## EDS COAL LIQUEFACTION PROCESS DEVELOPMENT

PHASE V

EDS Consolidation Program: Reactor Optimization Design Study

Interim Report

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#### Abstract

This is an Interim Report prepared under the U.S. Department of Energy Cooperative Agreement No. DE-FCU5-77ET10069 for EDS Coal Liquefaction Process Development - Phase V. Funding for the EDS Project is shared by U.S. Department of Energy, Exxon Company, U.S.A. (a division of Exxon Corporation), Electric Power Research Institute, Japan Coal Liquefaction Development Company, Phillips Coal Company, Anaconda Minerals Company, Ruhrkohle AG, and ENI. The agreement covers the period January 1, 1977 through December 31, 1985. The laboratory process research and development studies were conducted at various Exxon Research and Engineering (ER&E) facilities: Research and Development Division at Baytown, Texas; Products Research Division at Linden, New Jersey; and the Exxon Research and Development Laboratories at Baton Rouge, Louisiana. The engineering research and development studies were performed by the Exxon Engineering Petroleum and Synthetic Fuels and Technology Departments at Florham Park, New Jersey.

This report documents the results of a reactor optimization design study. The work was conducted as part of the EDS Consolidation Program. The design recommendations represent a consolidation of learnings accrued during previous phases of the EDS Project including results obtained from ECLP operations, from the ECLP Test Program, and from past EDS Study Design preparations.

## TABLE OF CONTENTS

			PAGE		
General Description					
Sum	mary of Res	ults	1		
•	Reactor Marketter We Calculation Solids Holdung Backmixing Evaluation Relative		2 3 7 7 13 18 18 23 26 27		
Con	clusions		29		
Ref	erences		31		
Tab	les				
+ + +	Table 1: Table 2: Table 3: Table 4: Table 5: Table 6:	Reactor Metal Volume Requirements Reactor Temperature Profile Calculations Summary of EDS Solids Holdup Data Liquefaction Reactor Process Information Evaluation of Reactor Configurations Relative Investments for Reactor Case Configurations	8 14 17 19 24 28		
Figu	ıres				
+	Figure 1: Figure 2:	Design Temperature vs. Internal Diameter for 12-inch Thickness Temperature vs. Hydrogen Partial	4		
	_	Pressure - Nelson Curve Limitations	6		
+	Figure 3:	EDS Liquefaction Reactor Temperature Profile	11		
+	Figure 4:	Schematic Effect of Backmixing on EDS Liquefaction Reactor Temperature Profile	12		
+	Figure 5:	Gas Holdup (Solids-Free) vs. Superficial Gas Velocity	20		
+	Figure 6: Figure 7:	Liquid Holdup vs. Superficial Gas Velocity Effect of Backmixing on ART Requirements	21 22		

## EDS CONSOLIDATION PROGRAM

## REACTOR OPTIMIZATION DESIGN STUDY

This report documents the results of a study to evaluate lique-faction reactor design requirements for a commercial-scale EDS plant. The work was conducted as part of the EDS Consolidation Program. The design recommendations represent a consolidation of learnings accrued during previous phases of the EDS Project including results obtained from ECLP operations, from the ECLP Test Program, and from past EDS Study Design preparations.

### General Description

As a result of EDS process development activities, information to improve the understanding of liquefaction reactor design requirements has become available. In particular, reactor tracer tests conducted at RCLU, CLPP, and ECLP have expanded the data base regarding reactor hydrodynamics and have resulted in the development of correlations which can be utilized to identify optimum liquefaction reactor design guidelines. This study utilizes these correlations to explore alternative reactor design configurations, relative to those typically used in past EDS study designs, to determine preferred commercial reactor design arrangements. This study also updates the commercial plant reactor design philosophy regarding reactor mechanical design and size constraints, reactor exotherm profile estimation techniques, reactor solids holdup guidelines, and reactor material selection alternatives.

## Summary of Results

The information currently available regarding reactor design criteria has been used to identify the considerations which should be evaluated when preparing EDS reactor design specifications. Conclusions and recommendations from this study are summarized as follows:

- Maximum reactor wall thicknesses are 12 inches based on state-of-theart fabrication ability. For typical EDS processing conditions and design limits, this translates into maximum reactor internal diameters of twelve feet.
- Reactors of fixed internal volume have the same weight and cost whether designed as long, small diameter vessels or as shorter, larger diameter vessels.
- Trail EDS reactors may substitute 1-1/4 Cr-0.5 Mo in place of 2-1/4 Cr-1 Mo as the base metal material. Hydrogen partial pressures in the trail reactors are low enough to allow this material replacement. However, this replacement is not necessarily cost-effective, and a selection of which material results in the lowest investment can only be made at the time of procurement.

- Guidelines are recommended for determining the reactor exotherm profile as necessary to meet a target average reactor temperature. The average reactor temperature has been defined as the average of the mid-volume temperatures for each of the reactors provided, based on use of a typical EDS exotherm profile uncorrected for backmixing effects.
- Available solids holdup data indicates that crushing feed coal to top sizes of 100 mesh or less may have substantial benefits. Smaller coal particle sizes directionally reduce solids holdup levels and result in more effective use of available reactor volume.
- For coal feed particle top sizes of 20-30 mesh, which are typical of those generally considered for EDS study designs, reactor superficial gas velocities should be maintained above 0.10 ft/sec. For these design conditions, solids holdup levels of no more than 20% should be achievable.
- Reactor diameter should be selected to achieve superficial gas velocities of 0.10 ft/sec. This allows optimum capture of hydrodynamic benefits which accrue from decreased gas holdup levels, while not placing the design in a region where solids holdup concerns might govern.
- Reactor staging should be provided to achieve Peclet numbers in the range of 10-15. This allows a reasonable approach to plug flow kinetics such that backmixing debits on conversion levels are not substantial.
- Processing conditions from the EDS Wyoming Coal Bottoms Recycle Study Design Addendum (Reference 1) were used to evaluate alternate reactor configurations. For these process conditions, the optimum design for processing 6,250 T/SD of dry coal provided two parallel trains, each containing two-twelve foot I.D. reactors. The relative investment for the recommended configuration was 80% relative to the reactor design specified for the Wyoming Addendum. The relative investment for the recommended configuration was 90% of that for a configuration identical to that provided for the Wyoming Addendum, if the Wyoming Addendum configuration were resized using the current understanding of reactor hydrodynamics.
- Consideration should be given to adjusting coal throughput per reactor train to allow meeting the 0.10 ft/sec superficial gas velocity criteria with a 12 foot I.D. reactor. This allows capture of economy-of-scale credits for other equipment pieces within the liquefaction process section.

## Reactor Mechanical Design and Size Constraints

When designing liquefaction reactors, it is typically costeffective to utilize the largest possible cross-sectional area. For a given process throughput, larger cross-sectional areas translate into lower superficial gas velocities and improved hydrodynamics. There is also the basic economy-of-scale size effect which generally favors building equipment as large as possible to limit the overall number of equipment pieces. As a result, identification of the maximum permissable reactor diameters from a mechanical design and procurement viewpoint must be considered.

