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MATHEMATICAL-MODELING STUDIES OF IN-SITU COAL GASIFICATION

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MATHEMATICAL-MODELING STUDIES OF IN-SITU COAL GASIFICATION

MODÉLISATION MATHÉMATIQUE DE LA GAZÉIFICATION SOUTERRAINE DU CHARBON

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SUMMARY

Commercialization of the in-situ or underground coal gasification (UCG) process has been impeded because of uncertainties with respect to its reliability and predictability. Modeling studies when combined with a well-designed field test program are the only avenue to a proper understanding of this technology. This paper reviews the latest developments in four important facets of the UCG process: reverse-combustion linking; gasification and resource recovery; water influx; and subsidence.

RÉSUMÉ

L'application commerciale du procédé de gazéification souterraine du charbon (UCG) a été retardée par les incertitudes portant sur sa fiabilité et sa reproductibilité. Seules des études de modélisation combinées à un programme bien conçu d'essais in-situ permettront de parvenir à une juste compréhension de cette technologie. Cet article rend compte des derniers développements concernant quatre aspects importants du procédé UCG: la liaison par combustion à contre-courant, la gazéification et la récupération du charbon, la pénétration de l'eau dans la cavité et l'affaissement des terrains.

INTRODUCTION

Underground coal gasification (UCG) is a promising technology for converting coal to a useful product gas by partially combusting it underground in the presence of water and a limited amount of oxygen. In particular, UCG is an attractive technology for recovering deep low rank coals which appears to offer many advantages with respect to its efficiency, resource recovery, economics, and minimal environmental impact. Despite the many advantages of the UCG process, its commercialization has been impeded because of uncertainties with respect to its reliability and predictability. Modeling studies combined with a well-designed field test program are necessary to develop the understanding of UCG required to advance it towards commercialization.

This paper will review modeling studies of four important facets of UCG technology: permeability enhancement or linking; gasification and resource recovery; water influx; and subsidence. Because of space limitation, this review will be confined to discussing those models whose predictions have been tested against UCG field test data. Furthermore, the emphasis in discussing these models will be on what they tell us about the UCG process rather than on the formulation and solution of the model equations. This review necessarily focuses on the UCG modeling and field test efforts in the U.S. which have concentrated primarily on the enormous subbituminous coal reserves in the western U.S. For a more comprehensive overview, the interested reader is referred to the reviews of Gregg and Edgar (1), the U.S. Department of Energy (2), and Krantz and Gunn (3).

THE LINKED VERTICAL WELL UCG PROCESS

Before discussing the modeling studies, a brief description of the UCG process will be given. A schematic of the UCG process is shown in Figure 1. Injection (well 1) and production (well 2) well bores are drilled into the coal seam as shown in panel A. The permeability of the coal seam then must be enhanced to ensure reasonable gasification rates and to avoid condensation of tars from the product gas as it passes through the cooler regions of the coal seam. This can be accomplished by reverse combustion, electrolinking, hydraulic fracturing, and directional drilling. Modeling studies of both reverse combustion and electrolinking have been published. The former will be discussed in the subsequent section whereas the latter is the subject of another paper by the authors at this conference (4).

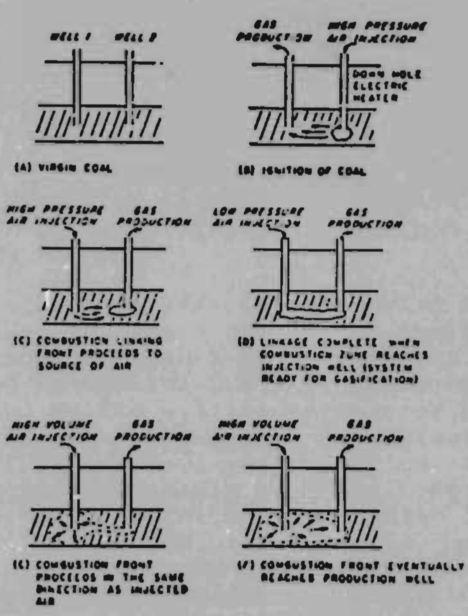

FIGURE 1. SEQUENCE OF EVENTS IN UCG PROCESS EMPLOYING REVERSE COMBUSTION LINKING

Reverse combustion linking is initiated by air injection and ignition of the coal at the production well as shown in panel B of Figure 1. The burn front is then drawn towards the injection well by shifting the air injection to the latter as shown in panel C. The coal is not completely consumed over a broad swath but only carbonized along one or more narrow channels or linkage paths. Linking is completed when the reverse combustion front reaches the bottom of the injection well as shown in panel D. It is then possible to inject air or oxygen at a high flow rate to effect gasification of a broad swath of the coal by forward combustion as shown in panels E and F.

