Canyon Ridge Consulting Report
CRC2011-0002
December 6, 2011

EOS7C-ECBM Version 1.0:

Additions for Enhanced Coal Bed Methane Including the Dusty Gas Model

Stephen W. Webb
Canyon Ridge Consulting LLC
10 Canyon Ridge Dr.
Sandia Park, NM 87047

This page intentionally blank.

CRC2011-0002
December 6, 2011

EOS7C-ECBM VERSION 1.0:

ADDITIONS FOR ENHANCED COAL BED METHANE INCLUDING THE DUSTY GAS MODEL

Stephen W. Webb
Canyon Ridge Consulting LLC
10 Canyon Ridge Dr
Sandia Park, NM 87047

Abstract

EOS7C is an equation of state module for the TOUGH2 program for CO_2 or N_2 in Methane (CH_4) Reservoirs. In the present work, additions have been made to the EOS7C Version 1.0 module to include the Enhanced Coal Bed Methane (ECBM) modifications developed by Webb (2003). In addition, the Dusty Gas Model for gas-phase diffusion (Webb, 2001) has been included.

The ECBM modifications to the EOS7C equation of state incorporate the extended Langmuir isotherm for sorbing gases, including the change in porosity associated with the sorbed gas mass. Comparison to hand calculations for pure gas and binary mixtures shows very good agreement. Application to a CO_2 well injection problem given by Law et al. (2002) shows reasonable agreement.

The Dusty Gas Model modifications add options to calculate gas diffusion using the Dusty-Gas Model including separate and coupled approaches. Comparison to low-permeability pure gas diffusion data shows excellent agreement. The results from the DGM are compared to the Fick's law behavior for diffusion across a capillary fringe. The differences between the models are small due to the relatively high permeability (10^{-11} m^2) of the problem.

This work was carried out through Lawrence Berkeley National Laboratory as part of the ZERT project, funded by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, National Energy Technology Laboratory, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Table of Contents

List of Figures

List of Tables

Nomenclature

b	Klinkenberg parameter
c	molar concentration
d	distance to the interface
D_i^K	Knudsen diffusion coefficient for component i
D_{ij}	binary diffusion coefficient for components i and j
G_s	gas storage capacity (sm^3/kg; scf/ton)
G_{sL}	dry, ash-free Langmuir storage capacity (sm^3/kg; scf/ton)
K_H	Henry's constant
N^D	molar diffusive flux
P	pressure (kPa, psia)
P_L	Langmuir pressure (kPa, psia)
R	gas constant
T	temperature
x	sorbed or liquid phase mole fraction
y	gas phase mole fraction
w_a	ash weight fraction
w_{we}	equilibrium moisture weight fraction

Greek

α	separation factor
τ	tortuosity
ϕ	porosity
θ	exponent on temperature correction factor

Subscripts

$1,2,\ldots$	component number
air	air
d	downstream
eff	effective value
g	gas value
i	interface, component
ℓ	liquid value
nc	number of components
P	value at P
T	value at T
u	upstream
0	reference conditions, all-gas value for the porous medium
β	saturation

Superscripts

g	gas value
i	interface
ℓ	liquid value
*	effective value

Acknowledgments

The opportunity for me to contribute to the ZERT project at Lawrence Berkeley National Laboratory was provided by Dr. Curtis M. Oldenburg (LBNL). I want to thank Curt for his interest, help, and comments during the preparation and testing of these code enhancements.

1.0 Introduction

EOS7C is an equation of state module for TOUGH2 for CO_2 or N_2 in Methane (CH_4) reservoirs. The TOUGH2 EOS7C Version 1.0 module for CO_2 (Oldenburg et al., 2004) has been enhanced to include the Enhanced Coal Bed Methane (ECBM) modifications developed by Webb (2003). In addition, the Dusty Gas Model for gas-phase diffusion (Webb, 2001) has been included. Each modification will be discussed separately.

1.1 Enhanced Coal Bed Modifications

Modifications have been made for the EOS7C module of TOUGH2 for Enhanced Coal Bed Methane (ECBM). In ECBM, CO_2 is pumped into methane-rich coal beds. Due to adsorption processes, the CO_2 is sorbed onto the coal, which displaces previously sorbed methane (CH_4). The released methane can then be recovered, at least partially offsetting the cost of CO_2 sequestration.

A number of papers discuss the mechanics of ECBM. Hall et al. (1994) compare their experimental data for adsorption of methane, nitrogen, and carbon dioxide and the binary mixtures on wet Fruitland coal with numerous models including the extended Langmuir and loading ratio (LRC) correlations, as well as three versions of 2-d EOS, the van der Waals, Eyring, and EOS-S. For the mixture data, the ideal adsorbed solution (IAS) approach is also evaluated. The details of the various models are beyond the scope of the present document, and the interested reader is referred to the original reference. For pure gas adsorption, Hall et al. showed that the extended Langmuir model performed the poorest with a %AAD (absolute average percent deviation) of about 2.5; the other models were similar to each other with a %AAD ranging from 0.6 to 1.8 for the various pure gases, or almost within the experimental uncertainty. For binary mixtures, the extended Langmuir and LRC models performed the poorest while the other models were about equal. The %AAD for the extended Langmuir model is 19 and 11 for the individual gases and 6 for the total. For the LRC, the corresponding %AAD values are 28, 6 and 8. For the other models, the average corresponding %AAD values are about 13, 9, and 5.

The relatively poor performance of the extended Langmuir model is probably due to the fact that it has only two model constants to fit the experimental data for pure gas adsorption, while the three other approaches have three model constants. Note that all the data fits were done for the pure gas adsorption data, not for the mixture data.

Arri et al. (1992) came to similar conclusions about the performance of the extended Langmuir model. The extended Langmuir model seems to perform well at 500 psia but not as well at 1000 and 1500 psia.

The overall conclusion can be reached that the extended Langmuir model provides a reasonable prediction of the adsorption processes of ECBM, especially for scoping studies. However, for more accurate predictions, investigation of the use of other more complex models may be necessary. The extended Langmuir model was also used by Zarrouk and Moore (2009) in their modification of TOUGH2 for ECBM.

1.2 Dusty Gas Model for Gas Diffusion

The TOUGH2 code, including the EOS7C module, includes simplified methods for gas diffusion based on a direct application of Fick’s law. Application of Fick’s law to gas diffusion in porous media has recently been questioned by a number of investigators including Thorstenson and Pollock (1989), Abriola et al. (1992), and Webb (1998). The Dusty Gas Model (DGM), which is a more fundamental approach to gas diffusion in porous media, is preferable to Fick’s law. The DGM is discussed in great detail by Mason and Malinauskas (1983) and Cunningham and Williams (1980). Webb (1998) compared the two approaches to comprehensive gas diffusion data in low-permeability graphite (2.13 x 10^{-18} m^2) obtained by Evans et al. (1962, 1963). The DGM predictions compared very well with the experimental data and to Graham’s laws, which are fundamental gas diffusion relationships for porous media. In contrast, the Fick’s law predictions did not obey Graham’s laws and did not compare well to the data.

Webb (1998) and Webb and Pruess (2003) showed that for a binary mixture, the DGM model can be rewritten in a form similar to Fick’s law. However, the coefficient in front of the mass fraction gradient is not a constant but is a function of the mass fractions of the components. Webb and Pruess (2003) showed that for trace gas diffusion, a simple modification of Fick’s law can be performed that will produce the same results as the DGM. However, for gas diffusion involving other than trace gases, the two approaches cannot be made equivalent. As shown by Webb and Pruess (2003), the differences between the two approaches (Fick’s Law and DGM) get larger as the permeability decreases.

Due to the fact that gas diffusion can be an important physical process in geologic CO_2 sequestration, the EOS7C module of TOUGH2 has been modified to include the DGM for gas diffusion as an option. Oldenburg et al. (2004) used a preliminary implementation of the DGM methods to simulate the mixing of CO_2 and CH_4 in depleted gas reservoirs, concluding that the DGM is needed for low permeability media, consistent with previous work.

2.0 Code Modifications

2.1 Enhanced Coal Bed Methane

For the purposes of this report, the extended Langmuir model is considered to be adequate for the prediction of ECBM. The extended Langmuir isotherm is given below (Law et al., 2002).

The gas storage capacity for a single gas species is given by the Langmuir relationship

$$G_s = G_{sL}\left[1-\left(w_a + w_{we}\right)\right]\frac{P}{P+P_L} \tag{1}$$

where

G_s	gas storage capacity (sm^3/kg-coal)
G_{sL}	dry, ash-free Langmuir storage capacity (sm^3/kg-coal)
w_a	ash weight fraction
w_{we}	equilibrium moisture weight fraction
P	pressure (Pa)
P_L	Langmuir pressure (Pa)

The individual Langmuir parameters from equation (1) are used to model multiple gas species through the extended Langmuir isotherm

$$G_{si} = G_{sLi}\left[1-\left(w_a + w_{we}\right)\right]\frac{\dfrac{P\,y_i}{P_{Li}}}{1+P\displaystyle\sum_{j=1}^{nc}\frac{y_j}{P_{Lj}}} \tag{2}$$

where

y	mole fraction of component i in the gas phase
i	component i
nc	number of components

Gas sorbtion is added to the basic mass balance equation in TOUGH2 as follows:

$$M_{gas}^{\kappa} = \phi\sum_{gas} S_{gas}\,\rho_{gas} X_{gas}^{\kappa} + \left(1-\phi\right)\rho_{coal}\,G_{si}\,\rho_{gas,STP} \tag{3}$$

where M_{gas}^{κ} is the mass of component κ in the gas phase per unit volume and ϕ is total fluid volume fraction including the sorbed gases. Standard (STP) conditions are assumed to be 1 atmosphere (101.325 kPa) and 60°F (15.56°C).

The sorbed gases lead to coal bed volume changes. The density of the sorbed gases determines the sorbed volume and resultant coal bed shrinkage or swelling. The sorbed gas density is not well defined. Arri et al. (1992) suggest that the sorbed gas density can be approximated by the liquid density at the atmospheric boiling point, which is 421. kg/m^3 for methane and 808 kg/m^3 for nitrogen. Because CO_2 is a solid at the atmospheric boiling point, they suggest the saturated liquid density at the triple point, or 1180 kg/m^3.

In order to include coalbed shrinking and swelling, the sorbed gases change the local porosity as determined by the sorbed gas density and the amount of gas sorbed. Two porosities or volumes are defined; the total fluid porosity (volume), which includes any sorbed gas volume, and the net fluid porosity (volume), which is the net value available for fluids. These terms are shown schematically in Figure 1.

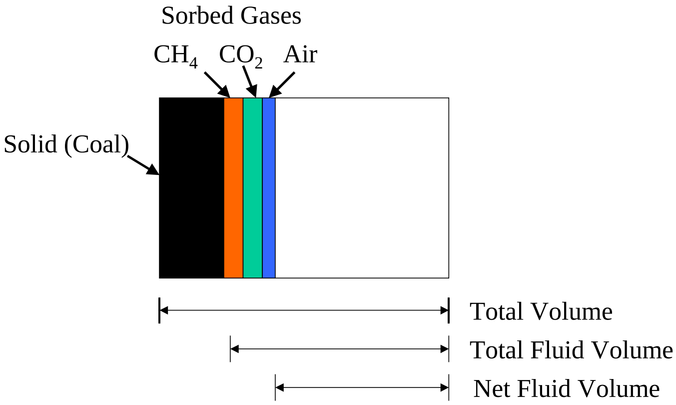


Figure 1. Volume Nomenclature

One thing to note is that the gas storage capacity per the above Langmuir isotherm is not a function of gas saturation. As long as there is any gas, the entire mass of coal in that element is available for gas storage without regard to the gas saturation. Therefore, for the same gas composition, the gas storage capacity is the same for a gas saturation of 0.01% or a gas saturation of 100%. This behavior has led to an option of a gas saturation dependent extended Langmuir isotherm, or

$$G_{si} = G_{sLi}\, S_g \left[1-\left(w_a + w_{we}\right)\right] \frac{\dfrac{P\, y_i}{P_{Li}}}{1 + P \displaystyle\sum_{j=1}^{nc} \frac{y_j}{P_{Lj}}} \tag{4}$$

When a phase change from two-phase to liquid-saturated conditions occurs, the gas saturation goes to zero and the handling of the sorbed mass becomes important. In the present code, this sorbed mass is saved and no further sorbtion or desorbtion occurs while the element is at full liquid saturation, and the sorbed mass is included in the mass balance. Because this sorbed mass is no longer dependent on the current element thermodynamic conditions, the value of this sorbed mass is written out as part of the SAVE file as detailed in the input section. When the gas phase returns to the element, the sorbed mass for liquid conditions is used in the gas phase mass balance, and the liquid phase sorbed mass is zeroed out.

2.2 Dusty Gas Model

The general form of the Dusty Gas Model for the gas diffusion of component i is given by (Thorstenson and Pollack, 1989)[1]

$$\sum_{j=1, j\neq i}^{n} \frac{y_i N_j^D - y_j N_i^D}{D_{ij}^*} - \frac{N_i^D}{D_i^{K*}} = \frac{\left(\nabla P_i - \rho_g g\right)}{RT} \tag{5}$$

where N^D is the molar diffusive flux, y is the gas phase mole fraction, D_{ij}^* is the effective binary diffusion coefficient, D^{K*} is the effective Knudsen diffusion coefficient, P is the pressure, R is the gas constant, and T is the temperature. The summation is over all components in the system except itself such that the diffusion of all gas components is coupled.

For a 3-component system and ignoring gravity for simplicity in this presentation, the set of equations becomes

$$-\left[\frac{1}{D_1^{K*}} + \frac{y_2}{D_{12}^*} + \frac{y_3}{D_{13}^*}\right] N_1^{D,g} + \frac{y_1}{D_{12}^*} N_2^{D,g} + \frac{y_1}{D_{13}^*} N_3^{D,g} = \frac{\nabla P_1}{RT} = \frac{P \nabla y_1}{RT} + \frac{y_1 \nabla P}{RT} \tag{6a}$$

$$\frac{y_2}{D_{21}^*} N_1^{D,g} - \left[\frac{y_1}{D_{21}^*} + \frac{1}{D_2^{K*}} + \frac{y_3}{D_{23}^*}\right] N_2^{D,g} + \frac{y_{21}}{D_{23}^*} N_3^{D,g} = \frac{\nabla P_2}{RT} = \frac{P \nabla y_2}{RT} + \frac{y_2 \nabla P}{RT} \tag{6b}$$

$$\frac{y_3}{D_{31}^*} N_1^{D,g} + \frac{y_3}{D_{32}^*} N_2^{D,g} - \left[\frac{y_1}{D_{31}^*} + \frac{y_2}{D_{32}^*} + \frac{1}{D_3^{K*}}\right] N_3^{D,g} = \frac{\nabla P_3}{RT} = \frac{P \nabla y_3}{RT} + \frac{y_3 \nabla P}{RT} \tag{6c}$$

where the two terms on the right-hand side represent ordinary and Knudsen diffusion driving forces, respectively. Note that self diffusion, D_{11}^*, is not explicitly included in the equation set. Self diffusion in gases is expressed by the Knudsen diffusion coefficient, D_i^{K*}, which is operative even if the gas only has a single component.

For a single component, the DGM equation reduces to

$$N_1^{D,g} = -D_1^{K^*} \frac{\nabla P_1}{RT} \tag{7}$$

where the Knudsen diffusion coefficient models the "slip" of the gas, or the Klinkenberg effect.

---

[1] For consistency with the ECBM nomenclature, the mole fraction in the gas phase is designated as y and the mole fraction in the liquid phase is designated as x.

As can be seen from equation (5), the diffusion of any single component may be strongly coupled with the diffusion of the other components. Therefore, in general, a single equation for the diffusion of a given component cannot be developed. Two exceptions are binary gas diffusion, where equations can be developed as given by Thorstenson and Pollock (1989), and trace gas diffusion, where an effective tortuosity can be defined for use with Fick's law (Webb and Pruess, 2003) that will give the same results as the DGM.

The above equations are for gas diffusion in the gas phase without considering the presence of a liquid phase. For diffusion of dissolved components in the liquid phase, a simple Fick's law model has been used. The model is different from that of Pruess et al. (1999), however, in that Fick's law is based on mole fractions rather than mass fractions. The present model gives equimolar diffusion in the liquid, while the model used by Pruess et al. (1999) gives equal and opposite mass fluxes. The diffusion fluxes for each dissolved component (including water) are given by

$$N_i^{D,\ell} = -D_{1i,\ell}^{*} c_\ell \nabla x_i \tag{8}$$

where i applies to all the components including water.

2.2.1 Coupling of Diffusive Fluxes

The above equations predict gas and liquid diffusion for uniform properties and under single-phase conditions. For nonuniform properties and multiphase conditions, the solution of the above equations becomes much more complicated. Pruess and Webb (1999) developed a multiphase diffusion scheme by invoking conservation of total flux across the interface, which leads to harmonic weighting of the strength coefficient. However, their diffusion equations were based on Fick's law, such that coupling between components in a given phase was not included. Only the coupling of gas and liquid diffusion was considered.

The general concept of a weighting scheme for diffusion is that the fluxes to and from an "interface" condition are equal. This "interface" condition is defined by this equality of fluxes. For simple cases, harmonic weighting is the resulting weighting scheme as discussed by Tsang and Pruess (1990). The same principle of conservation of mass flux, or diffusive flux, will be used in this case based on the combined gas and liquid rates. As discussed by Pruess and Webb (1999), the weighting scheme must consider the combined fluxes rather than each one individually.

For example, the DGM equation for component 1 can be written in terms of the unspecified interface conditions (mole fraction and pressure) as follows

$$-\left[\frac{1}{D_1^{K*}} + \frac{y_2}{D_{12}^{*}} + \frac{y_3}{D_{13}^{*}}\right] N_1^{D,g} + \frac{y_1}{D_{12}^{*}} N_2^{D,g} + \frac{y_1}{D_{13}^{*}} N_3^{D,g} = \frac{P}{RT}\frac{y_{1,i} - y_{1,u}}{d_u} + \frac{y_1}{RT}\frac{P_i - P_u}{d_u} \tag{9}$$

where subscript *i* denotes the interface condition, and d_u is the distance from element 1 to the interface, or the upstream length. Naturally, the properties of element 1 are used for the coefficients. Similarly, the downstream equation is

$$-\left[\frac{1}{D_1^{K*}}+\frac{y_2}{D_{12}^*}+\frac{y_3}{D_{13}^*}\right]N_1^{D,g}+\frac{y_1}{D_{12}^*}N_2^{D,g}+\frac{y_1}{D_{13}^*}N_3^{D,g}=\frac{P}{RT}\frac{y_{1,d}-y_{1,i}}{d_d}+\frac{y_1}{RT}\frac{P_d-P_i}{d_d} \tag{10}$$

and the properties of element 2 are used. Similar sets of equations can be written for each gas phase components and each liquid phase component.

The gas equations specify the interfacial mole fraction in terms of the gas mole fraction, while the liquid equations use the liquid mole fraction for the interface. The difference between the mole fractions is resolved by defining an effective value of Henry's constant, which is defined as

$$K_{H,i,eff}=K_{H,i}\frac{c_\ell}{c_g}=\frac{y_{g,i}}{x_{\ell,i}} \tag{11}$$

so the liquid interfacial mole fractions can be converted to gas interfacial mole fractions. $K_{H,i,eff}$ for the interface is calculated from the upstream and downstream elements based on the element mole fractions. Only elements with gas in them are considered. The value at the interface is estimated by harmonic weighting of the element values.

The values of the interfacial mole fractions and total interfacial pressure are calculated by invoking equal upstream and downstream total molar fluxes (gas plus liquid) to and from the interface for each component, as well as the requirement that the mole fractions sum to 1.0.

In a three-component system, the following relationships are calculated for each connection

diffusive gas flux from the upstream element to the interface (3 eqns)
diffusive gas flux from the interface to the downstream element (3 eqns)
diffusive liquid flux from the upstream element to the interface (3 eqns)
diffusive liquid flux from the interface to the downstream element (3 eqns)
gas + liquid flux to interface = gas + liquid flux away from interface
  for each component (3 eqns)
sum of interface mole fractions in gas phase equals 1.0 (1 eqn)

where the flux equations are the DGM or liquid diffusion equations.

The unknowns are

diffusive gas flux from the upstream element to the interface (3 unk)
diffusive gas flux from the interface to the downstream element (3 unk)
diffusive liquid flux from the upstream element to the interface (3 unk)
diffusive liquid flux from the interface to the downstream element (3 unk)

interface mole fractions (3 unk)
interface pressure (1 unk)

where the gas and liquid diffusive fluxes for each component are unknowns.

Therefore, for a three-component system, there are 16 equations and 16 unknowns. For a five-component system such as in EOS7C, there are 26 equations and 26 unknowns for the fully coupled solution.

Separate gas and liquid diffusion calculations are an option similar to the original model in Pruess et al. (1999) assuming that there is no coupling between the gas diffusion in the individual phases. Separate calculations are also performed if the fully coupled option was selected but there is no diffusion in a given phase for all components.

For the separate flux calculations, gas diffusion is calculated separately as is liquid diffusion. The separate gas diffusion equation set involves 16 equations and 16 unknowns. For liquid diffusion, the equation set includes 15 equations and 15 unknowns. There is no interface pressure unknown, and the mole fraction sum equation is deleted.

Solution is easily accomplished with standard matrix solvers. Checks are made that the upstream and downstream fluxes for each component have a relative error < 10^{-3} (typical values are 10^{-10} or less) and that the sum of the interface mole fractions is equal to 1.0 with the same relative error as the mass fluxes.

2.2.2 Gas Diffusion Coefficients

For ordinary diffusion, the effective diffusion coefficients are the binary gas values, such as those calculated by Fuller (see Reid et al., 1987), multiplied by the medium tortuosity, τ_0, and the saturation-dependent tortuosity, τ_β, as well as pressure and temperature correction factors. These parameters are the same as used by Pruess et al. (1999), or

$$D_{ij,PT} = D_{ij}(P_0, T_0)\frac{P_0}{P}\left(\frac{T+273.15}{273.15}\right)^{\theta} \tag{12}$$

where P_0 and T_0 are 10^5 Pa and 0^{o}C, respectively, and

$$D_{ij}^{*} = D_{ij,PT}\phi\tau_0\tau_\beta \tag{13}$$

For Knudsen diffusion, the coefficient is often calculated from the Klinkenberg coefficient, b_i, (Klinkenberg, 1941) using the following relationship (Thorstenson and Pollock, 1989)

$$D_i^K = \frac{kb_i}{\mu_i} \tag{14}$$

The Knudsen diffusion coefficients for different gases are related by

$$D_j^K = D_i^K \left(\frac{m_i}{m_j} \right)^{1/2} \tag{15}$$

where m is the molecular weight.

The Klinkenberg coefficient for air at 25°C has been correlated with the liquid permeability by Heid et al. (1950) using numerous samples from oil-field cores and can be written as follows

$$b_{air} = 0.11\, k_\ell^{-0.39} \tag{16}$$

where b_{air} is the Klinkenberg coefficient for air in Pa, and k_ℓ is the liquid-phase permeability in m^2. Note that the data used in this correlation have permeability values between 10^{-12} and 10^{-17} m^2. Subsequently, Jones and Owens (1980) measured permeabilities on low-permeability gas sands with permeabilities between 10^{-14} and 10^{-19} m^2; their correlation is

$$b_{air} = k_\ell^{-0.33} \tag{17}$$

Between 10^{-14} and 10^{-17} m^2 where the permeability data overlap, the values from both correlations are quite similar. Each correlation gives lower values than the other in the region it is most applicable. Therefore, a reasonable approach is to take the minimum Klinkenberg coefficient from the two correlations where the two correlations overlap.

The Knudsen diffusion coefficient for air is input into the code as the Klinkenberg parameter in the ROCKS block. Equation (15) is used to calculate the Knudsen diffusion coefficient for the various components. If the DGM is used, the input value is the Knudsen diffusion coefficient. The input value is assumed to be at 25°C similar to the Heid et al. correlation. The temperature correction to other conditions is given by

$$D_{i,T}^K = D_i^K (T_0) \left(\frac{T + 273.15}{298.15} \right)^{0.5} \tag{18}$$

If no value is input, the value is calculated from the Klinkenberg coefficient as determined above using equation 14. Note that there is no pressure correction because the Knudsen diffusion coefficient is independent of pressure (Mason and Malinauskas, 1983).

Because the Klinkenberg coefficient, and therefore the Knudsen diffusion coefficient, has been correlated in a porous medium, the porosity and tortuosity, τ_0, effects are already included in the value as discussed by Thorstenson and Pollock (1989). Therefore, only the saturation-dependent tortuosity, τ_β, is used to modify the Knudsen diffusion coefficient, or

$$D_i^{K*} = D_{i,T}^{K} \; \tau_\beta \tag{19}$$

The same equations and relationships for τ_0 and τ_β presented by Pruess et al. (2000) are used in the present model implementation, including the various options for the tortuosity coefficients. Because the tortuosity values τ_0 and τ_β have to be separately stored due to the Knudsen diffusion coefficient, the value of NB for diffusion is increased from 8 to 9. The various secondary parameters are stored as follows:

PAR (7)	Diffusion factor 1 ($\phi\tau_0$)
PAR (8)	Diffusion factor 2 (τ_β)
PAR (7)	Diffusion factor 3 ($D_\beta^\kappa(T,P)/D_\beta^\kappa(T_0,P_0)$)

The density has been taken out of the PAR(7) variable because the DGM calculations are in terms of moles.

2.2.3 Liquid Diffusion Coefficients

Methods for calculating liquid diffusion coefficients in a non-porous system are given by Reid et al. (1987), where typical values for water as the solvent are about 10^{-9} m^2/s at infinite dilution for room temperature conditions. Unlike gases, no pressure or temperature correction is applied. However, the tortuosity factors as given in equation (13) above are employed. When the Millington-Quirk relationship is selected for the saturation-dependent tortuosity, τ_β, the gas saturation is simply replaced by the liquid saturation; Jury et al. (1983) also used this approach to estimate the tortuosity for liquids.

2.2.4 Model Applicability

Note that there is a lower limit for Knudsen diffusion. The assumption in the above equations is that “slip” flow occurs, which can be modeled by the Klinkenberg factor. However, at very low permeabilities, other diffusion mechanisms become important such as configurational diffusion (Cunningham and Williams, 1980, Xiao and Wei, 1992). In configurational diffusion, the pore size is approximately equal to the size of the gas molecules, and the configuration of the molecules and molecule-surface effects become important. The permeability drops off drastically in the configurational diffusion range. Based on simple calculations, the transition between “slip” flow and configurational diffusion is of the order of 10^{-21}. Therefore, the applicability of the above Klinkenberg correction should be limited to media with liquid permeabilities of 10^{-21} m^2 and greater. If the porous medium has a lower value, the diffusion regime is probably configurational, and additional model modifications are required.

2.3 Changes to TOUGH2 Routines

The changes to TOUGH2 are in a number of subroutines. There are changes for the ECBM modifications and for the DGM. The changes and the appropriate subroutines are listed below.

- Changes in BALLA
    - Print ECBM Langmuir parameters
    - Added sorbed phase mass and volume to balance
- Changes in CONVER
    - Final converged porosity adjustment
- Changes in EOS
    - DGM changes including calculation of diffusion parameters
    - Added IE(16) options for DGM sample problems
- Changes in INPUT
    - New CBM Block
    - Changes to INCON Input for sorbed masses
    - New DGM Block
- Changes in MULTI
    - Change in porosity due to coalbed swelling/shrinkage
    - Mass split between gas phase and sorbed phase
    - DGM Model Implementation
- Changes in OUT
    - List the porosity changes and the sorbed masses
    - Reformatted to element output – added trace component mass fraction in liquid phase
- Changes in OUTDF
    - Changes to diffusion output to include DGM
- Changes to RELP
    - Added Law et al. relative permeability (IRP=9) for Law et al. sample problem
- Changes to RFILE
    - Changes to INCON processing for ECBM
- Changes in TOUGH2
    - Added array storage for ECBM and DGM
- Changes to WRIFI
    - Modified SAVE file format for ECBM
- New subroutine CBMGS
    - Extended Langmuir isotherm
- New subroutine BALCBM
    - Initial Sorbed Mass Calculations

This page intentionally blank.

3.0 Verification

3.1 Enhanced Coal Bed Methane

Verification of the modifications to TOUGH2 for the ECBM is provided through comparison of the output from the code to literature results. The first verification exercise compares the results from extended Langmuir isotherm calculations with the results presented by Arri et al. (1992). These results are for pure gas and binary gas sorption, where the extended Langmuir parameters are specified by Arri et al. (1992). The second verification exercise is for a sample problem presented by Law et al. (2002), which has been used for comparison of various ECBM simulators.

