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Fossil Fuel Conversion -- Measurement and Modeling

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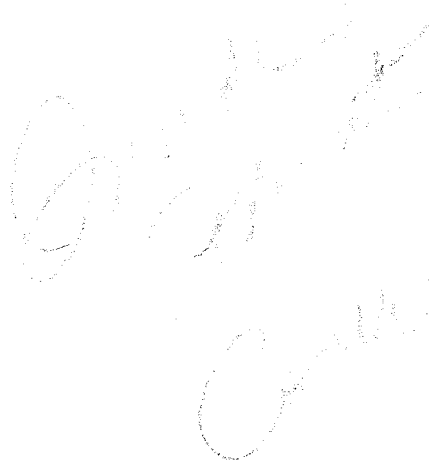
DISCLAIMER



PB.18 Fossil Fuel Conversion - Measurement And Modeling

CONTRACT INFORMATION

Contract Number: DE-AC21-93MC30040

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Period of Performance: September 14, 1993 to September 13, 1996

FY95 Program Schedule

		S	O	N	D	J	F	M	A	M	J	J	A
2.	Gasification Processes												
3.	Gas Phase Combustion												
4.	Fluidized-Bed Systems												
5.	Applications												

OBJECTIVES

The main objective of this program is to understand the chemical and physical mechanisms in coal conversion processes and incorporate this knowledge in computer-aided reactor engineering technology for the purposes of development, evaluation, design, scale up, simulation, control and feedstock evaluation in advanced coal conversion devices. To accomplish this objective, this program will: 1) provide critical data on the physical and chemical processes in fossil fuel gasifiers and combustors; 2) further develop a set of comprehensive codes; and 3) apply these codes to model various types of combustors and gasifiers (fixed-bed, transport reactor, and fluidized-bed for coal and gas turbines for natural gas).

BACKGROUND INFORMATION

To expand the utilization of coal, it is necessary to reduce the technical and economic risks inherent in using a feedstock which is highly variable and which sometimes exhibits unexpected and unwanted behavior. Reducing the risks can be achieved by establishing the technology to predict a coal's behavior in a process. This program is creating this predictive capability by merging technology developed at Advanced Fuel Research, Inc. (AFR) in predicting coal devolatilization behavior with technology developed at Brigham Young University (BYU) in comprehensive computer codes for modeling of entrained-bed and fixed-bed reactors and technology developed at the U.S. DOE-METC in comprehensive computer codes for fluidized-bed reactors. These advanced technologies will be further developed to provide: 1) a fixed-bed model capable of predicting combustion and gasification of large coal particles, 2) a transport reactor model, 3) a model for lean premixed combustion of natural gas, and 4) an improved fluidized-bed code with an advanced coal devolatilization chemistry submodel.

PROJECT DESCRIPTION

The program consists of five tasks: 1) Preparation of a Research Plan, 2) Modeling of Gasification Processes, 3) Modeling of Gas Phase Combustion, 4) Modeling of Fluidized Bed Systems, and 5) Applications. This paper describes the work performed during the second year of the contract.

RESULTS

Devolatilization of Large Coal Particles (AFR) - Fluidized-bed coal combustion and gasification systems normally use comparatively large size coal particles of several millimeters in diameter. Due to heat and/or mass transport limitations, such large coal particles have slower devolatilization rates compared to micron-sized particles used in pulverized coal combustion. This section reports the progress in developing a large coal particle devolatilization model (LCPD) for fixed-bed and fluidized-bed coal combustion and gasification. The model combines a heat transfer model with a general coal devolatilization model FG-DVC [1-3] which was developed for pulverized coal particles.

Coal particles are considered to be spherical in the model. The particle size is assumed to remain unchanged during the devolatilization, since two counteracting processes, weight loss and swelling, lead to negligible size changes for mm-size coal particles in fluidized beds [4]. This assumption implies that the coal particle density will decrease with time due to weight loss. The devolatilization is assumed to be thermally neutral in accordance with most of the data which indicate relatively small effects [5]. The mass transport is modeled by an existing mechanism in FG-DVC. The key components in the model are 1) a heat transfer submodel; 2) a coal devolatilization submodel, FG-DVC; 3) a coal physical property (thermal conductivity and specific heat) submodel by Merrick [5,]; and 4) a correlation for convective heat transfer from gas to the particle reported by Kunii and Levenspiel [7] and Kothari [8].

Model predictions are being compared with experimental data in the literature for model verification. Morris and Keairns [4] studied three American coals at high pressure (10 atm) in a laboratory small scale fluidized bed facility with inert fluidizing gas. They reported 50% and 95% methane devolatilization times corrected for in-bed gas dispersion time for an Indiana coal. Fig. 1 compares the model predictions with data on the variation of the methane devolatilization time with mean particle size. The model predicts quite well the 50% methane devolatilization time. The slight

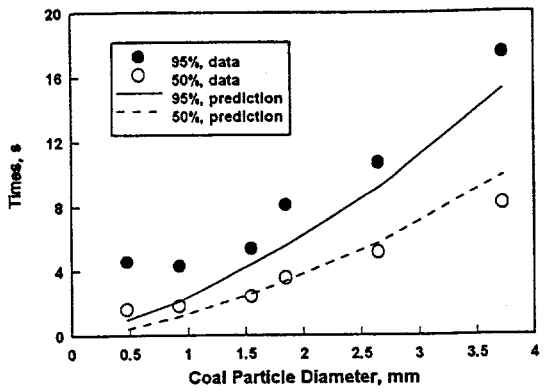

Fig. 1. Predicted and Measured [4] CH_4 Devolatilization Times as a Function of Particle Size.