MODELING STUDIES OF REVERSE COMBUSTION LINKING

The goal of modeling studies of reverse combustion linking is to discern the physics of the process and to develop predictive models for the flame speed and associated linking time, and the number and size of the linkage channels as functions of the gas injection rate and oxygen content, production well back pressure, and coal properties. Three types of models are required to predict these quantities. The fact that reverse combustion channels rather than propagating as a broad flame front has been shown by Krantz and Gunn (5, 6, 7) to be due to the inherent instability of the reverse combustion process. That is, reverse combustion is an unstable displacement process in which a high permeability region (the carbonized coal) displaces a low permeability region (the uncarbonized coal). It is unstable towards the propagation of narrow channels for a reason analogous to that which explains why water flooding of oil reservoirs is unstable to finger formation. Hence, the number of links initiated can be predicted by considering the initial stages of reverse combustion during which the front is expanding more or less radially about the production well; this analysis has been done by Bumb (8). The manner in which the diameter of the resulting reverse combustion links changes in response to changes in the flow rate and oxygen content of the injection gas can be addressed by a model which considers the stability of a planar reverse combustion flame sheet; this model has been developed by Gunn and Krantz (7), extended to higher pressures characteristic of linking at greater depths by Britten et al. (9), and applied to field test data by Krantz and Gunn (10). Finally, a process model for reverse combustion which predicts the flame temperature and speed, and product gas composition as a function of the injection flux within a channel has been advanced by Kotowski and Gunn (11) and extended to higher pressures by Britten et al. (9). The latter model utilizes the predictions of the stability theory models for the number and diameter of the reverse combustion channels in order to convert the total gas injection rate into a gas injection flux effective in each channel.

These modeling studies provide the following picture of the reverse combustion linking process. Bumb's (8) analysis for the initial stages of reverse combustion linking suggests that two to three channels are generated in shallow UCG burns in subbituminous coal such as those conducted by the U.S. Department of Energy in Wyoming. Gunn and Krantz' (7) analysis shows that the diameter of the channels increases markedly with increasing gas injection rate such that the gas flux in a channel remains nearly constant. For this reason, the flame speed and corresponding linking time remain fairly constant for a fixed well spacing despite wide variations in the gas injection rate, at least for shallow burns in subbituminous coals. These predictions are consistent with the Hanna, Wyoming, UCG field tests for which the time required to link the 18.3 m well spacing was approximately 10 days despite a fifteen-fold variation in gas injection rate. The manner in which changes in the process variables or physical properties affect the channel diameter can be understood solely in terms of how they affect the ratio of heat conduction into the carbonized region relative to heat convection downstream. Increasing this ratio decreases the channel diameter. For example, increasing the pressure for a fixed gas injection rate increases the rate of combustion of volatile matter and thereby decreases the thickness of the combustion zone. Hence, since this steepens the temperature gradient at the combustion front, it increases the heat conduction into the uncarbonized region and decreases the channel diameter. This prediction suggests that reverse combustion may not provide a satisfactory primary method for linking at high pressures since the resulting small links could easily plug due to condensation of tars. The process model of Kotowski and Gunn (11) indicates that under normal conditions, reverse combustion is oxygen-limited. Hence, for a fixed oxygen injection flux, the rate of combustion of volatile matter and correspondingly the rate of heat generation are predetermined for a fixed set of coal properties. The flame temperature is determined by the balance between heat generation and heat loss due to conduction into the uncarbonized coal and heat convection by the product gases. The flame speed is determined solely by how rapidly heat is conducted into the uncarbonized coal. The effect of any change in the process parameters or physical properties can be understood then solely in terms of how this change affects the heat generation relative to the heat loss. For example, increasing the pressure increases both the oxygen and fuel partial pressures thereby greatly accelerating the combustion reaction and steepening the temperature profile. This causes an increase in flame speed and a decrease in flame temperature.