3.1.1 Isotherms

Arri et al. (1992) present the results of isotherm calculations for pure gas and binary gas conditions for CH_4, CO_2, and N_2. The results from the present calculation are presented in the same English units used in the original reference for ease of comparison. Figure 2 shows the pure gas isotherm results; the extended Langmuir values are summarized in Table 1. The solid line is the isotherm given earlier by equation (1) with zero ash and moisture weight fractions, while the symbols are the results from the modified TOUGH2 code. The agreement is excellent.

Figures 3 through 6 present results for binary gas adsorption using the extended Langmuir isotherm constants given in Table 1. Figure 3 shows the CH_4-N_2 binary gas sorption isotherms at 500 psia calculated with the modified TOUGH2 program as given by the symbols. The solid lines are the results given by equation (2). Figure 4 presents the CH_4-CO_2 isotherm at 1000 psia. In both cases, the agreement is excellent between the analytical solution and the results from the modified TOUGH2 program.

The species splits in the gas phase and the sorbed phase are shown in Figures 5 and 6 for the two mixtures given above. These curves are independent of pressure because it is completely defined by the pure gas Langmuir isotherms as discussed by Arri et al. (1992). The separation factor, α, is given by

$$\alpha_i = \frac{\left({}^{x}\!/_{y} \right)_i}{\left({}^{x}\!/_{y} \right)_j} \qquad (20)$$

where x is the sorbed phase mole fraction and y is the gas phase mole fraction, and i and j are the two gases. The value of the separation factor can be calculated from (Arri, et al., 1992)

$$\alpha_i = \frac{\left(G_{sL} / P_L \right)_i}{\left(G_{sL} / P_L \right)_j} \qquad (21)$$

Table 1. Langmuir Parameters (Arri et al., 1992)

Gas	G_{SL}(SCF/ton)	p_L (psia)
CO_2	1128	204.5
CH_4	759	362.3
N_2	616	1458.

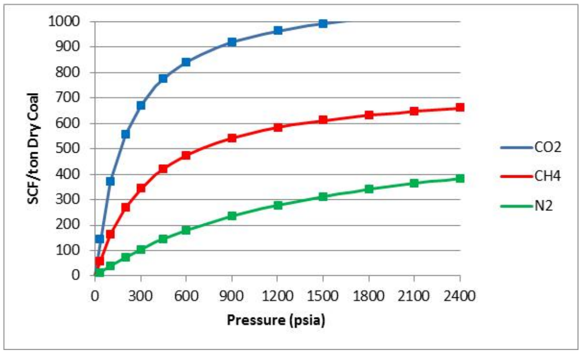


Figure 2. Pure Gas Isotherms

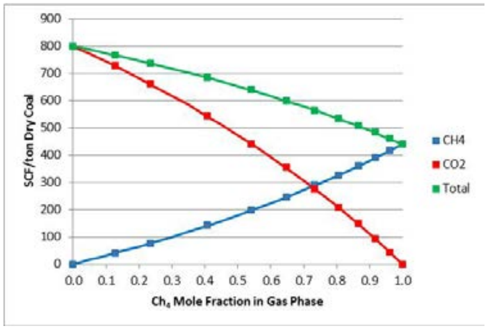


Figure 3. CH_4-CO_2 Sorption at 500 psia

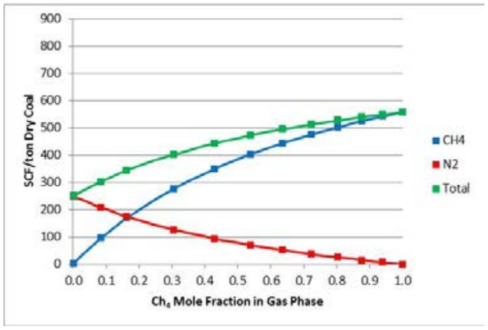


Figure 4. CH_4-N_2 Sorption at 1000 psia

Figure 5. CH_4-CO_2 Splits at 500 psia

Figure 6. CH_4-N_2 Splits at 1000 psia

which is not a function of pressure. For a binary gas mixture, equation can be rearranged to give the gas phase mole fraction of component i as

$$y_i = \left(1 + \alpha_i \frac{1 - x_i}{x_i}\right)^{-1} \tag{22}$$

which is the solid line in the figures. Again, the agreement between the results from the modified TOUGH2 code and the above equation is excellent.

3.1.2 Law et al. (2002) Problem

Law et al. (2002) have presented a comparison of ECBM simulators for two simplified problem sets. The first problem is a single-well CO_2 injection test, while the second problem is a five-spot CO_2-ECBM recovery process. The geometry and relative permeability functions are explicitly defined by Law et al. (2002); note that there is no capillary pressure. The first problem (single well CO_2 injection) will be analyzed with the modified TOUGH2 code in this section. Additional details including input and selected output are included in Appendix C.

The problem involves injecting pure CO_2 into a coal seam. Flow occurs in natural fractures that have a small natural porosity of 0.001 and a permeability of 3.65 millidarcies. The initial conditions of the reservoir are 7650 kPa, $45^{o}C$, and a gas saturation of 0.408 of pure CH_4. Coal matrix swelling/shrinkage is neglected. The problem chronology is an initial 15 days of CO_2 injection followed by a 45-day shut-in period, a 60-day production period, and a 62.5-day shut-in period.

The mesh is specified as a 29x1x1 cylindrical grid with given spacing as detailed in Table 2. The well radius is 0.0365 m. For this problem, a new relative permeability function had to be added to TOUGH2. The relative permeabilities for water and gas are specified as a tabular function of water saturation as given in Table 3. Details of the coalbed characteristics are given in Table 4, while the test parameter details are summarized in Table 5.

As mentioned above, no coal swelling or shrinking is included in the problem definition. This behavior is modeled by specifying the sorbed gas density as artificially high (10^{10} kg/m^3) in order to effectively disable effect of sorbed gases on the porosity.

Table 2.
Radial Grid System

i	Δr (m)	r (m)
1	0.9110	0.9110
2	1.1600	2.0710
3	1.3456	3.4166
4	1.5609	4.9775
5	1.8106	6.7881
6	2.1003	8.8884
7	2.4364	11.3248
8	2.8262	14.1510
9	3.2784	17.4294
10	3.8030	21.2324
11	4.4114	25.6438
12	5.1173	30.7611
13	5.9360	36.6971
14	6.8858	43.5829
15	7.9875	51.5704
16	9.2655	60.8359
17	10.7480	71.5839
18	12.4677	84.0516
19	14.4625	98.5141
20	16.7765	115.2906
21	19.4608	134.7514
22	22.5745	157.3259
23	26.1864	183.5123
24	30.3763	213.8886
25	35.2364	249.1250
26	40.8742	289.9992
27	47.4141	337.4133
28	55.0005	392.4138
29	61.4972	453.9110

Table 3.
Relative Permeability Relationships

Water Saturation	Relative Permeability	
	Water	Gas
1.00	1.000	0.000
0.975	0.814	0.0035
0.950	0.731	0.007
0.90	0.601	0.018
0.85	0.490	0.033
0.80	0.392	0.051
0.75	0.312	0.070
0.70	0.251	0.090
0.65	0.200	0.118
0.60	0.154	0.147
0.55	0.116	0.180
0.50	0.088	0.216
0.45	0.067	0.253
0.40	0.049	0.295
0.35	0.035	0.342
0.30	0.024	0.401
0.25	0.015	0.466
0.20	0.007	0.537
0.15	0.002	0.627
0.10	0.0013	0.720
0.05	0.0006	0.835
0.00	0.000	1.000

Table 4.
Coalbed Characteristics

Coal Seam Thickness	9 m
Top of Coal Seam	1253.6 m
Absolute Permeability of Natural Fractures	3.65 md
Relative Permeabilities	see Table 3
Porosity of Natural Fracture System	0.001
Effective Compressibility	1.45×10^{-7} kPa^{-1}
Initial Conditions	
Temperature	45^{o}C
Pressure (uniform)	7650 kPa
Gas Saturation	0.408 (100% CH_4)
Liquid Saturation	0.592
Pure Gas Adsorption Isotherms	
In-Situ Coal Density	1434 kg/m^3
In-Situ Moisture Content (by wt.)	0.0672
In-Situ Ash Content (by wt.)	0.156
CH_4 G_{sL}	0.0152 sm^3/kg
p_L	4688.5 kPa
CO_2 G_{sL}	0.0310 sm^3/kg
p_L	1903. kPa
N_2 G_{sL}	0.0150 sm^3/kg
p_L	27,241. kPa

Water Properties - Specified in Problem Definition – internal TOUGH2 properties used instead

Table 5.
Problem Parameters

Cylindrical Grid (r-θ-z):	29x1x1
Inner radius	0.0365 m
Outer Radius	454 m
Mesh	see Table 2

15-day CO_2 Injection period (0 - 15 days)
- CO_2 Injection Rate - 28,316.82 sm^3/d
- Maximum Bottom-Hole Pressure - 15,000 kPa

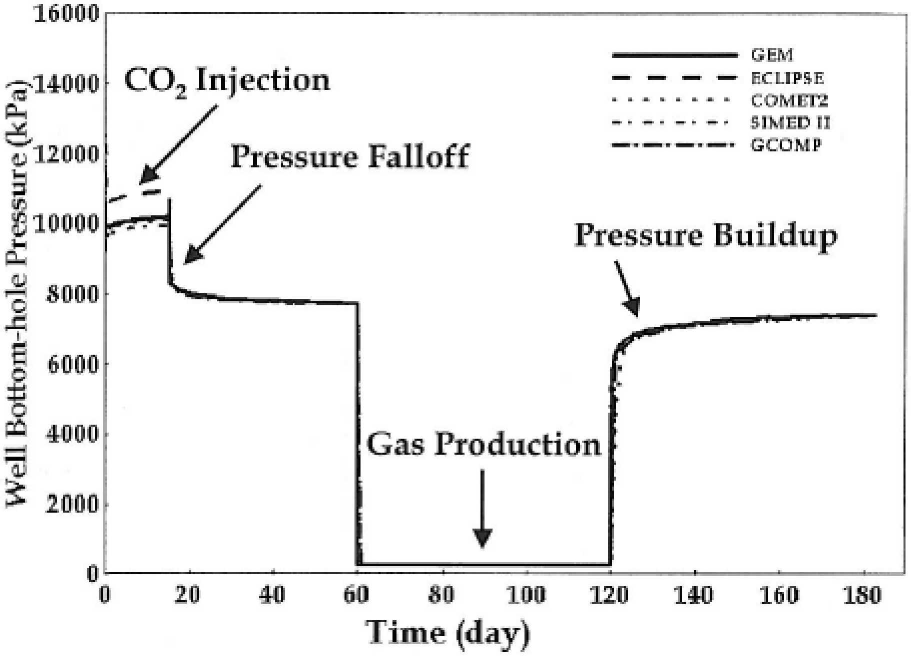
45-day Shut-In (15 - 60 days)
60-day Production period (60 - 120 days)
- Maximum Production rate - 100,000 sm^3/d
- Minimum Bottom-Hole Pressure - 275 kPa

62.5-day Shut-In Period (120 - 182.5 days)

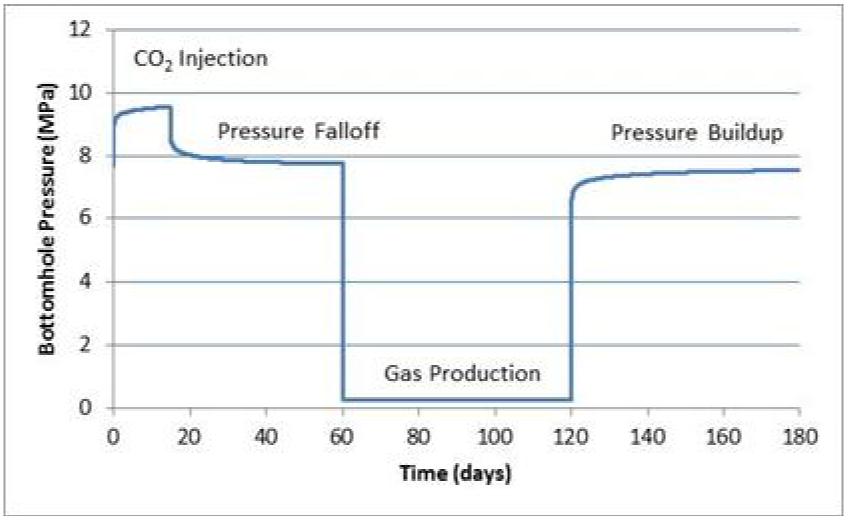
One of the parameters from the various codes that is compared in Law et al. (2002) is the initial gas-in-place for the CH_4. The values for the five codes range from 6.0315 x 10^7 to 6.1681 x 10^7 sm^3. The present code predicts 6.146 x 10^7 sm^3.

The predicted bottom-hole pressure as a function of time is shown in Figure 7. The general behavior compares well to the results presented by Law et al. (2002) except that the borehole pressure during CO_2 injection is slightly low. This difference may due to the treatment of the borehole, which was treated explicitly in the present simulations, or due to differences in CO_2 properties.

Figure 8 gives the gas production rate results. The flow rates of CH_4 and CO_2 are initially in agreement with the results given in Law et al. (2002). At about 64 days, however, the gas production predicted by the present code drops significantly when an element near the borehole changes from pure gas to two-phase conditions and the gas relative permeability decreases from 1.0 to 0.49. This decrease in gas production rate is not seen in the results presented by Law et al. (2002). Overall, the agreement is reasonable.

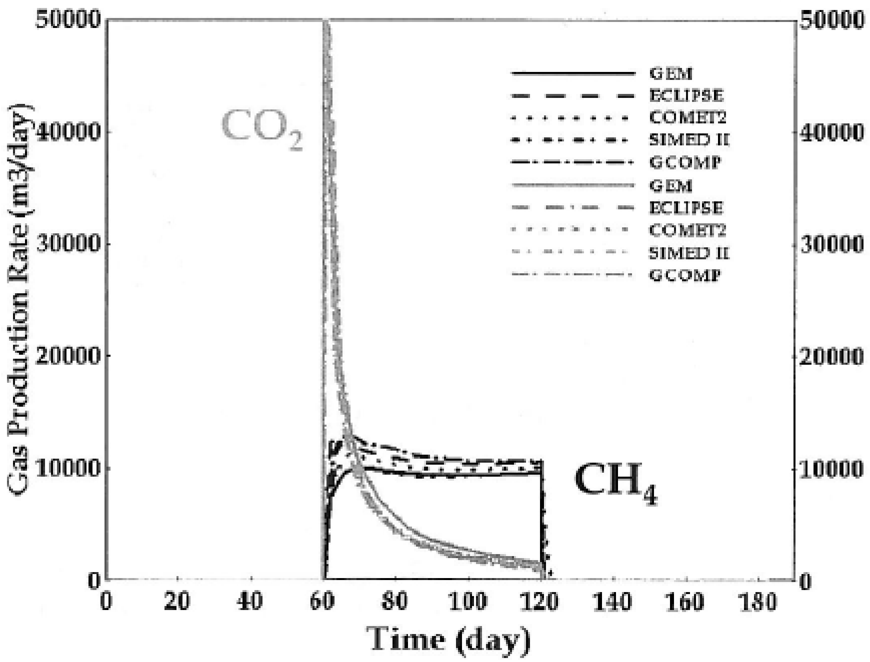


(a) Law et al. (2002)

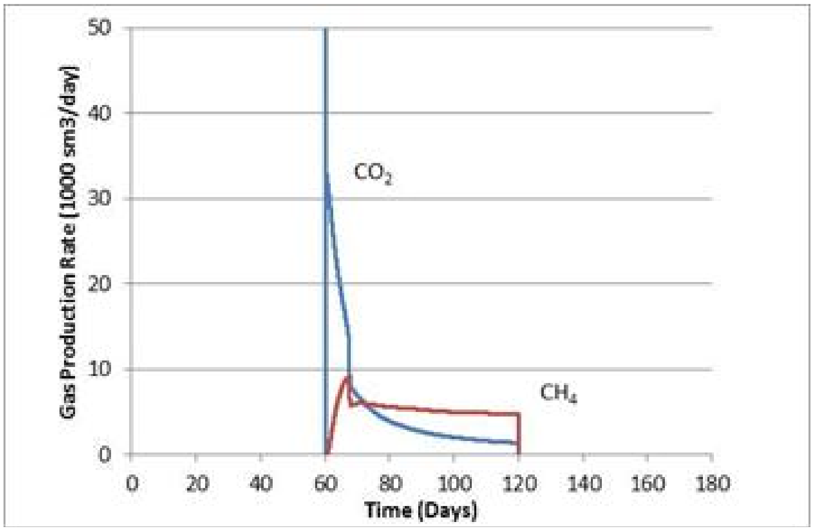


(b) Present Results

Figure 7. Well Bottom-Hole Pressure



(a) Law et al. (2002)



(b) Present Results

Figure 8. CH$_4$ and CO$_2$ Production Rates

3.2 Dusty Gas Model

The above model has been verified by comparison to a number of problems with known or hand-calculated solutions.

3.2.1 Single Gas

A simple two-volume problem with a single gas (CO_2) was modeled to check the Knudsen diffusion coefficient case. Conditions were a permeability of 10^{-12} m^2 (air Knudsen diffusion coefficient of 2.864 x 10^{-4} m^2/s at 25^oC), a temperature of 20^oC, and a pressure gradient of 0.1 Pa/m. The diffusion of air was evaluated by equation (7) as 4.183 x 10^{-10} kg/s, which agrees with the program output to within 0.5%.

3.2.2 Binary Gases

The DGM has been compared to the experimental data of Evans et al. (1962, 1963) for a low permeability (2.13 x 10^{-18} m^2) graphite by Webb (1998), which showed that the DGM compares well to the data while Fick's law does not. Some of these same data have been used in the present verification exercise. The trace gases were specified to be Argon and Helium as in the experiments. Two situations were considered: (1) zero pressure difference diffusion (Knudsen and ordinary diffusion only), and (2) combined advection and diffusion. Appendix D contains more details on the input and output for these simulations.

a. Zero Pressure Difference

For the zero pressure difference case, Mason and Malinauskas (1983) give a relationship for the mole flux of both gases as a function of total pressure, which assumes a linear variation in the mole fraction of both gases in the graphite. The experimental data compare well to the relationship. Figure 9 compares the results of the present modified version of TOUGH2 with the relationship of Mason and Malinauskas; the agreement is excellent.

b. Combined Advection and Diffusion

For this more general case, Mason et al. (1967) performed an integration of the DGM assuming a linear variation for the mole fraction as above. Iteration is required to obtain the desired fluxes. The experimental data compare very well to the integrated equation. Explicit equations describing the various curves were not presented, so the curves were extracted from the original figures of Mason and Malinauskas (1983). Comparison of the present modified version of TOUGH2 to these curves is given in Figure 10. The predictions compare very well to the curves. As mentioned above, the curves assume a linear mole fraction variation in their derivation, so the agreement is not expected to be perfect.

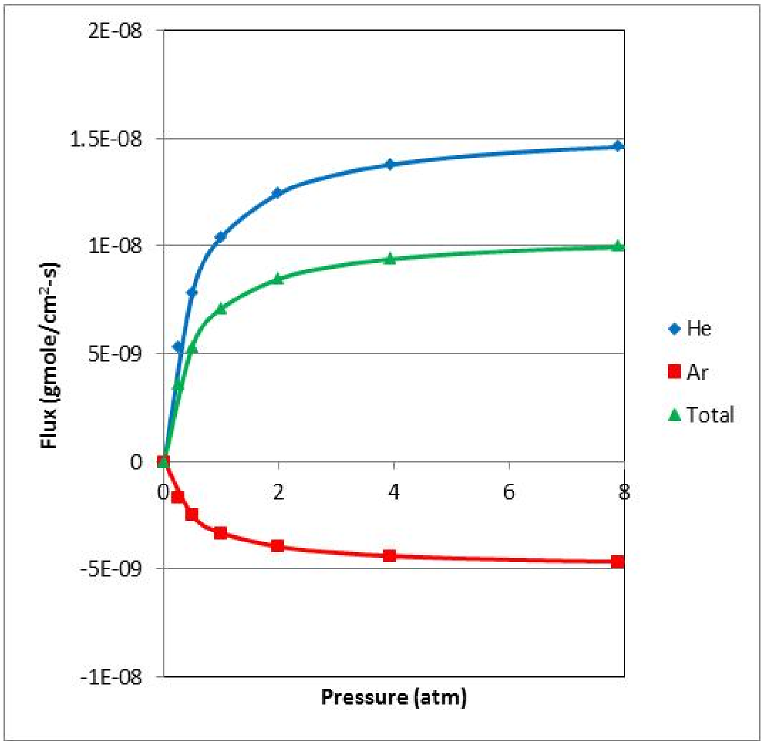


Figure 9. Verification for Zero Pressure Difference Diffusion

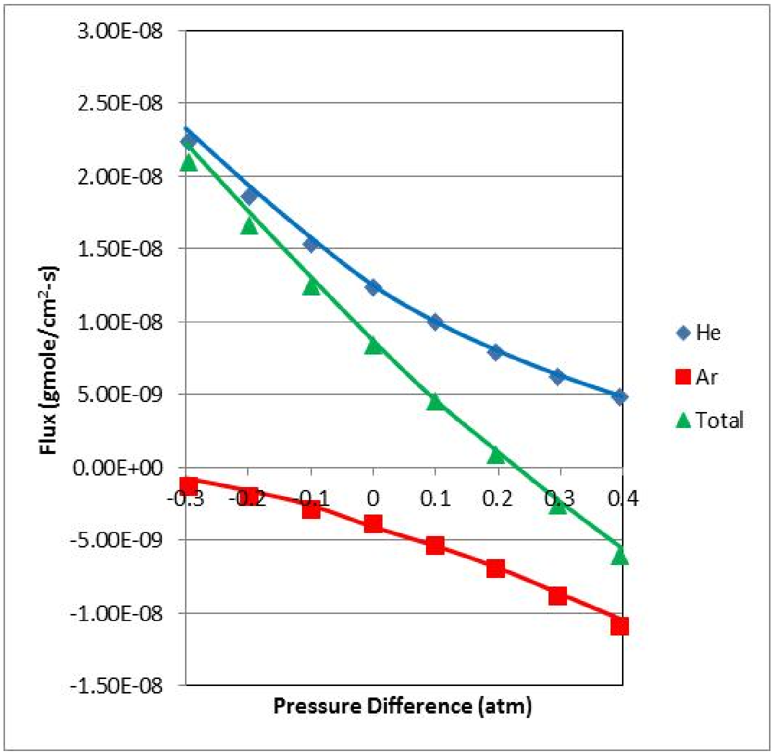


Figure 10. Verification for Combined Advection Plus Diffusion

3.2.3 Diffusion Across a Capillary Fringe

Pruess et al. (1999) presented a sample problem involving TCE and PCE diffusion across a capillary fringe. The problem consists of TCE and PCE in the gas phase at the solubility limits above the water table, which diffuses through the capillary fringe into the water table below. The original TOUGH2 results in Pruess et al. (1999) show considerable differences between the separate and coupled diffusion models. The calculation has been redone with the modified code to check the original implementation as well as to ascertain the differences between the previous Fick's law model and the present Dusty Gas Model for this problem. Appendix E gives more details about the simulations.

Figures 11 and 12 show the results for the original Fick's law approach and for the DGM. The differences between the results are minimal. As discussed by Webb (1998) and Webb and Pruess (2003), differences between Fick's law and the DGM are minimal at higher permeabilities (> 10^{-13} m^2) but they may increase to be orders of magnitude at lower values (~ 10^{-18} m^2). Therefore, the present problem is not a definitive test of the possible differences between Fick's law and the DGM.

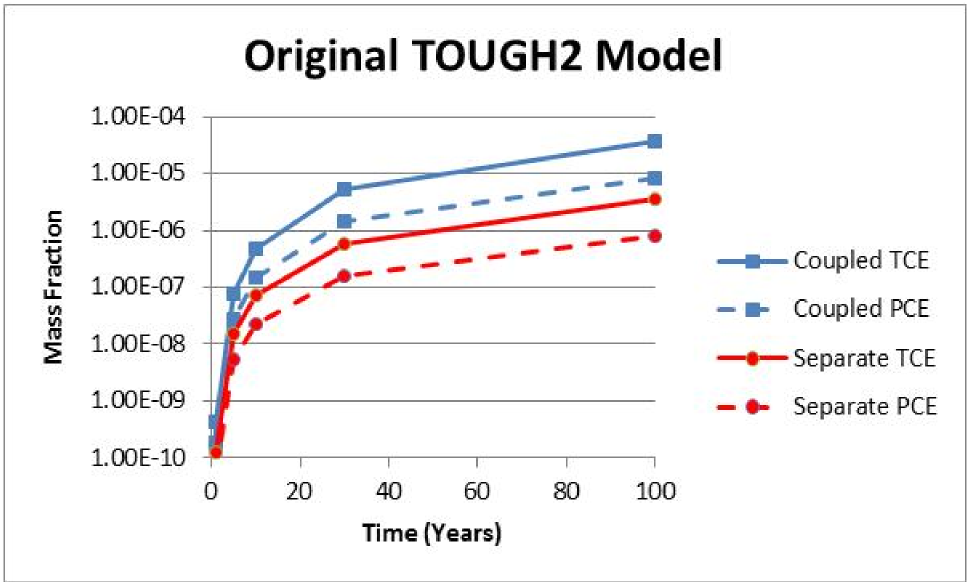


Figure 11. Original TOUGH2 Fick's Law Results

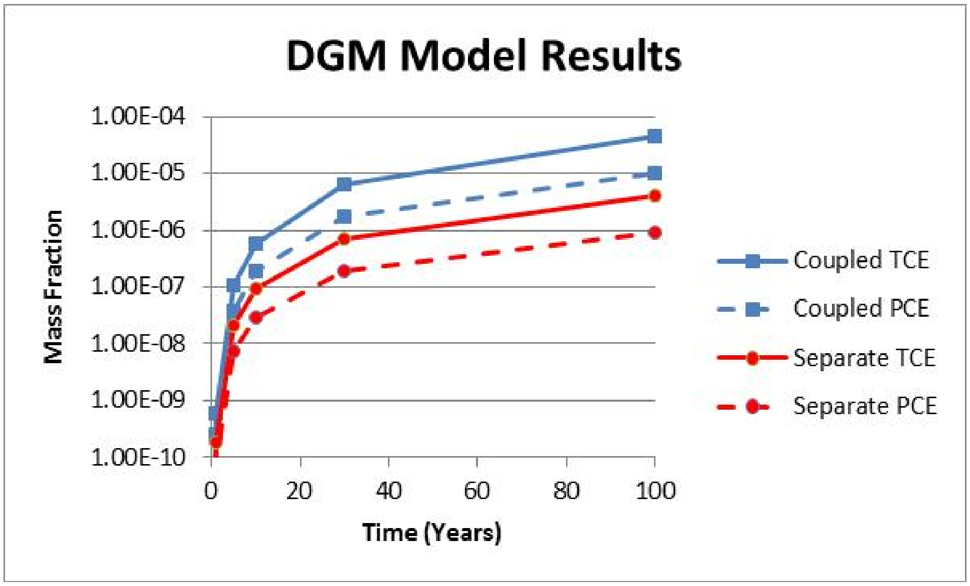


Figure 12. TOUGH2 DGM Results

This page intentionally blank.

4.0 Summary and Discussion

4.1 ECBM

ECBM code modifications have been successfully made to the TOUGH2-EOS7C code as demonstrated by the successful simulation of the Law et al. (2002) problem set 1. While the behavior is qualitatively similar to the behavior seen in Law et al. (2002), there are some quantitative differences that need to be investigated in the future. A comparison of the features of the various codes could help to identify the reason for the different behavior. Additional ECBM simulations are also recommended such as the Law et al. (2002) problem sets 2 and 2P for a 5-spot process.

The present version of the code includes the porosity change from ECBM. Additional modifications should be made to change the permeability and connection flow area based on the change in porosity. Zarrouk (2004) discusses a number of porosity-permeability relationships that could be implemented. A subset of these models should probably be added to the code. Changes to the connection flow area could be simply related to the porosity change based on an assumed flow geometry.

4.2 DGM

Implementation of the DGM compares very well to existing gas-phase diffusion data. The use of the DGM may be limited because the computer time increases significantly compared to the default Fick's law approach. For the Law et al. (2002) problem, the computer time increased by about a factor of three when the DGM model was used instead of the Fick's law approach. Improving the computational efficiency may be necessary before the DGM is used for large-scale problems. Using the trace gas approach of Webb and Pruess (2003) to reduce the equation set for trace gases may improve the computational efficiency.