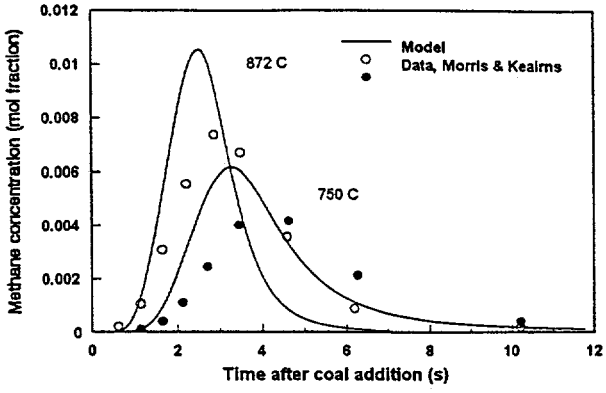

Fig. 2. Comparison of Predicted In-Bed CH_4 Concentration with Measured CH_4 Off-Gas Concentration [4] for 1.55 mm Coal Particles at 872°C in Fluidized Bed.

under-prediction of the 95% time is believed to be caused by the fact that coal particles used in the experiment had a range of particle sizes, which is not accurately described by an arithmetic mean particle size. This is more clearly shown when the methane concentration in bed is predicted and compared with the uncorrected off-gas data in Fig. 2. The time lag between the predicted and measured curves could arise from gas dispersion between the bed and the outlet. However, the contribution from larger particles in the size range could also lead to longer devolatilization times. Morris and Keairns [4] measured the dispersion time with a tracer method, and showed that the minimum dispersion time is 3 seconds. Since their off-gas data in Fig. 2 indicate that methane starts to be collected at the outlet as early as 1 second after coal addition, it is not clear how this information can be used to correct the off-gas data to derive the in-bed concentration. Given these uncertainties, the model predicts well both the evolution rate and the ultimate yield of methane of the large particles.

It appears that the heat transfer to coal particles in fixed and fluidized beds is difficult to model. Many investigators have reported correlations to calculate the Nusselt number from the particle Reynolds number. Gunn [9] pointed out that these values have several orders of magnitude difference at the same Reynolds number. Further work is needed to clarify this uncertainty.

Transport Reactor Modeling (AFR) - Significant progress has been made in developing a computational fluid dynamics (CFD) model for coal combustion and gasification in transport reactors (or circulating fluidized beds, CFBs). This work is being done using the BYU entrained-bed model (PCGC-2) as the framework. Since CFBs have much higher solid loadings than entrained beds, for which PCGC-2 was developed, major modifications have been made in the Lagrangian particle trajectory submodel. A stochastic particle turbulence dispersion model is used to model the particle dispersion. This modification is necessary because of the extensive gas-solid interactions in CFBs. Numerical modifications have also been made in the gas-phase aerodynamics model to handle the substantial interphase momentum exchange and pressure variations. This approach has been successful in cold flow modeling of CFBs. Model verification is being carried out based on a large set of experimental data from cold particle-laden flow data collected at the CCNY circulating fluidized-bed facility. Additional data are available from CFB research, which has been very active in the past decade. Fig. 3 illustrates a comparison of measurements and model predictions for the radial profile of void fraction at the 1/2 height of the CCNY reactor. The

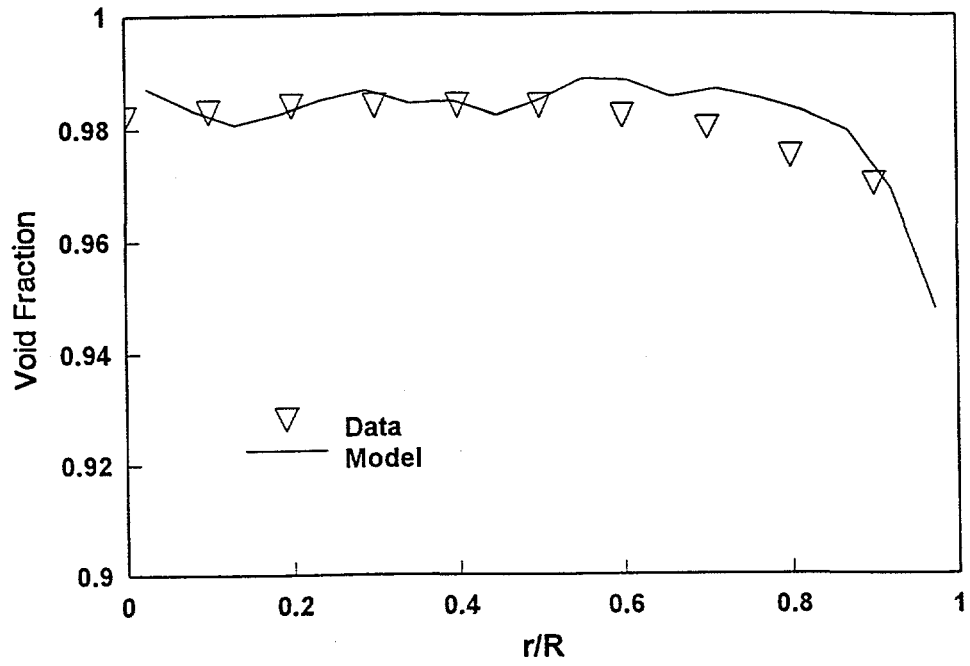

Fig. 3. Comparison of Calculated and Measured Void Fraction Distribution in a Transport Reactor.

comparison is surprisingly good. The model also predicts correctly the axial pressure drop and the particle velocity profile with downward flow near the reactor wall. The shape of the gas velocity profile is predicted but the discrepancy in the magnitude indicates a need for further investigation. It is planned to carry out systematic verification of the model with various flow conditions and to extend it to predict data for coal combustion and gasification.

The experimental work reported in the literature has revealed a unique gas-particle two-phase flow structure in CFBs. There is a dilute core coupled with a dense annulus. The masses (both gas and solids) in the core are rapidly transported upward while the annulus flow is slow but significantly downward-moving. There is no consensus on what causes this unique flow structure. Our calculations indicate that the turbulence structure plays an important role. Experimental observations have shown the intensive mass exchange between the core and the annulus. Such exchange is undoubtedly driven by the turbulence, since the average radial gas velocity is very low. Our calculations show two important phenomena. 1) When the turbulence is not homogeneous in the radial direction, solid particles tend to segregate in regions with low turbulence intensity. And 2) if the turbulence intensity in the core is high enough, particles will concentrate near the reactor wall.

