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14765

January 1985

RESTRICTED

ENGLISH

COAL GASIFICATION .

DP/IND/80/004

INDIA

Technical Report*

Mission 6-11 January 1985

Prepared for the Government of the Republic of India
by the United Nations Industrial Development Organization,
acting as executing agency for United Nations Development Programme

Based on the work of Morton M. Denn,
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United Nations Industrial Development Organization
Vienna

27 '85

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DP/IND/80/004 - Coal Gasification

Modelling of Coal Gasification Reactions

Hyderabad, India

I visited the regional research laboratory, Hyderabad from Sunday, January 6 through Friday, January 11, 1985. I gave one lecture on the application of modern finite element computational methods while at the laboratory, but the bulk of my time was spent in discussions with laboratory scientists and engineers associated with the coal gasification project. These discussions focussed on progress to date on reactor modelling and on obtaining experimental data from the gasifier, and on the plans for the coming year, experimental and theoretical.

The prediction of effluent properties from a moving bed coal gasifier is relatively insensitive to model details, and thus provides little insight into the usefulness of models for design and operation of the reactor. The main information that one needs for design and analysis is the location and magnitude of the maximum temperature in the gasifier. Such data are not available, and thus no existing model of a gasifier can be used with confidence for engineering analysis. The progress at Hyderabad since my last visit is quite gratifying, and suggests that profile data of the type necessary for model validation and application may be obtainable. We spent a good deal of time analysing the data obtained by shutting down the gasifier and removing sequential layers from the coal bed. Data analysis was not complete, but sufficient data were available to indicate that trends regarding the behaviour within the reactor were clearly correct, though interpretation of the data is not transparent. The data appeared to indicate that some mixing between zones took place while the reactor was being emptied. It is not at all clear why this should have occurred, nor where the mixing could have taken place. We agreed that it would be very useful to obtain data on the solids residence time distribution when the gasifier is operating normally, and to repeat the residence time distribution measurement when the gasifier is shut down and the solid layers sequentially removed; this will show if flow patterns during emptying are the same as the flow patterns during normal operation, and hence if the analysis of the solids can be related directly to the conditions at known spatial positions in the gasifier. If the latter is not true, then the residence time distribution measurements may indicate how to "unmix" the data in order to obtain the true profile within the reactor.

Plans are continuing, as they should, for the measurement of temperature profiles along the axis of the gasifier during operation. Such measurements provide the ultimate test of model validity, and are to be encouraged if they seem at all possible. The design of the experiment is not yet obvious; I have some concerns about possible gas by-passing because of the presence of the vertical thermocouple well, and it is essential to ensure that the design is such as to minimise this possibility, since it will give spurious temperature readings. I also have some concern about the effect of axial conduction along the thermocouple well on the measured profile; such conduction would lead to a broader temperature maximum than in fact exists. This effect can be readily checked by calculations using the profiles computed from the current model, and I believe that this will be done shortly.

The other planned experiments, in addition to normal operation of the gasifier on several other coals and analysis of the contents following quench, are a continuation of the work on gasification kinetics of Indian coals. This work clearly needs to be continued, since these kinetic data are not readily available and are required before application of any models that are to be used in design and analysis. Overall, I am in complete agreement with the experimental programme that is planned for the remainder of 1985.

The normal transients that occur during operation provide a great deal of information about the dynamical characteristics of the gasifier when it is perturbed slightly. Such data have been recorded on strip charts in the past, and there are plans to obtain normal operating data by electronic means in the coming months. We can anticipate that at some point in the future it may be desirable to develop a dynamical model for control purposes for the gasifiers, particularly if there are plans to use moving bed gasifiers as part of a combined-cycle power generating system, where the gasifier must respond to short-term transients. These dynamical data will be invaluable at that time, since they contain all of the information necessary for construction of a linear model. I do not recommend diverting manpower to such dynamical modelling now, but I believe that it is essential that data be stored in an easily-retrievable fashion (preferably on disc), so that the files for long runs can be recovered when needed in order to carry out the appropriate correlation analysis for development of transfer functions.

The modelling work is proceeding satisfactorily. The one-dimensional, homogeneous model for the gasifier developed in Hyderabad is operational, and the LBL/DOE model developed at Berkeley is now nearly operational in Hyderabad (with only a few inconsistencies in Fortran statements remaining to be found). The two codes, though they differ in small details with regard to the physics, give essentially the same predictions regarding reactor performance when tested with the input conditions. Progress is good on the development of a two-dimensional homogeneous reactor model in Hyderabad.

We spent a good deal of time discussing the development of appropriate equations for a one-dimensional heterogeneous model. There appear to be some problems in the published literature regarding the correct form for the equations, but I believe that we have these ironed out. The computational problem for implementation of such a model has never really been solved

satisfactorily, and some physical approximation has to be made at the bottom of the gasifier in order to solve the equations. Several such approximations have been described in the literature, and one or more of these will be implemented on the RRL model; it should be possible to test the variations among these approximations, since they do not differ considerably in structure of the problem solution. Ideally, the gasifier would be described by a two-dimensional, heterogeneous model, including the two-dimensional nature of the fluid mechanics. The required computational power for the solution of such equations does not exist at present in India, and I do not believe that such a modelling task should be attempted. We have discussed the possibility that my colleagues and I at Berkeley might undertake such a task as part of our own gasification programme, but that determination has not yet been made.

Overall, I am pleased with the progress that has been made at RRL during the past year. The personnel are clearly competent, and they are motivated to accomplish a great deal on this programme. The type of data that they are gathering has long been needed in this area, and the gasifier represents a unique experimental tool that will be of great value not only to the Indian gasification programme, but to the world-wide community interested in understanding the behaviour of this type of reactor. They should be encouraged to continue in the path that they have been following at RRL.

I understand that there are plans under the UNIDO programme for an RRL scientist to spend an additional man month with my group at Berkeley. Mr. M. M. Mallikarjunan should be the individual sent, since that would represent the most efficient use of our time at Berkeley and the most efficient transfer of knowledge and technology to the Hyderabad group. His first stay provided him with the necessary introduction to the personnel and the facilities at Berkeley, and a re-orientation and adjustment period will not be required. If someone new were to come then a substantial part of his stay would be spent learning his way around and in learning to use the Berkeley facilities, including the computer system. I am agreeable to a visit any time after July, under the same terms as the previous visit.