This page intentionally blank.

5.0 References

Abriola, L.M., C.-S. Fen, and H.W. Reeves, 1992, "Numerical simulation of unsteady organic vapor transport in porous media using the dusty gas model," Subsurface Contamination by Immiscible Fluids, edited by Weyer, Balkema, Rotterdam, pp. 195-202.

Arri, L.E., D. Yee, W.D. Morgan, and M.W. Jeansonne, 1992, "Modeling Coalbed Methane Production With Binary Gas Sorption," SPE 24363, SPE Rocky Mountain Regional meeting, Casper, Wyoming, May 18-21, 1992.

Cunningham, R.E., and R.J.J. Williams, 1980, Diffusion in Gases and Porous Media, Plenum, New York.

Evans, R.B., III, G.M. Watson, and J. Truitt, 1962, "Interdiffusion of gases in a low permeability graphite at uniform pressure," *J. Appl. Phys*., 33:2682-2688.

Evans, R.B., III, G.M. Watson, and J. Truitt, 1963, "Interdiffusion of gases in a low permeability graphite. II. Influence of pressure gradients," *J. Appl. Phys*., 34:2020-2026.

Hall, F.E., C. Ahou, K.A.M. Gasem, R.L. Robinson, Jr., and D. Yee, "Adsorption of Pure Methane, Nitrogen, and Carbon Dioxide and Their Binary Mixtures on Wet Fruitland Coal," SPE 29194, 1994 Eastern Regional Conference & exhibit, Charleston, West Virginia, November 8-10, 1994.

Heid, J.G., J.J. McMahon, R.F. Nielson, and S.T. Yuster, 1950, "Study of the Permeability of Rocks to Homogeneous Fluids," *API Drilling and Production Practice,* pp. 230-244.

Jones, F.O., and W.W. Owens, 1980, "A Laboratory Study of Low-Permeability Gas Sands," *J. Petroleum Technology*, pp. 1631-1640.

Jury, W.A., W.F. Spencer, and W.J. Farmer, 1983, "Behavior assessment model for trace organics in soil. I. Description of model," *J. Environ. Qual*., 12:558-564.

Klinkenberg, L.J., 1941, "The Permeability of Porous Media to Liquids and Gases," *API Drilling and Production Practice,* pp. 200-213.

Law, D. H.-S., L.G.H. van der Meer, and W.D. Gunter, 2002, "Numerical Simulator Comparison Study for Enhanced Coalbed Methane Recovert Processes, Part 1: Pure Carbon Dioxide Injection, SPE 75669, SPE Gas Technology Symposium, Calgary, Alberta, 30 April – 2 May 2002.

Mason, E.A., and A.P. Malinauskas, 1983, Gas transport in porous media: the dusty-gas model, Chem. Eng. Monograph 17, Elsevier, New York.

Mason, E.A., A.P. Malinauskas, and R.B. Evans, III, 1967, "Flow and Diffusion of Gases in Porous Media," *J. Chemical. Physics*, 46:3199-3216.

Oldenburg, C.M., S.W. Webb, K. Pruess, and G.J. Moridis, 2004, "Mixing of Stably Stratified Gases in Subsurface Reservoirs: A Comparison of Diffusion Models," *Transport in Porous Media*, 54:323-334.

Oldenburg, C.M., G.J. Moridis, N. Spycher, and K. Pruess, 2004, "EOS7C Version 1.0: TOUGH2 Module for Carbon Dioxide or Nitrogen in Natural Gas (Methane) Reservoirs," LBNL-56589, Lawrence Berkeley National Laboratory, Berkeley, CA.

Pruess, K., C.M. Oldenburg, and G. Moridis, 1999, "TOUGH2 User's Guide, Version 2.0," LBNL-43134, Lawrence Berkeley National Laboratory, Berkeley, CA.

Pruess, K., and S.W. Webb, 1999, "On Finite Difference Modeling of Diffusion of Phase-Partitioning Species under Multiphase Conditions," AGU Fall Meeting, Supplement to Eos, Transactions, AGU Volume 8, Number 46, pg. F385.

Reid, R.C., J.M. Prausnitz, and B.E. Poling, 1987, The Properties of Gases and Liquids, Fourth Edition, McGraw-Hill Book Company, New York.

Thorstenson, D.D., and D.W. Pollock, 1989, "Gas transport in unsaturated zones: multi-component systems and the adequacy of Fick's laws," *Water Resour. Res*., 25:477-507.

Tsang, Y.W., and K. Pruess, 1990, "Further Modeling Studies of Gas Movement and Moisture Migration at Yucca Mountain, Nevada," LBL-29127, Lawrence Berkeley Laboratory, Berkeley, CA.

Webb, S.W., 1996, "Gas-Phase Diffusion in Porous Media – Evaluation of an Advective-Dispersive Formulation and the Dusty-Gas Model Including Comparison to Data for Binary Mixtures," SAND96-1197, Sandia National Laboratories, Albuquerque, NM.

Webb, S.W., 1998, "Gas-Phase Diffusion in Porous Media – Evaluation of an Advective-Dispersive Formulation and the Dusty-Gas Model for Binary Mixtures," *J. Porous Media*, 1:187-199.

Webb, S.W., 2001, "Modification of TOUGH2 to include the Dusty Gas Model for Gas Diffusion," SAND2001-3214, Sandia National Laboratories, Albuquerque, NM.

Webb, S.W., 2003, "Modification of TOUGH2 for Enhanced Coal Bed Methane Simulations," SAND2003-0154, Sandia National Laboratories, Albuquerque, NM.

Webb, S.W., and K. Pruess, 2003, "The use of Fick's Law for modeling trace gas diffusion in porous media," *Transport in Porous Media*, 51:327-341.

Zarrouk, S.J., 2004, Simulation of Complex Multi-Phase Multi-Component, Reacting Flows in Porous Media, Doctoral Thesis in Engineering Science, The University of Auckland.

Zarrouk, S.J., and T.A. Moore, 2009, "Preliminary reservoir model of enhanced coalbed methane (ECBM) in a subbituminous coal seam, Huntly Coalfield, New Zealand. Int. J. of Coal Geology, 77:153-161.

Appendix A
Input for ECBM Modifications

The input for the ECBM modifications are in a new block named CBM. The extended Langmuir isotherm is only applied to specified materials, or rock types. The average in-situ moisture content, w_{we}, and average in-situ ash content, w_a, are input as are the Langmuir parameters p_L and Gs_L for each component. In the present case of EOS7R, there are 5 components. The sorbed gas density is also input to model coal swelling and shrinkage.

The input format is as follows:

CBM – Block for ECBM Input

CBM.1 format(A5)
MATCBM

MATCBM Material Name From ROCKS Block

CBM.2 format(2f10.4.i10)
w_a, w_{we}, *islcbm*

w_a ash weight fraction
w_{we} equilibrium moisture weight fraction
islcbm flag for gas saturation dependent extended Langmuir isotherm
= 0 - independent of gas saturation (default)
≠ 0 – gas storage capacity related to gas saturation

CBM.3 format(3e10.4)
G_{sL}, P_L, *rhosrb*

G_{sL} dry, ash-free Langmuir storage capacity (sm^3/kg-coal)
P_L Langmuir pressure (Pa)
rhosrb Sorbed Gas Density (kg/m^3)
enter 5 sets – 1 for each component (water, brine, ncg, trc, CH_4)

Note that while the Langmuir parameters for the water and brine components are not used, they must be input.

Additional sets of material names and corresponding properties can be added. The CBM block is terminated with a blank line.

INCON – modification of INCON Block

INCON.1 format(A3,I2,2I5,E15.8,i10)
EL,NE,NSEQ,NADD,PORX,IXL

EL,NE,NSEQ,NADD,PORX unchanged from original code
IXL flag for sorbed gas masses for liquid-saturated conditions
≠ 1, no sorbed gases (default)
= 1, non-zero sorbed gases

INCON.2 format(4e20.14)
X1, X2, X3, …

X1, X2, X3, … unchanged from original code
If IXL=1, read another line for the sorbed gas mass for components 3, 4, and 5

The SAVE block written out by TOUGH2 is automatically modified as above for sorbed gases for liquid-saturated conditions.

Appendix B
Input for Dusty Gas Model

Modifications to existing input parameters have been made as listed below.

MULTI

For the DGM, the value of NB should be equal to 9 for diffusion calculations. If an NB value of 8 is input, it is automatically changed to 9 internally.

PARAM

The value of MOP(24) triggers the different gas diffusion options as follows:

= 0 – Fully-coupled Fick's law Model (existing option)
= 1 – Separate Fick's law Model (existing option)
= 2 – Fully-coupled DGM (new option)
= 3 – Separate DGM (new option)

ROCKS

Knudsen diffusion coefficients for air are entered in the ROCKS BLOCK in the location reserved for the Klinkenberg parameter, b, in units of m^2/s at 25^oC. The MOP(24) value determines whether the input parameter is the Klinkenberg parameter (MOP(24)=0,1) or the Knudsen diffusion coefficient (MOP(24)=2,3). If the input is a Knudsen diffusion coefficient, the correction to the gas permeability for slip effects is not performed. If a Knudsen diffusion coefficient is not input and the DGM is selected, the value is calculated based on the minimum value from the Heid et al. (1950) and the Jones and Owens (1980) correlations as discussed earlier.

A new block to input the DGM ordinary diffusion coefficients has been added.

DGM – DGM gas diffusion coefficients

DGM.1-4 format(8e10.4)

Di-j – binary diffusion coefficient for components i and j (m^2/s)

first row:	D_{1-2}, D_{1-3}, D_{1-4}, D_{1-5}
second row:	D_{2-3}, D_{2-4}, D_{2-5}
third row:	D_{3-4}, D_{3-5}
fourth row:	D_{4-5}

diffusivity values for DGM assume $D_{j-i} = D_{i-j}$
gas diffusion coefficients from DIFFU BLOCK are not used.
liquid diffusion coefficients from DIFFU BLOCK are used.

This page intentionally blank.

Appendix C
Law et al. Problem

The details of the Law et al. (2002) problem including the results from the present version of the code are discussed in the main report. This Appendix present the input files and selected output.

The problem was simulated in three phases. The first simulation encompassed the 15-day CO_2 injection period and the 45-day shut-in phase. The second simulation was for the 60-day production period, while the third simulation looked at the following 62.5-day shut-in period.

First Simulation

The first simulation looked at the first 60 days including the initial CO_2 injection and the first shut-in period. The input file is shown in Figure C-1. Note that in addition to CO_2 injection, a very small amount of CH_4 is injected. EOS7C has shown convergence problems when gas component concentrations are zero or very small. To address this, a small amount of CH_4 is injected along with the CO_2 in order to ensure non-zero CH_4 concentration.

Figure C-2 shows the output at 1 second. Note that the mass fraction for all components in the liquid and gas phase are listed. The sorbed mass of each component in each element is shown along with the corresponding change in porosity. Finally, the component volume and mass distribution including the sorbed masses for the entire problem are summarized.

Second Simulation

The second simulation uses the SAVE file from the first simulation as input where the pressure in the borehole element (A1 1) is set to a constant value of 275 kPa. The volume of this element is increased to > 10^{50} m^3 so the conditions are a boundary condition. Figure C-3 shows the input file, while Figure C-4 shows the output at 1 second into the 60-day production period. Note that initially there are a number of messages that the solubility iteration failed. Iterating on solubility is necessary because EOS7C uses gas mass fractions to calculate gas-mixture properties, including solubility, which in turn controls gas mass fractions.

Third Simulation

The third simulation uses the SAVE file from the second simulation as input. The borehole element volume is changed back to the original value. Figures C-5 and C-6 show the input file and the output 1 second into the final shut-in period.

```
Law Problem 1 - Part A
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
coal     2  1434.e00      .001  3.65e-15  3.65e-15  3.65e-15      2.51      920.
  1.45e-10                    0.25
    9
    8           .457       .00  5.105e-4      1.e7        1.
bh       2  1434.e00       1.0  3.65e-09  3.65e-09  3.65e-09      2.51      920.
                              0.25
    5           .457       .15        1.       .10
    8           .457       .00  5.105e-4      1.e7        1.

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    5    5    2    8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   2  -5    100020 0 0000001000300 01
             5.184e6     1.e00      100.A1  1
     1.e-5    1.0e+0
             1.013e5                    0.                  0.                  0.
               10.50                   20.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2
        1.   1.296e6 157.788e6 315.576e6 946.728e6 3.15576e9
SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6                                                                1    1    1
     -1.e5




               28.96                                                  1.e-10

     0.e-0     0.e-1
     0.e-6     0.e-6     0.e-6    -1.e-6    -1.e-6     0.e-6
     1.e50       16.     0.e-6    -1.e-6                           1.0e-11
     1.e50       44.    -1.e-6     0.e-6                           4.0e-09

     diffusivity data are input as follows:
     first row:  water (gas, liq.)
     second row: brine (gas, liq.)
     third row:  ncg   (gas, liq.)
     fourth row: trc   (gas, liq.)
     fifth row:  ch4   (gas, liq.)
DIFFU----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
     1.e-6    1.e-10
     0.e-6    1.e-10
     1.e-6    1.e-10
     1.e-6    1.e-10
     1.e-6    1.e-10

     diffusivity values for DGM are input as follows (assumes Dj-i = Di-j):
     first row:   D1-2, D1-3, D1-4, D1-5
     second row:  D2-3, D2-4, D2-5
     third row:   D3-4, D3-5
     fourth row:  D4-5
DGM
    1.0e-6    1.0e-6    1.0e-6    1.0e-6
    1.0e-6    1.0e-6    1.0e-6
    1.0e-6    1.0e-6
    1.0e-6
CBM
coal
     0.156    0.0672
        0.        0.        0.
    0.0310   1903.e3  1180.e10
    0.0150  27241.e3   808.e10
    0.0152  4688.5e3   421.e10
```

```
ELEME ---    30   31    0    0   0.00000   453.911 mod
A1  1              20.3767E-010.8371E-02          0.1825E-01          -.4500E+01
A1  2              10.2347E+020.5206E+01          0.4738E+00          -.4500E+01
A1  3              10.9780E+020.2173E+02          0.1491E+01          -.4500E+01
A1  4              10.2088E+030.4640E+02          0.2744E+01          -.4500E+01
A1  5              10.3705E+030.8232E+02          0.4197E+01          -.4500E+01
A1  6              10.6023E+030.1338E+03          0.5883E+01          -.4500E+01
A1  7              10.9309E+030.2069E+03          0.7838E+01          -.4500E+01
A1  8              10.1392E+040.3094E+03          0.1011E+02          -.4500E+01
A1  9              10.2036E+040.4524E+03          0.1274E+02          -.4500E+01
A1 10              10.2927E+040.6505E+03          0.1579E+02          -.4500E+01
A1 11              10.4157E+040.9238E+03          0.1933E+02          -.4500E+01
A1 12              10.5847E+040.1299E+04          0.2344E+02          -.4500E+01
A1 13              10.8161E+040.1814E+04          0.2820E+02          -.4500E+01
A1 14              10.1132E+050.2516E+04          0.3373E+02          -.4500E+01
A1 15              10.1563E+050.3473E+04          0.4014E+02          -.4500E+01
A1 16              10.2149E+050.4775E+04          0.4758E+02          -.4500E+01
A1 17              10.2945E+050.6544E+04          0.5620E+02          -.4500E+01
A1 18              10.4024E+050.8943E+04          0.6621E+02          -.4500E+01
A1 19              10.5486E+050.1219E+05          0.7782E+02          -.4500E+01
A1 20              10.7465E+050.1659E+05          0.9128E+02          -.4500E+01
A1 21              10.1014E+060.2254E+05          0.1069E+03          -.4500E+01
A1 22              10.1376E+060.3057E+05          0.1250E+03          -.4500E+01
A1 23              10.1864E+060.4143E+05          0.1460E+03          -.4500E+01
A1 24              10.2524E+060.5608E+05          0.1704E+03          -.4500E+01
A1 25              10.3413E+060.7585E+05          0.1987E+03          -.4500E+01
A1 26              10.4613E+060.1025E+06          0.2315E+03          -.4500E+01
A1 27              10.6231E+060.1385E+06          0.2696E+03          -.4500E+01
A1 28              10.8411E+060.1869E+06          0.3137E+03          -.4500E+01
A1 29              10.1135E+070.2522E+06          0.3649E+03          -.4500E+01
A1 30              10.1472E+070.3270E+06          0.4232E+03          -.4500E+01

CONNE
A1  1A1  2                   10.1825E-050.4555E+000.2064E+01
A1  2A1  3                   10.4555E+000.5800E+000.5152E+02
A1  3A1  4                   10.5800E+000.6728E+000.1171E+03
A1  4A1  5                   10.6728E+000.7805E+000.1932E+03
A1  5A1  6                   10.7805E+000.9053E+000.2815E+03
A1  6A1  7                   10.9053E+000.1050E+010.3839E+03
A1  7A1  8                   10.1050E+010.1218E+010.5026E+03
A1  8A1  9                   10.1218E+010.1413E+010.6404E+03
A1  9A1 10                   10.1413E+010.1639E+010.8002E+03
A1 10A1 11                   10.1639E+010.1901E+010.9856E+03
A1 11A1 12                   10.1901E+010.2206E+010.1201E+04
A1 12A1 13                   10.2206E+010.2559E+010.1450E+04
A1 13A1 14                   10.2559E+010.2968E+010.1739E+04
A1 14A1 15                   10.2968E+010.3443E+010.2075E+04
A1 15A1 16                   10.3443E+010.3994E+010.2465E+04
A1 16A1 17                   10.3994E+010.4633E+010.2916E+04
A1 17A1 18                   10.4633E+010.5374E+010.3440E+04
A1 18A1 19                   10.5374E+010.6234E+010.4048E+04
A1 19A1 20                   10.6234E+010.7231E+010.4753E+04
A1 20A1 21                   10.7231E+010.8388E+010.5571E+04
A1 21A1 22                   10.8388E+010.9730E+010.6520E+04
A1 22A1 23                   10.9730E+010.1129E+020.7620E+04
A1 23A1 24                   10.1129E+020.1309E+020.8897E+04
A1 24A1 25                   10.1309E+020.1519E+020.1038E+05
A1 25A1 26                   10.1519E+020.1762E+020.1210E+05
A1 26A1 27                   10.1762E+020.2044E+020.1409E+05
A1 27A1 28                   10.2044E+020.2371E+020.1640E+05
A1 28A1 29                   10.2371E+020.2750E+020.1908E+05
A1 29A1 30                   10.2750E+020.3075E+020.2219E+05

INCON

INDOM
coal
             7650.e3                                     0.0
              10.408                 45.
bh
             7650.e3                                     0.0
                 1.0                 45.
```

```
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A1  1CO201    0    0    0    4     COM31
            0.       1.296e6       1.296e6         1.e10
         0.609         0.609            0.            0.
      430.65e3      430.65e3            0.            0.
A1  1CH401    0    0    0    4     COM51
            0.       1.296e6       1.296e6         1.e10
      0.609e-6      0.609e-6            0.            0.
      430.65e3      430.65e3            0.            0.

FOFT
A1  1
A1  2

COFT
A1  1A1  2

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure C-1. Law et al. (2002) Problem Input – Part 1

```
Law Problem 1 - Part A

         OUTPUT DATA AFTER (   1,  5)-2-TIME STEPS                                                    THE TIME IS 0.115741E-04 DAYS

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

 TOTAL TIME     KCYC   ITER  ITERC   KON        DX1M         DX2M         DX3M          MAX. RES.      NER    KER        DELTEX
0.100000E+01      1      5      5     2       0.21384E+05  0.88130E-21  0.23655E+00    0.17371E-07       1     3       0.10000E+01

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

                                                        NCG = CO2

ELEM.  INDEX     P           T          SL       XBRINE(LIQ)  XNCG(LIQ)   XTRC(LIQ)   XCH4(LIQ)   XNCG(GAS)   XTRC(GAS)   XCH4(GAS)      DG
                (PA)      (DEG-C)                                                                                                     (KG/M**3)

A1  1     1 0.76714E+07 0.45000E+02 0.00000E+00 0.88130E-21 0.53083E-02 0.00000E+00 0.93151E-03 0.23655E+00 0.00000E+00 0.76345E+00 0.62310E+02
A1  2     2 0.76714E+07 0.45000E+02 0.59195E+00 0.47802E-22 0.12557E-05 0.45272E-37 0.10372E-02 0.63991E-04 0.66246E-34 0.99853E+00 0.52353E+02
A1  3     3 0.76501E+07 0.45000E+02 0.59201E+00 0.79898E-27 0.84000E-12 0.87341E-42 0.10350E-02 0.42893E-10 0.12817E-38 0.99859E+00 0.52192E+02
A1  4     4 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.15640E-20 0.46937E-49 0.10350E-02 0.79864E-19 0.68878E-46 0.99859E+00 0.52191E+02
A1  5     5 0.76500E+07 0.45000E+02 0.59200E+00 0.10838E-35 0.69072E-32 0.59850E-59 0.10350E-02 0.35271E-30 0.87827E-56 0.99859E+00 0.52191E+02
A1  6     6 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.14446E-44 0.36307E-70 0.10350E-02 0.73767E-43 0.53279E-67 0.99859E+00 0.52191E+02
A1  7     7 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.22197E-57 0.16184E-81 0.10350E-02 0.11335E-55 0.23750E-78 0.99859E+00 0.52191E+02
A1  8     8 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.25743E-70 0.54451E-93 0.10350E-02 0.13145E-68 0.79905E-90 0.99859E+00 0.52191E+02
A1  9     9 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.22420E-83 0.13757-104 0.10350E-02 0.11448E-81 0.20188-101 0.99859E+00 0.52191E+02
A1 10    10 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.14630E-96 0.26044-116 0.10350E-02 0.74706E-95 0.38218-113 0.99859E+00 0.52191E+02
A1 11    11 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.71380-110 0.36863-128 0.10350E-02 0.36450-108 0.54096-125 0.99859E+00 0.52191E+02
A1 12    12 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.26007-123 0.38963-140 0.10350E-02 0.13280-121 0.57177-137 0.99859E+00 0.52191E+02
A1 13    13 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.70642-137 0.30704-152 0.10350E-02 0.36073-135 0.45057-149 0.99859E+00 0.52191E+02
A1 14    14 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.14304-150 0.18036-164 0.10350E-02 0.73040-149 0.26467-161 0.99859E+00 0.52191E+02
A1 15    15 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.21578-164 0.78930-177 0.10350E-02 0.11018-162 0.11583-173 0.99859E+00 0.52191E+02
A1 16    16 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.24244-178 0.25728-189 0.10350E-02 0.12380-176 0.37754-186 0.99859E+00 0.52191E+02
A1 17    17 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.20271-192 0.62405-202 0.10350E-02 0.10351-190 0.91576-199 0.99859E+00 0.52191E+02
A1 18    18 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.12615-206 0.11267-214 0.10350E-02 0.64417-205 0.16533-211 0.99859E+00 0.52191E+02
A1 19    19 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.58416-221 0.15135-227 0.10350E-02 0.29829-219 0.22210-224 0.99859E+00 0.52191E+02
A1 20    20 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.20122-235 0.15125-240 0.10350E-02 0.10275-233 0.22196-237 0.99859E+00 0.52191E+02
A1 21    21 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.51564-250 0.11244-253 0.10350E-02 0.26330-248 0.16500-250 0.99859E+00 0.52191E+02
A1 22    22 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.98239-265 0.62146-267 0.10350E-02 0.50165-263 0.91196-264 0.99859E+00 0.52191E+02
A1 23    23 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.13918-279 0.25543-280 0.10350E-02 0.71071-278 0.37483-277 0.99859E+00 0.52191E+02
A1 24    24 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.14660-294 0.78048-294 0.10350E-02 0.74857-293 0.11453-290 0.99859E+00 0.52191E+02
A1 25    25 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.11485-309 0.17738-307 0.10350E-02 0.58646-308 0.26030-304 0.99859E+00 0.52191E+02
A1 26    26 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.00000E+00 0.30138-321 0.10350E-02 0.00000E+00 0.44295-318 0.99859E+00 0.52191E+02
A1 27    27 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.10350E-02 0.00000E+00 0.00000E+00 0.99859E+00 0.52191E+02
A1 28    28 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.10350E-02 0.00000E+00 0.00000E+00 0.99859E+00 0.52191E+02
A1 29    29 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.10350E-02 0.00000E+00 0.00000E+00 0.99859E+00 0.52191E+02
A1 30    30 0.76500E+07 0.45000E+02 0.59200E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.10350E-02 0.00000E+00 0.00000E+00 0.99859E+00 0.52191E+02

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


ELEM.  INDEX    PHIS        PHIF      DPHINCG     DPHITRC     DPHICH4     MASST       MASSNCG     MASSTRC     MASSCH4
                                                                            (KG)        (KG)        (KG)        (KG)

 A1  1     1 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A1  2     2 0.10000E-02 0.10000E-02 -.19392E-15 -.99098E-47 -.16879E-11 0.16683E+03 0.53704E-01 0.18793E-32 0.16678E+03
 A1  3     3 0.10000E-02 0.10000E-02 -.12984E-21 -.19152E-51 -.16862E-11 0.69426E+03 0.14984E-06 0.15134E-36 0.69426E+03
 A1  4     4 0.10000E-02 0.10000E-02 -.24175E-30 -.10293E-58 -.16862E-11 0.14822E+04 0.59564E-15 0.17365E-43 0.14822E+04
 A1  5     5 0.10000E-02 0.10000E-02 -.10677E-41 -.13124E-68 -.16862E-11 0.26301E+04 0.46678E-26 0.39289E-53 0.26301E+04
 A1  6     6 0.10000E-02 0.10000E-02 -.22330E-54 -.79614E-80 -.16862E-11 0.42756E+04 0.15870E-38 0.38745E-64 0.42756E+04
 A1  7     7 0.10000E-02 0.10000E-02 -.34311E-67 -.35489E-91 -.16862E-11 0.66082E+04 0.37689E-51 0.26694E-75 0.66082E+04
 A1  8     8 0.10000E-02 0.10000E-02 -.39792E-80 -.11940-102 -.16862E-11 0.98814E+04 0.65360E-64 0.13430E-86 0.98814E+04
```

```
A1  9     9 0.10000E-02 0.10000E-02 -.34655E-93 -.30168-114 -.16862E-11 0.14453E+05 0.83258E-77 0.49628E-98 0.14453E+05
A1 10    10 0.10000E-02 0.10000E-02 -.22614-106 -.57109-126 -.16862E-11 0.20778E+05 0.78105E-90 0.13506-109 0.20778E+05
A1 11    11 0.10000E-02 0.10000E-02 -.11034-119 -.80835-138 -.16862E-11 0.29509E+05 0.54122-103 0.27151-121 0.29509E+05
A1 12    12 0.10000E-02 0.10000E-02 -.40199-133 -.85440-150 -.16862E-11 0.41506E+05 0.27735-116 0.40365-133 0.41506E+05
A1 13    13 0.10000E-02 0.10000E-02 -.10919-146 -.67328-162 -.16862E-11 0.57933E+05 0.10515-129 0.44397-145 0.57933E+05
A1 14    14 0.10000E-02 0.10000E-02 -.22110-160 -.39549-174 -.16862E-11 0.80357E+05 0.29533-143 0.36174-157 0.80357E+05
A1 15    15 0.10000E-02 0.10000E-02 -.33353-174 -.17308-186 -.16862E-11 0.11095E+06 0.61515-157 0.21858-169 0.11095E+06
A1 16    16 0.10000E-02 0.10000E-02 -.37475-188 -.56416-199 -.16862E-11 0.15255E+06 0.95030-171 0.97960-182 0.15255E+06
A1 17    17 0.10000E-02 0.10000E-02 -.31333-202 -.13684-211 -.16862E-11 0.20906E+06 0.10889-184 0.32562-194 0.20906E+06
A1 18    18 0.10000E-02 0.10000E-02 -.19499-216 -.24705-224 -.16862E-11 0.28565E+06 0.92589-199 0.80327-207 0.28565E+06
A1 19    19 0.10000E-02 0.10000E-02 -.90296-231 -.33189-237 -.16862E-11 0.38944E+06 0.58453-213 0.14712-219 0.38944E+06
A1 20    20 0.10000E-02 0.10000E-02 -.31104-245 -.33167-250 -.16862E-11 0.52992E+06 0.27399-227 0.20005-232 0.52992E+06
A1 21    21 0.10000E-02 0.10000E-02 -.79704-260 -.24656-263 -.16862E-11 0.71981E+06 0.95367-242 0.20201-245 0.71981E+06
A1 22    22 0.10000E-02 0.10000E-02 -.15185-274 -.13627-276 -.16862E-11 0.97678E+06 0.24656-256 0.15151-258 0.97678E+06
A1 23    23 0.10000E-02 0.10000E-02 -.21514-289 -.56010-290 -.16862E-11 0.13232E+07 0.47320-271 0.84358-272 0.13232E+07
A1 24    24 0.10000E-02 0.10000E-02 -.22660-304 -.17114-303 -.16862E-11 0.17917E+07 0.67488-286 0.34903-285 0.17917E+07
A1 25    25 0.10000E-02 0.10000E-02 -.17752-319 -.38897-317 -.16862E-11 0.24228E+07 0.71495-301 0.10727-298 0.24228E+07
A1 26    26 0.10000E-02 0.10000E-02 0.00000E+00 0.00000E+00 -.16862E-11 0.32746E+07 0.00000E+00 0.24746-312 0.32746E+07
A1 27    27 0.10000E-02 0.10000E-02 0.00000E+00 0.00000E+00 -.16862E-11 0.44232E+07 0.00000E+00 0.00000E+00 0.44232E+07
A1 28    28 0.10000E-02 0.10000E-02 0.00000E+00 0.00000E+00 -.16862E-11 0.59707E+07 0.00000E+00 0.00000E+00 0.59707E+07
A1 29    29 0.10000E-02 0.10000E-02 0.00000E+00 0.00000E+00 -.16862E-11 0.80570E+07 0.00000E+00 0.00000E+00 0.80570E+07
A1 30    30 0.10000E-02 0.10000E-02 0.00000E+00 0.00000E+00 -.16862E-11 0.10449E+08 0.00000E+00 0.00000E+00 0.10449E+08