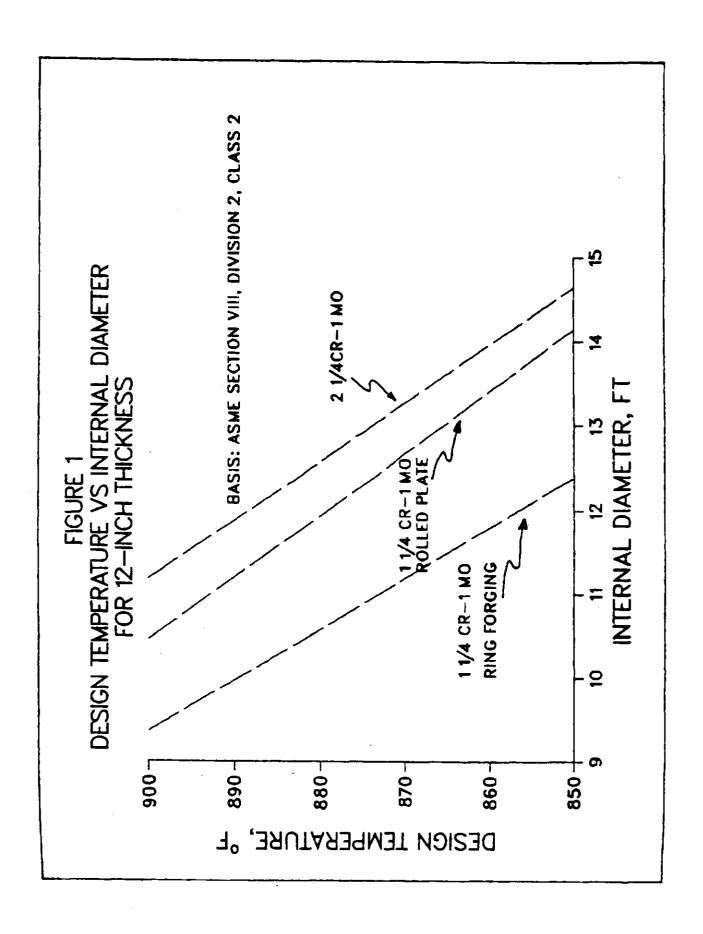
For EDS liquefaction design purposes, it has been determined that wall thickness represents the key constraint on reactor diameter. State-of-the-art fabrication ability indicates that 12-inch walls represent the maximum thickness which should be considered. This thickness has been provided for commercial petroleum industry vessels currently in operation. Although the quantity of world-wide vendors capable of providing 12-inch wall vessels is limited, sufficient vendors have this capability to ensure a competitive bidding environment.

The base reactor metal for liquefaction reactors is either 2-1/4 Cr-l Mo or 1-1/4 Cr-0.5 Mo (see "Reactor Material Selection Considerations" for more information). It is assumed that the reactors will be constructed in accordance with ASME Section VIII Codes, Division 2, Class 2. Figure 1 plots allowable reactor inside diameter vs. design temperature as constrained by the 12-inch wall thickness limitation. Information utilizes typical ASME Code stress values for 2-1/4 Cr-1 Mo and 1-1/4 Cr-0.5 Mo (two 1-1/4 Cr curves are presented – one assumes rolled plate construction while the other assumes ring forgings). These stress values may change based on review of fabrication procedures and methods of individual suppliers, but they should be representative for screening purposes.

Figure 1 indicates two basic points. First, allowable stress decreases rapidly as design temperature rises above 850°F. Up to 850°F, the rate of stress decrease vs. temperature increase is very flat such that increasing design temperature does not get severely debited by requirements for increased metal thickness (or conversely, through limitations of internal diameter if thickness is limited to 12 inches). However, above 850°F, which is representative of typical EDS liquefaction reactor design requirements, the negative effects of increasing design temperature are fairly severe. Secondly, internal reactor diameters of approximately 12 feet represent the maximum diameter for design conditions comparable to those used for the EDS Wyoming Bottoms Recycle Study Design Addendum (2-1/4 Cr-1 Mo base metal, 885°F design temperature). This 12-foot maximum diameter is utilized within this study as the effects of hydrodynamics and other design criteria are analyzed to determine optimum design configurations.

## Reactor Material Selection Considerations

The key variable associated with reactor base metal material selection is hydrogen partial pressure. Hydrogen partial pressure is typically highest for EDS liquefaction process conditions at the inlet to the first reactor, before hydrogen has been consumed during the coal conversion process. At this point, reaction temperatures are conversely at their lowest since the exothermic heat of reaction has not yet contributed to a temperature rise.



Directionally, this relationship of temperature and hydrogen partial pressure is favorable for materials selection. Selection of materials for hydrogen resistance is based on the use of Nelson curves – a family of empirically derived curves published and maintained by the API in Publication 941. Figure 2 depicts the Nelson curve information for 2-1/4 Cr-1 Mo and 1-1/4 Cr-0.5 Mo steels in the region of interest for EDS liquefaction reactor design. Information is also provided on Figure 2 to show the data points associated with the reactor design conditions used for the EDS Wyoming Bottoms Recycle Study Design Addendum. In this design, each liquefaction line contained three reactors in a series arrangement, with treat gas provided as quench for temperature control following the first and second reactors. The information shows that 2-1/4 Cr-1 Mo must be used as the base metal for the first reactor. However, 1-1/4 Cr-0.5 Mo can be substituted for 2-1/4 Cr-1 Mo as the base metal for the trail reactors.

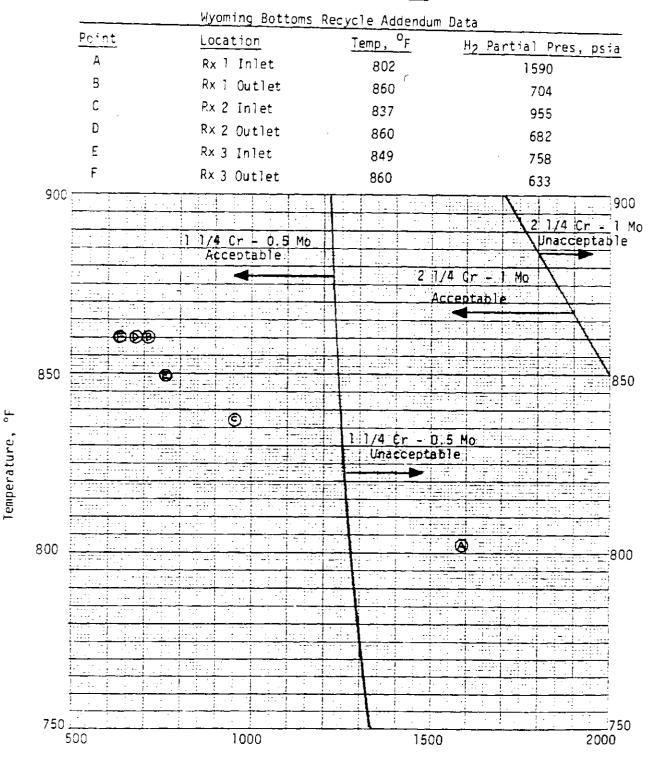
It should be noted that this relationship is specific to the Wyoming Addendum design, and the process conditions and treat gas rates which it describes. Directionally, this relationship should hold for all EDS designs, although each design should be checked for its selected process conditions and treat gas rate. Upset conditions should also be evaluated to ensure that the Nelson curve limits are not violated under any operational circumstances. Included in this evaluation should be the effect of backmixing on the temperature profile within each reaction stage. Backmixing effects tend to well mix the contents of each stage. As a result, stage inlet hydrogen partial pressures may occur at temperatures nearly equal to the stage outlet temperature. Backmixing effects on temperature are discussed in more detail later in this report.

Although 1-1/4 Cr-0.5 Mo is typically a lower cost material than 2-1/4 Cr-1Mo, this relationship does not always hold. The relative costs of these two metals varies with time depending on market demand and contractor's fabrication availability. At present, 1-1/4 Cr-0.5 Mo is approximately 10% cheaper per pound than 2-1/4 Cr-1 Mo.

