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Dear Mel:

SUBJECT: BMI-2104 Review

From the beginning of the peer review process on the subject work, I have been most impressed by the very substantial efforts undertaken by the principles (Batelle, Sandia, Oak Ridge) and your staff. I believe to a very considerable extent the work is based on the state of the art, but I also believe first that the state of the art is not very good and second in some cases the computer codes involved do not use the best information that has been developed over the past several years. I recognize that within the time constraints of the subject work it would have been both unwise and difficult to modify the computer programs. As such there was sufficient confusion in the review meeting of October 12, 13 because of changes in some input data and use of MARCH 2 for SURREY-1. Now that the draft reports are nearing completion, it would be appropriate for me to bring my observations to your attention.

To a large extent my observations are a result of my long standing research interests in aerosol mechanics, and my recent review of aerosol mechanics in nuclear reactor safety, Progress in Nuclear Energy 12, 1 (1983). I had provided your office a preprint of this paper at the first peer review meeting, and also Chris Ryder has a copy of the just published paper. Chris has indicated that he has found the review paper quite pertinent and useful, and it is my purpose in this note only to summarize some of my main observations.

It appears to me that realistic (or conservative) description of a whole generally requires a correspondingly more realistic description of the parts, especially when the processes are highly dynamic and not well understood. Exceptions exist, but in general the local error must be much less than the global error. Thus if the overall release results for the release fractions are to be accurate within an order of magnitude, than the aerosol codes should be accurate at least to the first order. To achieve this goal, advances in several aspects of aerosol mechanics must be made. I have noted below the specific areas where advances are needed,

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and I have also commented upon the aspects where the release study aerosol computer codes (TRAP-MELT, NAUA) do not use the state of the art information.

(i) Single Particle Aerosol Mechanics:

a) Condensation-Evaporation (Heat and Mass Transfer):

The computer programs use Mason's expression which is not valid for small aerosols. I have developed some better expressions, which have been verified for isothermal conditions. An approximate expression for non-isothermal conditions can be readily constructed by using the results reported in my review paper. I have presented such results in the past at NRC aerosol review group meetings. The theoretical results, however, need to be improved (for cross-effects, internal heat generation, strong condensation and evaporation, surface effects), and experimental verification must be carried out. The latter can be accomplished by using recently developed single particle electrodynamic balances (Davis) or the type of apparatus used by Dr. Thomas for NRC sponsored accommodation coefficients measurement work at this University.

b) Chemical Reactions and Chemisorption:

Relatively little information for particles and gases of interest is known. Again, I believe efforts of the type suggested in a) above must be initiated. In respect to a question that was raised at the October 12, 13 meeting, I believe the heat of vaporization (reaction) would be important if there is significant condensation (reaction) and should not be neglected a priori. Recent experimental evidence strongly suggests that condensing/evaporating environments can have strong synergestic effects on chemical reactions, and such evidence should be considered.

c) Thermophoresis, Diffusiophoresis, Photophoresis:

The codes are using relatively crude expressions for thermophoresis and diffusiophoresis. I have reported in my paper how better expressions for these effects can be constructed by using results that have become available in recent years. I have also noted that much additional theoretical and experimental effort is needed - because recently, controversies regarding even the qualitative aspects have arisen.

Photophoresis (or radio-phoresis) has not been accounted for in any of the codes. Either it should be established that it is not important or it should be accounted for.

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d) Deposition rates:

The models for deposition rates are entirely ad-hoc and serious questions can be raised regarding the expressions presently in use. I believe first, consistent phenomenology should be developed (starting from general space dependent forms of the aerosol equation), and the deposition coefficients should be defined unambiguously both from theoretical and experimental viewpoints. Also, new correlations for turbulent deposition have become available in the aerosol literature (for example, DeMota and Friedlander), and these should be considered in lieu of the expressions presently in use. Stefan flow and diffusiophoresis must also be considered.

e) Homogeneous Nucleation:

I detected a certain tendency on the part of the code developers-Batelle - to reference old texts as these are readily available. Much has occured in the past several years, and better expressions have become available. Even these latter expressions are undergoing revisions because of progress in kinetic theory and experimental aspects, and while the inclination of the code developers can be understood in view of immense pressures to get results, I think there must be a continuing NRC effort to have available the latest, critically appraised information, in a useable form.