         Law Problem 1 - Part A

                                                                               KCYC =    1  -  ITER =    5  -  TIME =0.100000E+01
    ELEM1  ELEM2  INDEX    FLOH      FLOH/FLOF       FLOF       FLO(BRINE)   FLO(GAS)     FLO(LIQ.)    VEL(GAS)     VEL(LIQ.)
                           (W)        (J/KG)        (KG/S)        (KG/S)      (KG/S)       (KG/S)      (M/S)        (M/S)

    A1  1  A1  2     1 -.178510E+06 0.785572E+06 -.227236E+00 0.000000E+00 -.227236E+00 0.000000E+00 -.176688E-02 0.000000E+00
    A1  2  A1  3     2 -.225277E+04 0.686491E+06 -.328157E-02 -.457270E-25 -.232497E-02 -.956596E-03 -.211248E-02 -.315698E-04
    A1  3  A1  4     3 -.133638E+02 0.686218E+06 -.194745E-04 -.454546E-32 -.137854E-04 -.568910E-05 -.552853E-05 -.825977E-07
    A1  4  A1  5     4 -.529265E-01 0.686231E+06 -.771265E-07 0.000000E+00 -.545969E-07 -.225296E-07 -.132709E-07 -.198260E-09
    A1  5  A1  6     5 -.148631E-03 0.686231E+06 -.216591E-09 -.685735E-46 -.153322E-09 -.632689E-10 -.255780E-10 -.382121E-12
    A1  6  A1  7     6 -.302324E-06 0.686231E+06 -.440557E-12 0.000000E+00 -.311865E-12 -.128692E-12 -.381494E-13 -.569932E-15
    A1  7  A1  8     7 0.437474E-09 0.686231E+06 0.637503E-15 0.000000E+00 0.451280E-15 0.186223E-15 0.421661E-16 0.629939E-18
    A1  8  A1  9     8 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1  9  A1 10     9 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 10  A1 11    10 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 11  A1 12    11 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 12  A1 13    12 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 13  A1 14    13 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 14  A1 15    14 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 15  A1 16    15 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 16  A1 17    16 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 17  A1 18    17 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 18  A1 19    18 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 19  A1 20    19 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 20  A1 21    20 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 21  A1 22    21 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 22  A1 23    22 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 23  A1 24    23 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 24  A1 25    24 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 25  A1 26    25 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 26  A1 27    26 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 27  A1 28    27 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 28  A1 29    28 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    A1 29  A1 30    29 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

```
         Law Problem 1 - Part A
                                                                               KCYC =    1  -  ITER =    5  -  TIME =0.100000E+01
MASS FLOW RATES (KG/S) FROM DIFFUSION

ELEM1 ELEM2  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP
              all   wv    all   br    all  ncg    all  trc    all  ch4
A1  1 A1  2 0.25170E-12 0.00000E+00 -.27935E-10 0.78012E-44 0.27683E-10
A1  2 A1  3 0.57579E-14 -.87375E-32 -.82939E-13 -.85630E-43 0.77181E-13
A1  3 A1  4 0.32538E-16 -.27440E-36 -.10442E-18 -.31118E-47 -.32434E-16
A1  4 A1  5 0.12886E-18 0.52939E-45 -.27652E-27 -.23785E-54 -.12886E-18
A1  5 A1  6 0.36176E-21 -.66496E-45 -.15340E-38 -.38095E-64 -.36179E-21
A1  6 A1  7 0.12124E-23 0.00000E+00 -.37722E-51 -.27172E-75 -.11869E-23
A1  7 A1  8 0.00000E+00 0.00000E+00 -.65420E-64 -.13671E-86 0.00000E+00
A1  8 A1  9 0.00000E+00 0.00000E+00 -.83334E-77 -.50520E-98 0.00000E+00
A1  9 A1 10 0.00000E+00 0.00000E+00 -.78177E-90 -.13749-109 0.00000E+00
A1 10 A1 11 0.00000E+00 0.00000E+00 -.54172-103 -.27639-121 0.00000E+00
A1 11 A1 12 0.00000E+00 0.00000E+00 -.27761-116 -.41091-133 0.00000E+00
A1 12 A1 13 0.00000E+00 0.00000E+00 -.10525-129 -.45195-145 0.00000E+00
A1 13 A1 14 0.00000E+00 0.00000E+00 -.29560-143 -.36824-157 0.00000E+00
A1 14 A1 15 0.00000E+00 0.00000E+00 -.61571-157 -.22251-169 0.00000E+00
A1 15 A1 16 0.00000E+00 0.00000E+00 -.95117-171 -.99722-182 0.00000E+00
A1 16 A1 17 0.00000E+00 0.00000E+00 -.10899-184 -.33148-194 0.00000E+00
A1 17 A1 18 0.00000E+00 0.00000E+00 -.92674-199 -.81771-207 0.00000E+00
A1 18 A1 19 0.00000E+00 0.00000E+00 -.58506-213 -.14976-219 0.00000E+00
A1 19 A1 20 0.00000E+00 0.00000E+00 -.27424-227 -.20365-232 0.00000E+00
A1 20 A1 21 0.00000E+00 0.00000E+00 -.95455-242 -.20564-245 0.00000E+00
A1 21 A1 22 0.00000E+00 0.00000E+00 -.24678-256 -.15423-258 0.00000E+00
A1 22 A1 23 0.00000E+00 0.00000E+00 -.47363-271 -.85874-272 0.00000E+00
A1 23 A1 24 0.00000E+00 0.00000E+00 -.67550-286 -.35531-285 0.00000E+00
A1 24 A1 25 0.00000E+00 0.00000E+00 -.71561-301 -.10920-298 0.00000E+00
A1 25 A1 26 0.00000E+00 0.00000E+00 -.56330-316 -.24936-312 0.00000E+00
A1 26 A1 27 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A1 27 A1 28 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A1 28 A1 29 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A1 29 A1 30 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

```
         Law Problem 1 - Part A

                                                                               KCYC =    1  -  ITER =    5  -  TIME =0.100000E+01
ELEMENT SOURCE INDEX      GENERATION RATE     ENTHALPY    FF(GAS)      FF(LIQ.)      P(WB)
                            (KG/S) OR (W)     (J/KG)                                 (PA)

 A1  1   CO2 1    1          0.609000E+00   0.430650E+06
 A1  1   CH4 1    2          0.609000E-06   0.430650E+06

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


********** VOLUME- AND MASS-BALANCES ********************************************************************************************

********** [KCYC,ITER] = [   1,  5] *****                                 THE TIME IS 0.100000E+01 SECONDS, OR 0.115741E-04 DAYS


               PHASES PRESENT
*************************************************************
 PHASES       *        GAS          AQUEOUS       ADSORBED
 VOLUME (M^3) * 0.23770431E+04 0.34489883E+04 0.98235242E-05
 MASS   (KG)  * 0.12406178E+06 0.34267399E+07 0.41357037E+08
*************************************************************

               COMPONENT MASS IN PLACE (KG)
***************************************************************************
 PHASES     *    GAS           AQUEOUS        ADSORBED        TOTAL
***************************************************************************
 COMPONENTS *
 WATER      * 0.17446455E+03 0.34231933E+07 0.00000000E+00 0.34233677E+07
 BRINE      * 0.20686535E-20 0.65988834E-21 0.00000000E+00 0.27285418E-20
 NCG        * 0.55527851E+00 0.17333148E-04 0.53704153E-01 0.60900000E+00
 TRC        * 0.33216906E-34 0.62496461E-36 0.18794284E-32 0.19132703E-32
 CH4        * 0.12388676E+06 0.35466388E+04 0.41357037E+08 0.41484470E+08
***************************************************************************

*********************************************************************************************************************************
```

Figure C-2. Selected Law et al. (2002) Problem Output – Part 1

```
Law Problem 1 - Part B
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
coal     2  1434.e00      .001  3.65e-15  3.65e-15  3.65e-15      2.51      920.
  1.45e-10                          0.25
    9
    8           .457       .00  5.105e-4      1.e7        1.
bh       2  1434.e00       1.0  3.65e-09  3.65e-09  3.65e-09      2.51      920.
                                    0.25
    5           .457       .15        1.       .10
    8           .457       .00  5.105e-4      1.e7        1.

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    5    5    2    8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3  -5    100020 0 0000001000300 01
   5.184e6  1.0368e7     1.e00      100.A1  1
     1.e-5    1.0e+0
             1.013e5                  0.                  0.                  0.
               10.50                 20.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1
  5184001.   1.296e6 157.788e6 315.576e6 946.728e6 3.15576e9
SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6                                                                1    1    1
     -1.e5




               28.96                                            1.e-10

     0.e-0     0.e-1
     0.e-6     0.e-6     0.e-6    -1.e-6    -1.e-6     0.e-6
     1.e50       16.     0.e-6    -1.e-6                       1.0e-11
     1.e50       44.    -1.e-6     0.e-6                       4.0e-09

     diffusivity data are input as follows:
     first row:  water (gas, liq.)
     second row: brine (gas, liq.)
     third row:  rn1   (gas, liq.)
     fourth row: rn2   (gas, liq.)
     fifth row:  air   (gas, liq.)
DIFFU----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
     1.e-6    1.e-10
     0.e-6    1.e-10
     1.e-6    1.e-10
     1.e-6    1.e-10
     1.e-6    1.e-10

     diffusivity values for DGM are input as follows (assumes Dj-i = Di-j):
     first row:   D1-2, D1-3, D1-4, D1-5
     second row:  D2-3, D2-4, D2-5
     third row:   D3-4, D3-5
     fourth row:  D4-5
DGM
    1.0e-6    1.0e-6    1.0e-6    1.0e-6
    1.0e-6    1.0e-6    1.0e-6
    1.0e-6    1.0e-6
    1.0e-6
CBM
coal
     0.156    0.0672
        0.        0.        0.
        0.        0.        0.
    0.0310   1903.e3  1180.e10
    0.0150  27241.e3   808.e10
    0.0152  4688.5e3   421.e10

ELEME ---    30   31    0    0  0.00000   453.911 mod
A1  1              20.3767E+510.8371E-02          0.1825E-01          -.4500E+01
A1  2              10.2347E+020.5206E+01          0.4738E+00          -.4500E+01
A1  3              10.9780E+020.2173E+02          0.1491E+01          -.4500E+01
A1  4              10.2088E+030.4640E+02          0.2744E+01          -.4500E+01
A1  5              10.3705E+030.8232E+02          0.4197E+01          -.4500E+01
A1  6              10.6023E+030.1338E+03          0.5883E+01          -.4500E+01
A1  7              10.9309E+030.2069E+03          0.7838E+01          -.4500E+01
A1  8              10.1392E+040.3094E+03          0.1011E+02          -.4500E+01
A1  9              10.2036E+040.4524E+03          0.1274E+02          -.4500E+01
A1 10              10.2927E+040.6505E+03          0.1579E+02          -.4500E+01
```

```
A1 11              10.4157E+040.9238E+03          0.1933E+02          -.4500E+01
A1 12              10.5847E+040.1299E+04          0.2344E+02          -.4500E+01
A1 13              10.8161E+040.1814E+04          0.2820E+02          -.4500E+01
A1 14              10.1132E+050.2516E+04          0.3373E+02          -.4500E+01
A1 15              10.1563E+050.3473E+04          0.4014E+02          -.4500E+01
A1 16              10.2149E+050.4775E+04          0.4758E+02          -.4500E+01
A1 17              10.2945E+050.6544E+04          0.5620E+02          -.4500E+01
A1 18              10.4024E+050.8943E+04          0.6621E+02          -.4500E+01
A1 19              10.5486E+050.1219E+05          0.7782E+02          -.4500E+01
A1 20              10.7465E+050.1659E+05          0.9128E+02          -.4500E+01
A1 21              10.1014E+060.2254E+05          0.1069E+03          -.4500E+01
A1 22              10.1376E+060.3057E+05          0.1250E+03          -.4500E+01
A1 23              10.1864E+060.4143E+05          0.1460E+03          -.4500E+01
A1 24              10.2524E+060.5608E+05          0.1704E+03          -.4500E+01
A1 25              10.3413E+060.7585E+05          0.1987E+03          -.4500E+01
A1 26              10.4613E+060.1025E+06          0.2315E+03          -.4500E+01
A1 27              10.6231E+060.1385E+06          0.2696E+03          -.4500E+01
A1 28              10.8411E+060.1869E+06          0.3137E+03          -.4500E+01
A1 29              10.1135E+070.2522E+06          0.3649E+03          -.4500E+01
A1 30              10.1472E+070.3270E+06          0.4232E+03          -.4500E+01

CONNE
A1  1A1  2                   10.1825E-050.4555E+000.2064E+01
A1  2A1  3                   10.4555E+000.5800E+000.5152E+02
A1  3A1  4                   10.5800E+000.6728E+000.1171E+03
A1  4A1  5                   10.6728E+000.7805E+000.1932E+03
A1  5A1  6                   10.7805E+000.9053E+000.2815E+03
A1  6A1  7                   10.9053E+000.1050E+010.3839E+03
A1  7A1  8                   10.1050E+010.1218E+010.5026E+03
A1  8A1  9                   10.1218E+010.1413E+010.6404E+03
A1  9A1 10                   10.1413E+010.1639E+010.8002E+03
A1 10A1 11                   10.1639E+010.1901E+010.9856E+03
A1 11A1 12                   10.1901E+010.2206E+010.1201E+04
A1 12A1 13                   10.2206E+010.2559E+010.1450E+04
A1 13A1 14                   10.2559E+010.2968E+010.1739E+04
A1 14A1 15                   10.2968E+010.3443E+010.2075E+04
A1 15A1 16                   10.3443E+010.3994E+010.2465E+04
A1 16A1 17                   10.3994E+010.4633E+010.2916E+04
A1 17A1 18                   10.4633E+010.5374E+010.3440E+04
A1 18A1 19                   10.5374E+010.6234E+010.4048E+04
A1 19A1 20                   10.6234E+010.7231E+010.4753E+04
A1 20A1 21                   10.7231E+010.8388E+010.5571E+04
A1 21A1 22                   10.8388E+010.9730E+010.6520E+04
A1 22A1 23                   10.9730E+010.1129E+020.7620E+04
A1 23A1 24                   10.1129E+020.1309E+020.8897E+04
A1 24A1 25                   10.1309E+020.1519E+020.1038E+05
A1 25A1 26                   10.1519E+020.1762E+020.1210E+05
A1 26A1 27                   10.1762E+020.2044E+020.1409E+05
A1 27A1 28                   10.2044E+020.2371E+020.1640E+05
A1 28A1 29                   10.2371E+020.2750E+020.1908E+05
A1 29A1 30                   10.2750E+020.3075E+020.2219E+05

INCON -- INITIAL CONDITIONS FOR   30 ELEMENTS AT TIME  0.518400E+07
A1  1           0.10000000E+01
 0.2750000000000E+06 0.1602888385780E-27 0.9999990001911E+00 0.3168568899443E-51
 0.9998089379860E-06 0.4500000000000E+02
A1  2           0.10000136E-02
 0.7743664241503E+07 0.4811165636323E-18 0.9999991370482E+00 0.1911719905639E-47
 0.8629518109750E-06 0.4500000000000E+02
A1  3           0.10000136E-02
 0.7743663893911E+07 0.1318713159337E-18 0.9999991234901E+00 0.5003991423966E-44
 0.8765099178187E-06 0.4500000000000E+02
A1  4           0.10000136E-02
 0.7743662991331E+07 0.8534702199149E-19 0.9999991144762E+00 0.2546394716046E-40
 0.8855237906300E-06 0.4500000000000E+02
A1  5           0.10000136E-02
 0.7743661279602E+07 0.2278790433689E-19 0.9999991077060E+00 0.1672271019552E-36
 0.8922939493019E-06 0.4500000000000E+02
A1  6           0.10000136E-02
 0.7743658395326E+07 0.1877007942890E-17 0.9999991020493E+00 0.1296849815342E-32
 0.8979503541390E-06 0.4500000000000E+02
A1  7           0.10000136E-02
 0.7743653838796E+07 0.7188530711316E-18 0.9999990966919E+00 0.1115809083918E-28
 0.9029842832312E-06 0.4500000000000E+02
A1  8           0.10000136E-02
 0.7743646921701E+07 0.2711226717536E-17 0.9999987120099E+00 0.9889328629321E-25
 0.9076944474855E-06 0.4500000000000E+02
A1  9           0.10000136E-02
 0.7743636703395E+07 0.5537188282405E-14 0.4446466990279E-01 0.1772677205593E-23
 0.1090031061271E+02 0.4500000000000E+02
A1 10           0.10000136E-02
```

```
 0.7743616188437E+07 0.1687917365216E-14 0.4446406037316E-01 0.1438508384716E-19
 0.1085155667760E+02 0.4500000000000E+02
A1 11           0.10000136E-02
 0.7743582712347E+07 0.2713924489972E-15 0.4292333902344E-01 0.1018904771155E-19
 0.1081216181643E+02 0.4500000000000E+02
A1 12           0.10000136E-02
 0.7743531367601E+07 0.3880865305626E-16 0.1341765803872E-01 0.1688417364370E-19
 0.1072859362446E+02 0.4500000000000E+02
A1 13           0.10000136E-02
 0.7743481724222E+07 0.6305199099004E-17 0.7525783796166E-03 0.3991236862590E-19
 0.1069402774906E+02 0.4500000000000E+02
A1 14           0.10000135E-02
 0.7743409889581E+07 0.1792783393140E-17 0.2273542713190E-04 0.5355160070700E-19
 0.1066899568812E+02 0.4500000000000E+02
A1 15           0.10000135E-02
 0.7743292489188E+07 0.2228032492982E-17 0.4824117462080E-06 0.5840820344845E-19
 0.1063887935496E+02 0.4500000000000E+02
A1 16           0.10000135E-02
 0.7743103516966E+07 0.1224163986657E-17 0.7442861453709E-08 0.5390724943385E-19
 0.1060612752922E+02 0.4500000000000E+02
A1 17           0.10000135E-02
 0.7742806279558E+07 0.1167982401736E-17 0.8532112200822E-10 0.3754163752586E-19
 0.1057287235852E+02 0.4500000000000E+02
A1 18           0.10000134E-02
 0.7742346452855E+07 0.7653021819923E-18 0.7401494566775E-12 0.1847659224015E-19
 0.1053971245890E+02 0.4500000000000E+02
A1 19           0.10000133E-02
 0.7741642233678E+07 0.3472470236095E-18 0.4926499756633E-14 0.6374861719984E-20
 0.1050843027784E+02 0.4500000000000E+02
A1 20           0.10000131E-02
 0.7740581305936E+07 0.2203513517528E-17 0.2538585020184E-16 0.1560085505786E-20
 0.1047916590514E+02 0.4500000000000E+02
A1 21           0.10000129E-02
 0.7738999325668E+07 0.7344304057019E-19 0.1015745428556E-18 0.2741087445899E-21
 0.1045034221329E+02 0.4500000000000E+02
A1 22           0.10000126E-02
 0.7736650615921E+07 0.2654492688939E-19 0.3140554378576E-21 0.3473255212479E-22
 0.1042305843262E+02 0.4500000000000E+02
A1 23           0.10000121E-02
 0.7733231831248E+07 0.1117827428419E-18 0.7407434562950E-24 0.3158165258146E-23
 0.1040012628641E+02 0.4500000000000E+02
A1 24           0.10000114E-02
 0.7728398576917E+07 0.5837289668767E-19 0.1300973871649E-26 0.2026538258512E-24
 0.1038763221590E+02 0.4500000000000E+02
A1 25           0.10000104E-02
 0.7722068347140E+07 0.2491296747741E-19 0.1646156372194E-29 0.8951432895663E-26
 0.1038746743264E+02 0.4500000000000E+02
A1 26           0.10000094E-02
 0.7714491022283E+07 0.2216132630573E-20 0.1435865704778E-32 0.2627196047295E-27
 0.1039303773404E+02 0.4500000000000E+02
A1 27           0.10000081E-02
 0.7706136806354E+07 0.8457864995717E-20 0.8150628414191E-36 0.4873204346150E-29
 0.1039755651792E+02 0.4500000000000E+02
A1 28           0.10000069E-02
 0.7697675319375E+07 0.3312799534649E-20 0.2772537650423E-39 0.5291326898384E-31
 0.1040018530601E+02 0.4500000000000E+02
A1 29           0.10000058E-02
 0.7690256495902E+07 0.4153392758103E-20 0.4913146717978E-43 0.2937744311484E-33
 0.1040179589505E+02 0.4500000000000E+02
A1 30           0.10000052E-02
 0.7685709510268E+07 0.1117147094709E-20 0.3413386015705E-47 0.6302161496768E-36
 0.1040266218685E+02 0.4500000000000E+02
+++
                               0.51840000E+07

INDOM

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A1  1CO201    0    0    0    4     COM31
            0.        1.296e6       1.296e6         1.e10
         0.609         0.609           0.            0.
      430.65e3      430.65e3           0.            0.
A1  1CH401    0    0    0    4     COM51
            0.        1.296e6       1.296e6         1.e10
      0.609e-6      0.609e-6           0.            0.
      430.65e3      430.65e3           0.            0.

