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UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, D.C. 20555-0001

NOV 19 1999

Purdue Research Foundation
ATTN: Edie Doland
1063 Hovde Hall, Purdue University
West Lafayette, IN 47907-1063

Dear Ms. Doland :

SUBJECT: MODIFICATION NO. 6 TO TASK ORDER NO. 2 ENTITLED "MODULARIZATION OF TRAC-P" UNDER CONTRACT NO. NRC-04-97-046

In accordance with Section G.4, Task Order Procedures, of the subject contract, this letter definitizes Task Order No. 2 Modification No. 6. This effort shall be performed in accordance with the enclosed Statement of Work. Task 17 is not included in the estimated cost for this task order modification and shall remain on hold until a subsequent mod is issued.

The period of performance for Task Order No. 2 is changed to run from September 30, 1997 to November 30, 2000. The total estimated cost for full performance of this task order is increased by $394,734 from $1,245,743 to $1,640,477. $400,000 in incremental funding is hereby allotted to Task Order No. 2. This action changes the total cumulative funds obligated for performance of this task order from $940,561.60 to $1,340,561.60. The Contractor shall not incur costs for this task order which exceed the cumulative obligated amount of $1,340,561.60. All other terms and conditions of Task Order No. 2 remain unchanged.

Accounting data for Task Order No. 2 mod 6 is as follows:

B&R No.: 06015110135
Job Code: W-6749
BOC Code: 252A
RES ID: RES-C00-326
Appropriation No.: 31X0200
Amount Obligated by This Action: $400,000
FY 97 Obligated Amount:$ 162,000
FY 98 Obligated Amount:$ 300,012
FY 99 Obligated Amount:$ 478,549.60
FY 00 Obligated Amount: $ 400,000
Total Cumulative Obligations:$1,340,561.60

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Purdue

Contract No. NRC-04-97-046
Task Order No. 2 Mod 6

Please indicate your acceptance of this task order by having an official, authorized to bind your organization, execute three copies of this document in the space provided and return two copies to the Contract Specialist. You should retain the third copy for your records. The issuance of this task order does not amend any terms or conditions of the subject contract.

Your contacts during the course of this task order are:

Technical Matters: James Han, Project Officer
(301) 415-6773

Contractual Matters: Stephen Pool, Contract Specialist
(301) 415-8168

Sincerely,

Stephen M. Pool, Contracting Officer
Contract Management Branch No. 1
Division of Contracts and Property
Management
Office of Administration

ACCEPTED: TASK ORDER NO. 2 Mod 6

NAME

DEC 7 1999

DATE

Jeffrey H. Wilson
Treasurer

TITLE

Modification (No. ~~3~~ 6) to ~~the Statement of Work of~~ to Task Order #2, "Modularization of TRAC-P," under Contract # NRC-04-97-046 and Job Code W6749, "Thermal-Hydraulic Research"

Work Requirements

Modify the existing Tasks 2, 5, 12, and 15 and add new Tasks 16 through 21 as listed below. Note that all the following tasks will be performed by Penn State and the only exception is Task 17 that will be jointly performed by Penn State and Purdue University. However, <u>do not work on Task 17 until further notice from NRC</u>.

Task 2. Modularization of Component Communication

Coding will be developed to modularize the communication between components. Boundary information will be provided to each component at initialization and at each time step in a consistent and organized fashion. A communication manager subroutine will be called during initialization to provide the location of the required boundary data for each component, so that at every time step, the proper information is provided to each component. The deliverables of this task include the documentation specified in Subtask 1.5 and a working version of TRAC-M with the required modifications.

Estimated Level of effort: 1 staff month (in addition to the previous estimate of 4 s/m)
Estimated Completion Date: May 31, 2000 (new date)

Task 5. Provide Technical Assistance

This task provides technical assistance to NRC. Examples include technical presentations and tutorial session on the TRAC-M code, conference calls, meetings, and written correspondence to help the NRC staff gain adequate expertise to perform code development and maintenance functions.