This conclusion calls for a careful reconsideration of turbulence models. In addition, gas-particle turbulence interactions, particle-particle interactions, and particle-wall interactions may need to be further considered in the model.

Fluidized-Bed Model (AFR) - A reduced version of the FG-DVC model (FGDVC-RES) has been developed as a submodel for an existing fluidized-bed code, MFIX, developed at METC. FGDVC-RES employs only one ordinary differential equation to model the total devolatilization weight

loss, while coal dependent information (elemental compositions of char, tar and gas, rates and yields of char, tar and gas species) is provided through their correlations to the total weight loss. These correlations are given by a pre-calculation with the standard FG-DVC model based on the knowledge of nominal reactor conditions (pressure, temperature heating rate). This approach allows CFD codes to use FG-DVC as a submodel (in this case, MFIX) without the formidable computation burden of calculating the detailed devolatilization rates while retaining the predictive capability of the standard FG-DVC model. A version of FGDVC-RES is currently being integrated with MFIX at METC and will also be integrated at BYU with the fixed-bed code (FBED-1) under development there (see below).

Nitrogen Evolution from Small and Large Coal Particles (AFR) - Three bituminous coals were studied in this part of the project: Mettiki #2, Mapco #2, and Consol #2. Their proximate and ultimate analyses are given below (wt.% daf; ash and volatile matter on a dry basis; oxygen by difference):

Coal	Ash	VM	C	H	N	S	O
Mettiki	13.8	18.8	89.6	4.8	1.4	2.0	2.3
Mapco	8.3	37.8	83.2	5.4	1.5	.78	9.1
Consol	11.2	35.8	84.8	5.6	1.5	2.0	6.1

These coals are being considered for use in the METC Gasification Product Improvement Facilities (GPIF). Experiments were carried out in a TG-FTIR system (thermogravimetric analysis combined with Fourier-transform infrared analysis of volatile products) using the procedure described in a previous publication [10]. In a typical experiment, a coal sample is placed in a flow of helium and heated at 30 K/min to 1173 K. Then the sample is held at the final temperature for three minutes. During this temperature excursion, weight loss is continuously monitored, and infrared spectra of the released gases are obtained once every forty-one seconds. To study the effect of particle size on the release of ammonia (NH_3) and hydrogen cyanide (HCN), samples with two particle diameters, d_p, were prepared for TG-FTIR testing: $d_p < 0.150$ mm; and $d_p \approx 5$ mm. In each run, the sample size was approximately the same (m_s = 57-59 mg).

A strong influence of particle size on volatile-nitrogen evolution has been observed for all three coals. In Fig. 4, HCN and NH_3 evolution curves are shown as thick lines for the particle-size range 0-150 mm. As in the previous study of nitrogen release [11], a bimodal NH_3 evolution pattern can be seen. This is attributable to the primary and secondary ammonia release (the low- and high-temperature NH_3 peaks, respectively). According to the proposed model, coal-bound nitrogen (coal-N) is first released as HCN and (primary) ammonia, and this stage is followed by HCN reaction with char-hydrogen to form secondary ammonia as a product (Fig. 5).

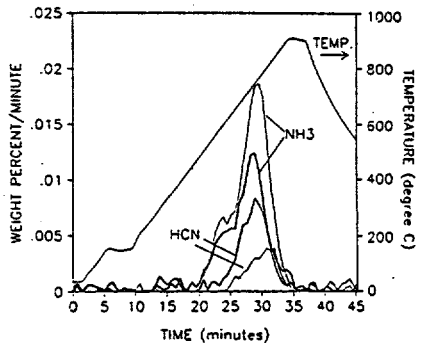

Fig. 4. Nitrogen Evolution Patterns During Pyrolysis of Mettiki Coal. Thick Lines: d_p < 0.150 mm; Thin Lines: $d_p \approx$ 5 mm.

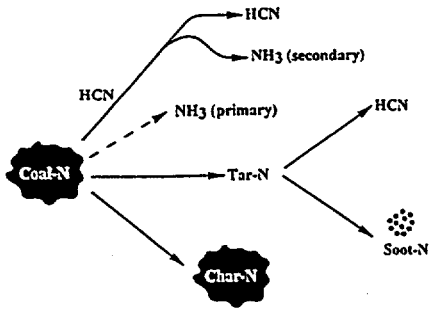

Fig. 5. Nitrogen Evolution From Coal During Pyrolysis.

If this mechanism is correct, then an increase in the particle size, and thus also in gas residence time within the particle, would lead to an increase in secondary-NH_3 release at the expense of the HCN peak. The primary ammonia peak should remain unchanged, or only weakly affected, as the amount of primary ammonia formation should not depend on the gas diffusion path length within the particle. This is precisely what is seen in Fig. 4, where the large-particle evolution curves are shown as thin lines. It should also be noted that the release of secondary-NH_3 and HCN occurs at the same time, which is in agreement with the proposed mechanism. The heterogeneous HCN-to-NH_3 conversion scheme is offered as an alternative to the gas-phase HCN hydrogenation mechanism suggested by Baumann and Möller [12]. If the HCN-to-NH_3 conversion were indeed a gas-phase reaction involving molecular hydrogen, then it would be difficult to justify the particle-size dependence, unless H_2 evolution happens to be particle size dependent. The collected data certainly provide strong evidence in favor of the heterogeneous scheme. Nitrogen evolution curves similar to those shown in Fig. 4 were also obtained in the case of Mapco and Consol coals.

Modeling of hydrogen cyanide and ammonia release during coal pyrolysis - The objective of this work is to demonstrate the potential of the FG-DVC model for predictive modeling of HCN and NH_3 release during coal pyrolysis. The FG-DVC model combines a functional group (FG) model for gas evolution and a statistical depolymerization, vaporization and cross-linking (DVC) model for tar formation. The model has been developed at Advanced Fuel Research, Inc., and described in several publications [1-3].