On the negative side, 1-1/4 Cr-0.5 Mo is a lower strength material than 2-1/4 Cr-1 Mo. This can be inferred from the information provided in Figure 1. Therefore, for a given internal reactor diameter, a greater quantity of 1-1/4 Cr-0.5 Mo metal is required relative to 2-1/4 Cr-1 Mo. This at least partially counteracts the incentives for use of 1-1/4 Cr-0.5 Mo based on its typically lower cost.

In summary, the above information indicates that use of 1-1/4 Cr-0.5 Mo instead of 2-1/4 Cr-1 Mo as the base metal for trail liquefaction reactors has potential as a cost reduction step. However, a key variable in determining if this modification is cost effective is the relative cost of the two metals at the time of procurement. At procurement time, vendors should be asked to quote relative purchase prices for both base metals (assuming a check of Nelson curve limitations for the selected process conditions allows the use of 1-1/4 Cr-0.5 Mo) and a selection of the most cost-effective option can then be made.

FIGURE 2
TEMPERATURE VS. HYDROGEN PARTIAL PRESSURE
NELSON CURVE LIMITATIONS



Hydrogen Partial Pressure, psia

## Reactor Weight vs. Reactor Volume Parameters

Reactor investment requirements are closely related to the quantity of metal required to fabricate the vessel. Approximately 90% of a reactor's investment is associated with material costs. It is therefore important to understand the relationship between reactor metal weight and reactor volume parameters.

Hydrodynamic effects indicate that long, small diameter reactors are directionally favored to allow approach to plug flow kinetics. However, appropriate staging can be provided, even for short, large diameter reactors to eliminate this as a factor of major concern. More importantly, short, large diameter reactors are favored to allow reducing gas holdup levels (which increases the effective reactor volume available for slurry).

For a reactor of fixed volume, straight-side metal requirements are identical for a short, large diameter reactor or for a long, small diameter reactor. This relationship is supported by information in Table 1. Reactor volume is directly proportional to length times diameter squared. For fixed design temperature, pressure, and material requirements, straight-side metal requirements are also directly proportional to length times diameter squared. As a result, adjustment of reactor dimensions to achieve an optimum design can concentrate solely on hydrodynamic correlations and their impact on reactor volume requirements. Reactor weight requirements are unaffected by the relationship of length and diameter used to achieve the required reactor volume.

Table 1 also indicates the relationship of head metal volume with diameter. Head metal volume (assuming hemispherical heads) is directly proportional to diameter cubed. This indicates that there is some advantage to smaller diameter vessels. However, the metal volume required for hemispherical heads typically represents 5% or less of the overall reactor metal volume requirements. Therefore, head metal volume requirements in relation to straight-side metal requirements are insignficant.

## Calculation of Average Reactor Temperature

RCLU and CLPP, the small pilot plants used to develop the yield data base for EDS, contain reactors which basically operate in an isothermal mode (RCLU is fully isothermal while CLPP typically exhibits a temperature rise equal to approximately one-half of that expected for an adiabatic design). As a result, the yield data base is related to an average reaction temperature. When operated adiabatically, as demonstrated at ECLP, the reaction exotherm results in a temperature profile with the rate of temperature rise dependent on degree of conversion, type of reaction products, and the quantity of process fluids. Translating this exotherm profile into an equivalent average reaction temperature, to allow utilization of the broad smaller pilot plant data base for conversion determations, can be accomplished in a variety of ways.

#### TABLE 1

## REACTOR METAL VOLUME REQUIREMENTS

#### Reactor Straight-Side

+ Reactor Volume

$$V_{R} = L \left(\frac{\pi}{4} D_{i}^{2}\right)$$

$$\therefore V_{R} \propto L D_{i}^{2}$$

+ Reactor Metal Volume

$$t = \frac{P D_{1}}{2 (SE - 0.6 P)}$$

$$V_{m} = L (\frac{\pi}{4} D_{0}^{2} - \frac{\pi}{4} D_{1}^{2})$$

$$D_{0} = D_{1} + 2t$$

$$V_{m} = L (\frac{\pi}{4})[(D_{1} + 2t)^{2} - D_{1}^{2}]$$

$$= L (\frac{\pi}{4})(D_{1}^{2} + 4t D_{1} + 4t^{2} - D_{1}^{2})$$

$$= L\pi t (D_{1} + t)$$

$$= L\pi \left[\frac{P D_{1}}{2(SE - 0.6 P)}[D_{1} + \frac{P D_{1}}{2(SE - 0.6 P)}]\right]$$

$$= \frac{L\pi P}{2(SE - 0.6 P)}[D_{1}^{2} + \frac{P D_{1}^{2}}{2(SE - 0.6 P)}]$$

$$= \frac{\pi P}{2(SE - 0.6 P)}[1 + \frac{P}{2(SE - 0.6 P)}] L D_{1}^{2}$$

$$\therefore V_{m} \alpha L D_{1}^{2}$$

$$\therefore V_{m} \alpha V_{R}$$

#### TABLE 1 (Cont'd)

## Reactor Heads - Metal Volume

+ Basis: Two Heads per Reactor

$$V_{s} = \frac{1}{6} \pi 0^{3}$$

$$t_{s} = \frac{P D_{i}}{4 (SE - 0.1 P)}$$

$$V_{m,s} = \frac{1}{6} \pi D_{0}^{3} - \frac{1}{6} \pi D_{i}^{3}$$

$$D_{0} = D_{i} + 2t_{s}$$

$$V_{m,s} = \frac{\pi}{6} [(D_{i} + 2t_{s})^{3} - D_{i}^{3}]$$

$$= \frac{\pi}{6} [6t D_{i}^{2} + 12t^{2} D_{i} + 8t^{3}]$$

$$= \frac{\pi}{6} \left\{ \frac{6 P D_{i}^{3}}{4 (SE - 0.1 P)} + \frac{12 P^{2} D_{i}^{3}}{[4 (SE - 0.1 P)]^{2}} + \frac{8 P^{3} D_{i}^{3}}{[4 (SE - 0.1 P)]^{3}} \right\}$$

$$= \frac{\pi}{6} \left\{ \frac{3P}{2} \left( \frac{1}{SE - 0.1 P} \right) + \frac{3P^{2}}{4} \left( \frac{1}{SE - 0.1 P} \right)^{2} + \frac{P^{3}}{8} \left( \frac{1}{SE - 0.1 P} \right)^{3} \right\} D_{i}^{3}$$

$$\therefore V_{m,s} \alpha D_{i}^{3}$$

#### Definition of Parameters

VR = Reactor Volume, in<sup>3</sup>

L = Reactor Straight Side, in

Di = Reactor Inside Diameter, in

t = Reactor Wall Thickness, in

P = Design Pressure, psig

S = Metal Stress, psi

E = Weld Efficiency = 1.0

D = Reactor Outside Diameter, in

VM = Reactor metal Straight-Side Volume, in<sup>3</sup>

VM = Sphere Volume, in<sup>3</sup>

ts = Hemispherical Head Thickness, in

VM = Reactor Metal Sphere Volume, in<sup>3</sup> (two heads)

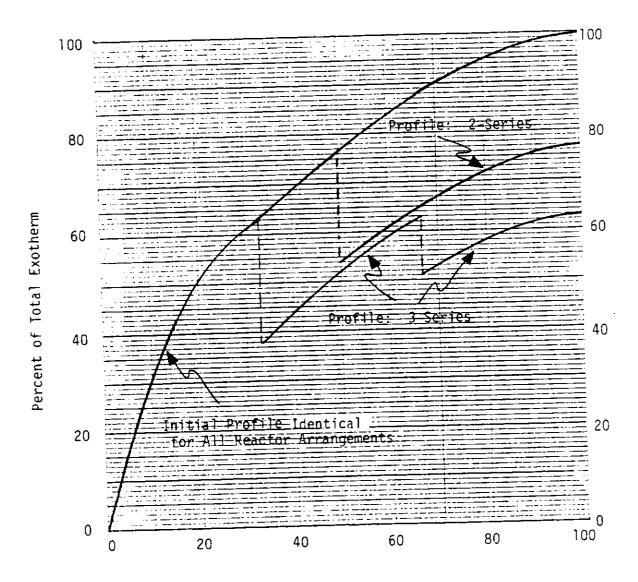
Techniques to determine the heat release and overall reaction temperature rise for EDS liquefaction have been developed and are well documented (Reference 2). The basic shape of the overall exotherm profile, with no intermediate quench assumed, has also been identified and is shown as Figure 3. Figure 3 is based on observed ECLP temperature profiles corrected for heat losses and is believed to represent a reasonable estimate of the profile shape which could be expected for commercial-scale reactors.

