUMMARY OF MOST SIGNIFICANT INFORMATION. IF DOCUMENT INCLUDES A SIGNIFICANT BIBLIOGRAPHY OR LITERATURE SURVEY, CITE IT HERE. SPELL OUT ACRONYMS ON FIRST REFERENCE.) (CONTINUE ON SEPARATE PAGE, IF NECESSARY.)

The underlying equations used in the fire models HAZARD I and CONRAD2 are examined to establish a prototype method for sensitivity analysis applied to currently available zone fire models. Generic differential equations are derived which can supplement existing equations in fire models to estimate the time-varying sensitivity of model outputs. The implications on the validity of the solutions obtained and on the computing resources necessary to obtain such sensitivity information is discussed. The results of the proposed analytical approach is compared with estimates from finite difference analyses for the CONRAD2 model. These finite difference methods, while more computing intensive, provide more believable results that the analytical approaches examined.

KEY WORDS (MAXIMUM OF 9; 28 CHARACTERS AND SPACES EACH; SEPARATE WITH SEMICOLONS; ALPHABETIC ORDER; CAPITALIZE ONLY PROPER NAMES)

finite difference theory; fire models; sensitivity analysis; zone models

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