2. Two Particle Aerosol Mechanics:

The difficulties that we have with single particle mechanics, affect very strongly the two particle mechanics. In addition, new difficulties also arise. We all realize that the coagulation coefficients are poorly known, but progress has been made in the past years. Specifically the following should be considered:

a) Brownian Coagulation (β_B):

All expressions that are available at this time have limitations. But I believe the expression I have given in my review paper perhaps is a good representation of the ideas advanced by Fuchs. I believe NAUA's expression should be examined carefully.

b) Gravitation Coagulation (β_G):

Under NRC sponsorship, my students and I have conducted extensive work in this area. Our expressions are radically different from those being used in NAUA (TRAP-MELT). Based on some work we have done with our ASTD aerosol behavior program, I believe that there should be serious questions about the expressions being used in BMI-2104 codes.

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c) Turbulent Coagulation (β_T):

This is most difficult to quantify, but is likely to be important in primary coolant systems. T. K. Enomoto is looking at this question in detail in conjunction with his Ph.D. thesis under my supervision, and I should be able to communicate a paper to your office within the next couple of months. I believe, many questions will require much further investigations as several assumptions have been made. Also, calculations corresponding to postulated PCS conditions must be made.

d) Synergism:

The assumption $\beta = \beta_B + \beta_G + \beta_T$ that the codes use, is unverified and has no scientific basis. All published work and our own investigations make it clear that synergism can be strong, and diffusiophoresis, thermophoresis, diffusion, kundsen drag forces, etc. can influence the calculated results markedly.

Efforts should be made to obtain better understanding of synergism, and improved β should be developed.

3. a) <u>The Aerosol Behavior Equation</u>:

The BMI-2104 codes use aerosol behavior equation that is based on strong "contraction of description". There must be some examination of the manner in which effects of shape, velocities, structure, spatial dependence, densities etc. are "averaged" to arrive at the equation. This will help define the coagulation coefficients and the deposition rates in some clear fashion. While resolution of all the questions will require much time and effort, some progress can be made in reasonably short time.

I am not convinced that the aerosol equations are being solved in the best possible manners. With condensation, the equations become hyperbolic, and there is no recognition of this fact in the algorithms being used in the BMI-2104 codes. Based on my own experience with ASTD, I have little doubt that the BMI-2104 codes would yield useless results for strong condensation (evaporation) conditions. I believe with some effort the situation can be, and should be, improved.

I would suggest in this conjunction that a class of problems must be used for computational benchmarking of the computer codes. Some analytical solutions are available, more are being developed, and the NRC must make sure that the codes use efficient numerical schemes that yield accurate results.

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Personally, I would recommend that efforts must be initiated for incorporating explicitly the spatial dependence of aerosol distribution especially in the PCS. I do not think that the TRAP-MELT approximations are consistent in this regard.

I recognize that NRC is a participant in several large scale experimental efforts (MARVIKEN, TREAT, CSTF, NSPP) which will be crucial to understanding of aerosol behavior in nuclear reactor accidents. I also think for data interpretation, guidance of experiments, and eventual development of the source terms that would meet critical unbiased scientific appraisals, the BMI-2104 codes are not adequate. I would like to urge, therefore, that a long range program that would seek to advance the state of the art through better theoretical modeling efforts and small separate effects tests should also be developed. Such a program should be complimentary to the large scale experimental efforts now underway.

No doubt every effort should be made to modify the present codes so that the known deficiencies are modified. I would recommend reactivation and much further strengthening of the efforts that had sought to prepare detailed and critical compilation of theoretical expressions and physical properties data as they pertain to aerosol behavior in severe accidents.

I have appreciated the opportunities for participation in the peer review meetings, and the sustained NRC support of my aerosol research work at this University. Some of the perspectives that I have developed, are result of this work. If I can assist you further, please do not hesitate to call upon me.

Sincerely,

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