Information is also plotted on Figure 3 which indicates how the overall exotherm profile can be distributed for a series arrangement of liquefaction reactors when intermediate quench injection is used to control maximum reaction temperatures. Information is provided for reactor arrangements which include two reactors in series or three reactors in series. These two arrangements are typical of configurations which are considered for commercial plant designs. This plot assumes that the outlet temperature from each of the reactors in series is controlled to the same temperature. The resulting 'saw-tooth' pattern illustrates the effects of intermediate quenching, where the slopes of the profiles are assumed to remain identical to that of the overall exotherm profile shape.

Recently, information has been developed which allows further adjustment of the exotherm profile to account for backmixing effects. information indicates that for each reaction stage (note that each commercialscale reactor will likely have two or three stages to allow approaching plug flow reaction conditions), the temperature rapidly increases and then flattens out for the majority of the reactor stage volume at a level nearly equivalent to the stage outlet temperature. This effect is schematically indicated by Figure 4, which has been developed assuming a reactor configuration containing three reactors in series with two stages per reactor. As indicated, backmixing raises average reactor temperatures, which in turn increases the reaction rate and the total heat release. For a given average reactor temperature, accounting for backmixing directionally allows a reduction in reactor inlet and outlet temperatures and a reduction in quench requirements. Ignoring backmixing effects results in a design which is slightly conservative since reactor outlet temperatures, and therefore design temperatures, are somewhat higher than actually required to achieve a given average reactor temperature. In addition, the first reactor inlet temperature, which corresponds to the furnace coil outlet temperature and is therefore related to furnace duty, is somewhat higher than necessary. The degree of conservatism is small, however, and ignoring backmixing effects does not have a significant impact on design requirements.

The information discussed above summarizes the items which should be considered when determining the appropriate technique for identifying the exotherm profile required to achieve conversion levels associated with average reactor temperatures as predicted by small scale EDS pilot plants. The recommended technique for commercial plant designs involves using the predicted overall EDS reaction exotherm profile shape, uncorrected for backmixing effects related to intra-reactor staging. The average overall reaction temperature should be calculated as the average of the mid-volume temperatures for each of the reactors provided in the selected series arrangement for each liquefaction processing train. (Note that other methods can be used to calculate average reactor temperature; other techniques result in temperature profiles for a given exotherm which are not sub-

# FIGURE 3 EDS LIQUEFACTION REACTOR TEMPERATURE PROFILE



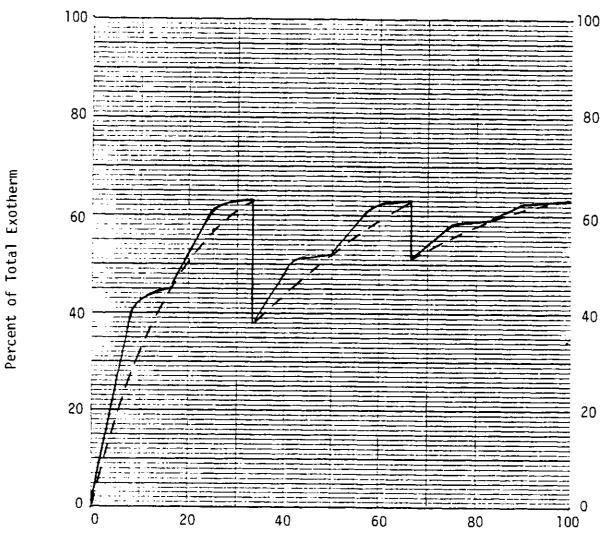
Relative Reactor Position, %

## FIGURE 4

## SCHEMATIC EFFECT OF BACKMIXING ON EDS REACTOR TEMPERATURE PROFILE

Basis: Three Reactors in Series, Two Stages Per Reactor
Dotted Line: Exotherm Profile Without Backmixing

Solid Line; Exotherm Profile With Backmixing



Relative Reactor Position, %

substantially different.) Correcting for backmixing effects has little impact on the resulting temperature profile, and the additional complexity of including this correction does not significantly change the results in terms of their impact on design requirements.

In general, outlet temperatures should be set equal to a constant value for each of the reactors in the selected series configuration. This results in all reactors having the same design temperature. An alternative calculation approach, which limits the first reactor's outlet temperature to a value less than the trail reactors' outlet temperatures, has some benefits in that it reduces the quench requirements needed for exotherm control and also lowers the required inlet temperature to the first reactor (which allows investment savings in the low flux portion of the slurry preheat furnace). However, this approach also requires a higher trail reactor design temperature (at least for the last trail reactor) and increases the wall thickness and cost of the trail reactor(s) relative to the reactors provided in the constant outlet temperature approach. The recommended approach allows purchase of identical reactors and eliminates the need for different mechanical design specifications for each reactor. This ability to purchase multiple, identical reactors rather than individual, different reactors has some difficult-to-quantify cost benefits.

Table 2 provides formulas for determining exotherm profiles based on the guidelines discussed above. Formulas are provided for configurations which contain either two or three reactors in series. To utilize the formulas, the total exothermic temperature rise must be known as well as the average reaction temperature required to achieve the selected conversion. Table 2 also contains a sample calculation based on the 92°F total exothermic temperature rise and the 840°F average reactor temperature used for the EDS Wyoming Coal Bottoms Recycle Study Design Addendum.

## Solids Holdup

Oversized inert particles which originate with the feed coal or which are formed in-situ due to calcium carbonate deposition can create a solids phase in the liquefaction reactors separate from the gas and slurry phases. Prescence of a solids phase reduces the effective reactor volume available for coal conversion. Minimizing solids holdup, either through improved control of oversize inert particles present in the coal feed or through periodic withdrawal of solids, reduces the reactor volume required to accomplish coal conversion.

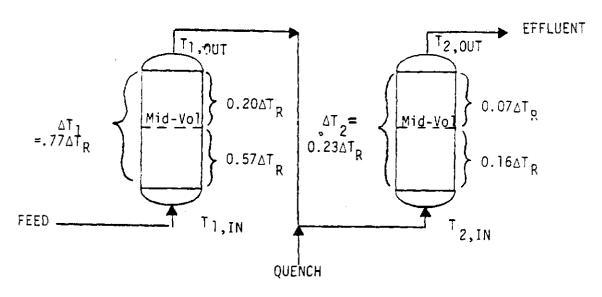
Only a limited amount of solids holdup data is available from the EDS pilot plants. The available data indicate that typical values for solids holdup were in the range of 10-20% for the various pilot plants. These values are representative of those used when calculating actual residence times for yield correlation purposes.

Theoretical considerations indicate that solids holdup is closely related to superficial gas velocity and to particle size of the solids. For a given particle size distribution, higher superficial gas velocities improve the system's ability to remove particles through the normal flow path. In a similar manner, for a fixed superficial gas velocity, smaller particles are more easily fluidized and removed.