FOFT
A1  1
A1  2
```

```
COFT
A1  1A1  2

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure C-3. Law et al. (2002) Problem Input – Part 2

```
Law Problem 1 - Part B

          OUTPUT DATA AFTER (   1,  2)-2-TIME STEPS                                                        THE TIME IS 0.600000E+02 DAYS

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

  TOTAL TIME     KCYC   ITER  ITERC   KON        DX1M         DX2M         DX3M          MAX. RES.      NER    KER        DELTEX
 0.518400E+07      1      2      2     2      0.36345E+05  0.48112E-18  0.31291E-08    0.31350E-05       2     3       0.10000E+01

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

                                                                          NCG = CO2

 ELEM.  INDEX     P           T          SL       XBRINE(LIQ)  XNCG(LIQ)   XTRC(LIQ)   XCH4(LIQ)   XNCG(GAS)   XTRC(GAS)   XCH4(GAS)       DG
                (PA)      (DEG-C)                                                                                                      (KG/M**3)

 A1  1     1 0.27500E+06 0.45000E+02 0.00000E+00 0.16029E-27 0.25729E-02 0.21255E-55 0.12864E-09 0.10000E+01 0.31686E-51 0.99981E-06 0.46326E+01
 A1  2     2 0.77073E+07 0.45000E+02 0.00000E+00 0.00000E+00 0.44423E-01 0.34253E-50 0.31346E-08 0.10000E+01 0.18682E-47 0.85982E-06 0.22775E+03
 A1  3     3 0.77432E+07 0.45000E+02 0.00000E+00 0.13030E-18 0.44517E-01 0.92171E-47 0.32168E-08 0.10000E+01 0.50042E-44 0.87647E-06 0.23002E+03
 A1  4     4 0.77437E+07 0.45000E+02 0.00000E+00 0.85283E-19 0.44518E-01 0.46905E-43 0.32503E-08 0.10000E+01 0.25464E-40 0.88552E-06 0.23005E+03
 A1  5     5 0.77437E+07 0.45000E+02 0.00000E+00 0.22788E-19 0.44518E-01 0.30803E-39 0.32752E-08 0.10000E+01 0.16723E-36 0.89229E-06 0.23005E+03
 A1  6     6 0.77437E+07 0.45000E+02 0.00000E+00 0.18770E-17 0.44518E-01 0.23888E-35 0.32960E-08 0.10000E+01 0.12969E-32 0.89795E-06 0.23005E+03
 A1  7     7 0.77437E+07 0.45000E+02 0.00000E+00 0.71885E-18 0.44518E-01 0.20553E-31 0.33144E-08 0.10000E+01 0.11158E-28 0.90298E-06 0.23005E+03
 A1  8     8 0.77436E+07 0.45000E+02 0.00000E+00 0.27112E-17 0.44518E-01 0.18216E-27 0.33317E-08 0.10000E+01 0.98893E-25 0.90769E-06 0.23005E+03
 A1  9     9 0.77436E+07 0.45000E+02 0.99689E-01 0.55372E-14 0.44465E-01 0.17727E-23 0.27912E-08 0.99949E+00 0.96304E-21 0.75986E-06 0.23033E+03
 A1 10    10 0.77436E+07 0.45000E+02 0.14844E+00 0.16879E-14 0.44464E-01 0.14385E-19 0.19958E-07 0.99949E+00 0.78150E-17 0.54334E-05 0.23033E+03
 A1 11    11 0.77436E+07 0.45000E+02 0.18784E+00 0.27139E-15 0.42923E-01 0.10189E-19 0.46598E-04 0.98598E+00 0.56604E-17 0.13502E-01 0.21231E+03
 A1 12    12 0.77435E+07 0.45000E+02 0.27141E+00 0.38809E-16 0.13418E-01 0.16884E-19 0.76799E-03 0.49899E+00 0.16850E-16 0.50006E+00 0.80524E+02
 A1 13    13 0.77435E+07 0.45000E+02 0.30597E+00 0.63052E-17 0.75258E-03 0.39912E-19 0.10298E-02 0.37352E-01 0.56514E-16 0.96129E+00 0.54250E+02
 A1 14    14 0.77434E+07 0.45000E+02 0.33100E+00 0.17928E-17 0.22735E-04 0.53552E-19 0.10443E-02 0.11503E-02 0.77581E-16 0.99746E+00 0.52927E+02
 A1 15    15 0.77433E+07 0.45000E+02 0.36112E+00 0.22280E-17 0.48241E-06 0.58408E-19 0.10448E-02 0.24423E-04 0.84678E-16 0.99859E+00 0.52887E+02
 A1 16    16 0.77431E+07 0.45000E+02 0.39387E+00 0.12242E-17 0.74429E-08 0.53907E-19 0.10448E-02 0.37682E-06 0.78155E-16 0.99861E+00 0.52884E+02
 A1 17    17 0.77428E+07 0.45000E+02 0.42713E+00 0.11680E-17 0.85321E-10 0.37542E-19 0.10447E-02 0.43198E-08 0.54430E-16 0.99861E+00 0.52882E+02
 A1 18    18 0.77423E+07 0.45000E+02 0.46029E+00 0.76530E-18 0.74015E-12 0.18477E-19 0.10447E-02 0.37476E-10 0.26790E-16 0.99861E+00 0.52879E+02
 A1 19    19 0.77416E+07 0.45000E+02 0.49157E+00 0.34725E-18 0.49265E-14 0.63749E-20 0.10446E-02 0.24946E-12 0.92441E-17 0.99861E+00 0.52873E+02
 A1 20    20 0.77406E+07 0.45000E+02 0.52083E+00 0.22035E-17 0.25386E-16 0.15601E-20 0.10445E-02 0.12856E-14 0.22626E-17 0.99861E+00 0.52866E+02
 A1 21    21 0.77390E+07 0.45000E+02 0.54966E+00 0.73443E-19 0.10157E-18 0.27411E-21 0.10443E-02 0.51445E-17 0.39762E-18 0.99861E+00 0.52854E+02
 A1 22    22 0.77367E+07 0.45000E+02 0.57694E+00 0.26545E-19 0.31406E-21 0.34733E-22 0.10441E-02 0.15910E-19 0.50398E-19 0.99861E+00 0.52836E+02
 A1 23    23 0.77332E+07 0.45000E+02 0.59987E+00 0.11178E-18 0.74074E-24 0.31582E-23 0.10437E-02 0.37537E-22 0.45846E-20 0.99861E+00 0.52811E+02
 A1 24    24 0.77284E+07 0.45000E+02 0.61237E+00 0.58373E-19 0.13010E-26 0.20265E-24 0.10432E-02 0.65955E-25 0.29437E-21 0.99861E+00 0.52775E+02
 A1 25    25 0.77221E+07 0.45000E+02 0.61253E+00 0.24913E-19 0.16462E-29 0.89514E-26 0.10426E-02 0.83503E-28 0.13013E-22 0.99861E+00 0.52728E+02
 A1 26    26 0.77145E+07 0.45000E+02 0.60696E+00 0.22161E-20 0.14359E-32 0.26272E-27 0.10418E-02 0.72887E-31 0.38231E-24 0.99861E+00 0.52671E+02
 A1 27    27 0.77061E+07 0.45000E+02 0.60244E+00 0.84579E-20 0.81506E-36 0.48732E-29 0.10409E-02 0.41406E-34 0.70991E-26 0.99860E+00 0.52609E+02
 A1 28    28 0.76977E+07 0.45000E+02 0.59981E+00 0.33130E-20 0.27725E-39 0.52913E-31 0.10400E-02 0.14096E-37 0.77167E-28 0.99860E+00 0.52546E+02
 A1 29    29 0.76903E+07 0.45000E+02 0.59820E+00 0.41534E-20 0.49132E-43 0.29377E-33 0.10392E-02 0.24995E-41 0.42884E-30 0.99860E+00 0.52491E+02
 A1 30    30 0.76857E+07 0.45000E+02 0.59734E+00 0.11175E-20 0.34134E-47 0.63022E-36 0.10387E-02 0.17373E-45 0.92052E-33 0.99860E+00 0.52457E+02

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


 ELEM.  INDEX    PHIS        PHIF      DPHINCG     DPHITRC     DPHICH4     MASST       MASSNCG     MASSTRC     MASSCH4
                                                                            (KG)        (KG)        (KG)        (KG)

 A1  1     1 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A1  2     2 0.10000E-02 0.10000E-02 -.43557E-11 -.40170E-60 -.20891E-17 0.12063E+04 0.12063E+04 0.76177E-46 0.20642E-03
 A1  3     3 0.10000E-02 0.10000E-02 -.43597E-11 -.10770E-56 -.21315E-17 0.50312E+04 0.50312E+04 0.85104E-42 0.87760E-03
 A1  4     4 0.10000E-02 0.10000E-02 -.43597E-11 -.54803E-53 -.21535E-17 0.10742E+05 0.10742E+05 0.92458E-38 0.18930E-02
 A1  5     5 0.10000E-02 0.10000E-02 -.43597E-11 -.35990E-49 -.21700E-17 0.19060E+05 0.19060E+05 0.10774E-33 0.33847E-02
 A1  6     6 0.10000E-02 0.10000E-02 -.43597E-11 -.27910E-45 -.21837E-17 0.30985E+05 0.30985E+05 0.13583E-29 0.55372E-02
 A1  7     7 0.10000E-02 0.10000E-02 -.43597E-11 -.24014E-41 -.21960E-17 0.47890E+05 0.47890E+05 0.18063E-25 0.86062E-02
 A1  8     8 0.10000E-02 0.10000E-02 -.43597E-11 -.21283E-37 -.22074E-17 0.71611E+05 0.71611E+05 0.23938E-21 0.12936E-01
```

```
A1  9     9 0.10000E-02 0.10000E-02 -.43586E-11 -.20732E-33 -.18484E-17 0.10472E+06 0.10472E+06 0.34105E-17 0.15844E-01
A1 10    10 0.10000E-02 0.10000E-02 -.43586E-11 -.16824E-29 -.13217E-16 0.15054E+06 0.15054E+06 0.39788E-13 0.16287E+00
A1 11    11 0.10000E-02 0.10000E-02 -.42746E-11 -.12114E-29 -.32653E-13 0.21025E+06 0.20968E+06 0.40690E-13 0.57147E+03
A1 12    12 0.10000E-02 0.10000E-02 -.17875E-11 -.29797E-29 -.99924E-12 0.14793E+06 0.12333E+06 0.14077E-12 0.24597E+05
A1 13    13 0.10000E-02 0.10000E-02 -.11489E-12 -.85809E-29 -.16493E-11 0.67730E+05 0.11064E+05 0.56583E-12 0.56666E+05
A1 14    14 0.10000E-02 0.10000E-02 -.34994E-14 -.11650E-28 -.16926E-11 0.81131E+05 0.46743E+03 0.10656E-11 0.80663E+05
A1 15    15 0.10000E-02 0.10000E-02 -.74271E-16 -.12712E-28 -.16939E-11 0.11148E+06 0.13698E+02 0.16053E-11 0.11146E+06
A1 16    16 0.10000E-02 0.10000E-02 -.11459E-17 -.11732E-28 -.16939E-11 0.15325E+06 0.29058E+00 0.20372E-11 0.15325E+06
A1 17    17 0.10000E-02 0.10000E-02 -.13136E-19 -.81707E-29 -.16939E-11 0.21002E+06 0.45649E-02 0.19443E-11 0.21002E+06
A1 18    18 0.10000E-02 0.10000E-02 -.11396E-21 -.40215E-29 -.16938E-11 0.28696E+06 0.54110E-04 0.13075E-11 0.28696E+06
A1 19    19 0.10000E-02 0.10000E-02 -.75853E-24 -.13876E-29 -.16938E-11 0.39120E+06 0.49103E-06 0.61507E-12 0.39120E+06
A1 20    20 0.10000E-02 0.10000E-02 -.39088E-26 -.33960E-30 -.16937E-11 0.53229E+06 0.34432E-08 0.20484E-12 0.53229E+06
A1 21    21 0.10000E-02 0.10000E-02 -.15641E-28 -.59676E-31 -.16936E-11 0.72297E+06 0.18715E-10 0.48893E-13 0.72297E+06
A1 22    22 0.10000E-02 0.10000E-02 -.48365E-31 -.75631E-32 -.16934E-11 0.98097E+06 0.78529E-13 0.84087E-14 0.98097E+06
A1 23    23 0.10000E-02 0.10000E-02 -.11409E-33 -.68788E-33 -.16931E-11 0.13286E+07 0.25095E-15 0.10360E-14 0.13286E+07
A1 24    24 0.10000E-02 0.10000E-02 -.20042E-36 -.44157E-34 -.16927E-11 0.17987E+07 0.59692E-18 0.90054E-16 0.17987E+07
A1 25    25 0.10000E-02 0.10000E-02 -.25367E-39 -.19515E-35 -.16922E-11 0.24314E+07 0.10216E-20 0.53816E-17 0.24314E+07
A1 26    26 0.10000E-02 0.10000E-02 -.22133E-42 -.57310E-37 -.16915E-11 0.32851E+07 0.12048E-23 0.21361E-18 0.32851E+07
A1 27    27 0.10000E-02 0.10000E-02 -.12568E-45 -.10638E-38 -.16908E-11 0.44355E+07 0.92411E-27 0.53557E-20 0.44355E+07
A1 28    28 0.10000E-02 0.10000E-02 -.42769E-49 -.11558E-40 -.16901E-11 0.59848E+07 0.42448E-30 0.78551E-22 0.59848E+07
A1 29    29 0.10000E-02 0.10000E-02 -.75813E-53 -.64210E-43 -.16895E-11 0.80731E+07 0.10154E-33 0.58886E-24 0.80731E+07
A1 30    30 0.10000E-02 0.10000E-02 -.52681E-57 -.13780E-45 -.16891E-11 0.10468E+08 0.91505E-38 0.16389E-26 0.10468E+08


         Law Problem 1 - Part B

                                                                               KCYC =    1  -  ITER =    2  -  TIME =0.518400E+07
    ELEM1  ELEM2  INDEX    FLOH      FLOH/FLOF       FLOF       FLO(BRINE)   FLO(GAS)     FLO(LIQ.)    VEL(GAS)     VEL(LIQ.)
                           (W)        (J/KG)        (KG/S)       (KG/S)       (KG/S)       (KG/S)      (M/S)        (M/S)

    A1  1  A1  2     1 0.524907E+06 0.423884E+06 0.123833E+01 0.000000E+00 0.123833E+01 0.000000E+00 0.263431E+01 0.000000E+00
    A1  2  A1  3     2 0.279088E+05 0.423086E+06 0.659648E-01 0.000000E+00 0.659648E-01 0.000000E+00 0.556636E-02 0.000000E+00
    A1  3  A1  4     3 0.690254E+03 0.423076E+06 0.163151E-02 0.000000E+00 0.163151E-02 0.000000E+00 0.605636E-04 0.000000E+00
    A1  4  A1  5     4 0.797751E+01 0.423075E+06 0.188560E-04 0.000000E+00 0.188560E-04 0.000000E+00 0.424248E-06 0.000000E+00
    A1  5  A1  6     5 -.739569E+01 0.423075E+06 -.174808E-04 0.000000E+00 -.174808E-04 0.000000E+00 -.269935E-06 0.000000E+00
    A1  6  A1  7     6 -.139912E+02 0.423076E+06 -.330701E-04 0.000000E+00 -.330701E-04 0.000000E+00 -.374451E-06 0.000000E+00
    A1  7  A1  8     7 -.239748E+02 0.423076E+06 -.566678E-04 0.000000E+00 -.566678E-04 0.000000E+00 -.490108E-06 0.000000E+00
    A1  8  A1  9     8 -.389010E+02 0.423076E+06 -.919481E-04 0.000000E+00 -.919481E-04 0.000000E+00 -.624123E-06 0.000000E+00
    A1  9  A1 10     9 -.608516E+02 0.424053E+06 -.143500E-03 -.235396E-21 -.143458E-03 -.425119E-07 -.864508E-06 -.536352E-09
    A1 10  A1 11    10 -.921651E+02 0.424007E+06 -.217367E-03 -.189842E-21 -.217254E-03 -.112471E-06 -.112384E-05 -.773690E-09
    A1 11  A1 12    11 -.130207E+03 0.435929E+06 -.298688E-03 -.143769E-21 -.298158E-03 -.529745E-06 -.143972E-05 -.236334E-08
    A1 12  A1 13    12 -.900694E+02 0.670875E+06 -.134256E-03 -.674243E-22 -.132519E-03 -.173735E-05 -.155774E-05 -.444311E-08
    A1 13  A1 14    13 -.115785E+03 0.854308E+06 -.135531E-03 -.220059E-22 -.132041E-03 -.349012E-05 -.201665E-05 -.660155E-08
    A1 14  A1 15    14 -.179879E+03 0.863776E+06 -.208248E-03 -.128078E-22 -.201103E-03 -.714407E-05 -.273710E-05 -.104684E-07
    A1 15  A1 16    15 -.270489E+03 0.856089E+06 -.315959E-03 -.324458E-22 -.301396E-03 -.145625E-04 -.361868E-05 -.164647E-07
    A1 16  A1 17    16 -.395096E+03 0.845087E+06 -.467522E-03 -.354752E-22 -.438543E-03 -.289792E-04 -.469167E-05 -.253939E-07
    A1 17  A1 18    17 -.565600E+03 0.830393E+06 -.681123E-03 -.661833E-22 -.624458E-03 -.566646E-04 -.599201E-05 -.388135E-07
    A1 18  A1 19    18 -.797452E+03 0.812602E+06 -.981355E-03 -.817669E-22 -.874513E-03 -.106843E-03 -.756967E-05 -.577115E-07
    A1 19  A1 20    19 -.111013E+04 0.792594E+06 -.140063E-02 -.669994E-22 -.120769E-02 -.192944E-03 -.945175E-05 -.831126E-07
    A1 20  A1 21    20 -.152828E+04 0.768517E+06 -.198861E-02 -.755937E-21 -.164555E-02 -.343060E-03 -.116604E-04 -.118994E-06
    A1 21  A1 22    21 -.207913E+04 0.740672E+06 -.280709E-02 -.438525E-22 -.220999E-02 -.597095E-03 -.142403E-04 -.167684E-06
    A1 22  A1 23    22 -.279068E+04 0.706961E+06 -.394743E-02 -.273884E-22 -.291566E-02 -.103178E-02 -.171176E-04 -.236204E-06
    A1 23  A1 24    23 -.366317E+04 0.676267E+06 -.541675E-02 -.185102E-21 -.376085E-02 -.165591E-02 -.200040E-04 -.312264E-06
    A1 24  A1 25    24 -.463808E+04 0.657777E+06 -.705115E-02 -.136824E-21 -.470718E-02 -.234397E-02 -.221673E-04 -.371136E-06
    A1 25  A1 26    25 -.557199E+04 0.657458E+06 -.847505E-02 -.702953E-22 -.565338E-02 -.282167E-02 -.228688E-04 -.383164E-06
    A1 26  A1 27    26 -.627201E+04 0.665658E+06 -.942227E-02 -.670651E-23 -.639605E-02 -.302622E-02 -.219275E-04 -.356141E-06
    A1 27  A1 28    27 -.645930E+04 0.672230E+06 -.960876E-02 -.253377E-22 -.661300E-02 -.299576E-02 -.192793E-04 -.305171E-06
    A1 28  A1 29    28 -.572265E+04 0.675980E+06 -.846570E-02 -.859472E-23 -.587144E-02 -.259426E-02 -.146339E-04 -.228148E-06
    A1 29  A1 30    29 -.360466E+04 0.678135E+06 -.531554E-02 -.669843E-23 -.370278E-02 -.161276E-02 -.791186E-05 -.122282E-06

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

```
         Law Problem 1 - Part B

                                                                               KCYC =    1  -  ITER =    2  -  TIME =0.518400E+07
MASS FLOW RATES (KG/S) FROM DIFFUSION

ELEM1 ELEM2  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP
              all   wv    all   br    all  ncg    all  trc    all  ch4
A1  1 A1  2 0.97371E-22 0.00000E+00 0.46860E-15 0.62527E-56 -.46860E-15
A1  2 A1  3 -.32742E-21 0.00000E+00 -.61364E-15 0.18441E-51 0.61364E-15
A1  3 A1  4 0.18805E-20 0.00000E+00 -.62856E-15 0.17673E-47 0.62856E-15
A1  4 A1  5 0.40887E-20 0.00000E+00 -.66850E-15 0.16509E-43 0.66850E-15
A1  5 A1  6 0.36611E-19 0.00000E+00 -.70154E-15 0.16081E-39 0.70150E-15
A1  6 A1  7 0.47169E-16 0.00000E+00 -.78122E-15 0.16269E-35 0.73405E-15
A1  7 A1  8 0.62538E-13 0.00000E+00 -.63314E-13 0.16275E-31 0.77523E-15
A1  8 A1  9 0.75851E-10 0.00000E+00 -.75829E-10 0.14420E-27 -.22138E-13
A1  9 A1 10 0.72046E-15 -.39869E-25 -.61023E-12 0.10191E-23 0.60951E-12
A1 10 A1 11 0.14349E-11 -.29969E-25 -.15736E-08 -.25098E-24 0.15722E-08
A1 11 A1 12 0.25784E-10 -.15569E-25 -.24046E-07 0.55240E-24 0.24020E-07
A1 12 A1 13 0.12779E-10 -.53678E-26 -.11860E-07 0.10188E-23 0.11847E-07
A1 13 A1 14 0.81545E-12 -.98750E-27 -.74300E-09 0.43228E-24 0.74219E-09
A1 14 A1 15 0.25552E-13 0.12020E-27 -.21543E-10 0.13575E-24 0.21517E-10
A1 15 A1 16 0.11541E-14 -.35164E-27 -.42787E-12 -.11601E-24 0.42671E-12
A1 16 A1 17 0.89917E-15 -.24919E-28 -.61246E-14 -.38987E-24 0.52254E-14
A1 17 A1 18 0.12726E-14 -.22316E-27 -.64677E-16 -.41715E-24 -.12079E-14
A1 18 A1 19 0.17993E-14 -.28182E-27 -.51561E-18 -.24280E-24 -.17988E-14
A1 19 A1 20 0.25050E-14 0.14974E-26 -.31497E-20 -.88497E-25 -.25050E-14
A1 20 A1 21 0.34354E-14 -.20331E-26 -.14785E-22 -.21501E-25 -.34354E-14
A1 21 A1 22 0.46919E-14 -.52847E-28 -.53715E-25 -.36291E-26 -.46919E-14
A1 22 A1 23 0.63219E-14 0.11154E-27 -.15143E-27 -.43592E-27 -.63219E-14
A1 23 A1 24 0.84919E-14 -.77396E-28 -.33514E-30 -.38252E-28 -.84919E-14
A1 24 A1 25 0.10994E-13 -.50476E-28 -.57888E-33 -.24645E-29 -.10994E-13
A1 25 A1 26 0.13369E-13 -.33836E-28 -.74535E-36 -.11248E-30 -.13369E-13
A1 26 A1 27 0.15064E-13 0.90771E-29 -.66655E-39 -.34229E-32 -.15064E-13
A1 27 A1 28 0.15512E-13 -.73560E-29 -.38534E-42 -.65181E-34 -.15512E-13
A1 28 A1 29 0.13764E-13 0.11916E-29 -.13273E-45 -.72067E-36 -.13764E-13
A1 29 A1 30 0.86759E-14 -.43747E-29 -.24195E-49 -.41308E-38 -.86759E-14
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

```
         Law Problem 1 - Part B

                                                                               KCYC =    1  -  ITER =    2  -  TIME =0.518400E+07

                                                        IE(14) = 1 (H FROM SUPST AND ZEVSREAL)

ELEM.  INDEX    P            T           SL         DX1         DX2       H(GAS)       ZFAC        K(GAS)      K(LIQ.)    VIS(GAS)
                                                                          (J/KG)                                          (PA S)

A1  1     1 0.27500E+06 0.45000E+02 0.00000E+00 0.19271E-45 -.28115E-70 0.51731E+06 0.98763E+00 0.10000E+01 0.00000E+00 0.15765E-04
A1  2     2 0.77073E+07 0.45000E+02 0.00000E+00 -.36345E+05 -.48112E-18 0.42388E+06 0.56304E+00 0.10000E+01 0.00000E+00 0.22608E-04
A1  3     3 0.77432E+07 0.45000E+02 0.00000E+00 -.47867E+03 -.15749E-20 0.42309E+06 0.56008E+00 0.10000E+01 0.00000E+00 0.22712E-04
A1  4     4 0.77437E+07 0.45000E+02 0.00000E+00 -.56198E+01 -.64037E-22 0.42308E+06 0.56004E+00 0.10000E+01 0.00000E+00 0.22713E-04
A1  5     5 0.77437E+07 0.45000E+02 0.00000E+00 -.71363E-01 -.23099E-25 0.42308E+06 0.56004E+00 0.10000E+01 0.00000E+00 0.22713E-04
A1  6     6 0.77437E+07 0.45000E+02 0.00000E+00 -.18833E-01 -.43531E-24 0.42308E+06 0.56004E+00 0.10000E+01 0.00000E+00 0.22713E-04
A1  7     7 0.77437E+07 0.45000E+02 0.00000E+00 -.18445E-01 0.10331E-24 0.42308E+06 0.56004E+00 0.10000E+01 0.00000E+00 0.22713E-04
A1  8     8 0.77436E+07 0.45000E+02 0.00000E+00 -.18439E-01 -.63740E-24 0.42308E+06 0.56004E+00 0.10000E+01 0.00000E+00 0.22713E-04
A1  9     9 0.77436E+07 0.45000E+02 0.99689E-01 -.18435E-01 0.15396E-23 0.42412E+06 0.55893E+00 0.72071E+00 0.12957E-02 0.22718E-04
A1 10    10 0.77436E+07 0.45000E+02 0.14844E+00 -.18425E-01 0.11416E-23 0.42413E+06 0.55895E+00 0.62990E+00 0.19782E-02 0.22718E-04
A1 11    11 0.77436E+07 0.45000E+02 0.18784E+00 -.18408E-01 0.42635E-24 0.43636E+06 0.59243E+00 0.55889E+00 0.57838E-02 0.21810E-04
A1 12    12 0.77435E+07 0.45000E+02 0.27141E+00 -.18384E-01 0.17857E-24 0.67711E+06 0.85417E+00 0.43817E+00 0.18853E-01 0.14681E-04
A1 13    13 0.77435E+07 0.45000E+02 0.30597E+00 -.18360E-01 0.24478E-25 0.87173E+06 0.88688E+00 0.39395E+00 0.25314E-01 0.13353E-04
A1 14    14 0.77434E+07 0.45000E+02 0.33100E+00 -.18325E-01 0.12927E-24 0.88753E+06 0.88810E+00 0.36441E+00 0.30821E-01 0.13302E-04
A1 15    15 0.77433E+07 0.45000E+02 0.36112E+00 -.18268E-01 -.67847E-25 0.88803E+06 0.88814E+00 0.33155E+00 0.38114E-01 0.13300E-04
A1 16    16 0.77431E+07 0.45000E+02 0.39387E+00 -.18177E-01 0.17904E-26 0.88804E+06 0.88814E+00 0.30076E+00 0.47284E-01 0.13300E-04
A1 17    17 0.77428E+07 0.45000E+02 0.42713E+00 -.18033E-01 0.13519E-27 0.88804E+06 0.88814E+00 0.27221E+00 0.58766E-01 0.13300E-04
A1 18    18 0.77423E+07 0.45000E+02 0.46029E+00 -.17810E-01 0.11669E-24 0.88805E+06 0.88815E+00 0.24539E+00 0.71321E-01 0.13300E-04
A1 19    19 0.77416E+07 0.45000E+02 0.49157E+00 -.17469E-01 0.40818E-24 0.88805E+06 0.88815E+00 0.22224E+00 0.84459E-01 0.13300E-04
A1 20    20 0.77406E+07 0.45000E+02 0.52083E+00 -.16954E-01 -.93474E-26 0.88806E+06 0.88816E+00 0.20100E+00 0.99667E-01 0.13299E-04
A1 21    21 0.77390E+07 0.45000E+02 0.54966E+00 -.16185E-01 -.71640E-26 0.88808E+06 0.88818E+00 0.18025E+00 0.11581E+00 0.13299E-04
A1 22    22 0.77367E+07 0.45000E+02 0.57694E+00 -.15042E-01 0.35686E-27 0.88810E+06 0.88821E+00 0.16222E+00 0.13648E+00 0.13298E-04
A1 23    23 0.77332E+07 0.45000E+02 0.59987E+00 -.13382E-01 -.79451E-27 0.88813E+06 0.88824E+00 0.14708E+00 0.15390E+00 0.13297E-04
A1 24    24 0.77284E+07 0.45000E+02 0.61237E+00 -.11053E-01 0.57776E-27 0.88818E+06 0.88829E+00 0.13983E+00 0.16538E+00 0.13295E-04
A1 25    25 0.77221E+07 0.45000E+02 0.61253E+00 -.80718E-02 -.33977E-24 0.88824E+06 0.88836E+00 0.13973E+00 0.16553E+00 0.13293E-04
A1 26    26 0.77145E+07 0.45000E+02 0.60696E+00 -.46257E-02 0.31126E-33 0.88831E+06 0.88844E+00 0.14296E+00 0.16041E+00 0.13290E-04
A1 27    27 0.77061E+07 0.45000E+02 0.60244E+00 -.97720E-03 -.10796E-25 0.88839E+06 0.88852E+00 0.14558E+00 0.15625E+00 0.13287E-04
A1 28    28 0.76977E+07 0.45000E+02 0.59981E+00 0.25609E-02 0.17349E-24 0.88848E+06 0.88861E+00 0.14712E+00 0.15386E+00 0.13284E-04
A1 29    29 0.76903E+07 0.45000E+02 0.59820E+00 0.55178E-02 -.32454E-29 0.88855E+06 0.88869E+00 0.14819E+00 0.15264E+00 0.13281E-04
A1 30    30 0.76857E+07 0.45000E+02 0.59734E+00 0.72523E-02 0.34842E-24 0.88859E+06 0.88874E+00 0.14876E+00 0.15198E+00 0.13280E-04

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

```
         Law Problem 1 - Part B

                                                                               KCYC =    1  -  ITER =    2  -  TIME =0.518400E+07
ELEMENT SOURCE INDEX      GENERATION RATE     ENTHALPY    FF(GAS)      FF(LIQ.)      P(WB)
                            (KG/S) OR (W)     (J/KG)                                 (PA)

 A1  1   CO2 1    1          0.000000E+00   0.000000E+00 0.000000E+00 0.000000E+00
 A1  1   CH4 1    2          0.000000E+00   0.000000E+00 0.000000E+00 0.000000E+00

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


********** VOLUME- AND MASS-BALANCES ********************************************************************************************

********** [KCYC,ITER] = [   1,  2] *****                                  THE TIME IS 0.518400E+07 SECONDS, OR 0.600000E+02 DAYS


               PHASES PRESENT
*************************************************************
 PHASES       *        GAS          AQUEOUS       ADSORBED
 VOLUME (M^3) * 0.23770266E+04 0.34490120E+04 0.98900904E-05
 MASS   (KG)  * 0.12708589E+06 0.34268415E+07 0.42143068E+08
*************************************************************

               COMPONENT MASS IN PLACE (KG)
***************************************************************************
 PHASES     *    GAS          AQUEOUS        ADSORBED        TOTAL
***************************************************************************
 COMPONENTS *
 WATER      * 0.17463422E+03 0.34231931E+07 0.00000000E+00 0.34233678E+07
 BRINE      * 0.31814352E-14 0.23272795E-11 0.00000000E+00 0.23304609E-11
 NCG        * 0.27197389E+04 0.84575982E+02 0.78633692E+06 0.78914124E+06
 TRC        * 0.25971959E-12 0.21787018E-14 0.96253540E-11 0.98872523E-11
 CH4        * 0.12419152E+06 0.35637752E+04 0.41356731E+08 0.41484487E+08
***************************************************************************

*********************************************************************************************************************************
```

Figure C-4. Selected Law et al. (2002) Problem Output – Part 2

```
Law Problem 1 - Part C
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
coal     2  1434.e00      .001  3.65e-15  3.65e-15  3.65e-15      2.51      920.
  1.45e-10                          0.25
    9
    8           .457       .00  5.105e-4      1.e7        1.
bh       2  1434.e00       1.0  3.65e-09  3.65e-09  3.65e-09      2.51      920.
                                    0.25
    5           .457       .15        1.       .10
    8           .457       .00  5.105e-4      1.e7        1.