The nitrogen-evolution modeling is based on the following assumptions:

- Both HCN and NH_3 can be formed as primary coal pyrolysis products. The original coal-N is divided into inventories that potentially produce HCN, NH_3, and char-N.
- NH_3 is additionally produced by a secondary reaction between HCN and char-surface hydrogen. The time scale of this reaction is governed by the gas residence time within a particle, which is evaluated by a gas transport subroutine.
- Primary HCN and NH_3 formation mechanisms follow first-order kinetics with distributed activation energies. The secondary NH_3 formation from HCN is assumed to be first order in HCN and second order in surface hydrogen.
- As pyrolysis progresses, tar-N evolves from HCN, NH_3, and char-N producing inventories.
- The sizes of the HCN- and NH_3-producing inventories, as well as the kinetic parameters for nitrogen evolution, are determined by a laboratory TG-FTIR experiment.
- Tar-cracking reactions are neglected, except for the initial stage, which is treated using the same kinetics as those for coal pyrolysis.
- Frequency factors for all pyrolytic reactions are assumed to be of order 10^{12}-10^{14} s^{-1} [13].

The input to the model is: (1) coal elemental analysis; and (2) low heating rate pyrolysis data collected for a given coal in a TG-FTIR experiment. The latter data are used to

determine the kinetic parameters for nitrogen evolution during pyrolysis.

Modeling of fluidized-bed pyrolysis data has been attempted in this study. Four Australian bituminous coals were used, and their elemental compositions are shown in the table below (wt.% daf; ash and VM dry basis; oxygen by difference). The fluidized-bed pyrolyzer and experimental conditions have been described elsewhere [13,14].

Coal	Ash	VM	C	H	N	S	O
A	12.1	39.8	83.6	5.4	1.9	1.1	8.1
B	13.6	23.8	87.4	4.6	1.7	.32	5.9
C	11.2	20.3	88.5	4.7	1.8	.48	4.5
D	13.0	16.0	88.7	4.6	2.0	.57	4.2

HCN and NH_3 yields for coal B are plotted as a function of temperature in Fig. 6. It can be seen that the HCN evolution increases with temperature, whereas NH_3 yields exhibit a maximum at about 1050 K. It should be noted that the model accurately predicts both trends. The maximum in NH_3 yields can be qualitatively explained by a decrease in HCN residence time within the particle at elevated temperatures. As temperature increases, so does the rate of evolution of HCN and other species. Since transport rates within the particle increase with the volume of gases evolved, HCN is more rapidly shuttled out of the particle. As a consequence, the reduced HCN residence time leads to smaller quantities of secondary NH_3. The reason for the slight underprediction of NH_3 release near the maximum is believed to be related to inaccuracies in estimating the gas residence time within the particle. Work on improving the sub-model describing gas diffusion through the porous particle is under way.

Results for coals A, C, and D are similar to those shown in Fig. 6, except that the model underpredicts HCN yields at higher temperatures for coal A. This is due to the tar cracking reactions, which are not accounted for by the model. Tar formation is more important in the case of the more volatile coal A than for the higher-rank coals B, C, and D.

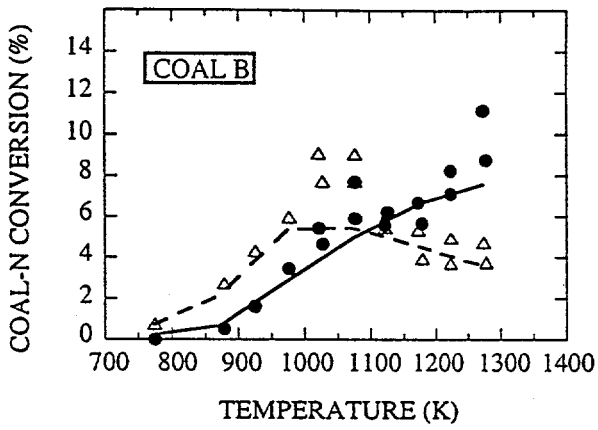

Fig. 6. HCN (•) and NH_3 (Δ) Yields in Fluidized-Bed Pyrolysis of Coal B. Solid and Dotted Lines are Model Predictions for HCN and NH_3, Respectively.

Oxidation Rates for Large Coal Particles at High Pressures (BYU) - Fixed-and fluidized-bed combustion and gasification processes are typically done with large coal particles at high pressures but the previously available fixed-bed codes use kinetic rates derived from small particle experiments at atmospheric pressure. Thus, work was conducted to measure kinetic rates for large coal particles at high pressures.

In a previous project, a unique experimental facility was constructed to obtain oxidation rates of large particles at high temperatures and high pressures. It consists of a cantilever beam balance insert for the BYU High Pressure Controlled Profile (HPCP) reactor. The balance unit measures the mass loss of the particles as they oxidize in the HPCP reactor. It includes a force transducer, a ceramic cantilever beam, and a platinum wire-mesh sample basket. The basket is secured to the cantilever beam and

extends into the reactor tube through one of the optical access ports of the HPCP reactor. This facility permits measurements of the oxidation and gasification rates of char particles at pressures up to 17 atm and temperatures up to 1700 K. It was successfully demonstrated by measuring the effects of pressure on oxidation rates of mm-sized Utah bituminous and North Dakota lignite char particles.