#### TABLE 2

## REACTOR TEMPERATURE PROFILE CALCULATIONS

#### TWO REACTORS IN SERIES



$$T_{AVG} \stackrel{\text{SET}}{=} \frac{T_{1,0UT} - 0.20 \, \Delta T_{R}}{2} + \frac{T_{2,0UT} - 0.07 \, \Delta T_{R}}{2}$$

$$T_{AVG} = \frac{T_{1,0UT} + T_{2,0UT}}{2} - 0.135 \, \Delta T_{R}$$
when  $T_{1,0UT} = T_{2,0UT}$ 

$$T_{AVG} = T_{1,0UT} - 0.135 \, \Delta T_{R}$$

$$T_{1,0UT} = T_{2,0UT} = T_{AVG} + 0.135 \, \Delta T_{R}$$

$$T_{1,0UT} = T_{2,0UT} = 840^{\circ}F$$

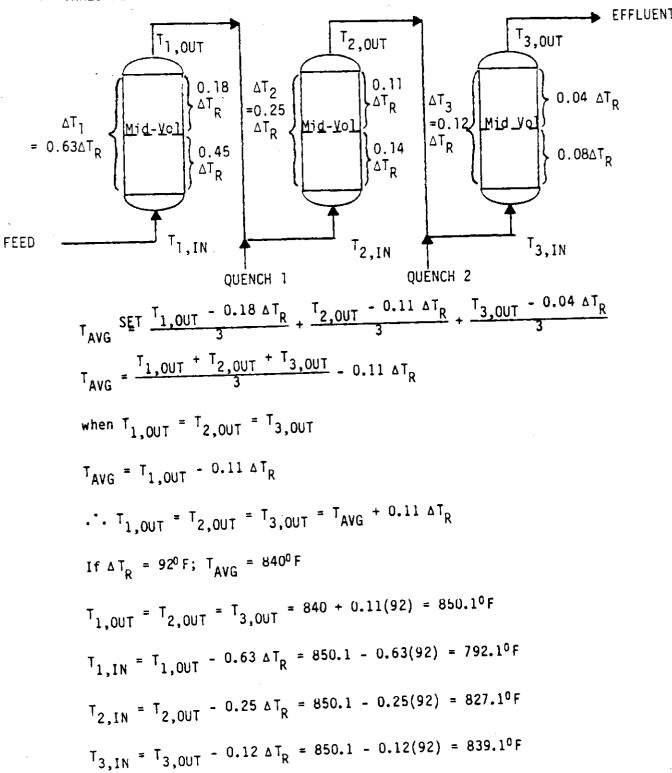
$$T_{1,0UT} = T_{2,0UT} = 840 + 0.135(92) = 852.4^{\circ}F$$

$$T_{1,1N} = T_{1,0UT} - 0.77 \, \Delta T_{R} = 852.4 - 0.77(92) = 781.6^{\circ}F$$

$$T_{2,1N} = T_{2,0UT} - 0.23 \, \Delta T_{R} = 852.4 - 0.23(92) = 831.2^{\circ}F$$

## TABLE 2 (CONT'U)

## THREE REACTORS IN SERIES



Evaluating EDS pilot plant data indicates that this relationship of particle size and superficial gas velocity as it applies to solids hold-up does hold – at least directionally. Table 3 summarizes information obtained at the three EDS pilot plants during tracer tests. Typical coal feed particle top sizes (99%-) for the pilot plants are 16 mesh for ECLP, 30 mesh for CLPP, and 100 mesh for RCLU. Reactor geometry also results in the following pattern for representative superficial gas velocities: 0.18 ft/sec for ECLP, 0.10 ft/sec for CLPP, and 0.05 ft/sec for RCLU. The largest pilot plant has the largest particle sizes at the highest superficial gas velocity, while the smaller pilot plants have progressively smaller particle sizes at progressively lower superficial gas velocities. As a result, despite the range of conditions, all pilot plants have been able to sustain equilibrium solids holdups which are approximately in the same range of 10-20%.

Although the above analysis is non-rigorous, the information it provides can be used to identify a potentially substantial cost-reduction design modification. Crushing coal very fine (100 mesh or smaller) for commercial applications should directionally reduce the level of solids holdup and possibly eliminate solids holdup as a concern. Superficial gas velocities of approximately 0.10 ft/sec are desirable for commercial designs to allow capture of hydrodynamic credits (through reduction of yas holdup to low values). CLPP data is available at similar conditions, and with coal particle top sizes of approximately 30 mesh resulted in solids holdup levels in the range of 15-20%. Crushing to finer sizes (e.g., 100 mesh top size) should reduce solids holdup to lower levels.

Reducing solids holdup directly results in savings in liquefaction reactor investment. Lowering solids holdup by 10% lowers the required reactor volume by 10%. If solids holdup can be reduced to very low equilibrium levels through coal particle size reduction, elimination of the reactor solids withdrawal facilities also becomes possible. (Note that concerns regarding calcium carbonate growth for low rank coals must also be considered before this change is implemented.) Smaller coal feed particle sizes also are favorable in terms of their impact on slurry saltation calculations and their impact on feed pump operability. Recent data also indicates that smaller coal particle sizes improve conversion - at least for some low rank coals. On the negative side, smaller coal feed particles sizes directionally increase the investment and operating costs for the coal crushing equipment. This change also potentially impacts on the coal drying technique used prior to liquefaction, since crushing to fine particle sizes can not be accomplished without first removing at least the coal surface moisture. This requires at least a partial gas swept mill drying step prior to slurry drying for final coal moisture removal.

Since the data base regarding solids holdup is limited, it is premature to recommend smaller coal feed particle sizes and use of low solids holdup levels for design purposes. In addition to improving the limited solids holdup data base, a more detailed evaluation of the cost effects of smaller coal particle sizes should be conducted. Such an evaluation is outside the scope of this study. When conducted, it should

TABLE 3
SUMMARY OF EDS SOLIDS HOLDUP DATA(1)

Unit	Typical Coal Top Size,	mesh	Vgas, ft/sec	Vliq, ft/sec	Solids Holdup
ECLP	16		0.15 0.19	0.052 0.054	0.21 0.20 0.06
		Avg =	$\frac{0.21}{0.18}$	0.057 0.054	0.16
CLPP	30		0.06 0.071 0.103 0.113 0.124 0.107 0.112	0.016 0.014 0.019 0.018 0.017 0.017	0.15 0.15 0.20 0.20 0.20 0.15
		Avg =	$\frac{0.104}{0.10}$	$\frac{0.019}{0.017}$	$\frac{0.27}{0.18}$
RCLU	100	Avg =	0.028 0.045 0.075 0.05	0.0069 0.0061 0.005 0.006	0.12 0.10 0.08 0.10

consider the crushing costs as well as the integrated plant effects that might result (i.e., gas swept mill vs. slurry drying, yield effects as related to coal size, oxidation effects and their impact on yields if gas swept mill drying is required, etc.).

Present evaluations should continue to assume equilibrium solids holdup levels of 20% when determining required reactor volumes. Coal feed top sizes on the order of 20-30 mesh should then be sufficiently small to allow reduction of superficial gas velocities to levels of approximately 0.10 ft/sec. Superficial gas velocities in this range allow capture of hydrodynamic credits which result from gas holdup decreases. Provision of solids withdrawal facilities should allow sustaining solids holdup levels of 20%, even for lower rank coals which exhibit calcium carbonate particle growth.

#### Gas Holdup Effects

The following analysis of the effects of gas holdup on reactor design is based on liquefaction process conditions equivalent to those used for the EDS Wyoming Coal Bottoms Recycle Study Design Addendum. The results are directionally correct for analyses of EDS reactor designs for other process conditions.