FORWARD COMBUSTION GASIFICATION AND RESOURCE RECOVERY MODELS

Process models for forward combustion gasification seek to predict the gas production rate, heating value, composition, and temperature. Two such successful process models have been developed by Gunn and Whitman (12) and Thorsness and Rosza (13). Both models visualize forward gasification as a packed bed process with intimate contact between the solid and gas. The Gunn and Whitman model, which is more widely used because it is easier to implement numerically, assumes local thermal equilibrium between the solid and gas, and assumes the process to be pseudo-steady-state in a coordinate system translated at a constant combustion front velocity. The more complicated Thorsness and Rosza model does not make these assumptions but demonstrates that they are indeed quite reasonable. Both models predict the Hanna and Hoe Creek, Wyoming, UCG field test data quite well.

These models indicate that the forward combustion gasification process consists of three zones. In the gasification zone, the coal char combustion reactions quickly consume the available oxygen to create temperatures of approximately 1400 K in subbituminous coal. The temperature drops off rapidly downstream of the combustion front due to the endothermic steam-char reaction, which becomes quite slow at temperatures below 1000 K, such that the entire gasification zone is typically only 20 cm or so in thickness. In the zone approximately 20 cm thick wherein the temperature drops from 1000 K to 600 K, devolatilization becomes the principal reaction. This is followed by a very thick zone wherein drying of the coal occurs.

Since both process models discussed above are one-dimensional models, they cannot predict the resource recovery or areal sweep of the combustion front through the coal seam. Several areal sweep models for two-well UCG burns have been developed. That of Jennings et al. (14) is the simplest of these models to implement and has been shown to predict the resource recovery patterns of the Hanna, Wyoming, UCG field tests quite well. This model numerically solves the Darcy flow equation for source-sink flow between the expanding gasification cavity and the production well. The two-dimensional cavity boundary is advanced locally at each time increment assuming that the local flame front velocity is related to the local oxidant flux by the linear relationship determined from the one-dimensional process model of Gunn and Whitman (12).

MODELING STUDIES OF WATER INFLUX

Water plays a vital role in the UCG process by being the principal source of hydrogen for the steam-char gasification reaction. Both the Russian UCG operations as well as those conducted on subbituminous coal by the U.S. Department of Energy in Wyoming indicate that there is frequently sufficient natural water influx to obviate the need to inject steam into the process. Indeed, this is one of the advantages of UCG since it may eliminate the need for injecting high quality surface water such as is required for surface gasifiers. However, excessive water influx robs heat from the endothermic steam-char reaction and thereby lowers the product gas heating value. The product gas heating value during the Hanna, Wyoming, field tests showed a steady decline presumably due to progressively increasing water influx. The process model calculations of Gunn and Whitman (12) indicate that an optimum water influx between 0.1 and 0.2 moles of water per mole of injected air exists for the Hanna coal used in these field tests.

For quite some time, the source of the relatively large water influx observed in the Wyoming field tests remained a mystery. Indeed, it is readily established that the amount of free or bound water and elemental hydrogen present initially in the coal gasified is grossly insufficient to satisfy the hydrogen balance on the overall UCG process. Furthermore, the permeability of western U.S. coals is quite low and the UCG operating pressure is always maintained sufficiently close to hydrostatic to insure that relatively little water enters the UCG process by permeation. In addition, simple drying of the coal and overburden surrounding the UCG cavity can account for a negligible amount of water influx. This follows from the fact that heat from the hot gasification cavity surface must be conducted through a progressively increasing thickness as the drying front recedes into the surrounding coal or overburden.

A successful water influx model then was developed by Krantz and coworkers (15, 16) which incorporated two principal mechanisms for water influx: permeation, and spalling enhanced drying. The permeation component in this model allows for permeation into the complex cavity-link geometry, capillary pressure effects, and a time-varying pressure history. In the spalling enhanced drying component of this model, it is postulated that small pieces of coal or rock break off or spall near the steam front as a result of thermal and/or mechanical stresses. In this manner, new cavity roof surface is exposed to the high temperature cavity thus leading to higher thermal gradients and faster drying rates. Due to this spalling of small fragments from the roof, at any instant of time the roof will be composed of surface elements which have been exposed to the hot cavity for various times. The distribution of exposure times for these elements is known as the surface-age distribution. Each element of the roof is is drying at its own rate dictated by its age and described by the appropriate solution to the unsteady-state, one-dimensional drying equation for a water-saturated porous medium. The average drying rate is given as the weighted average of each elemental area where the weighting function is the surface-age distribution. This average drying rate, which differs for each stratum of coal or rock, can be determined either by field test studies or by a laboratory core characterization technique. The permeation component of this model requires a knowledge of the cavity and link surface area, whereas the spalling enhanced drying component requires a knowledge of the surface area of the cavity roof. These are determined by an appropriate areal sweep coal consumption model.