During the past year, the facility was overhauled and a new round of experiments was begun. The experiments are being conducted with Consol #2, Mapco #2, and Mettiki #2 coals. As discussed above, these coals are to be used for the PyGas™ gasifier under the DOE/METC Gasification Product Improvement Facility (GPIF) project. Parametric experiments were performed by measuring mass loss and gas temperature versus time for coal samples of 0.1, 0.2, and 0.3 grams, at temperatures of 900, 1050, and 1200 K, and Reynolds numbers of 63, 126, and 252 all at atmospheric pressure. This resulted in 39 runs; 20 additional runs at the average values of the parameters were also performed to check the reproducibility of the experiment. The results are still being analyzed but the following statements can be made at present. The experiments ran typically for 15 minutes and could be divided into devolatilization, oxidation, and decay zones. The devolatilization zone had the greatest mass loss rate while the oxidation zone had the greatest mass loss. The cube root of mass declined linearly with time for all coals as shown in Figure 7 and as previously observed. This is consistent with a thick ash layer model. Ash layers formed and usually remained in place around the char particles. Additional parametric experiments will be performed at higher pressures such as 5 and possibly 10 atmospheres. The experimental results will be analyzed and correlated and, based on these results, a new model of large coal particle oxidation at high pressures will be developed.

Advanced Fixed-Bed Model Development and Evaluation (BYU) - Some coals such as caking coals, cannot be readily gasified in traditional fixed-beds. Therefore, novel configurations have been proposed to gasify caking coals. One such complex configuration is a high-pressure, air-blown, dry-ash, staged gasifier of the PyGas™ gasification process, which is under development for the DOE/METC Gasification Product Improvement Facility (GPIF) project. Another such complex configuration is used in the DOE Clean Coal Technology's (CCT) ENCOAL mild coal gasification process. There is a need for a general, advanced, computer model that can be used as a reliable design and analysis tool capable of simulating both traditional and emerging novel configurations such as the staged gasifier of the GPIF project and the rotary fixed beds of the ENCOAL project.

The overall approach in developing such a model is to improve and extend the comprehensive, one-dimensional fixed-bed code (FBED-1) developed previously to (1) include provisions for countercurrent, cocurrent and possible crosscurrent flows as well as for the additions and withdrawals of gases at multiple locations in the bed, (2) incorporate the advanced submodels being developed in other projects for coal devolatilization, oxidation, and gasification processes for large coal particles in fixed beds, (3) incorporate an efficient and robust numerical method appropriate for stiff, non-linear problems and (4) evaluate the advanced fixed-bed code by comparing its predictions with the experimental data for temperature, pressure, and composition profiles in fixed beds available from the literature and from the developers.

Accomplishments this year include additional sensitivity analysis of the FBED-1 model to study the effects of the devolatilization

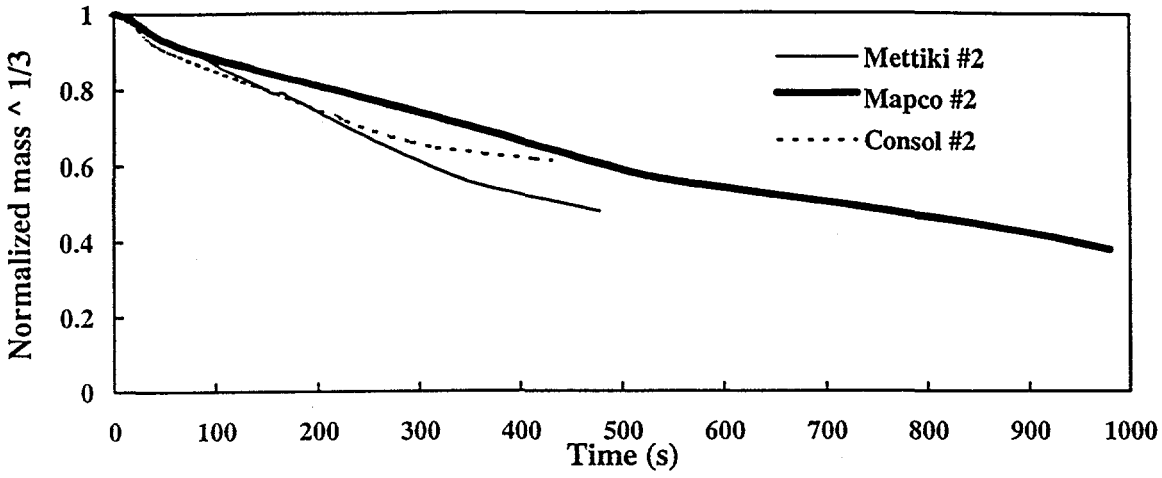

Fig. 7. Cube Root of Normalized Mass Loss vs. Time For Coal Sample of 0.2g at 900K, 126 Re, and 1 atm.

submodels, the oxidation and gasification submodels, and the gas phase chemistry options. Based on this analysis, the recommended options for the FBED-1 model are: the FG-DVC submodel for devolatilization, the Shell Progressive (SP) submodel for oxidation and gasification, and a partial chemical equilibrium option for the gas phase. The partial equilibrium option involves keeping tar non-reactive and gases non-reactive below a switch temperature, although both are kept in thermal equilibrium. Also, the fixed-bed model, FBED-1, was extended to handle a cocurrent flow pattern. Modifications were made to allow for additions and withdrawals of gases at multiple locations in the bed, but the preliminary results indicated a need for full kinetic treatment of gas phase chemistry, which is now under consideration. Also, under consideration is a reduced version of the FG-DVC devolatilization submodel, FG-DVC-RES, which is computationally more efficient than the standard version, FG-DVC.

The modified FBED-1 code with the cocurrent flow option was successfully used to simulate the PyGas™ staged gasifier using preliminary input data proposed by CRSS, Inc. and again using more recent design geometry and input data. The geometry of the gasifier required separate simulation of five flow regions, with the results of one region being used as the input for the following region. The simulations were done for the all-rank oxidation and gasification kinetics at atmospheric pressure, for the Pittsburgh #8 kinetics at atmospheric pressure, and for the Pittsburgh #8 kinetics at 41 atm. Simulation results for the latter case, which show detailed profiles for both cocurrent and countercurrent sections of the gasifier, are displayed in Figure 8.

Additional improvements will be made in the FBED-1 model to improve its industrial utility as a design and analysis tool. These improvements will include incorporation of a large particle devolatilization version of FG-DVC called LCPD (see above) and a large particle oxidation submodel being developed under this project. A robust solution method suitable for stiff, non-linear problems of fixed-bed systems will be implemented. The model will be evaluated by comparison with experimental data and by application to gasifiers of interest such as the PyGas™ gasifier.