Estimated Level of Effort: 2 staff months (in additional to the previous estimate of 2 s/m)
Estimated Completion Date: November 30, 2000 (new date)

Task 12. Development Error Resolution

Under Task 2, the solution procedure as well as the component communication has been revamped in a more modularized and parallelized manner. During these drastic modifications, a number of long standing code bugs were located and corrected. It is highly probable that some others were introduced in these tasks and a number of other long standing bugs exist in areas not touched by this effort. Given the high level of testing thus far, these two classes of bugs can be expected to be relatively subtle, and careful interpretation of final test results will be necessary to locate and correct such bugs. In addition, the final round of testing can be expected to reveal various modeling deficiencies and coding inefficiencies that should be corrected before final release. Task 12 is dedicated to the detection and resolution of these problems. Submit resolution reports and code modifications to the NRC configuration control as per the currently invoked procedures. Deliverables include patch files for code modifications, resolution reports, test plan, and results.

Estimated Level of Effort: 3.5 staff months (in addition to the previous estimate of 6 s/m)
Estimated Completion Date: November 30, 2000 (new date)

Task 15. Assessment

As a means of measuring the success of the BWR consolidation activity and the improvements made to the TRAC-M code under this contract, code simulation fidelity must be assessed and compared to that of TRAC-B. An example report will be provided to the contractor to serve as an example of the information required in the letter reports generated under this task. The following TRAC-B calculations will be completed and documented as per the NRC SQA procedures:

1. BWR/6 Small Break on Ta29zl
2. BWR/6 Simplified Model of MSIV w/o Scram- Steady State
3. BWR/6 Simplified Model of MSIV w/o Scram- Transient
4. BWR/6 Simplified Model of MSIV w/o Scram- Restart
5. BWR/6 Large Break on Ta29xl
6. Some separate-effects tests to be specified by NRC

Deliverables include letter reports in both text and electronic format, and Input decks in electronic format.

Estimated Level of Effort: 5 staff months (in addition to the previous estimate of 10 s/m)
Estimated Completion Date: November 30, 1999 (new date)

Task 16. Higher Order Numerical Methods

Incorporation of the External Component has facilitated coupling the consolidated code to other tools, such as CFD codes. CFD codes utilize higher-order differencing schemes, whereas the consolidated code is limited to a first-order technique. Unfortunately, when coupling two different order numerical schemes, numerically-induced bifurcations may be generated at the location of the coupling if strong gradients are present. Therefore, it may be necessary to incorporate higher-order numerics into the consolidated code.

First-order differencing limits the ability of the code to preserve gradients in physical properties, such as boron concentration and thermal and density fronts. A second-order method would ameliorate this limitation, improving the code's prediction of boron concentration and physical properties (such as density and temperature) that influence the core power predicted by a coupled kinetics code. These gradients also influence instability predictions and a less numerically diffusive scheme would improve the code's ability to model these transients. Instability calculations are now performed only with the semi-implicit method, due to the high diffusion of the SETS scheme. However, SETS allows the code to run at larger time steps. It may be possible to run stability cases with SETS if a higher order scheme were used. This would result in a faster running code and would allow the semi-implicit option to be removed from the code, which would reduce the maintenance effort. (Note that RELAP5 currently has a method to sharpen the thermal gradient. This would not be needed if a higher order differencing scheme were implemented, [illegible] consolidation.)

In order to efficiently couple the TRAC code to a CFD code and to minimize numerical diffusion to better represent gradients in physical properties, higher-order numerics should be incorporated into TRAC. This work has been facilitated by the modularization of the hydraulic component to hydraulic component communication in the code as well as the modularization of the solution procedure. Before the optimal means of providing this capability is determined, a pilot study of various approaches should be done so that final incorporation into TRAC is done efficiently and the run-time is not dramatically hindered.