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    5    5    2    8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3  -5    100020 0 0000001000300 01  3
  1.0368e7  1.5768e7     1.e00      100.A1  1
     1.e-5    1.0e+0
            1.013e5                 0.                  0.                  0.
              10.50                20.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1
 10368001.   1.296e6 157.788e6 315.576e6 946.728e6 3.15576e9
SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6                                                                 1    1    1
     -1.e5




              28.96                                             1.e-10

     0.e-0     0.e-1
     0.e-6     0.e-6     0.e-6    -1.e-6    -1.e-6     0.e-6
     1.e50       16.     0.e-6    -1.e-6                           1.0e-11
     1.e50       44.    -1.e-6     0.e-6                           4.0e-09

     diffusivity data are input as follows:
     first row:  water (gas, liq.)
     second row: brine (gas, liq.)
     third row:  rn1   (gas, liq.)
     fourth row: rn2   (gas, liq.)
     fifth row:  air   (gas, liq.)
DIFFU----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
     1.e-6    1.e-10
     0.e-6    1.e-10
     1.e-6    1.e-10
     1.e-6    1.e-10
     1.e-6    1.e-10

     diffusivity values for DGM are input as follows (assumes Dj-i = Di-j):
     first row:   D1-2, D1-3, D1-4, D1-5
     second row:  D2-3, D2-4, D2-5
     third row:   D3-4, D3-5
     fourth row:  D4-5
DGM
    1.0e-6    1.0e-6    1.0e-6    1.0e-6
    1.0e-6    1.0e-6    1.0e-6
    1.0e-6    1.0e-6
    1.0e-6
CBM
coal
     0.156    0.0672
        0.        0.        0.
        0.        0.        0.
    0.0310   1903.e3  1180.e10
    0.0150  27241.e3   808.e10
    0.0152  4688.5e3   421.e10

ELEME ---    30   31    0    0   0.00000   453.911 mod
A1  1              20.3767E-010.8371E-02          0.1825E-01          -.4500E+01
A1  2              10.2347E+020.5206E+01          0.4738E+00          -.4500E+01
A1  3              10.9780E+020.2173E+02          0.1491E+01          -.4500E+01
A1  4              10.2088E+030.4640E+02          0.2744E+01          -.4500E+01
A1  5              10.3705E+030.8232E+02          0.4197E+01          -.4500E+01
A1  6              10.6023E+030.1338E+03          0.5883E+01          -.4500E+01
A1  7              10.9309E+030.2069E+03          0.7838E+01          -.4500E+01
A1  8              10.1392E+040.3094E+03          0.1011E+02          -.4500E+01
A1  9              10.2036E+040.4524E+03          0.1274E+02          -.4500E+01
A1 10              10.2927E+040.6505E+03          0.1579E+02          -.4500E+01
```

```
A1 11              10.4157E+040.9238E+03          0.1933E+02          -.4500E+01
A1 12              10.5847E+040.1299E+04          0.2344E+02          -.4500E+01
A1 13              10.8161E+040.1814E+04          0.2820E+02          -.4500E+01
A1 14              10.1132E+050.2516E+04          0.3373E+02          -.4500E+01
A1 15              10.1563E+050.3473E+04          0.4014E+02          -.4500E+01
A1 16              10.2149E+050.4775E+04          0.4758E+02          -.4500E+01
A1 17              10.2945E+050.6544E+04          0.5620E+02          -.4500E+01
A1 18              10.4024E+050.8943E+04          0.6621E+02          -.4500E+01
A1 19              10.5486E+050.1219E+05          0.7782E+02          -.4500E+01
A1 20              10.7465E+050.1659E+05          0.9128E+02          -.4500E+01
A1 21              10.1014E+060.2254E+05          0.1069E+03          -.4500E+01
A1 22              10.1376E+060.3057E+05          0.1250E+03          -.4500E+01
A1 23              10.1864E+060.4143E+05          0.1460E+03          -.4500E+01
A1 24              10.2524E+060.5608E+05          0.1704E+03          -.4500E+01
A1 25              10.3413E+060.7585E+05          0.1987E+03          -.4500E+01
A1 26              10.4613E+060.1025E+06          0.2315E+03          -.4500E+01
A1 27              10.6231E+060.1385E+06          0.2696E+03          -.4500E+01
A1 28              10.8411E+060.1869E+06          0.3137E+03          -.4500E+01
A1 29              10.1135E+070.2522E+06          0.3649E+03          -.4500E+01
A1 30              10.1472E+070.3270E+06          0.4232E+03          -.4500E+01

CONNE
A1  1A1  2                   10.1825E-050.4555E+000.2064E+01
A1  2A1  3                   10.4555E+000.5800E+000.5152E+02
A1  3A1  4                   10.5800E+000.6728E+000.1171E+03
A1  4A1  5                   10.6728E+000.7805E+000.1932E+03
A1  5A1  6                   10.7805E+000.9053E+000.2815E+03
A1  6A1  7                   10.9053E+000.1050E+010.3839E+03
A1  7A1  8                   10.1050E+010.1218E+010.5026E+03
A1  8A1  9                   10.1218E+010.1413E+010.6404E+03
A1  9A1 10                   10.1413E+010.1639E+010.8002E+03
A1 10A1 11                   10.1639E+010.1901E+010.9856E+03
A1 11A1 12                   10.1901E+010.2206E+010.1201E+04
A1 12A1 13                   10.2206E+010.2559E+010.1450E+04
A1 13A1 14                   10.2559E+010.2968E+010.1739E+04
A1 14A1 15                   10.2968E+010.3443E+010.2075E+04
A1 15A1 16                   10.3443E+010.3994E+010.2465E+04
A1 16A1 17                   10.3994E+010.4633E+010.2916E+04
A1 17A1 18                   10.4633E+010.5374E+010.3440E+04
A1 18A1 19                   10.5374E+010.6234E+010.4048E+04
A1 19A1 20                   10.6234E+010.7231E+010.4753E+04
A1 20A1 21                   10.7231E+010.8388E+010.5571E+04
A1 21A1 22                   10.8388E+010.9730E+010.6520E+04
A1 22A1 23                   10.9730E+010.1129E+020.7620E+04
A1 23A1 24                   10.1129E+020.1309E+020.8897E+04
A1 24A1 25                   10.1309E+020.1519E+020.1038E+05
A1 25A1 26                   10.1519E+020.1762E+020.1210E+05
A1 26A1 27                   10.1762E+020.2044E+020.1409E+05
A1 27A1 28                   10.2044E+020.2371E+020.1640E+05
A1 28A1 29                   10.2371E+020.2750E+020.1908E+05
A1 29A1 30                   10.2750E+020.3075E+020.2219E+05

INCON -- INITIAL CONDITIONS FOR   30 ELEMENTS AT TIME  0.103680E+08
A1  1           0.10000000E+01
 0.2750000000000E+06 0.1602888385780E-27 0.9999990001911E+00 0.3168568899497E-51
 0.9998089379860E-06 0.4500000000000E+02
A1  2           0.99967356E-03
 0.5398176757523E+07 0.1183600146397E-17 0.8568857209277E-02 0.2348022330739E-20
 0.1049002069567E+02 0.4500000000000E+02
A1  3           0.99973802E-03
 0.5842870103326E+07 0.1180129878545E-17 0.9069703402601E-02 0.2541324963116E-20
 0.1048161911536E+02 0.4500000000000E+02
A1  4           0.99977154E-03
 0.6074078360544E+07 0.1181517993261E-17 0.9271089396350E-02 0.2642389611750E-20
 0.1047735525057E+02 0.4500000000000E+02
A1  5           0.99979471E-03
 0.6233964831855E+07 0.1179381534318E-17 0.9321566004644E-02 0.2713244155382E-20
 0.1047427620680E+02 0.4500000000000E+02
A1  6           0.99981291E-03
 0.6359449151570E+07 0.1180850080530E-17 0.9230823836713E-02 0.2770240843410E-20
 0.1047158417260E+02 0.4500000000000E+02
A1  7           0.99982816E-03
 0.6464685273857E+07 0.1149292780106E-17 0.8967603461296E-02 0.2819865602997E-20
 0.1046889831820E+02 0.4500000000000E+02
A1  8           0.99984148E-03
 0.6556514033096E+07 0.1211887960362E-17 0.8472528729576E-02 0.2865313536439E-20
 0.1046593866407E+02 0.4500000000000E+02
A1  9           0.99985339E-03
 0.6638650750849E+07 0.1154504419243E-17 0.7657410934490E-02 0.2907870535859E-20
 0.1046244030646E+02 0.4500000000000E+02
A1 10           0.99986421E-03
```

```
 0.6713289275208E+07 0.1159807797445E-17 0.6405329112028E-02 0.2946336857788E-20
 0.1045813691679E+02 0.4500000000000E+02
A1 11           0.99987415E-03
 0.6781794681209E+07 0.1193156563130E-17 0.4605306188873E-02 0.2973567044929E-20
 0.1045285499926E+02 0.4500000000000E+02
A1 12           0.99988332E-03
 0.6845035016714E+07 0.1244079218795E-17 0.2312830611395E-02 0.2966300339368E-20
 0.1044728212476E+02 0.4500000000000E+02
A1 13           0.99989190E-03
 0.6904161635313E+07 0.1352174585275E-17 0.2635782506930E-03 0.2865100175615E-20
 0.1044279989186E+02 0.4500000000000E+02
A1 14           0.99990005E-03
 0.6960952679940E+07 0.1531644383431E-17 0.1073253988269E-04 0.2592638428701E-20
 0.1044119719074E+02 0.4500000000000E+02
A1 15           0.99990804E-03
 0.7015939137998E+07 0.1558036712642E-17 0.2793779613642E-06 0.2228884091592E-20
 0.1043985661056E+02 0.4500000000000E+02
A1 16           0.99991582E-03
 0.7069440431346E+07 0.1244886351726E-17 0.4997056269413E-08 0.1793589988891E-20
 0.1043837908201E+02 0.4500000000000E+02
A1 17           0.99992345E-03
 0.7121725896351E+07 0.8342295573407E-18 0.6377911637881E-10 0.1314820001295E-20
 0.1043671521662E+02 0.4500000000000E+02
A1 18           0.99993084E-03
 0.7172962552118E+07 0.1053959770778E-17 0.5983431816136E-12 0.8440181497593E-21
 0.1043483913062E+02 0.4500000000000E+02
A1 19           0.99993814E-03
 0.7223279084604E+07 0.1040656944983E-17 0.4218474294639E-14 0.4486244514524E-21
 0.1043274206130E+02 0.4500000000000E+02
A1 20           0.99994527E-03
 0.7272746608883E+07 0.7004524488190E-18 0.2268942243139E-16 0.1834463519816E-21
 0.1043044233486E+02 0.4500000000000E+02
A1 21           0.99995234E-03
 0.7321354946182E+07 0.3352384703342E-19 0.9382789434369E-19 0.5346147027227E-22
 0.1042799747138E+02 0.4500000000000E+02
A1 22           0.99995929E-03
 0.7368995208732E+07 0.6260654213552E-19 0.2981464069687E-21 0.1053807486223E-22
 0.1042551288146E+02 0.4500000000000E+02
A1 23           0.99996602E-03
 0.7415435297029E+07 0.1264809862383E-18 0.7219805603820E-24 0.1370919000368E-23
 0.1042313541133E+02 0.4500000000000E+02
A1 24           0.99997252E-03
 0.7460241238126E+07 0.6375630833583E-19 0.1308795599708E-26 0.1167463016721E-24
 0.1042101824508E+02 0.4500000000000E+02
A1 25           0.99997861E-03
 0.7502798871012E+07 0.2306969103100E-19 0.1733645758704E-29 0.6471678822913E-26
 0.1041921515288E+02 0.4500000000000E+02
A1 26           0.99998443E-03
 0.7542303882058E+07 0.1760040045669E-19 0.1624409504733E-32 0.2312616435726E-27
 0.1041752806495E+02 0.4500000000000E+02
A1 27           0.99998948E-03
 0.7577728588996E+07 0.2540949704497E-20 0.1030546964168E-35 0.5204294213640E-29
 0.1041546655302E+02 0.4500000000000E+02
A1 28           0.99999385E-03
 0.7607669568796E+07 0.3447060381879E-20 0.4132326567891E-39 0.7006337182962E-31
 0.1041292896948E+02 0.4500000000000E+02
A1 29           0.99999709E-03
 0.7630206431180E+07 0.9038555112236E-21 0.9165912334157E-43 0.5012308608115E-33
 0.1041052188805E+02 0.4500000000000E+02
A1 30           0.99999895E-03
 0.7642593867603E+07 0.4469354352466E-21 0.8320064703198E-47 0.1426781826557E-35
 0.1040902122990E+02 0.4500000000000E+02
+++
                               0.10368000E+08

INDOM

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A1  1CO201    0    0    0    4     COM31
            0.       1.296e6       1.296e6         1.e10
         0.609         0.609            0.            0.
      430.65e3      430.65e3            0.            0.
A1  1CH401    0    0    0    4     COM51
            0.       1.296e6       1.296e6         1.e10
      0.609e-6      0.609e-6            0.            0.
      430.65e3      430.65e3            0.            0.

FOFT
A1  1
A1  2
```

```
COFT
A1  1A1  2

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure C-5. Law et al. (2002) Problem Input – Part 3

```
Law Problem 1 - Part C

          OUTPUT DATA AFTER (   1,  4)-2-TIME STEPS                                                   THE TIME IS 0.120000E+03 DAYS

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

  TOTAL TIME     KCYC   ITER  ITERC   KON          DX1M         DX2M         DX3M          MAX. RES.      NER    KER        DELTEX
 0.103680E+08      1      4      4     2       0.20590E+06  0.11897E-17  0.99707E+00    0.75242E-09       1     5      0.10000E+01

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

                                                         NCG = CO2

 ELEM.  INDEX     P           T          SL       XBRINE(LIQ)  XNCG(LIQ)   XTRC(LIQ)   XCH4(LIQ)   XNCG(GAS)   XTRC(GAS)   XCH4(GAS)     DG
                 (PA)      (DEG-C)                                                                                                    (KG/M**3)

 A1  1     1 0.48090E+06 0.45000E+02 0.27396E-03 0.11897E-17 0.29312E-02 0.86172E-22 0.26147E-04 0.84028E+00 0.93705E-18 0.14932E+00 0.63752E+01
 A1  2     2 0.53983E+07 0.45000E+02 0.51000E+00 0.11836E-17 0.85690E-02 0.23483E-20 0.61124E-03 0.43039E+00 0.35657E-17 0.56817E+00 0.50213E+02
 A1  3     3 0.58429E+07 0.45000E+02 0.51838E+00 0.11801E-17 0.90697E-02 0.25413E-20 0.65321E-03 0.42993E+00 0.35678E-17 0.56873E+00 0.54763E+02
 A1  4     4 0.60741E+07 0.45000E+02 0.52264E+00 0.11815E-17 0.92711E-02 0.26424E-20 0.67561E-03 0.42797E+00 0.35751E-17 0.57074E+00 0.57056E+02
 A1  5     5 0.62340E+07 0.45000E+02 0.52572E+00 0.11794E-17 0.93216E-02 0.27132E-20 0.69266E-03 0.42373E+00 0.35901E-17 0.57501E+00 0.58483E+02
 A1  6     6 0.63594E+07 0.45000E+02 0.52842E+00 0.11808E-17 0.92308E-02 0.27702E-20 0.70859E-03 0.41605E+00 0.36170E-17 0.58271E+00 0.59350E+02
 A1  7     7 0.64647E+07 0.45000E+02 0.53110E+00 0.11493E-17 0.89676E-02 0.28199E-20 0.72571E-03 0.40323E+00 0.36614E-17 0.59553E+00 0.59707E+02
 A1  8     8 0.65565E+07 0.45000E+02 0.53406E+00 0.12119E-17 0.84725E-02 0.28653E-20 0.74602E-03 0.38272E+00 0.37315E-17 0.61604E+00 0.59494E+02
 A1  9     9 0.66387E+07 0.45000E+02 0.53756E+00 0.11545E-17 0.76574E-02 0.29079E-20 0.77174E-03 0.35057E+00 0.38392E-17 0.64817E+00 0.58577E+02
 A1 10    10 0.67133E+07 0.45000E+02 0.54186E+00 0.11598E-17 0.64053E-02 0.29463E-20 0.80544E-03 0.30078E+00 0.40004E-17 0.69793E+00 0.56773E+02
 A1 11    11 0.67818E+07 0.45000E+02 0.54715E+00 0.11932E-17 0.46053E-02 0.29736E-20 0.84936E-03 0.22528E+00 0.42291E-17 0.77337E+00 0.53939E+02
 A1 12    12 0.68450E+07 0.45000E+02 0.55272E+00 0.12441E-17 0.23128E-02 0.29663E-20 0.90223E-03 0.11971E+00 0.45009E-17 0.87883E+00 0.50271E+02
 A1 13    13 0.69042E+07 0.45000E+02 0.55720E+00 0.13522E-17 0.26358E-03 0.28651E-20 0.94938E-03 0.14381E-01 0.46167E-17 0.98407E+00 0.47129E+02
 A1 14    14 0.69610E+07 0.45000E+02 0.55880E+00 0.15316E-17 0.10733E-04 0.25926E-20 0.96062E-03 0.58644E-03 0.41796E-17 0.99787E+00 0.47112E+02
 A1 15    15 0.70159E+07 0.45000E+02 0.56014E+00 0.15580E-17 0.27938E-06 0.22289E-20 0.96686E-03 0.15183E-04 0.35663E-17 0.99845E+00 0.47499E+02
 A1 16    16 0.70694E+07 0.45000E+02 0.56162E+00 0.12449E-17 0.49971E-08 0.17936E-20 0.97272E-03 0.27006E-06 0.28481E-17 0.99848E+00 0.47893E+02
 A1 17    17 0.71217E+07 0.45000E+02 0.56328E+00 0.83423E-18 0.63779E-10 0.13148E-20 0.97842E-03 0.34285E-08 0.20726E-17 0.99849E+00 0.48278E+02
 A1 18    18 0.71730E+07 0.45000E+02 0.56516E+00 0.10540E-17 0.59834E-12 0.84402E-21 0.98399E-03 0.31997E-10 0.13209E-17 0.99850E+00 0.48656E+02
 A1 19    19 0.72233E+07 0.45000E+02 0.56726E+00 0.10407E-17 0.42185E-14 0.44862E-21 0.98944E-03 0.22445E-12 0.69723E-18 0.99851E+00 0.49028E+02
 A1 20    20 0.72727E+07 0.45000E+02 0.56956E+00 0.70045E-18 0.22689E-16 0.18345E-21 0.99478E-03 0.12013E-14 0.28316E-18 0.99852E+00 0.49394E+02
 A1 21    21 0.73214E+07 0.45000E+02 0.57200E+00 0.33524E-19 0.93828E-19 0.53461E-22 0.10000E-02 0.49439E-17 0.81974E-19 0.99853E+00 0.49753E+02
 A1 22    22 0.73690E+07 0.45000E+02 0.57449E+00 0.62607E-19 0.29815E-21 0.10538E-22 0.10051E-02 0.15637E-19 0.16054E-19 0.99854E+00 0.50106E+02
 A1 23    23 0.74154E+07 0.45000E+02 0.57686E+00 0.12648E-18 0.72198E-24 0.13709E-23 0.10101E-02 0.37695E-22 0.20754E-20 0.99855E+00 0.50450E+02
 A1 24    24 0.74602E+07 0.45000E+02 0.57898E+00 0.63756E-19 0.13088E-26 0.11675E-24 0.10149E-02 0.68038E-25 0.17568E-21 0.99856E+00 0.50782E+02
 A1 25    25 0.75028E+07 0.45000E+02 0.58078E+00 0.23070E-19 0.17336E-29 0.64717E-26 0.10194E-02 0.89759E-28 0.96832E-23 0.99857E+00 0.51098E+02
 A1 26    26 0.75423E+07 0.45000E+02 0.58247E+00 0.17600E-19 0.16244E-32 0.23126E-27 0.10236E-02 0.83789E-31 0.34421E-24 0.99857E+00 0.51391E+02
 A1 27    27 0.75777E+07 0.45000E+02 0.58453E+00 0.25409E-20 0.10305E-35 0.52043E-29 0.10274E-02 0.52980E-34 0.77099E-26 0.99858E+00 0.51654E+02
 A1 28    28 0.76077E+07 0.45000E+02 0.58707E+00 0.34471E-20 0.41323E-39 0.70063E-31 0.10305E-02 0.21185E-37 0.10339E-27 0.99859E+00 0.51877E+02
 A1 29    29 0.76302E+07 0.45000E+02 0.58948E+00 0.90386E-21 0.91659E-43 0.50123E-33 0.10329E-02 0.46891E-41 0.73744E-30 0.99859E+00 0.52044E+02
 A1 30    30 0.76426E+07 0.45000E+02 0.59098E+00 0.44694E-21 0.83201E-47 0.14268E-35 0.10342E-02 0.42515E-45 0.20958E-32 0.99859E+00 0.52136E+02

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


 ELEM.  INDEX    PHIS        PHIF      DPHINCG     DPHITRC     DPHICH4     MASST       MASSNCG     MASSTRC     MASSCH4
                                                                            (KG)        (KG)        (KG)        (KG)

 A1  1     1 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A1  2     2 0.99967E-03 0.99967E-03 -.13240E-11 -.54151E-30 -.97500E-12 0.46303E+03 0.36669E+03 0.10269E-15 0.96338E+02
 A1  3     3 0.99974E-03 0.99974E-03 -.13636E-11 -.55860E-30 -.10062E-11 0.19879E+04 0.15736E+04 0.44142E-15 0.41428E+03
 A1  4     4 0.99977E-03 0.99977E-03 -.13761E-11 -.56747E-30 -.10237E-11 0.42904E+04 0.33906E+04 0.95738E-15 0.89987E+03
 A1  5     5 0.99979E-03 0.99979E-03 -.13733E-11 -.57438E-30 -.10395E-11 0.76253E+04 0.60038E+04 0.17195E-14 0.16215E+04
 A1  6     6 0.99981E-03 0.99981E-03 -.13542E-11 -.58117E-30 -.10580E-11 0.12307E+05 0.96243E+04 0.28283E-14 0.26827E+04
 A1  7     7 0.99983E-03 0.99983E-03 -.13139E-11 -.58893E-30 -.10824E-11 0.18674E+05 0.14432E+05 0.44298E-14 0.42421E+04
 A1  8     8 0.99984E-03 0.99984E-03 -.12438E-11 -.59867E-30 -.11168E-11 0.26976E+05 0.20431E+05 0.67334E-14 0.65449E+04
```

```
A1  9     9 0.99985E-03 0.99985E-03 -.11311E-11 -.61146E-30 -.11665E-11 0.37173E+05 0.27174E+05 0.10059E-13 0.99988E+04
A1 10    10 0.99986E-03 0.99986E-03 -.95711E-12 -.62839E-30 -.12388E-11 0.48323E+05 0.33057E+05 0.14862E-13 0.15266E+05
A1 11    11 0.99987E-03 0.99987E-03 -.70081E-12 -.64945E-30 -.13420E-11 0.57863E+05 0.34377E+05 0.21814E-13 0.23487E+05
A1 12    12 0.99988E-03 0.99988E-03 -.36066E-12 -.66936E-30 -.14769E-11 0.61238E+05 0.24883E+05 0.31623E-13 0.36354E+05
A1 13    13 0.99989E-03 0.99989E-03 -.42011E-13 -.66576E-30 -.16035E-11 0.59140E+05 0.40457E+04 0.43901E-13 0.55094E+05
A1 14    14 0.99990E-03 0.99990E-03 -.17113E-14 -.60207E-30 -.16243E-11 0.77636E+05 0.22858E+03 0.55069E-13 0.77407E+05
A1 15    15 0.99991E-03 0.99991E-03 -.44435E-16 -.51525E-30 -.16300E-11 0.10727E+06 0.81954E+01 0.65072E-13 0.10726E+06
A1 16    16 0.99992E-03 0.99992E-03 -.79280E-18 -.41274E-30 -.16350E-11 0.14793E+06 0.20104E+00 0.71668E-13 0.14793E+06
A1 17    17 0.99992E-03 0.99992E-03 -.10094E-19 -.30123E-30 -.16398E-11 0.20331E+06 0.35078E-02 0.71678E-13 0.20331E+06
A1 18    18 0.99993E-03 0.99993E-03 -.94474E-22 -.19253E-30 -.16445E-11 0.27860E+06 0.44859E-04 0.62599E-13 0.27860E+06
A1 19    19 0.99994E-03 0.99994E-03 -.66453E-24 -.10190E-30 -.16491E-11 0.38087E+06 0.43018E-06 0.45170E-13 0.38087E+06
A1 20    20 0.99995E-03 0.99995E-03 -.35662E-26 -.41496E-31 -.16535E-11 0.51965E+06 0.31413E-08 0.25029E-13 0.51965E+06
A1 21    21 0.99995E-03 0.99995E-03 -.14715E-28 -.12044E-31 -.16578E-11 0.70771E+06 0.17607E-10 0.98680E-14 0.70771E+06
A1 22    22 0.99996E-03 0.99996E-03 -.46658E-31 -.23647E-32 -.16620E-11 0.96280E+06 0.75758E-13 0.26291E-14 0.96280E+06
A1 23    23 0.99997E-03 0.99997E-03 -.11275E-33 -.30645E-33 -.16661E-11 0.13075E+07 0.24800E-15 0.46155E-15 0.13075E+07
A1 24    24 0.99997E-03 0.99997E-03 -.20399E-36 -.26001E-34 -.16700E-11 0.17745E+07 0.60754E-18 0.53025E-16 0.17745E+07
A1 25    25 0.99998E-03 0.99998E-03 -.26970E-39 -.14363E-35 -.16737E-11 0.24048E+07 0.10862E-20 0.39608E-17 0.24048E+07
A1 26    26 0.99998E-03 0.99998E-03 -.25227E-42 -.51158E-37 -.16770E-11 0.32569E+07 0.13732E-23 0.19068E-18 0.32569E+07
A1 27    27 0.99999E-03 0.99999E-03 -.15979E-45 -.11479E-38 -.16801E-11 0.44072E+07 0.11749E-26 0.57795E-20 0.44072E+07
A1 28    28 0.99999E-03 0.99999E-03 -.63992E-49 -.15417E-40 -.16826E-11 0.59581E+07 0.63512E-30 0.10477E-21 0.59581E+07
A1 29    29 0.10000E-02 0.10000E-02 -.14180E-52 -.11009E-42 -.16845E-11 0.80491E+07 0.18992E-33 0.10096E-23 0.80491E+07
A1 30    30 0.10000E-02 0.10000E-02 -.12865E-56 -.31306E-45 -.16855E-11 0.10445E+08 0.22346E-37 0.37234E-26 0.10445E+08

         Law Problem 1 - Part C

                                                                               KCYC =    1  -  ITER =    4  -  TIME =0.103680E+08
    ELEM1  ELEM2  INDEX    FLOH      FLOH/FLOF       FLOF       FLO(BRINE)   FLO(GAS)     FLO(LIQ.)    VEL(GAS)     VEL(LIQ.)
                           (W)        (J/KG)        (KG/S)       (KG/S)       (KG/S)       (KG/S)      (M/S)        (M/S)

    A1  1  A1  2     1 0.480165E+05 0.633468E+06 0.757994E-01 0.150480E-19 0.630856E-01 0.127138E-01 0.124265E+01 0.121722E-01
    A1  2  A1  3     2 0.497828E+05 0.630933E+06 0.789035E-01 0.156417E-19 0.656493E-01 0.132542E-01 0.483257E-01 0.500027E-03
    A1  3  A1  4     3 0.496182E+05 0.630049E+06 0.787530E-01 0.156743E-19 0.654867E-01 0.132663E-01 0.205376E-01 0.218369E-03
    A1  4  A1  5     4 0.493860E+05 0.630161E+06 0.783705E-01 0.156525E-19 0.650987E-01 0.132718E-01 0.121506E-01 0.131623E-03
    A1  5  A1  6     5 0.490476E+05 0.631326E+06 0.776899E-01 0.156778E-19 0.644132E-01 0.132767E-01 0.817712E-02 0.899025E-04
    A1  6  A1  7     6 0.485456E+05 0.633866E+06 0.765866E-01 0.152646E-19 0.633049E-01 0.132817E-01 0.589101E-02 0.656094E-04
    A1  7  A1  8     7 0.478108E+05 0.638343E+06 0.748982E-01 0.161024E-19 0.616111E-01 0.132871E-01 0.442286E-02 0.498541E-04
    A1  8  A1  9     8 0.467617E+05 0.645632E+06 0.724277E-01 0.153468E-19 0.591347E-01 0.132930E-01 0.340937E-02 0.388875E-04
    A1  9  A1 10     9 0.453158E+05 0.657034E+06 0.689703E-01 0.154249E-19 0.556708E-01 0.132995E-01 0.267517E-02 0.308883E-04
    A1 10  A1 11    10 0.434433E+05 0.674197E+06 0.644370E-01 0.158769E-19 0.511304E-01 0.133066E-01 0.212407E-02 0.248481E-04
    A1 11  A1 12    11 0.413173E+05 0.697818E+06 0.592093E-01 0.165656E-19 0.458938E-01 0.133155E-01 0.169966E-02 0.201987E-04
    A1 12  A1 13    12 0.396246E+05 0.721075E+06 0.549521E-01 0.180230E-19 0.416232E-01 0.133289E-01 0.137569E-02 0.166117E-04
    A1 13  A1 14    13 0.393746E+05 0.723237E+06 0.544422E-01 0.204783E-19 0.410721E-01 0.133702E-01 0.113638E-02 0.138536E-04
    A1 14  A1 15    14 0.392917E+05 0.722184E+06 0.544067E-01 0.209205E-19 0.409793E-01 0.134275E-01 0.945342E-03 0.116318E-04
    A1 15  A1 16    15 0.391992E+05 0.720788E+06 0.543838E-01 0.168070E-19 0.408830E-01 0.135008E-01 0.790028E-03 0.981876E-05
    A1 16  A1 17    16 0.390831E+05 0.719130E+06 0.543477E-01 0.113385E-19 0.407562E-01 0.135916E-01 0.662961E-03 0.833100E-05
    A1 17  A1 18    17 0.389328E+05 0.717183E+06 0.542857E-01 0.144381E-19 0.405868E-01 0.136989E-01 0.557682E-03 0.709391E-05
    A1 18  A1 19    18 0.387325E+05 0.714935E+06 0.541763E-01 0.143798E-19 0.403583E-01 0.138180E-01 0.469943E-03 0.605817E-05
    A1 19  A1 20    19 0.384585E+05 0.712409E+06 0.539837E-01 0.976241E-20 0.400464E-01 0.139373E-01 0.396307E-03 0.518297E-05
    A1 20  A1 21    20 0.380742E+05 0.709676E+06 0.536500E-01 0.470512E-21 0.396149E-01 0.140351E-01 0.333951E-03 0.443383E-05
    A1 21  A1 22    21 0.375254E+05 0.706873E+06 0.530864E-01 0.881250E-21 0.390104E-01 0.140760E-01 0.280639E-03 0.378297E-05
    A1 22  A1 23    22 0.367324E+05 0.704189E+06 0.521627E-01 0.177176E-20 0.381546E-01 0.140081E-01 0.234566E-03 0.320790E-05
    A1 23  A1 24    23 0.355843E+05 0.701822E+06 0.507027E-01 0.877670E-21 0.369367E-01 0.137660E-01 0.194184E-03 0.269004E-05
    A1 24  A1 25    24 0.339320E+05 0.699843E+06 0.484852E-01 0.306405E-21 0.352035E-01 0.132817E-01 0.158328E-03 0.221763E-05
    A1 25  A1 26    25 0.315902E+05 0.697982E+06 0.452593E-01 0.220036E-21 0.327576E-01 0.125018E-01 0.126171E-03 0.178545E-05
    A1 26  A1 27    26 0.283342E+05 0.695577E+06 0.407348E-01 0.289134E-22 0.293558E-01 0.113790E-01 0.970834E-04 0.139063E-05
    A1 27  A1 28    27 0.238888E+05 0.692470E+06 0.344979E-01 0.337159E-22 0.247168E-01 0.978107E-02 0.703562E-04 0.102252E-05
    A1 28  A1 29    28 0.179236E+05 0.689451E+06 0.259969E-01 0.675931E-23 0.185186E-01 0.747831E-02 0.454279E-04 0.669226E-06
    A1 29  A1 30    29 0.100317E+05 0.687543E+06 0.145907E-01 0.189302E-23 0.103551E-01 0.423555E-02 0.218832E-04 0.325082E-06

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