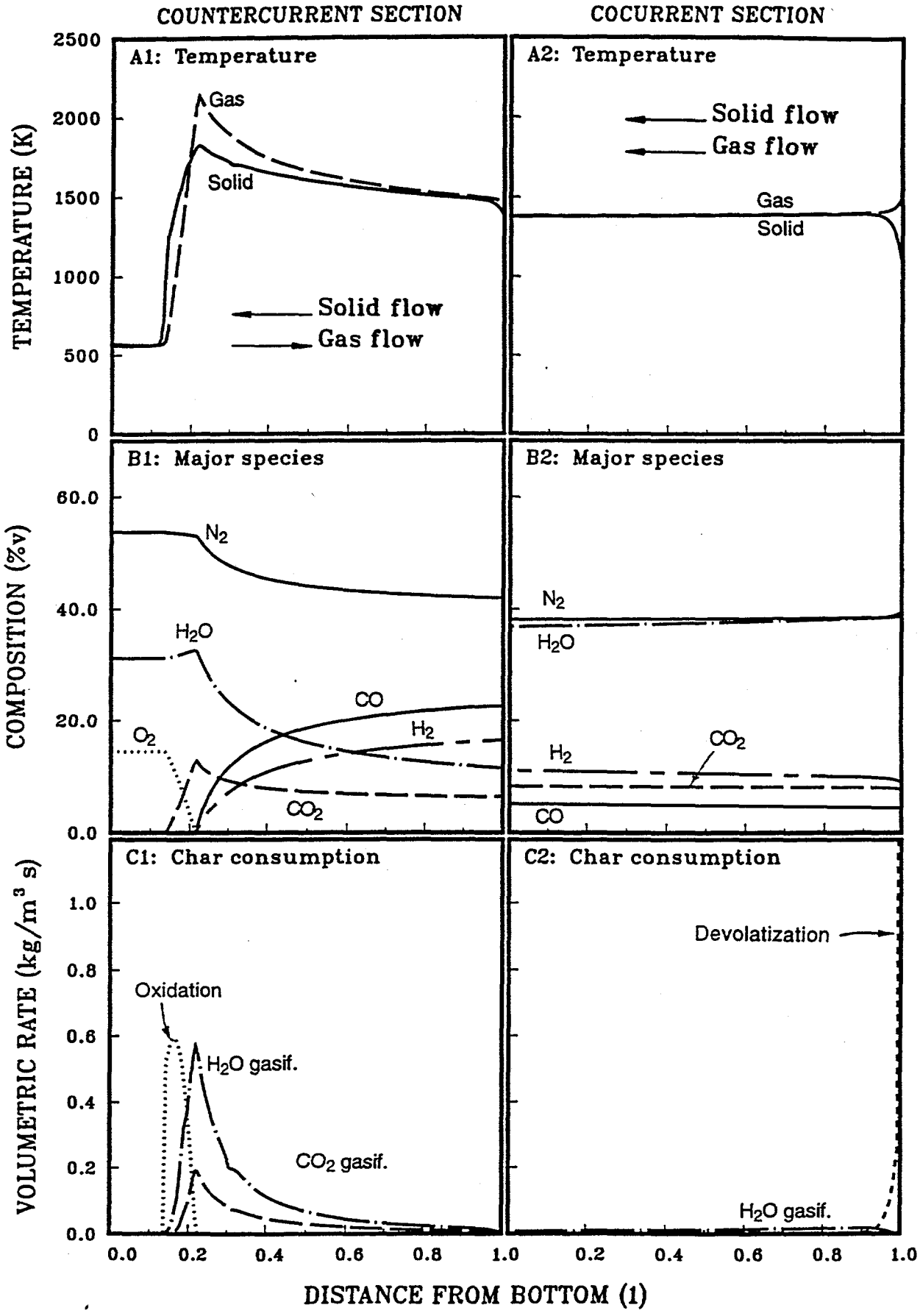

Fig. 8. FBED-1 Predictions for the PyGas Gasifier for the Pittsburgh #8 Kinetics at 41 atm.

Application of ACERC Combustion and Gasification Codes and AFR Diagnostic Capabilities to Systems of Interest to METC (BYU/AFR) - The Hague coal combustor is a part of the Kennebunk Test Facility, an externally-fired, combined cycle demonstration facility being built by Hague International under funding from the DOE Morgantown Energy Technology Center. The Hague coal combustor is a two-stage, down-fired combustor. A collar divides the first stage from the second and also provides access ports for the second stage air. The first stage operates fuel-rich to reduce NO_x emissions. To complete combustion, the remaining combustion air is added in the second stage. Successful operation of the downstream units, the slag screen and the ceramic heat exchanger, depends strongly on the performance of the combustor.

The performance of the combustor was predicted by a three-dimensional, coal combustion code, PCGC-3. The gas flow is solved in the Eulerian framework, using a finite-difference formulation of the Navier-Stokes equations coupled with the energy conservation equation. The particle transport is solved separately in the Lagrangian framework, and the two phases are coupled through various source terms. The turbulent, Reynolds stresses are approximated by an effective eddy viscosity. The conservation equations are closed by the Prandtl mixing length model, the standard k-ε model, or the nonlinear k-ε model. The gas phase reactions are assumed to be fast and limited by turbulent mixing rates only. Thus, the reaction rates are calculated using locally instantaneous equilibrium based on the degree of mixing of the relevant species. The extent of mixing between inlet gas streams is described by a conserved scalar variable, mixture fraction. The fluctuations of the mixture fraction are modeled by a probability density function. Particle reactions such as drying, devolatilization, oxidation, and gasification are included. Devolatilization is modeled by a single-step or a two-step model. Oxidation and gasification rates are determined from Arrhenius-type expressions. Radiative heat transfer between gases, particles, and walls is modeled by a discrete-ordinates method. Formation of thermal and fuel NO_x is included. The Zel'dovich mechanism is used for the thermal NOx and global reaction rates based on the de Soëte rates were used for the fuel NO_x. Formation and capture of SO_x species by a sorbent can also be modeled if needed.

