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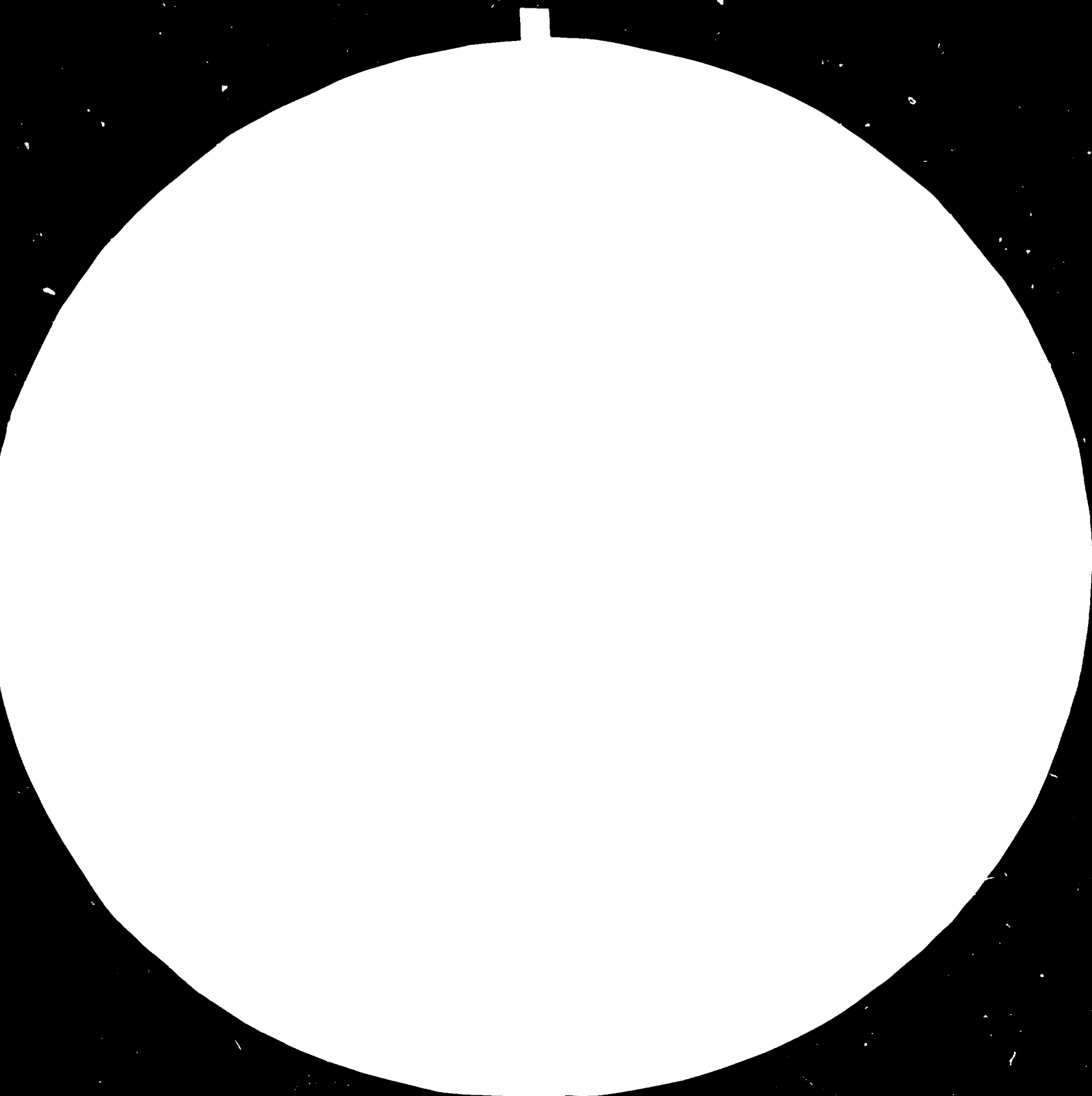
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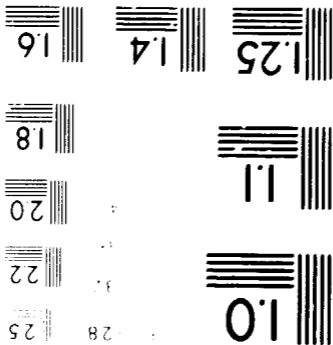
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Technical Report*

Mission 9-20 January 1984

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Based on the work of Morton M. Denn,
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During the period from January 9 - 20, 1984, the UNIDO consultant visited the Regional Research Laboratory, Hyderabad (RRLH), working on the coal gasification project. During that period four lectures have been presented relating to fundamental concepts of coal gasifier modeling and numerous discussions with RRLH scientists took place in both large and small groups.