Table 4 summarizes the process information associated with the liquefaction reactor design for the Wyoming Addendum. The Wyoming Addendum provided three reactors in a series arrangement. Quench gas was injected after the first and second reactor to control the exothermic heat of reaction and limit the reactor outlet temperatures to a level of 850.1°F. (Calculated per exotherm guidelines to achieve 840°F 'average' reactor temperature.) Treat gas rate to the first reactor was set to provide twice the hydrogen consumed by reaction in the first reactor.

The ratio of superficial gas to superficial liquid velocities, as indicated for each of the three reactors in Table 4, can be used with EDS hydrodynamic correlations to develop Figure 5. Figure 5 plots gas holdup (on a solids-free basis) vs. superficial gas velocity. The information in Figure 5 can then be used to develop Figure 6, which shows the relationship of liquid holdup to superficial gas velocity when solids holdup is assumed to be 20%. The data indicates that if the reactor diameter is selected to meet a superficial gas velocity of 0.10 ft/sec, approximately 60% of the reactor volume is available for promotion of the coal conversion reaction. If superficial gas velocities are doubled, at an average value of 0.20 ft/sec, only 45% of the reactor volume represents liquid holdup.

## Backmixing Effects on Reaction Kinetics

Backmixing effects must also be considered when designing EDS liquefaction reactors. However, backmixing effects can almost be completely negated, and plug flow kinetics can be approached, by use of intrareactor distributors. Figure 7 was developed from EDS backmixing correlations and RCLU yield model predictions to show the effects of backmixing on

TABLE 4 LIQUEFACTION REACTOR PROCESS INFORMATION

Basis: EDS Wyoming Coal Bottoms Recycle Study Design Addendum

S/C/B/VGO = 1.6/1.0/0.5/0.2

Treat Rate: Set at twice consumption entering the first reactor

with inter-reactor quench provided following the first

and second reactors.

Temperature Profile: Reactor 1, 792.1 + 850.1°F

Reactor 2, 827.1 + 850.1°F Reactor 3, 839.1 + 850.1°F

Coal Feed Rate: 6250 T/SD dry coal to each liquefaction line

		Vapor, ft <sup>3</sup> /sec	Liquid, ft <sup>3</sup> /sec	V/L Ratio
Rx 1,	Inlet	13.88	8.29	1.67
	Outlet	16.05	8.47	1.89
	Average	14.96	8.38	1.79
Rx 2,	Inlet	19.70	8.04	2.45
	Outlet	22.84	7.73	2.97
	Average	21.27	7.88	2.70
Rx 3,	Inlet	22.36	7.68	2.91
	Outlet	25.47	7.43	3.43
	Average	23.91	7.56	3.16

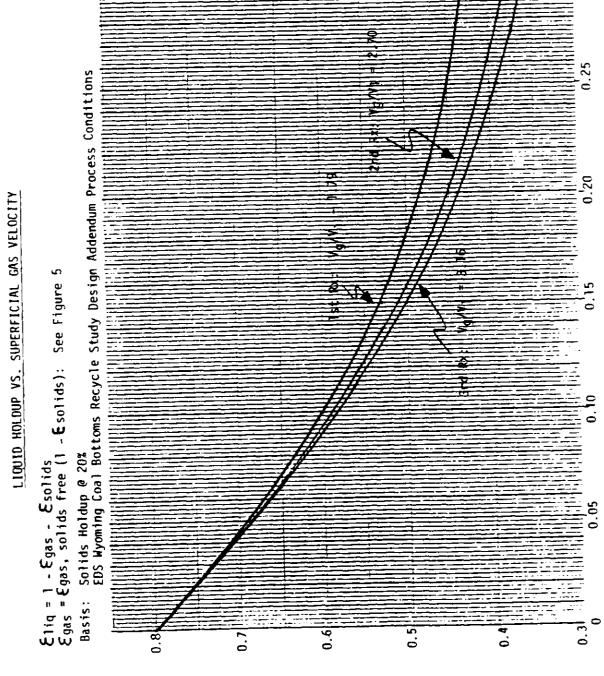
FIGURE 5

Basis: EDS Wyoming Coal Bottoms Recycle Study Design Addendum Process Conditions - 1.32 V<sub>gas</sub> GAS HOLDUP (SOLIDS-FREE) VS. SUPERFICIAL GAS VELOCITY  $(V_{gas} + V_{liq} + 0.33) - \sqrt{(V_{gas} + V_{liq} + 0.33)^2}$ 0.20 n Egas, sf 0.500.40 0.300.20 0.10

Gas Superficial Velocity, ft/sec

Gas Holdup (Solids-Free), Fraction

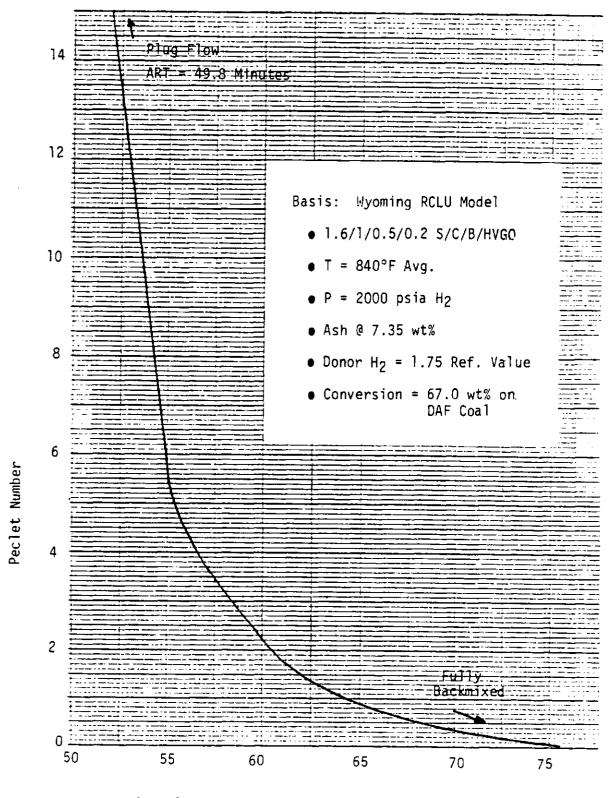
FIGURE 6



Liquid Holdup, Fraction

FIGURE 7

EFFECT OF BACKMIXING ON ART REQUIREMENTS



Actual Required Residence Time, Minutes

actual required residence time to achieve a target conversion level. Figure 7 was structured to match the EDS Wyoming Bottoms Recycle Addendum conversion level of 67.0 wt% on dry, ash-free coal.

Backmixing effects are characterized by the Peclet number. For a completely mixed reactor, the Peclet number is zero. For a plug flow reactor, the Peclet number is infinite. As indicated by Figure 7, plug flow conditions are approached if the Peclet number has a value greater than 10. Backmixing results in a significant increase in required actual residence time to achieve target conversion when the Peclet number is less than 5. For typical EDS reactor design configurations, Peclet numbers in the range of 10-15 can be achieved by providing reasonable staging arrangements. For a reactor configuration of three reactors in series, providing one intermediate distributor per each reactor results in six reaction stages and a Peclet number greater than 10.

Although staging can be used to approach plug flow kinetics, calculation of the Peclet number for each considered reactor configuration should still be performed. The calculated Peclet number should then be used to adjust the required actual residence time for the configuration being evaluated. As indicated by Figure 7, this adjustment will be small since the actual required residence time to achieve target conversion only increases by approximately one minute (from a base value of 52 minutes) as Peclet number decreases from 15 to 10.