The simulations were conducted using the following options and parameters: the standard k-ε turbulence model, the single-step devolatilization model, the oxidation model, and the devolatilization and oxidation rate constants for a hvAb coal such as Pittsburgh #8. The computational grid was constructed of 86,240 cells (110 x 28 x 28). The mass balance closure was within 0.01% and the energy balance closure within 4.79%. The gas velocity vectors in an axial section through the center line are shown in Figure 9. These first results are preliminary in nature.

Additional simulations will be performed to yield better convergence and to confirm grid size independence. Simulations will also be performed to investigate the effects of coal kinetic rates, inlet conditions such as flow rate and swirl of primary and secondary air, boundary conditions such as wall temperature, and design elements. The specific, devolatilization and oxidation rates of coal fired at the Kennebunk Test Facility will be measured by AFR and BYU and used in the new computations.

Submodel for Lean Premixed Combustion of Natural Gas in Industrial Gas Turbines (BYU) - A submodel for lean, premixed combustion (LPC) of natural gas in industrial gas turbines is being developed for implementation into a general, comprehensive gas turbine combustion model being developed under independent funding. The submodel must incorporate finite-rate chemistry

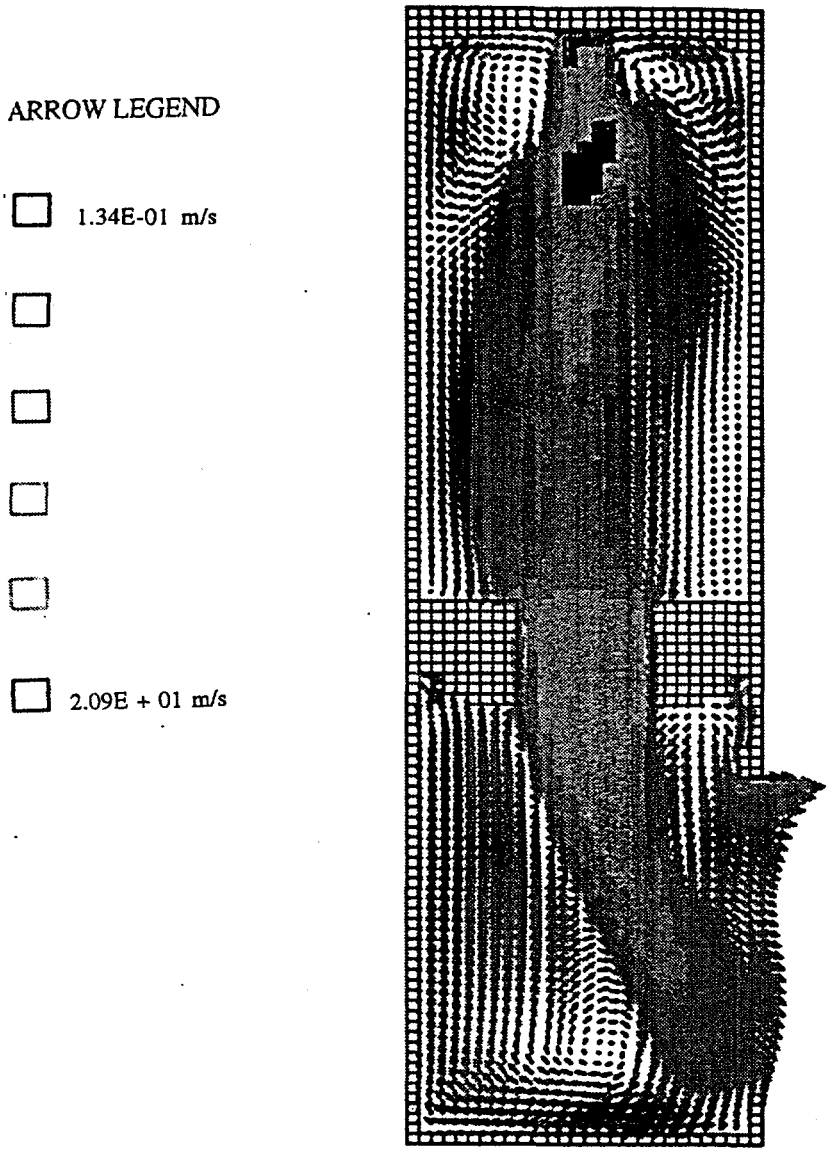

Fig. 9. PCGC-3 Prediction of the Gas Velocity Field for the Hague Coal Combustor at the Axial Section Through the Center Line.

and predict NO_x and CO emissions at conditions approaching fuel-lean blowout (0.4 to 0.6 stoichiometric ratio in the primary zone). Proper accounting for the effects of chemistry/turbulence interactions is important. The Monte Carlo probability density function (pdf) method [15] has been selected as a basis for the submodel.

A partially-stirred reactor (PaSR) model has been used to investigate the pdf method and to help evaluate reduced kinetic schemes. In the PaSR [16], there is a finite rate, given by a mixing frequency, at which the reactive fluids are mixed on a molecular level, as well as a finite rate at which they react after being mixed. Both the mixing and reaction time scales are important in the PaSR. Chemical mechanisms of varying complexity for CH_4-air have been tested with the PaSR model at conditions typical of gas turbines. Figures 10a and b show lean premixed CH_4-air combustion (equivalence ratio = 0.378, pressure = 30 atm, inlet temperature = 1200 K) predictions of mean temperature and CO mass fraction, respectively.