TRAC code will be stripped down to minimize its complexity, leaving just the minimal coding required to run SETS and SEMI-IMPLICIT schemes for a network consisting of both one-dimensional and three-dimensional components. The numerical scheme will be modified to provide a second-order differencing technique, while leaving the first order technique in place. This approach will provide the ability to judge the benefit and detriment of the higher-order technique. Factors should include numerical diffusion, run-time and numerical stability. Test cases should be devised to test these factors and should be run with both schemes to determine the most advantageous differencing method. Implementation is also a concern and the code architecture should also be studied and discussed to ensure that when incorporated into TRAC, the coding is readable and extendable. Provide a letter report to NRC to summarize the results of this study. All coding must be done in F90 and should be portable across all NRC platforms (SUN, SGI, HP, DEC Alpha, Windows NT, IBM AIX). Deliverables include a letter report in both text and electronic format, and pilot code developed during this study in electronic format.

Estimated Level of Effort: 7 staff months
Estimated Completion Date: November 30, 2000

Task 17. Shared Memory Parallelization

NRC will survey the industry to determine which shared memory application program interface (API) is supported by the most F90 compilers on NRC platforms (SUN Solaris, IBM AIX, SGI, HP, DEC Alpha, and NT). The selected API will be used to increase the speed of the parallelized code (this involves splitting do-loops over components to different processors) on shared memory machines. The coarse grain parallel coding using PVM will be modified (ie, splitting up vessel from the one-dimensional loops) to utilize the external component interface (ECI) to pass only the required information to enhance the speed of the code running on distributed and shared memory machines. Currently, if using ECI to run TRAC processes, multiple input decks must be created with the proper information in each deck for each processor. A more user-friendly approach should be developed so that the user need only input the component numbers for which each processor to perform the solution. SQA procedures must be followed.

Estimated Level of Effort: 9 staff months (= 7 s/m for Purdue University + 2 s/m for Penn State for solution procedure assistance)
Estimated Completion Date: April 30, 2001 (to be revised)

Task 18. Time Step Driver Routines

The External Component developed under this contract allows the code to be coupled to other processes. [illegible] step information must be communicated to the central process so that the minimum value is chosen and all the processes run at this value. Therefore, the TRAC Time step driver routines must be re-written so that they can receive and send this information efficiently. SQA procedures must be followed.

Estimated Level of Effort: 1.5 staff months

Estimated Completion Date: November 30, 2000

Task 19. Water Packer Logic

Detection of water packing event is flawed in the code, limiting its robustness and increasing its run-time. This logic will be reviewed and a more robust method will be incorporated into the code so that the events can be detected and mitigated. This work will be performed by the NRC staff member with assistance from the contractor (namely, Penn State).

Estimated Level of Effort: 1 staff month
Estimated Completion Date: November 30, 2000

Task 20. Fill and Break Modifications

Fill and Break components should be modified so that the treatment of time levels is similar to that of the other hydraulic components (e.g., use of TimeUpGen1D logic), eradicating the need to overwrite terms in the pressure equation in low level subroutine such as tf1ds. These components should have an entry in the CompSeg, etc... arrays so that they function as 1 cell/mesh components with special equation sets, allowing implicit feedback of the Fill and Break properties on the solution (properties and derivatives are evaluated during the iteration). SQA procedures must be followed.

Estimated Level of Effort: 2.5 staff months
Estimated Completion Date: November 30, 2000

Task 21. Code Execution Interruption Logic

When the code detects a failure, several means of halting execution are utilized. A consistent set of logic should be developed to assign a level of severity to the error, messages written to a specified set of files and the code execution halted in a particular manner. This work will improve the code readability, facilitate the diagnosis of bugs, and assist the user in de-bugging an input deck. SQA procedures must be followed.

Estimated Level of effort: 1.5 staff months
Estimated Completion Date: November 30, 2000

Meetings and Travel:

The contractor will attend three meetings at the NRC office in Rockville, Maryland. For planning purposes, each meeting will involve two people and last for two days. However, any travel must be approved in advance by the NRC Technical Monitor.