```
         Law Problem 1 - Part C

                                                                                KCYC =    1  -  ITER =    4  -  TIME =0.103680E+08
MASS FLOW RATES (KG/S) FROM DIFFUSION

ELEM1 ELEM2  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP
              all   wv    all   br    all  ncg    all  trc    all  ch4
A1  1 A1  2 -.20348E-11 -.64330E-31 -.90092E-10 0.57818E-27 0.92127E-10
A1  2 A1  3 -.32593E-12 -.41150E-30 -.10377E-11 0.50064E-29 0.13637E-11
A1  3 A1  4 -.26651E-12 0.32039E-30 -.85717E-11 0.31861E-28 0.88382E-11
A1  4 A1  5 -.19853E-12 -.71602E-30 -.26265E-10 0.93412E-28 0.26463E-10
A1  5 A1  6 -.95458E-13 0.62754E-30 -.58958E-10 0.20638E-27 0.59054E-10
A1  6 A1  7 0.66190E-13 -.16102E-28 -.11365E-09 0.39318E-27 0.11358E-09
A1  7 A1  8 0.31720E-12 0.36600E-28 -.20034E-09 0.68367E-27 0.20002E-09
A1  8 A1  9 0.69920E-12 -.37486E-28 -.33283E-09 0.11129E-26 0.33213E-09
A1  9 A1 10 0.12637E-11 0.38080E-29 -.52782E-09 0.17055E-26 0.52655E-09
A1 10 A1 11 0.20321E-11 0.26050E-28 -.79106E-09 0.23921E-26 0.78902E-09
A1 11 A1 12 0.28243E-11 0.43011E-28 -.10589E-08 0.27212E-26 0.10560E-08
A1 12 A1 13 0.26858E-11 0.97895E-28 -.10001E-08 0.10978E-26 0.99739E-09
A1 13 A1 14 0.23940E-12 0.17122E-27 -.12902E-09 -.40805E-26 0.12878E-09
A1 14 A1 15 -.10571E-12 0.26137E-28 -.54453E-11 -.58353E-26 0.55510E-11
A1 15 A1 16 -.11806E-12 -.32037E-27 -.14486E-12 -.69636E-26 0.26293E-12
A1 16 A1 17 -.11585E-12 -.43258E-27 -.26273E-14 -.76278E-26 0.11848E-12
A1 17 A1 18 -.11326E-12 0.23794E-27 -.33828E-16 -.74714E-26 0.11330E-12
A1 18 A1 19 -.11064E-12 -.14788E-28 -.31876E-18 -.62447E-26 0.11064E-12
A1 19 A1 20 -.10791E-12 -.38783E-27 -.22491E-20 -.41629E-26 0.10791E-12
A1 20 A1 21 -.10499E-12 -.77893E-27 -.12073E-22 -.20260E-26 0.10499E-12
A1 21 A1 22 -.10172E-12 0.34758E-28 -.49717E-25 -.66357E-27 0.10172E-12
A1 22 A1 23 -.97910E-13 0.77964E-28 -.15708E-27 -.14045E-27 0.97910E-13
A1 23 A1 24 -.93312E-13 -.78041E-28 -.37821E-30 -.19051E-28 0.93312E-13
A1 24 A1 25 -.87604E-13 -.51466E-28 -.68188E-33 -.16619E-29 0.87604E-13
A1 25 A1 26 -.80409E-13 -.70176E-29 -.89819E-36 -.93317E-31 0.80409E-13
A1 26 A1 27 -.71257E-13 -.19596E-28 -.83574E-39 -.33503E-32 0.71257E-13
A1 27 A1 28 -.59471E-13 0.11978E-29 -.52545E-42 -.75283E-34 0.59471E-13
A1 28 A1 29 -.44230E-13 -.34162E-29 -.20866E-45 -.10087E-35 0.44230E-13
A1 29 A1 30 -.24585E-13 -.63383E-30 -.46858E-49 -.73297E-38 0.24585E-13
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

```
         Law Problem 1 - Part C
                                                                               KCYC =    1  -  ITER =    4  -  TIME =0.103680E+08
                                                        IE(14) = 1 (H FROM SUPST AND ZEVSREAL)

ELEM.  INDEX    P            T           SL         DX1         DX2       H(GAS)       ZFAC        K(GAS)      K(LIQ.)    VIS(GAS)
                                                                          (J/KG)                                          (PA S)

A1  1     1 0.48090E+06 0.45000E+02 0.27396E-03 0.20590E+06 0.11897E-17 0.59814E+06 0.98409E+00 0.10000E+01 0.10000E+01 0.14469E-04
A1  2     2 0.53983E+07 0.45000E+02 0.51000E+00 0.15438E+03 -.35318E-23 0.72223E+06 0.89768E+00 0.20880E+00 0.93601E-01 0.13517E-04
A1  3     3 0.58429E+07 0.45000E+02 0.51838E+00 0.33324E+00 0.44013E-24 0.71926E+06 0.89052E+00 0.20277E+00 0.98293E-01 0.13655E-04
A1  4     4 0.60741E+07 0.45000E+02 0.52264E+00 -.18234E-01 -.25179E-24 0.71846E+06 0.88702E+00 0.19970E+00 0.10068E+00 0.13724E-04
A1  5     5 0.62340E+07 0.45000E+02 0.52572E+00 -.19030E-01 0.96799E-25 0.71913E+06 0.88489E+00 0.19748E+00 0.10241E+00 0.13764E-04
A1  6     6 0.63594E+07 0.45000E+02 0.52842E+00 -.18970E-01 -.13450E-23 0.72149E+06 0.88360E+00 0.19554E+00 0.10391E+00 0.13780E-04
A1  7     7 0.64647E+07 0.45000E+02 0.53110E+00 -.18827E-01 0.16905E-23 0.72616E+06 0.88307E+00 0.19361E+00 0.10542E+00 0.13771E-04
A1  8     8 0.65565E+07 0.45000E+02 0.53406E+00 -.18597E-01 -.10550E-23 0.73416E+06 0.88334E+00 0.19148E+00 0.10707E+00 0.13733E-04
A1  9     9 0.66387E+07 0.45000E+02 0.53756E+00 -.18260E-01 0.49221E-25 0.74713E+06 0.88453E+00 0.18896E+00 0.10903E+00 0.13659E-04
A1 10    10 0.67133E+07 0.45000E+02 0.54186E+00 -.17783E-01 0.26707E-24 0.76760E+06 0.88679E+00 0.18586E+00 0.11144E+00 0.13538E-04
A1 11    11 0.67818E+07 0.45000E+02 0.54715E+00 -.17123E-01 0.28679E-24 0.79910E+06 0.89010E+00 0.18206E+00 0.11440E+00 0.13370E-04
A1 12    12 0.68450E+07 0.45000E+02 0.55272E+00 -.16630E-01 0.44122E-24 0.84390E+06 0.89396E+00 0.17821E+00 0.11807E+00 0.13176E-04
A1 13    13 0.69042E+07 0.45000E+02 0.55720E+00 -.15913E-01 0.53291E-24 0.88974E+06 0.89683E+00 0.17525E+00 0.12147E+00 0.13031E-04
A1 14    14 0.69610E+07 0.45000E+02 0.55880E+00 -.15287E-01 0.56659E-25 0.89539E+06 0.89659E+00 0.17419E+00 0.12269E+00 0.13032E-04
A1 15    15 0.70159E+07 0.45000E+02 0.56014E+00 -.14789E-01 -.48841E-24 0.89510E+06 0.89599E+00 0.17331E+00 0.12371E+00 0.13049E-04
A1 16    16 0.70694E+07 0.45000E+02 0.56162E+00 -.14442E-01 -.46769E-24 0.89458E+06 0.89539E+00 0.17233E+00 0.12483E+00 0.13067E-04
A1 17    17 0.71217E+07 0.45000E+02 0.56328E+00 -.14269E-01 0.18349E-24 0.89407E+06 0.89481E+00 0.17123E+00 0.12610E+00 0.13084E-04
A1 18    18 0.71730E+07 0.45000E+02 0.56516E+00 -.14296E-01 -.81674E-26 0.89357E+06 0.89424E+00 0.16999E+00 0.12752E+00 0.13101E-04
A1 19    19 0.72233E+07 0.45000E+02 0.56726E+00 -.14546E-01 -.15403E-24 0.89308E+06 0.89369E+00 0.16861E+00 0.12912E+00 0.13118E-04
A1 20    20 0.72727E+07 0.45000E+02 0.56956E+00 -.15034E-01 -.22254E-24 0.89259E+06 0.89315E+00 0.16709E+00 0.13086E+00 0.13135E-04
A1 21    21 0.73214E+07 0.45000E+02 0.57200E+00 -.15760E-01 0.71336E-26 0.89212E+06 0.89262E+00 0.16548E+00 0.13272E+00 0.13152E-04
A1 22    22 0.73690E+07 0.45000E+02 0.57449E+00 -.16700E-01 0.11439E-25 0.89166E+06 0.89210E+00 0.16384E+00 0.13461E+00 0.13168E-04
A1 23    23 0.74154E+07 0.45000E+02 0.57686E+00 -.17790E-01 -.81140E-26 0.89120E+06 0.89160E+00 0.16227E+00 0.13642E+00 0.13184E-04
A1 24    24 0.74602E+07 0.45000E+02 0.57898E+00 -.18915E-01 -.37361E-26 0.89077E+06 0.89112E+00 0.16087E+00 0.13803E+00 0.13200E-04
A1 25    25 0.75028E+07 0.45000E+02 0.58078E+00 -.19921E-01 -.34879E-27 0.89036E+06 0.89066E+00 0.15968E+00 0.13940E+00 0.13215E-04
A1 26    26 0.75423E+07 0.45000E+02 0.58247E+00 -.20646E-01 -.64421E-27 0.88997E+06 0.89024E+00 0.15857E+00 0.14068E+00 0.13229E-04
A1 27    27 0.75777E+07 0.45000E+02 0.58453E+00 -.20983E-01 0.24789E-28 0.88963E+06 0.88987E+00 0.15721E+00 0.14225E+00 0.13241E-04
A1 28    28 0.76077E+07 0.45000E+02 0.58707E+00 -.20902E-01 -.38893E-28 0.88934E+06 0.88955E+00 0.15553E+00 0.14417E+00 0.13252E-04
A1 29    29 0.76302E+07 0.45000E+02 0.58948E+00 -.20505E-01 -.29193E-29 0.88913E+06 0.88932E+00 0.15394E+00 0.14600E+00 0.13260E-04
A1 30    30 0.76426E+07 0.45000E+02 0.59098E+00 -.20109E-01 0.94896E-33 0.88901E+06 0.88919E+00 0.15295E+00 0.14714E+00 0.13264E-04

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

```
         Law Problem 1 - Part C

                                                                               KCYC =    1  -  ITER =    4  -  TIME =0.103680E+08
ELEMENT SOURCE INDEX      GENERATION RATE     ENTHALPY    FF(GAS)      FF(LIQ.)      P(WB)
                            (KG/S) OR (W)     (J/KG)                                 (PA)

 A1  1   CO2 1    1          0.000000E+00   0.000000E+00 0.000000E+00 0.000000E+00
 A1  1   CH4 1    2          0.000000E+00   0.000000E+00 0.000000E+00 0.000000E+00

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


********** VOLUME- AND MASS-BALANCES ********************************************************************************************

********** [KCYC,ITER] = [   1,  4] *****                                 THE TIME IS 0.103680E+08 SECONDS, OR 0.120000E+03 DAYS


               PHASES PRESENT
*************************************************************
 PHASES       *        GAS          AQUEOUS       ADSORBED
 VOLUME (M^3) * 0.24166090E+04 0.34093473E+04 0.97885702E-05
 MASS   (KG)  * 0.12457760E+06 0.33872263E+07 0.41325400E+08
*************************************************************

               COMPONENT MASS IN PLACE (KG)
***************************************************************************
 PHASES     *    GAS          AQUEOUS        ADSORBED        TOTAL
***************************************************************************
 COMPONENTS *
 WATER      * 0.17718627E+03 0.33836986E+07 0.00000000E+00 0.33838758E+07
 BRINE      * 0.11164848E-16 0.19798750E-12 0.00000000E+00 0.19799867E-12
 NCG        * 0.12405885E+03 0.54432497E+02 0.17959557E+06 0.17977406E+06
 TRC        * 0.10030833E-13 0.16590340E-15 0.54877186E-12 0.55896860E-12
 CH4        * 0.12427635E+06 0.34732110E+04 0.41145805E+08 0.41273554E+08
***************************************************************************

*********************************************************************************************************************************
```

Figure C-6. Selected Law et al. (2002) Problem Output – Part 3

Appendix D
Binary Gas Problem for He-Ar

As discussed in Mason and Malinauskas (1983), the binary gas diffusion data from Evans et al. (1962. 1963) are for a low-permeability (2.13 x 10^{-18} m^2) graphite system 0.447 cm thick with a porosity of 0.11 and a porosity-tortuosity factor of 1.42 x 10^{-4} (Evans et al., 1962). Mason and Malinauskas (1983) analyzed the experiments using a constant He-Ar gas viscosity of 228. x 10^{-7} Pa-s.

The input and output for the binary gas diffusion problem is summarized in this appendix. In order to facilitate this simulation on other computers, a special value of IE(16) (Oldenburg et al. 2004) of 10 has been programmed. When IE(16) equals 10, the ncg properties are set to Argon, the CH_4 properties are set to Helium, the gases are assumed to be perfect gases (compressibility factor of 1.0), and the gas-phase viscosity is set equal to 228. x 10^{-7} Pa-s, consistent with the Evans et al. (1962, 1963) experiments.

Figure D-1 shows the input file for a combined advection and diffusion problem where the average pressure is 1.96 atm (198.6 kPa) and the pressure difference across the graphite is -0.39 atm (-40. kPa).

```
*He(ch4)/Ar(ncg) Test Problem - 5 components
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
vados    2  2600.e00      0.11  2.13e-18  2.13e-18  2.13e-18      2.51      920.
                                 1.29e-3  1.460e-8
    7           .457       .15        1.       .10
    7           .457       .00  5.105e-4      1.e7        1.

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    5    5    2    9
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   32000     10020 00 000020000400 06
              1.e7      100.                          9.81
     1.e-5
             1.986E5  .0000000000000E+00                0.5                 0.0
              0.5000  .2500000000000E+02
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6
      0.01 31.5576e6 157.788e6 315.576e6 946.728e6 3.15576e9
SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6                                                                1    1   10
     -1.e5

     0.e-0     0.e-1
     0.e-6     0.e-6     0.e-6    -1.e-6    -1.e-6     0.e-6
     1.e50     28.96     0.e-6    -1.e-6                       2.10e-08
     1.e50     28.96    -1.e-6     0.e-6                       1.18e-08

     diffusivity data are input as follows:
     first row:  water (gas, liq.)
     second row: brine (gas, liq.)
     third row:  ncg   (gas, liq.)
     fourth row: trc   (gas, liq.)
     fifth row:  ch4   (gas, liq.)
DIFFU----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
     1.e-6    1.e-10
     0.e-6    1.e-10
     1.e-6    1.e-10
     1.e-6    1.e-10
     1.e-6    1.e-10

     diffusivity values for DGM are input as follows (assumes Dj-i = Di-j):
     first row:   D1-2, D1-3, D1-4, D1-5
     second row:  D2-3, D2-4, D2-5
     third row:   D3-4, D3-5
     fourth row:  D4-5
DGM
    1.0e-9    1.0e-9    1.0e-9    1.0e-9
    1.0e-9    1.0e-9    1.0e-9
    1.0e-9   7.46e-5
    1.0e-9
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1          vados .1000E+11 .0000E+01           .5000E+00 .5000E+00-.5000E+00
A21 1          vados .1000E-02 .0000E+00           .5000E+00 .5000E+00-.1500E+01
A31 1          vados .1000E-02 .0000E+01           .5000E+00 .5000E+00-.5000E+00
A41 1          vados .1000E-02 .0000E+00           .5000E+00 .5000E+00-.1500E+01
A51 1          vados .1000E-02 .0000E+01           .5000E+00 .5000E+00-.5000E+00
A61 1          vados .1000E-02 .0000E+00           .5000E+00 .5000E+00-.1500E+01
A71 1          vados .1000E-02 .0000E+01           .5000E+00 .5000E+00-.5000E+00
A81 1          vados .1000E-02 .0000E+00           .5000E+00 .5000E+00-.1500E+01
A91 1          vados .1000E-02 .0000E+01           .5000E+00 .5000E+00-.5000E+00
AA1 1          vados .1000E-02 .0000E+00           .5000E+00 .5000E+00-.1500E+01
AB1 1          vados .1000E-02 .0000E+00           .5000E+00 .5000E+00-.1500E+01
AC1 1          vados .1000E+11 .0000E+00           .5000E+00 .5000E+00-.1500E+01

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1A21 1                   1 0.0000001 0.0002235 1.000e-00
A21 1A31 1                   1 0.0002235 0.0002235 1.000e-00
A31 1A41 1                   1 0.0002235 0.0002235 1.000e-00
A41 1A51 1                   1 0.0002235 0.0002235 1.000e-00
A51 1A61 1                   1 0.0002235 0.0002235 1.000e-00
A61 1A71 1                   1 0.0002235 0.0002235 1.000e-00
A71 1A81 1                   1 0.0002235 0.0002235 1.000e-00
A81 1A91 1                   1 0.0002235 0.0002235 1.000e-00
A91 1AA1 1                   1 0.0002235 0.0002235 1.000e-00
AA1 1AB1 1                   1 0.0002235 0.0002235 1.000e-00
AB1 1AC1 1                   1 0.0002235 0.0000001 1.000e-00
```

```
INCON -- INITIAL CONDITIONS FOR   19 ELEMENTS AT TIME   .100000E-08
A11 1
             1.786E5                 0.0             0.99703                 0.0
             0.00297               25.00
A21 1
             1.986E5                 0.0                0.99                 0.0
                0.01               25.00
A31 1
             1.986E5                 0.0                0.99                 0.0
                0.01               25.00
A41 1
             1.986E5                 0.0                0.99                 0.0
                0.01               25.00
A51 1
             1.986E5                 0.0                0.99                 0.0
                0.01               25.00
A61 1
             1.986E5                 0.0                0.99                 0.0
                0.01               25.00
A71 1
             1.986E5                 0.0                0.99                 0.0
                0.01               25.00
A81 1
             1.986E5                 0.0                0.99                 0.0
                0.01               25.00
A91 1
             1.986E5                 0.0                0.99                 0.0
                0.01               25.00
AA1 1
             1.986E5                 0.0                0.99                 0.0
                0.01               25.00
AB1 1
             1.986E5                 0.0                0.99                 0.0
                0.01               25.00
AC1 1
             2.186E5                 0.0               0.077                 0.0
               0.923               25.00

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure D-1. He-Ar Advection plus Advection Problem Input

```
*He(ch4)/Ar(ncg) Test Problem - 5 components

          OUTPUT DATA AFTER (  32,  2)-2-TIME STEPS                                                   THE TIME IS 0.115741E+03 DAYS

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

  TOTAL TIME     KCYC   ITER  ITERC   KON        DX1M         DX2M         DX3M          MAX. RES.      NER    KER        DELTEX
 0.100000E+08     32      2     94     2       0.26817E-02  0.30881E-23  0.38490E-07    0.66456E-06       2     3       0.46311E+07

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


 ELEM.  INDEX      P           T         SL        XBRINE(LIQ)  XNCG(LIQ)   XTRC(LIQ)   XCH4(LIQ)   XNCG(GAS)   XTRC(GAS)   XCH4(GAS)      DG
                 (PA)      (DEG-C)                                                                                                     (KG/M**3)

 A11 1     1 0.17860E+06 0.25000E+02 0.00000E+00 0.28300E-22 0.22616E-02 0.31554E-42 0.29154E-06 0.99703E+00 0.69415E-40 0.29700E-02 0.28031E+01
 A21 1     2 0.18013E+06 0.25000E+02 0.00000E+00 0.00000E+00 0.19628E-02 0.93628E-35 0.16731E-05 0.98067E+00 0.23343E-32 0.19334E-01 0.24729E+01
 A31 1     3 0.18349E+06 0.25000E+02 0.00000E+00 0.90817E-26 0.14514E-02 0.95357E-35 0.40760E-05 0.93892E+00 0.30789E-32 0.61078E-01 0.19089E+01
 A41 1     4 0.18710E+06 0.25000E+02 0.00000E+00 0.00000E+00 0.10654E-02 0.97285E-35 0.59480E-05 0.88538E+00 0.40366E-32 0.11462E+00 0.14851E+01
 A51 1     5 0.19093E+06 0.25000E+02 0.00000E+00 0.72939E-26 0.77429E-03 0.99275E-35 0.74204E-05 0.81805E+00 0.52387E-32 0.18195E+00 0.11676E+01
 A61 1     6 0.19494E+06 0.25000E+02 0.00000E+00 0.00000E+00 0.55489E-03 0.10138E-34 0.85921E-05 0.73551E+00 0.67139E-32 0.26449E+00 0.93023E+00
 A71 1     7 0.19908E+06 0.25000E+02 0.00000E+00 0.12534E-25 0.38961E-03 0.10354E-34 0.95372E-05 0.63746E+00 0.84653E-32 0.36254E+00 0.75340E+00
 A81 1     8 0.20332E+06 0.25000E+02 0.00000E+00 0.62477E-26 0.26511E-03 0.10576E-34 0.10312E-04 0.52521E+00 0.10471E-31 0.47479E+00 0.62209E+00
 A91 1     9 0.20764E+06 0.25000E+02 0.00000E+00 0.00000E+00 0.17127E-03 0.10801E-34 0.10958E-04 0.40203E+00 0.12672E-31 0.59797E+00 0.52496E+00
 AA1 1    10 0.21200E+06 0.25000E+02 0.00000E+00 0.97976E-26 0.10046E-03 0.11028E-34 0.11507E-04 0.27299E+00 0.14977E-31 0.72701E+00 0.45349E+00
 AB1 1    11 0.21640E+06 0.25000E+02 0.00000E+00 0.00000E+00 0.46946E-04 0.11257E-34 0.11983E-04 0.14418E+00 0.17278E-31 0.85582E+00 0.40124E+00
 AC1 1    12 0.21860E+06 0.25000E+02 0.00000E+00 0.48441E-26 0.23681E-04 0.11372E-34 0.12207E-04 0.77000E-01 0.18479E-31 0.92300E+00 0.37899E+00

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


 ELEM.  INDEX     PHIS        PHIF      DPHINCG     DPHITRC     DPHICH4     MASST       MASSNCG     MASSTRC     MASSCH4
                                                                            (KG)        (KG)        (KG)       (KG)

 A11 1     1 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A21 1     2 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A31 1     3 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A41 1     4 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A51 1     5 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A61 1     6 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A71 1     7 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A81 1     8 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A91 1     9 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 AA1 1    10 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 AB1 1    11 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 AC1 1    12 0.11000E+00 0.11000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00

          *He(ch4)/Ar(ncg) Test Problem - 5 components

                                                                                KCYC =   32  -  ITER =    2  -  TIME =0.100000E+08
     ELEM1  ELEM2  INDEX    FLOH      FLOH/FLOF       FLOF       FLO(BRINE)   FLO(GAS)     FLO(LIQ.)    VEL(GAS)     VEL(LIQ.)
                            (W)        (J/KG)        (KG/S)       (KG/S)       (KG/S)       (KG/S)      (M/S)        (M/S)

     A11 1  A21 1     1 0.603432E-01 0.381540E+05 0.158157E-05 0.000000E+00 0.158157E-05 0.000000E+00 0.581416E-05 0.000000E+00
     A21 1  A31 1     2 0.100557E+00 0.751172E+05 0.133867E-05 0.000000E+00 0.133867E-05 0.000000E+00 0.637524E-05 0.000000E+00
     A31 1  A41 1     3 0.137451E+00 0.122537E+06 0.112171E-05 0.000000E+00 0.112171E-05 0.000000E+00 0.686635E-05 0.000000E+00
     A41 1  A51 1     4 0.170427E+00 0.182314E+06 0.934801E-06 0.000000E+00 0.934801E-06 0.000000E+00 0.727860E-05 0.000000E+00
     A51 1  A61 1     5 0.199331E+00 0.255940E+06 0.778819E-06 0.000000E+00 0.778819E-06 0.000000E+00 0.761117E-05 0.000000E+00
     A61 1  A71 1     6 0.224415E+00 0.344109E+06 0.652164E-06 0.000000E+00 0.652164E-06 0.000000E+00 0.786930E-05 0.000000E+00
     A71 1  A81 1     7 0.246273E+00 0.446412E+06 0.551672E-06 0.000000E+00 0.551672E-06 0.000000E+00 0.806189E-05 0.000000E+00
     A81 1  A91 1     8 0.265833E+00 0.561448E+06 0.473477E-06 0.000000E+00 0.473477E-06 0.000000E+00 0.819932E-05 0.000000E+00
```

```
    A91 1  AA1 1     9 0.284595E+00 0.688039E+06 0.413632E-06 0.000000E+00 0.413632E-06 0.000000E+00 0.829194E-05 0.000000E+00
    AA1 1  AB1 1    10 0.305790E+00 0.829829E+06 0.368497E-06 0.000000E+00 0.368497E-06 0.000000E+00 0.834913E-05 0.000000E+00
    AB1 1  AC1 1    11 0.321204E+00 0.920466E+06 0.348958E-06 0.000000E+00 0.348958E-06 0.000000E+00 0.837041E-05 0.000000E+00

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


         *He(ch4)/Ar(ncg) Test Problem - 5 components

                                                                               KCYC =   32  -  ITER =    2  -  TIME =0.100000E+08
MASS FLOW RATES (KG/S) FROM DIFFUSION

ELEM1 ELEM2  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP
              gas   wv    gas   br    gas  ncg    gas  trc    gas  ch4    liq   wv    liq   br    liq  ncg    liq  trc    liq  ch4

A11 1 A21 1 0.00000E+00 0.75457E-31 -.18860E-05 0.16715E-37 0.10308E-05 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A21 1 A31 1 0.88075E-21 0.24015E-31 -.15919E-05 0.16285E-37 0.97961E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A31 1 A41 1 0.19508E-20 0.23412E-31 -.13282E-05 0.15879E-37 0.93279E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A41 1 A51 1 0.12307E-20 0.10798E-31 -.10997E-05 0.15510E-37 0.89128E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A51 1 A61 1 0.28632E-21 0.10564E-31 -.90785E-06 0.15178E-37 0.85538E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A61 1 A71 1 0.51357E-21 0.11022E-31 -.75075E-06 0.14886E-37 0.82493E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A71 1 A81 1 0.10043E-20 0.15195E-31 -.62476E-06 0.14630E-37 0.79944E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A81 1 A91 1 0.86343E-21 0.42975E-32 -.52537E-06 0.14407E-37 0.77825E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A91 1 AA1 1 0.24900E-21 0.46491E-32 -.44794E-06 0.14212E-37 0.76066E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
AA1 1 AB1 1 0.33834E-22 0.45915E-32 -.38815E-06 0.14040E-37 0.74600E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
AB1 1 AC1 1 0.67284E-22 0.21694E-35 -.36189E-06 0.13958E-37 0.73928E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

         *He(ch4)/Ar(ncg) Test Problem - 5 components

                                                                               KCYC =   32  -  ITER =    2  -  TIME =0.100000E+08

                                                        IE(14) = 1 (H FROM SUPST AND ZEVSREAL)


ELEM.  INDEX    P            T           SL         DX1         DX2       H(GAS)       ZFAC        K(GAS)      K(LIQ.)    VIS(GAS)
                                                                          (J/KG)                                          (PA S)

A11 1     1 0.17860E+06 0.25000E+02 0.00000E+00 0.26817E-02 -.30881E-23 0.23634E+05 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
A21 1     2 0.18013E+06 0.25000E+02 0.00000E+00 0.24781E-02 0.00000E+00 0.38154E+05 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
A31 1     3 0.18349E+06 0.25000E+02 0.00000E+00 0.20121E-02 0.88337E-28 0.75117E+05 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
A41 1     4 0.18710E+06 0.25000E+02 0.00000E+00 0.15005E-02 0.00000E+00 0.12254E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
A51 1     5 0.19093E+06 0.25000E+02 0.00000E+00 0.95751E-03 0.19145E-27 0.18231E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
A61 1     6 0.19494E+06 0.25000E+02 0.00000E+00 0.39597E-03 0.00000E+00 0.25594E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
A71 1     7 0.19908E+06 0.25000E+02 0.00000E+00 -.17362E-03 0.32997E-26 0.34411E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
A81 1     8 0.20332E+06 0.25000E+02 0.00000E+00 -.74344E-03 0.17414E-26 0.44641E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
A91 1     9 0.20764E+06 0.25000E+02 0.00000E+00 -.13082E-02 0.00000E+00 0.56145E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
AA1 1    10 0.21200E+06 0.25000E+02 0.00000E+00 -.18646E-02 0.76095E-26 0.68804E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
AB1 1    11 0.21640E+06 0.25000E+02 0.00000E+00 -.24109E-02 -.81113E-26 0.82983E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04
AC1 1    12 0.21860E+06 0.25000E+02 0.00000E+00 -.26817E-02 0.59558E-34 0.92047E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.22800E-04

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