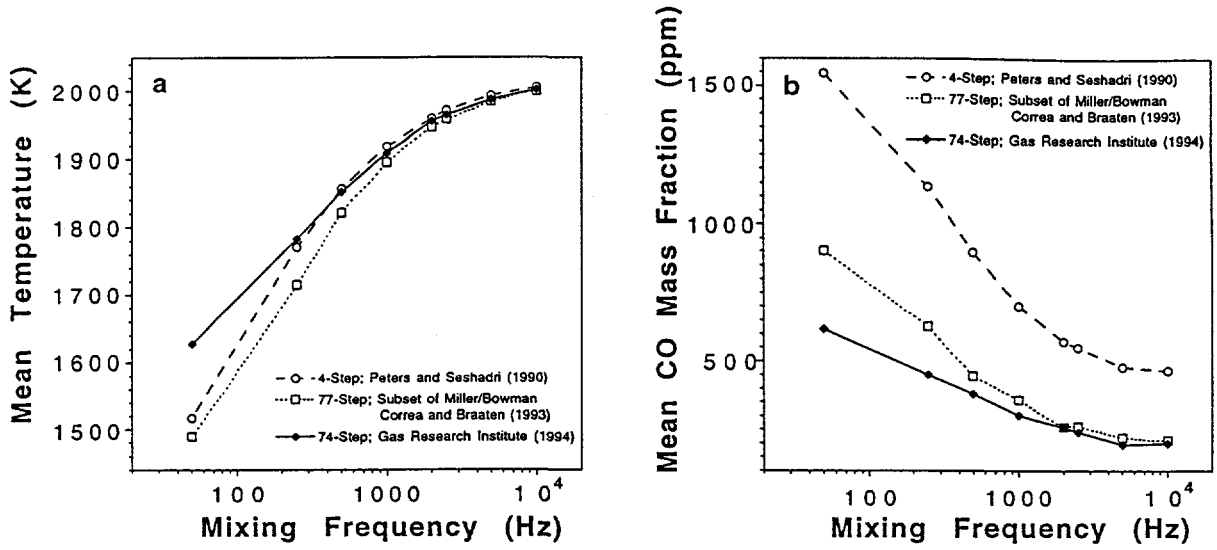

Fig. 10. (a) Predicted Mean Temperature and (b) CO Mass Fraction vs Mixing Frequency for Reduced and Detailed Chemical Mechanisms.

A velocity-scalar pdf submodel [17] has been tested and is being incorporated into an existing combustion flow code. The velocity-scalar pdf method is more accurate than the scalar-only pdf method and avoids the assumption of gradient diffusion. The chemistry was modeled with a single reaction progress variable, using Model A from the work of Chen and Kollmann [18]. Figure 11 shows scatterplots of particle position for non-premixed, adiabatic combustion of hydrogen and oxygen. The two-dimensional, axisymmetric jet enters at the left, and the flow is from left to right. The bottom edge of the figure represents the centerline of the reactor, and the outside wall is at a radial location of 0.2 m. There is a recirculation zone in the upper left corner. Each dot represents a pdf fluid "particle." Approximately 108,000 fluid particles were used in the calculation. A 20 x 20 grid was used in the flow code. Only one out of every five particles is shown.

During the next year, the submodel will be refined and extended to three dimensions. The model will be tested with kinetic schemes for LPC provided by independent work, and the submodel will also be incorporated into an unstructured flow code and applied to gas turbine configurations.

FUTURE WORK

Work during the next year will include: completion of verification of the FGDVC-RES model for fixed and fluidized beds; 2) completion of the large coal particle devolatilization (LCPD) version of the FG-DVC model; 3) completion of the CFB model development; 4) completion of the integration of FGDVC-RES with the MFIX model; 5) complete development of nitrogen devolatilization submodel; 6) complete development of large particle oxidation model; 7) complete integration of advanced submodels for large particles (oxidation, devolatilization) and improved numerical methods into FBED-1; 8) continue refinements of solution technique for LPC codes; 9) completion of case applications; 10) delivery of computer models to METC.

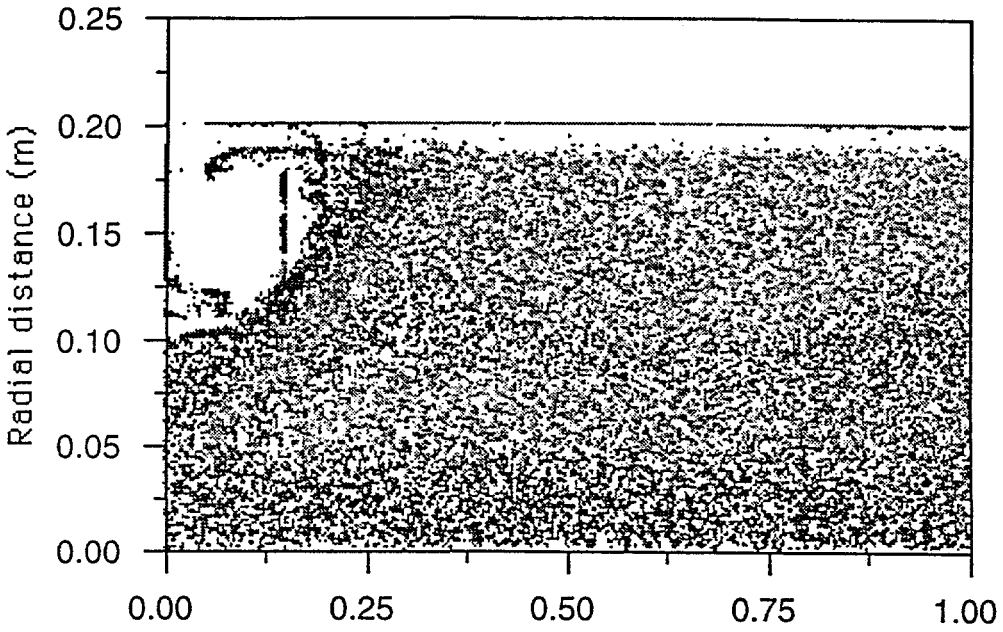

Fig. 11. Scatterplot of Instantaneous Particle Position for Velocity-Scalar pdf Simulations of Non-Premixed Combustion of Hydrogen and Oxygen.

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