## **Evaluation of Reactor Configurations**

The background information previously discussed can now be consolidated to evaluate alternative reactor design configurations. The reactor configuration used for the EDS Wyoming Coal Bottoms Recycle Study Design Addendum, which consisted of three twelve-foot internal diameter reactors in series per liquefaction line, has been used as the base point. Table 5 is provided to show comparative design values for the different configurations which have been considered. Information provided for each configuration includes reactor diameter, number of reactors, total reactor straight-side requirements, and total reactor metal volume.

For the base configuration, each of the three twelve-foot internal diameter reactors is 155 feet in length. Since superficial gas velocities are relatively high, in the range of 0.13-0.21 ft/sec, gas holdup levels are also high, averaging 32% for the three reactors. The Peclet number is 13.1, indicating that back-mixing effects have been adequately controlled by use of six total reaction stages (one inter-reactor distributor per reactor). The total metal volume requirement, including hemispherical heads, is 18,700 ft<sup>3</sup> for this configuration. Note that the reactor length specified for the Wyoming Addendum, which did not reflect the latest hydrodynamic knowledge discussed in this report, was 180 feet.

Case 1 describes a configuration which includes two parallel reactor trains with each train containing three reactors in series. The reactor diameter of 8.5 feet was selected since the resulting superficial velocities match those from the Base Case (i.e., the cross-sectional area of two-8.5 foot I.D. reactors is identical to that of one-12 foot I.D.

EVALUATION OF REACTOR CONFIGURATIONS

20 20 15 15 15 15 15 15 15 15 15 15 15 15 15	0.055	0.023	52.9 55.5 333 14.200 0.76
CASE 7 2 x 2 8 4 11.8 20 21 59	0.083	0.035	7.2 54.1 94.5 378 15,600 0.83
CASE 6  2 x 2  12  4  12  11.8  20 21 21 59	0.083	0.035 0.033	11.3 52.8 92 368 15,200 0.81
CASE 5 2 x 3 12 6 11.8 11.8 19 61	0.066 0.094 0.106	0.037 0.035 0.033	11.3 52.8 61 366 15,500 0.83
CASE 4 2 x 3 12 6 11 10.8 20 22 22 58	0.079 0.112 0.126	0.044 0.042 0.046	52.8 76 456 15.900 0.85
CASE 3 2 x 3 12 6 10 9.8 20 26 54	0.095 0.135 0.152	0.053 0.050 0.048	52.6 95 570 16,100 0.86
CASE 2 2 x 3 12 6 6 9 8.8 20 20 30 50	0.118 0.167 0.188	0.066 0.062 0.060	52.3 131 786 17,700 0.95
2 x 3 12 12 6 8.5 8.4 8.4	0.132	0.070 0.067 14.7	52,1 154 924 18,500 0,99
20 20 32 48	0.188	0.070	52.4 155 465 18,700 Base es heads.
Configuration, Parallel x Series Total Stages Total No. Reactors Reactor Diam., ft Reactor Wall Thickness, in. Solids Holdup, \$ (Avg) Gas Holdup, \$ (Avg) Liquid Holdup, \$ (Avg) Superficial Gas Vel, ft/sec	Superficial Liq. Vel., ft/sec	Ax 3 (Avg)  Overall Peclet Number  ARI, Minutes	Reactor Length, ft (Each) Total Reactor Straight-Side, ft Total Reactor Metal Volume, ft <sup>3</sup> (1) Total Reactor Metal Vol. Ratio to Base Note 1: Total reactor metal volume include

## Notes for Table 5:

1. Basis: EDS Wyoming Coal Bottoms Recycle Study Design Addendum Process Conditions

TAYG = 840°F S/C/B/HVGO = 1.6/1.0/0.5/0.2 P = 2000 psia H<sub>2</sub> Partial Pressure (nominal) Conversion = 67.0 wt% on DAF Coal Coal Feed Rate = 6,250 T/SD Dry Coal

Temperature Profile: Base Case, Cases 1-5

Rx 1: 792.1 + 850.1°F Rx 2: 827.1 + 850.1°F Rx 3: 839.1 + 850.1°F

Temperature Profile: Cases 6-8 Rx 1: 781.6 → 852.4°F Rx 2: 831.2 → 852.4°F

Treat Gas Supplied at Twice Consumption for the 1st Reactor; as Necessary for Exotherm Control to Trail Reactors

2. Actual Residence Time requirement is based on the use of Figure 7 for the indicated Peclet numbers.

reactor). As a result, gas holdup effects for Case 1 are identical to those of the Base Case. Since the L/D ratio of the reactors for Case 1 is greater than for the Base Case, the overall Peclet number is somewhat higher (14.7 vs. 13.1) and the reaction kinetics are slightly improved. Therefore, the actual residence time (ART) to achieve the target conversion level is smaller (52.1 minutes vs. 52.4 minutes for the Base Case). The overall metal volume requirement for Case 1 is essentially identical to the Base Case requirement. However, there are diseconomy-of-scale effects associated with providing six reactors instead of the three reactors for the Base Case configuration.

Cases 2 through 5 describe reactor configurations identical to Case 1. However, the reactor diameter is progressively increased from 9 to 12 feet to allow capture of credits associated with decreasing gas holdups. Case 5, which assumes 12 foot I.D. reactors, has the lowest gas holdup and results in the lowest requirement for reactor metal volume. The Case 5 metal requirement is 83% of the Base Case requirement, indicating that lowering gas holdup through use of maximum diameter reactors has significant cost benefits.

Case 6 describes a reactor configuration which provides two parallel reactor trains, but with each train containing two reactors instead of the three reactors assumed for Case 5. Reactor diameter is set equal to the maximum allowable value of 12 feet. As indicated, the hydrodynamic effects are almost identical to those of Case 5, and the required metal volume is slightly less (reflecting the need for only 8 reactor heads instead of the 12 heads required for Case 5). The main advantage Case 6 has relatative to Case 5 is the need to provide only four reactors instead of six.

Case 7 is similar to Case 6, except for the number of reactor stages. Case 7 assumes two stages per reactor vessel (four stages per each parallel line of two reactors) while Case 6 assumes three stages per reactor vessel. As a result, Case 7 has incremental backmixing relative to Case 6, and requires a higher residence time (54.1 vs. 52.8 minutes for Case 6). This comparison indicates that the additional staging provided for Case 6, which results in a Peclet number in the target range of 10-15, is justified.

Case 8 describes a reactor configuration which provides three parallel liquefaction trains, with each train containing two reactors in series. Reactor diameter is maintained at the twelve foot maximum. Case 8 has the lowest gas holdup value (15%) of any of the cases and therefore makes the most effective use of reactor volume. It also has the lowest reactor metal volume requirement, equivalent to 76% of the Base Case value. However, Case 8 requires six reactor vessles relative to the four reactor vessels required for Case 6. Also important, the superficial gas velocities for Case 8 are very low -- 0.055 ft/sec for the first reactor. For all cases analyzed, the solids holdup value has been assumed to be 20%. At gas velocities as low as those which result from the Case 8 configuration, the ability to maintain an equilibrium solids holdup level of 20% may require substantial solids withdrawal or very fine crushing of the feed coal. As indicated in the discussion of 'Solids Holdup', the data base regarding the relationship of superficial gas velocities and coal particle

sizes to equilibrium solids holdup levels is somewhat limited. However, reactor designs which result in superficial gas velocities far below 0.10 ft/sec should be avoided until the parameters which impact on solids holdup are better understood. Note that Case 6 has a superficial gas velocity of 0.083 ft/sec for the first reactor although the average superficial gas velocity over the entire reactor system is approximately 0.10 ft/sec.

## Relative Investments for Reactor Configurations

Table 6 indicates relative investments for the reactor configurations which were evaluated. The Base Case investment serves as the base value for all comparisons. For economy-of-scale considerations, investment proration slope exponents of 0.7, 0.8, and 0.9 were evaluated. An exponent value of 0.8 is estimated to represent the most appropriate value. The proration slope exponents have been applied to the metal volume requirements per reactor as indicated by Table 5. Number of reactor vessels per configuration has also been considered in the relative investment comparison.