The level of competence of those involved in the program is generally high. Those working on the modeling aspects of the program have adequate experience in the general area of reactor modeling. The staff operating the pilot plant is clearly competent, and appears to be quite sensitive to the particular experimental needs of a program that is integrated with a modeling effort.

The goal of this (or any) reactor modeling program is to develop mathematical models that will enable analysis of changing operating conditions, feedstock, and perhaps even reactor configuration, with the goal of using inexpensive computer experimentation to guide the selection of actual experimental conditions on a small scale or pilot plant system. This is the established procedure throughout most of the chemical and petrochemical industry, though it has made little inroad to date in coal conversion technology. There are several levels of models that are useful in the analysis of moving bed coal gasification reactors of the type under study at RRLH. The various modeling levels provide different amounts of information. The selection of a particular level of model depends on both the amount of experimental information that is available or that can be obtained, and on the computational facilities that are available.

The RRLH staff has made a good start on the development of what might be characterized as a first-level model: one dimensional (neglecting radial effects), and homogeneous (treating solid and gas phases as being at the same temperature). The available computational facilities at RRLH are ideally suited for this type of model, but it has severe limitations. First, the one-dimensional

approximation is probably not relevant to a small-diameter gasifier like the one that has been installed at RRLH, though it is undoubtedly appropriate for current generation large-diameter moving bed gasifiers. Second, there is some question as to the ability of a homogeneous model to predict lower bounds on blast gas temperature for reactor operability because of the effect of heat transfer effects in the lower portion of the gasifier. The latter prediction is quite important, in view of the economic considerations associated with the heating of the blast gas.

I have recommended that the modeling effort proceed in two ways: development of a one-dimensional, two-phase (different gas and solid temperature) model, and development of a simple single-phase (two-dimensional) model. Either of these should be within the scope of computational facilities available at RRLH, though I believe that each will stretch those facilities to the utmost. I have been informed that more extensive computational facilities are available at nearby locations, but I do not know the capabilities of these facilities, or the extent to which they will be available. Neither of these extended models will give a complete picture of what is happening in the gasifier, but each should provide information that will supplement the simpler one-dimensional single-phase model that has now been implemented. I believe that the ultimate goal of a full two-phase, two-dimensional model is beyond the computational facilities currently available at RRLH, and it should not be pursued at the present time.

The entire field of moving bed gasifier modeling suffers from a paucity of experimental measurements. Measurements of reactor effluent composition are commonly available for well-characterized coals, but such measurements are easily shown to be insensitive to important events happening within the reactor. In particular, such measurements are not indicative of the maximum temperature experienced by the coal, and the maximum temperature is perhaps the single most important operating variable in a dry-ash moving bed gasifier. Some specific uncertainties in the modeling of these gasifiers need to be resolved if the models developed at RRLH or elsewhere are to be truly useful in reactor analysis. The experimental data that are particularly needed for such resolution of modeling uncertainties are temperature profiles along the axis of the reactor, from the grate to the top, identifying the location and temperature of the combustion zone. The engineers in the pilot plant believe that it may be possible to obtain such

measurements in their gasifier, and I have encouraged them to do so. I see this as the highest priority experiment from the point of view of modeling (though perhaps it is less important from the point of view of answering the more basic question of the potential of this gasifier for the conversion of Indian coal). There are specific technical questions regarding the implementation of such an experiment, and we have discussed these in some detail.