This water influx model has been shown to predict the cumulative water influx for four Wyoming UCG field tests within 11 percent. The model also suggests an air or oxygen injection strategy whereby a nearby constant product gas heating value can be maintained for water influx conditions characteristic of those of the Wyoming field tests.

MODELING STUDIES OF SUBSIDENCE

Subsidence is the adjustment made by the earth in response to the removal of mass from the subsurface. It is of considerable concern in UCG because of its potential effects on the environment and its possible implications for the success of the UCG process itself. Several finite element numerical codes have been applied to predicting subsidence in UCG with only very limited success. For example, in the case of the Hoe Creek (Wyoming) III UCG field test, these codes predicted at most only a few centimeters of surface subsidence when in fact massive chimneying-type subsidence propagated to the surface. The authors argued that these finite element codes failed because they did not incorporate a realistic cavity geometry which evolves as a result of both gasification of the coal as well as spalling of the overlying coal and roof rock. Finite element codes are unable to predict this spalling accurately since it occurs on a scale of only a few centimeters and is influenced by random variations in the properties of the overburden strata which precludes obtaining reliable thermomechanical property data for these numerical codes. An alternative approach is to use a phenomenological model such as the "spalling enhanced drying model" described in the preceding section in order to predict the upward growth of the gasification cavity. This has been done by Levie et al. (17, 18) who have predicted the UCG cavity shape for the Hanna II Phases II and III, and Hanna III field tests in Wyoming, all of which have been recently cored in order to determine the actual post-burn cavity shape. Figure 2 shows the cavity dome profile along the line of centers between

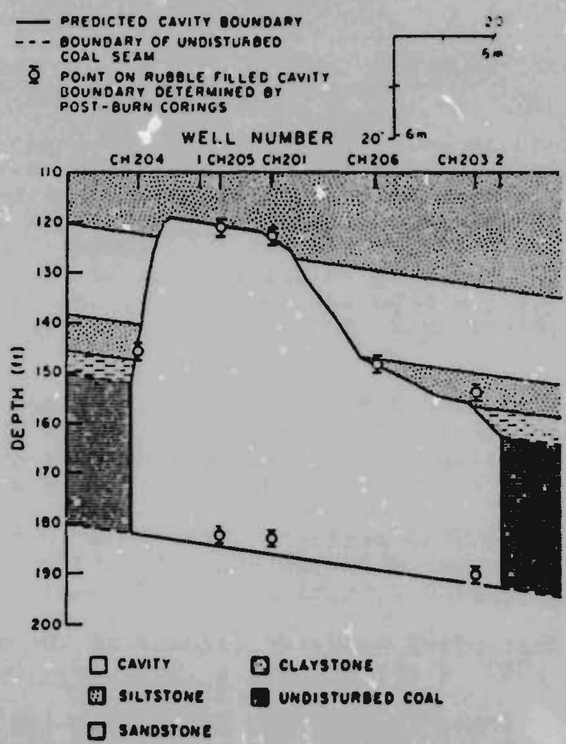

FIGURE 2. CAVITY PROFILE ALONG LINE-OF-CENTERS BETWEEN INJECTION AND PRODUCTION WELLS FOR THE HANNA III UCG FIELD TEST

the injection (well 1) and production (well 2) wells for the Hanna III field test. The data points (defined by a core hole number CH---) locate the cavity boundary as inferred from post-burn coring, whereas the model predictions are shown by the solid line.

CONCLUSIONS

This brief review indicates that considerable progress has been made in modeling reverse combustion linking, forward combustion gasification and resource recovery, water influx, and subsidence for relatively shallow UCG burns in subbituminous coals. The extent to which these models can be applied to deep UCG operations or to UCG in bituminous coals remains to be determined.

Space considerations did not permit discussing modeling studies of the UCG process economics. The interested reader is referred to the most recent such study by Boysen and Gunn (19).

Finally, it was not possible to discuss the authors' opinion as to the proper direction for further modeling studies. This topic has been addressed in a recent paper of Gunn and Krantz (20).

ACKNOWLEDGMENTS

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