Table 6 indicates that Case 6 is the most favorable (for a proration exponent of 0.8) in terms of reactor investment costs. For this reactor configuration, which provides two parallel reaction lines with each line containing two twelve-foot I.D. reactors, the investment requirement is 90% of the Base Case investment requirement. The key benefits realized by the Case 6 configuration can be attributed to use of the maximum allowable reactor diameter of 12 feet in a parallel line reactor arrangement, while providing the smallest number of reactor vessels. Use of the parallel arrangement with maximum allowable reactor diameter allows the optimum capture of reduced gas holdup incentives. Providing the smallest quantity of reactors (for a configuration which captures the gas holdup incentives) results in economy-of-scale benefits.

As mentioned, the relative investment for the recommended Case 6 configuration is 90% of that for the Base Case configuration which matches that provided for the Wyoming Addendum, when the Wyoming Addendum configuration is evaluated using the current understanding of hydrodynamics. The investment for the recommended configuration is 80% relative to the design actually specified for the Wyoming Addendum, which did not benefit from the current hydrodynamic data base.

## Throughput Considerations

Coal throughput is another variable which can be adjusted. The parametric case studies evaluated assumed 6250 T/SD of dry coal feed per liquefaction line since this was representative of values typically considered for EDS study designs. Although Case 6 was identified as the preferred reactor configuration of those analyzed, some concern was expressed (based on the current understanding of solids holdup estimates) that the superficial gas velocity was somewhat low and could result in a solids holdup level higher than the 20% value assumed. The superficial gas velocity can be revised by either decreasing reactor diameter or by increasing throughput.

TABLE 6

RELATIVE INVESTMENTS FOR REACTOR CASE CONFIGURATIONS

onent 0.9	<u> </u>	1.06	1.02	0.94	0.93	0.91	0.85	0,87	0.84
Proration Exponent 0.1 0.8 0.	< BASE	1.14	1.10	1.02	1.01	0.99	0.90	0.92	0.92
		1.22	1.19	1.11	1.10	1.08	0.94	96.0	1.02
Volume Per Rx (ft <sup>3</sup> )	6230	3080	2950	2680	2650	2580	3800	3900	2370
Internal Diameter, ft	12	8.5	6	10	11	12	12	12	12
Number of Reactors	က	9	9	9	9	9	4	4	9
Reactor Configuration Parallel x Series (Stages)	1 x 3 (6)	2 x 3 (12)	2 x 3 (12)	2 x 3 (12)	$2 \times 3 (12)$	2 x 3 (12)	2 x 2 (12)	2 x 2 (8)	3 × 2 (12)
Case	Base Case	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8

Investments prorated from the Base Case, using appropriate ratios of reactor metal volume per reactor with the indicated proration exponent and number of reactors. Note:

Example for Case 6 with proration exponent of 0.80:

Case 6 Relative Inv = 
$$(\frac{8A5E}{3})(\frac{3800}{6230})^{0.8}(4) = 0.90$$
 Base

Increasing throughput would be the preferred method of meeting minimum superficial gas velocity requirements. As previously indicated, metal volume is the key parameter used to determine relative reactor investments for heavy-walled vessels (defined as those with wall thicknesses greater than six inches). Therefore, once hydrodynamic requirements have been fixed (in this instance, to meet a minimum allowable superficial gas velocity of 0.10 ft/sec), there is no difference in reactor cost per unit of effective conversion volume for a case of lower throughput and smaller diameter or a case of higher throughput and larger diameter. This assumes that the cases being compared are similar enough so that each has the same number of reactor vessels, and that the differences in head metal volume requirements are insignificant. This results since hydrodynamics are identical for the two cases, and therefore liquid holdup values are identical. Another way of comparing the cases is to say that the volume of reactor metal per unit of coal throughput is identical for the two cases.

The increased throughput approach is preferred, however, because of the economy-of-scale impact on other equipment within the liquefaction section of the plant. Increasing reactor throughput means that all support equipment is also larger, and these equipment pieces are benefitted by economy-of-scale criteria. This reasoning is valid until maximum size constraints for other equipment are reached. For example, if increasing throughput result in the need for two reactor effluent separators instead of one, evaluation of these investment effects must also be considered.

#### Conclusions

The following major conclusions have been reached by this evaluation of EDS reactor design criteria. The comments are discussed in what is judged to be a reasonable rank order of importance.

- Available solids holdup data indicated that crushing feed coal to top sizes of 100 mesh or less may have substantial benefits in reactor design optimization. Smaller coal particles sizes directionally allow designing for lower superficial gas velocities, and therefore lower gas holdups, to maintain a fixed solids holdup level. Or, smaller coal particle sizes allow designing for lower solids holdup levels, and therefore result in more effective use of available reactor volume, for fixed levels of superficial gas velocities.
- For coal feed particle top sizes of 20-30 mesh, which are typical of those which generally have been considered for past EDS study designs, reactor superficial gas velocities should not be less than 0.10 ft/ sec. For these design conditions, solids holdup level of 20% should be used for design calculations which follow these design criteria.
- Reactor diameter should be selected to achieve superficial gas velocities of 0.10 ft/sec when using the criteria discussed above. This allows optimum capture of hydrodynamic benefits which result from decreases in gas holdup levels.
- Consideration should be given to adjusting design throughput to allow meeting the 0.10 ft/sec superficial gas velocity criteria with a 12-

foot internal diameter reactor. This allows capture of economy-ofscale credits for other equipment pieces within the liquefaction process section.

- Reactor staging should be provided to achieve Peclet numbers in the range of 10-15. This allows a reasonable approach to plug flow kinetics such that backmixing effects on conversion are not substantial.
- Reducing the number of reactor vessels is desirable. Although the kinetics and metal volume requirements for a configuration which includes three-12 foot I.D. reactrs in series or two-12 foot I.D. reactors in series are nearly identical, it is always preferrable to have a smaller number of vessels.
- Guidelines are presented for determining reactor temperature profiles to meet average reactor temperatures as predicted from small, isothermal EDS pilot plants.
- Maximum reactor wall thicknesses are 12 inches based on state-of-theart fabrication ability. This translates into a maximum reactor internal diameter of 12 feet for design conditions typical for the EDS process.
- Use of 1-1/4 Cr-0.5 Mo instead of 2-1/4 Cr-1 Mo as the base metal for trail EDS reactors has potential as a cost saving modification. Material selection should be made at the time of procurement based on actual vendor bids.
- A reactor of fixed volume has the same weight and cost whether designed as a long, small diameter vessel or as a shorter, larger diameter vessel.

The guidelines discussed in this study were used to design a reactor configuration based on the EDS Wyoming Coal Bottoms Recycle Study Design Addendum process requirements. The recommended design configuration to process 6,250 T/SD of dry coal (one-quarter of the total plant's lique-faction feed) provided two parallel trains, each containing two-twelve foot I.D. reactors in series. The relative cost of this configuration was 90% when compared to the single parallel train containing three-twelve foot I.D. reactors, as provided in the Wyoming Addendum (when the Addendum configuration was also evaluated using the current understanding of hydrodynamic effects). The relative cost of the recommended configuration was 80% when compared to the actual reactor design specified for the Wyoming Addendum.

#### References

- "EDS Wyoming Coal Bottoms Recycle Study Design Addendum," Interim Report No. 2893-123.
- 2. EDS Coal Liquefaction Process Development Quarterly Technical Progress Report, January 1 March 31, 1983, FE-2893-110, pgs. 10-16.