There are some proprietary computer programs whose availability would greatly aid the RRLH modeling program, and I recommend their acquisition, if at all possible at a reasonable price. Programs developed under my direction at the University of Delaware, owned by the Electric Power Research Institute, would be quite helpful in developing an RRLH code for the two-dimensional model. Based on informal conversations that I have had with the EPRI project manager, Dr. George Quentin, I believe that it might be possible to license these programs at negligible cost in return for an agreement to exchange technical information obtained on the gasifier. I do not know if such an arrangement, if possible, would be considered to be in the best interests of UNIDO or RRLH, but it seems to me that it would be. The programs were developed under EPRI Research Project 1268-1, Report EPRI AP-2576. The work was done for the Electric Power Research Institute, Clean Gaseous Fuels Program, Advanced Power Systems Division, 3412 Hillview Avenue, Palo Alto, California 94304. Dr. Quentin reports to Neville Holt, whom Dr. Vaidyeswaran knows, and the approach to EPRI should probably be made to Dr. Holt. I should not make the EPRI contact because I have been involved in a minor controversy with their licensing people over the question of ownership of an earlier computer program. (There is no doubt regarding EPRI ownership of this particular set of programs.)

There is a second program that has been developed by my student, Gregory Dow, at the Lawrence Berkeley Laboratory, under the sponsorship of the United States Department of Energy, Morgantown Energy Technology Center. This program has not yet been documented or even provided to METC. It is a highly efficient version of a one-dimensional, single-phase gasifier model, and in that sense it simply duplicates what has been done at RRLH, but is undoubtedly far more computationally efficient and is in a modular form that facilitates changes and improvements with increasing understanding of the gasifier. This work is done for a program at METC headed by Dr. Mahdev Ghate, who is acquainted with

Dr. Vaidyeswaran. I will approach Dr. Ghaté directly regarding permission to transmit this program to RRLH. If I am unsuccessful, then perhaps an official approach from UNIDO will be needed. I should point out that officials at METC are quite sensitive to the question of use and ownership of computer programs whose development they have sponsored.

It is my view that the modeling program at RRLH can proceed in a satisfactory manner for a number of months without my further involvement, but that additional personal collaboration would be helpful at periodic intervals. We have informally agreed on a schedule that would bring Mr. M. M. Mallikarjunan to work with me in Berkeley during the month of June, and then for me to return to RRLH during the last week of December. The least complicated way to handle Mr. Mallikarjunan's visit is to do it informally, through the College of Chemistry at the University of California. A request should be sent directly to me, Department of Chemical Engineering, University of California, Berkeley, California 94720, requesting that I accommodate Mr. Mallikarjunan in my laboratory for a period of up to four weeks. With the approval of my chairman and dean I can have visitors to my laboratory and provide them with facilities at no expense. I am willing to do this, since I do not expect the computer time to be excessive or to involve computations that cannot be justified under my existing research contract on coal gasification. This will be done with the understanding that any work done here will be considered to be non-proprietary, and anything that I deem to be publishable will be published with acknowledgment to the partial support of the U. S. Department of Energy, as well as to UNIDO for the support of Mr. Mallikarjunan's trip. We cannot accommodate him here under any other conditions.

I have one other observation to make regarding my stay at the Laboratory. I spent some time discussing research with other research groups at RRLH in areas in which I have some competence. The overall quality of work seems high. One thing did concern me greatly, however. I noted a dangerous lack of safety precautions in some laboratories (not, I wish to emphasize, in the coal gasification pilot plant). Such simple precautions as the chaining of gas cylinders were not observed. This represents an extraordinary disregard for the lives and safety of the workers in that laboratory, particularly given the possibility of earthquakes. Such an attitude towards safety would not be tolerated in any American laboratory with which I am acquainted, university or industry.

In summary, the portion of the gasification program on gasifier modeling appears to be progressing in a satisfactory manner, and will also profit from cooperation with the scientists responsible for the pilot plant. The planned experimental program on measurement of temperature profiles along the axis of the gasifier, if successful, will represent a major breakthrough in the understanding of such systems and in the ability to use models in an effective manner. The proposed time scale for Mr. Mallikarjunan's visit to Berkeley in June and my return to RRLH during the last week in December appeared to be about right for the logical progression of the program.