```
********** VOLUME- AND MASS-BALANCES ********************************************************************************************

********** [KCYC,ITER] = [  32,  2] *****                                  THE TIME IS 0.100000E+08 SECONDS, OR 0.115741E+03 DAYS


               PHASES PRESENT
*************************************************************
 PHASES       *        GAS          AQUEOUS       ADSORBED
 VOLUME (M^3) * 0.22000000E+10 0.00000000E+00 0.00000000E+00
 MASS   (KG)  * 0.35002595E+10 0.00000000E+00 0.00000000E+00
*************************************************************

               COMPONENT MASS IN PLACE (KG)
***************************************************************************
 PHASES     *    GAS          AQUEOUS        ADSORBED        TOTAL
***************************************************************************
 COMPONENTS *
 WATER      * -.29025216E-06 0.00000000E+00 0.00000000E+00 -.29025216E-06
 BRINE      * 0.87261531E-13 0.00000000E+00 0.00000000E+00 0.87261531E-13
 NCG        * 0.31063084E+10 0.00000000E+00 0.00000000E+00 0.31063084E+10
 TRC        * 0.77037196E-23 0.00000000E+00 0.00000000E+00 0.77037196E-23
 CH4        * 0.39395108E+09 0.00000000E+00 0.00000000E+00 0.39395108E+09
***************************************************************************

**********************************************************************************************************************************
```

Figure D-2. Selected He-Ar Advection plus Advection Problem Output

Appendix E
Diffusion Across Capillary Fringe

The problem is based on the TOUGH2 capillary fringe sample problem given by Pruess et al.(1999). Similar to the Dusty Gas Model simulations for He-Ar, a special value of IE(16) has been implemented to change the physical properties. For IE(16)=11, the ncg gas is PCE and CH4 is air with respective values of Henry's constant of 1.18 x 10^{-8} and 1.0 x 10^{-10} Pa^{-1}, and the gases are assumed to be perfect gases (compressibility factor of 1.0). The TCE properties are input through the trc gas input in the SELECT block.

The input file for the coupled DGM problem is shown in Figure E-1, while the final output results are given in Figure E-2.

```
*rdica* ... diffusion in a 1-D column across a capillary fringe
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
vados    2  2600.e00       .35    1.e-11   1.0e-11    1.e-11      2.51      920.
                                    0.25 0.7886e-4
    7           .457       .15        1.       .10
    7           .457       .00  5.105e-4      1.e7        1.
trapp    2  2600.e00       .35    0.e-11    0.e-11    0.e-11      2.51      920.
                                    0.25 0.7886e-4
    7           .457       .15        1.       .10
    7           .457       .00  5.105e-4      1.e7        1.
atmos    2  2600.e00       .35    1.e-11   1.0e-11    1.e-11      2.51      920.
                                     1.0 0.7886e-4
    7           .457       .15        1.       .10
    1             0.        0.        1.
aquif    2  2600.e00       .35    1.e-11   1.0e-11    1.e-11      2.51      920.
                                    0.25 0.7886e-4
    7           .457       .15        1.       .10
    7           .457       .00  5.105e-4      1.e7        1.

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    5    5    2    9
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3 200     99910 0 0000020000400 00  3
           3.15576e9        1.          A51 1           9.81
     1.e-5
             1.013e5                  0.                  0.                  0.
               10.50                20.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6
        1. 31.5576e6 157.788e6 315.576e6 946.728e6 3.15576e9
SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6                                                                1    1   11
     -1.e5

     0.e-0     0.e-1
     0.e-6     0.e-6     0.e-6    -1.e-6    -1.e-6     0.e-6

     1.e50   131.389    -1.e-6     0.e-6                      2.10e-08

     diffusivity data are input as follows:
     first row:  water (gas, liq.)
     second row: brine (gas, liq.)
     third row:  rn1   (gas, liq.)
     fourth row: rn2   (gas, liq.)
     fifth row:  air   (gas, liq.)
DIFFU----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
     1.e-6    1.e-10
     0.e-6    1.e-10
     1.e-6    1.e-10
     1.e-6    1.e-10
     1.e-6    1.e-10

     diffusivity values for DGM are input as follows (assumes Dj-i = Di-j):
     first row:   D1-2, D1-3, D1-4, D1-5
     second row:  D2-3, D2-4, D2-5
     third row:   D3-4, D3-5
     fourth row:  D4-5
DGM
    1.0e-6    1.0e-6    1.0e-6    1.0e-6
    1.0e-6    1.0e-6    1.0e-6
    1.0e-6    1.0e-6
    1.0e-6
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1          vados .1000E+01 .1000E+01           .5000E+00 .5000E+00-.5000E+00
A21 1          vados .1000E+01 .0000E+00           .5000E+00 .5000E+00-.1500E+01
A31 1          vados .1000E+01 .0000E+00           .5000E+00 .5000E+00-.2500E+01
A41 1          vados .1000E+01 .0000E+00           .5000E+00 .5000E+00-.3500E+01
A51 1          vados .1000E+01 .0000E+00           .5000E+00 .5000E+00-.4500E+01
A61 1          vados .1000E+01 .0000E+00           .5000E+00 .5000E+00-.5500E+01
A71 1          vados .1000E+01 .0000E+00           .5000E+00 .5000E+00-.6500E+01
A81 1          vados .1000E+01 .0000E+00           .5000E+00 .5000E+00-.7500E+01
A91 1          vados .1000E+01 .0000E+00           .5000E+00 .5000E+00-.8500E+01
AA1 1          vados .1000E+01 .0000E+00           .5000E+00 .5000E+00-.9500E+01
AB1 1          vados .1000E+01 .0000E+00           .5000E+00 .5000E+00-.1050E+02
AC1 1          aquif .1000E+01 .0000E+00           .5000E+00 .5000E+00-.1150E+02
AD1 1          aquif .1000E+01 .0000E+00           .5000E+00 .5000E+00-.1250E+02
AE1 1          aquif .1000E+01 .0000E+00           .5000E+00 .5000E+00-.1350E+02
AF1 1          aquif .1000E+01 .1000E+01           .5000E+00 .5000E+00-.1450E+02
ina 0
```

```
con 0          trapp
top 0          atmos        1.
bot 0          aquif        1.

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
con 0A51 1                   1     1.e-9        .5     1.e-1
top 0A11 1                   3     1.e-9        .5        1.        1.
A11 1A21 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
A21 1A31 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
A31 1A41 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
A41 1A51 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
A51 1A61 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
A61 1A71 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
A71 1A81 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
A81 1A91 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
A91 1AA1 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
AA1 1AB1 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
AB1 1AC1 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
AC1 1AD1 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
AD1 1AE1 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
AE1 1AF1 1                   3 .5000E+00 .5000E+00 .1000E+01 .1000E+01
AF1 1bot 0                   3        .5     1.e-9        1.        1.

INCON -- INITIAL CONDITIONS FOR   19 ELEMENTS AT TIME   .100000E-08
A11 1            .35000000E+00
  .1011830232536E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1084703339434E+02  .2000000000000E+02
A21 1            .35000000E+00
  .1011947147937E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1084652396067E+02  .2000000000000E+02
A31 1            .35000000E+00
  .1012064076966E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1084617651200E+02  .2000000000000E+02
A41 1            .35000000E+00
  .1012181019624E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1084590472686E+02  .2000000000000E+02
A51 1            .35000000E+00
  .1012297975914E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1084567823274E+02  .2000000000000E+02
A61 1            .35000000E+00
  .1012414945837E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1084548237028E+02  .2000000000000E+02
A71 1            .35000000E+00
  .1012531929394E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1084530856830E+02  .2000000000000E+02
A81 1            .35000000E+00
  .1012648926587E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1084513459288E+02  .2000000000000E+02
A91 1            .35000000E+00
  .1012765937418E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1084379900072E+02  .2000000000000E+02
AA1 1            .35000000E+00
  .1012882961888E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1077531383894E+02  .2000000000000E+02
AB1 1            .35000000E+00
  .1013000000000E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1020000000000E+02  .2000000000000E+02
AC1 1            .35000000E+00
  .1095699993696E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .9999999993101E-12  .2000000000000E+02
AD1 1            .35000000E+00
  .1193636094320E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .9999999994380E-12  .2000000000000E+02
AE1 1            .35000000E+00
  .1291572631693E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .9999999999067E-12  .2000000000000E+02
AF1 1            .35000000E+00
  .1389509605809E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .9999999996652E-12  .2000000000000E+02
ina 0            .35000000E+00
  .1013000000000E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .1050000000000E+02  .2000000000000E+02
con 0            .35000000E+00
  .1012297975914E+06  .0000000000000E+00           2.0063e-4           1.0998e-3
  .1084567823274E+02  .2000000000000E+02
top 0            .35000000E+00
  .1011771700865E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .9899948379529E+00  .2000000000000E+02
bot 0            .35000000E+00
  .1438478256741E+06  .0000000000000E+00  1.000000000000E-15  1.000000000000E-15
  .9999999999008E-12  .2000000000000E+02
```

```
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
       00.
NX       1        1.0
NY       1        1.0
NZ      15        1.0


ENDFI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure E-1. Capillary Fringe Problem Input

```
*rdica* ... diffusion in a 1-D column across a capillary fringe

          OUTPUT DATA AFTER (  37,  3)-2-TIME STEPS                                                    THE TIME IS 0.365250E+05 DAYS

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

  TOTAL TIME     KCYC   ITER  ITERC   KON        DX1M         DX2M         DX3M          MAX. RES.      NER    KER        DELTEX
 0.315576E+10     37      3     90     2       0.43471E-01  0.00000E+00  0.14908E-05    0.11884E-07       1      5       0.31902E+09

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


 ELEM.  INDEX     P           T          SL       XBRINE(LIQ)  XNCG(LIQ)   XTRC(LIQ)   XCH4(LIQ)   XNCG(GAS)   XTRC(GAS)   XCH4(GAS)      DG
                 (PA)      (DEG-C)                                                                                                     (KG/M**3)

 A11 1     1 0.10118E+06 0.20000E+02 0.14449E+00 0.00000E+00 0.98592E-05 0.53944E-04 0.15818E-04 0.50972E-02 0.15671E-01 0.96498E+00 0.12116E+01
 A21 1     2 0.10120E+06 0.20000E+02 0.15351E+00 0.00000E+00 0.29921E-04 0.16371E-03 0.15673E-04 0.14969E-01 0.46020E-01 0.92522E+00 0.12523E+01
 A31 1     3 0.10121E+06 0.20000E+02 0.15387E+00 0.00000E+00 0.50448E-04 0.27603E-03 0.15525E-04 0.24429E-01 0.75106E-01 0.88712E+00 0.12939E+01
 A41 1     4 0.10122E+06 0.20000E+02 0.15417E+00 0.00000E+00 0.71365E-04 0.39047E-03 0.15374E-04 0.33466E-01 0.10289E+00 0.85072E+00 0.13363E+01
 A51 1     5 0.10123E+06 0.20000E+02 0.15441E+00 0.00000E+00 0.92676E-04 0.50708E-03 0.15220E-04 0.42103E-01 0.12944E+00 0.81593E+00 0.13795E+01
 A61 1     6 0.10125E+06 0.20000E+02 0.15461E+00 0.00000E+00 0.92655E-04 0.50656E-03 0.15223E-04 0.42093E-01 0.12931E+00 0.81608E+00 0.13795E+01
 A71 1     7 0.10126E+06 0.20000E+02 0.15478E+00 0.00000E+00 0.92635E-04 0.50606E-03 0.15226E-04 0.42084E-01 0.12918E+00 0.81622E+00 0.13795E+01
 A81 1     8 0.10127E+06 0.20000E+02 0.15496E+00 0.00000E+00 0.92616E-04 0.50556E-03 0.15229E-04 0.42075E-01 0.12905E+00 0.81635E+00 0.13795E+01
 A91 1     9 0.10129E+06 0.20000E+02 0.15629E+00 0.00000E+00 0.92599E-04 0.50508E-03 0.15231E-04 0.42066E-01 0.12893E+00 0.81649E+00 0.13795E+01
 AA1 1    10 0.10130E+06 0.20000E+02 0.22448E+00 0.00000E+00 0.92579E-04 0.50455E-03 0.15234E-04 0.42057E-01 0.12879E+00 0.81663E+00 0.13796E+01
 AB1 1    11 0.10131E+06 0.20000E+02 0.79744E+00 0.00000E+00 0.89756E-04 0.45164E-03 0.15297E-04 0.41246E-01 0.11662E+00 0.82947E+00 0.13637E+01
 AC1 1    12 0.10957E+06 0.20000E+02 0.10000E+01 0.00000E+00 0.87772E-06 0.40137E-05 0.22444E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.35821E-01
 AD1 1    13 0.11936E+06 0.20000E+02 0.10000E+01 0.00000E+00 0.35403E-07 0.15524E-06 0.11200E-07 0.00000E+00 0.00000E+00 0.00000E+00 0.18175E-01
 AE1 1    14 0.12916E+06 0.20000E+02 0.10000E+01 0.00000E+00 0.11743E-08 0.50327E-08 0.42330E-09 0.00000E+00 0.00000E+00 0.00000E+00 0.17304E-01
 AF1 1    15 0.13895E+06 0.20000E+02 0.10000E+01 0.00000E+00 0.33975E-10 0.14375E-09 0.14203E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.17271E-01
 ina 0    16 0.10130E+06 0.20000E+02 0.50000E+00 0.00000E+00 0.10000E-14 0.10000E-14 0.15909E-04 0.52499E-12 0.29499E-12 0.98553E+00 0.11931E+01
 con 0    17 0.10123E+06 0.20000E+02 0.15432E+00 0.00000E+00 0.20063E-03 0.10998E-02 0.14428E-04 0.78719E-01 0.24247E+00 0.66801E+00 0.15983E+01
 top 0    18 0.10118E+06 0.20000E+02 0.00000E+00 0.00000E+00 0.19077E-17 0.33950E-17 0.16005E-04 0.10000E-14 0.10000E-14 0.98999E+00 0.11949E+01
 bot 0    19 0.14385E+06 0.20000E+02 0.10000E+01 0.00000E+00 0.10000E-14 0.10000E-14 0.10000E-11 0.00000E+00 0.00000E+00 0.00000E+00 0.17270E-01

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


 ELEM.  INDEX    PHIS        PHIF      DPHINCG     DPHITRC     DPHICH4     MASST       MASSNCG     MASSTRC     MASSCH4
                                                                            (KG)        (KG)        (KG)        (KG)

 A11 1     1 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A21 1     2 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A31 1     3 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A41 1     4 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A51 1     5 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A61 1     6 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A71 1     7 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A81 1     8 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 A91 1     9 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 AA1 1    10 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 AB1 1    11 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 AC1 1    12 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 AD1 1    13 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 AE1 1    14 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 AF1 1    15 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 ina 0    16 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 con 0    17 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 top 0    18 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 bot 0    19 0.35000E+00 0.35000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
```

```
         *rdica* ... diffusion in a 1-D column across a capillary fringe

                                                                               KCYC =   37  -  ITER =    3  -  TIME =0.315576E+10
    ELEM1  ELEM2  INDEX    FLOH      FLOH/FLOF       FLOF       FLO(BRINE)   FLO(GAS)     FLO(LIQ.)    VEL(GAS)     VEL(LIQ.)
                            (W)       (J/KG)        (KG/S)       (KG/S)       (KG/S)       (KG/S)      (M/S)        (M/S)

    con 0  A51 1     1 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
    top 0  A11 1     2 0.478006E-03 0.929432E+06 0.514299E-09 0.000000E+00 0.514299E-09 0.000000E+00 0.141759E-08 0.000000E+00
    A11 1  A21 1     3 -.707613E-03 0.929432E+06 -.761339E-09 0.000000E+00 -.761339E-09 0.000000E+00 -.209852E-08 0.000000E+00
    A21 1  A31 1     4 -.753447E-03 0.967697E+06 -.778598E-09 0.000000E+00 -.778550E-09 -.476247E-13 -.209842E-08 -.887912E-15
    A31 1  A41 1     5 -.799893E-03 0.100507E+07 -.795856E-09 0.000000E+00 -.795778E-09 -.775877E-13 -.207680E-08 -.144308E-14
    A41 1  A51 1     6 -.846558E-03 0.104121E+07 -.813054E-09 0.000000E+00 -.812943E-09 -.110755E-12 -.205499E-08 -.205605E-14
    A51 1  A61 1     7 -.106431E-04 0.106167E+07 -.100248E-10 0.000000E+00 -.987789E-11 -.146942E-12 -.241946E-10 -.272344E-14
    A61 1  A71 1     8 -.105177E-04 0.105788E+07 -.994221E-11 0.000000E+00 -.976057E-11 -.181641E-12 -.239127E-10 -.336230E-14
    A71 1  A81 1     9 -.103569E-04 0.105385E+07 -.982773E-11 0.000000E+00 -.961017E-11 -.217567E-12 -.235489E-10 -.402279E-14
    A81 1  A91 1    10 -.101612E-04 0.104951E+07 -.968180E-11 0.000000E+00 -.942706E-11 -.254734E-12 -.231047E-10 -.470472E-14
    A91 1  AA1 1    11 -.990224E-05 0.104436E+07 -.948164E-11 0.000000E+00 -.918473E-11 -.296903E-12 -.225461E-10 -.543665E-14
    AA1 1  AB1 1    12 -.958568E-05 0.795352E+06 -.120521E-10 0.000000E+00 -.864962E-11 -.340250E-11 -.230992E-10 -.433798E-13
    AB1 1  AC1 1    13 -.226160E-05 0.839548E+05 -.269383E-10 0.000000E+00 0.000000E+00 -.269383E-10 0.000000E+00 -.966785E-13
    AC1 1  AD1 1    14 -.231115E-05 0.839626E+05 -.275260E-10 0.000000E+00 0.000000E+00 -.275260E-10 0.000000E+00 -.787774E-13
    AD1 1  AE1 1    15 -.231434E-05 0.839718E+05 -.275609E-10 0.000000E+00 0.000000E+00 -.275609E-10 0.000000E+00 -.788771E-13
    AE1 1  AF1 1    16 -.231473E-05 0.839810E+05 -.275625E-10 0.000000E+00 0.000000E+00 -.275625E-10 0.000000E+00 -.788813E-13
    AF1 1  bot 0    17 -.231497E-05 0.839902E+05 -.275624E-10 0.000000E+00 0.000000E+00 -.275624E-10 0.000000E+00 -.788806E-13

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

         *rdica* ... diffusion in a 1-D column across a capillary fringe

                                                                               KCYC =   37  -  ITER =    3  -  TIME =0.315576E+10
MASS FLOW RATES (KG/S) FROM DIFFUSION

ELEM1 ELEM2  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP
              gas   wv    gas   br    gas  ncg    gas  trc    gas  ch4    liq   wv    liq   br    liq  ncg    liq  trc    liq  ch4

con 0 A51 1 0.26319E-10 0.00000E+00 -.10657E-08 -.32898E-08 0.27036E-08 0.24464E-24 0.00000E+00 -.28546E-24 -.15673E-23 0.20692E-26
top 0 A11 1 0.90627E-09 0.00000E+00 0.10610E-08 0.32630E-08 -.32002E-08 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A11 1 A21 1 -.15725E-10 0.00000E+00 0.10675E-08 0.32830E-08 -.19681E-08 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
A21 1 A31 1 -.15842E-10 0.00000E+00 0.10753E-08 0.33070E-08 -.19825E-08 -.93246E-25 0.00000E+00 0.10914E-24 0.59713E-24 -.77759E-27
A31 1 A41 1 -.15959E-10 0.00000E+00 0.10831E-08 0.33310E-08 -.19969E-08 -.14678E-24 0.00000E+00 0.17179E-24 0.93997E-24 -.12238E-26
A41 1 A51 1 -.16077E-10 0.00000E+00 0.10909E-08 0.33551E-08 -.20113E-08 -.20689E-24 0.00000E+00 0.24213E-24 0.13249E-23 -.17246E-26
A51 1 A61 1 -.13207E-12 0.00000E+00 -.15534E-11 -.16851E-10 0.87202E-11 0.10415E-26 0.00000E+00 -.30365E-27 -.75371E-26 0.40103E-28
A61 1 A71 1 -.13304E-12 0.00000E+00 -.15148E-11 -.16579E-10 0.85781E-11 0.12457E-26 0.00000E+00 -.35630E-27 -.90236E-26 0.48676E-28
A71 1 A81 1 -.13433E-12 0.00000E+00 -.14655E-11 -.16230E-10 0.83953E-11 0.14515E-26 0.00000E+00 -.40446E-27 -.10528E-25 0.57845E-28
A81 1 A91 1 -.13562E-12 0.00000E+00 -.14058E-11 -.15805E-10 0.81725E-11 0.23526E-26 0.00000E+00 -.63393E-27 -.17092E-25 0.95983E-28
A91 1 AA1 1 -.11741E-12 0.00000E+00 -.13373E-11 -.15309E-10 0.78886E-11 0.10802E-25 0.00000E+00 -.29451E-26 -.78312E-25 0.41057E-27
AA1 1 AB1 1 0.55309E-13 0.00000E+00 -.12657E-11 -.14706E-10 0.73630E-11 0.19214E-18 0.00000E+00 -.72163E-19 -.13513E-17 0.15803E-20
AB1 1 AC1 1 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.10652E-12 0.00000E+00 -.11774E-12 -.59298E-12 -.19967E-13
AC1 1 AD1 1 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.65795E-14 0.00000E+00 -.73580E-14 -.33705E-13 -.18627E-14
AD1 1 AE1 1 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.27095E-15 0.00000E+00 -.29900E-15 -.13121E-14 -.94143E-16
AE1 1 AF1 1 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.91609E-17 0.00000E+00 -.99610E-17 -.42708E-16 -.35737E-17
AF1 1 bot 0 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.55231E-18 0.00000E+00 -.59356E-18 -.25114E-17 -.23066E-18
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

         *rdica* ... diffusion in a 1-D column across a capillary fringe

                                                                               KCYC =   37  -  ITER =    3  -  TIME =0.315576E+10

                                                        IE(14) = 1 (H FROM SUPST AND ZEVSREAL)
```

```
ELEM.  INDEX    P            T           SL         DX1         DX2       H(GAS)       ZFAC        K(GAS)      K(LIQ.)    VIS(GAS)
                                                                          (J/KG)                                          (PA S)

A11 1     1 0.10118E+06 0.20000E+02 0.14449E+00 0.37499E-04 0.00000E+00 0.92943E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.10996E-04
A21 1     2 0.10120E+06 0.20000E+02 0.15351E+00 0.33421E-03 0.00000E+00 0.96775E+06 0.10000E+01 0.99065E+00 0.49118E-12 0.11055E-04
A31 1     3 0.10121E+06 0.20000E+02 0.15387E+00 0.92806E-03 0.00000E+00 0.10052E+07 0.10000E+01 0.98967E+00 0.79935E-12 0.11115E-04
A41 1     4 0.10122E+06 0.20000E+02 0.15417E+00 0.18164E-02 0.00000E+00 0.10413E+07 0.10000E+01 0.98889E+00 0.11404E-11 0.11178E-04
A51 1     5 0.10123E+06 0.20000E+02 0.15441E+00 0.29940E-02 0.00000E+00 0.10762E+07 0.10000E+01 0.98823E+00 0.15118E-11 0.11243E-04
A61 1     6 0.10125E+06 0.20000E+02 0.15461E+00 0.45846E-02 0.00000E+00 0.10760E+07 0.10000E+01 0.98771E+00 0.18682E-11 0.11243E-04
A71 1     7 0.10126E+06 0.20000E+02 0.15478E+00 0.67086E-02 0.00000E+00 0.10758E+07 0.10000E+01 0.98724E+00 0.22377E-11 0.11243E-04
A81 1     8 0.10127E+06 0.20000E+02 0.15496E+00 0.93538E-02 0.00000E+00 0.10756E+07 0.10000E+01 0.98678E+00 0.26636E-11 0.11243E-04
A91 1     9 0.10129E+06 0.20000E+02 0.15629E+00 0.12505E-01 0.00000E+00 0.10754E+07 0.10000E+01 0.98322E+00 0.85293E-11 0.11242E-04
AA1 1    10 0.10130E+06 0.20000E+02 0.22448E+00 0.16173E-01 0.00000E+00 0.10752E+07 0.10000E+01 0.80326E+00 0.14612E-05 0.11242E-04
AB1 1    11 0.10131E+06 0.20000E+02 0.79744E+00 0.43471E-01 0.00000E+00 0.10563E+07 0.10000E+01 0.47640E-02 0.82043E-01 0.11215E-04
AC1 1    12 0.10957E+06 0.20000E+02 0.10000E+01 -.33173E-05 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.10000E+01 0.10000E+01
AD1 1    13 0.11936E+06 0.20000E+02 0.10000E+01 -.23692E-05 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.10000E+01 0.10000E+01
AE1 1    14 0.12916E+06 0.20000E+02 0.10000E+01 -.14215E-05 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.10000E+01 0.10000E+01
AF1 1    15 0.13895E+06 0.20000E+02 0.10000E+01 -.47384E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.10000E+01 0.10000E+01
ina 0    16 0.10130E+06 0.20000E+02 0.50000E+00 0.00000E+00 0.00000E+00 0.91001E+06 0.10000E+01 0.22250E+00 0.29961E-02 0.10967E-04
con 0    17 0.10123E+06 0.20000E+02 0.15432E+00 0.00000E+00 0.00000E+00 0.12268E+07 0.10000E+01 0.98848E+00 0.13634E-11 0.11590E-04
top 0    18 0.10118E+06 0.20000E+02 0.00000E+00 0.00000E+00 0.00000E+00 0.90259E+06 0.10000E+01 0.10000E+01 0.00000E+00 0.10965E-04
bot 0    19 0.14385E+06 0.20000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.10000E+01 0.10000E+01

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


********** VOLUME- AND MASS-BALANCES *********************************************************************************************

********** [KCYC,ITER] = [  37,  3] *****                                   THE TIME IS 0.315576E+10 SECONDS, OR 0.365250E+05 DAYS


               PHASES PRESENT
*************************************************************
 PHASES       *        GAS          AQUEOUS       ADSORBED
 VOLUME (M^3) * 0.30089429E+01 0.22410571E+01 0.00000000E+00
 MASS   (KG)  * 0.40236538E+01 0.22373140E+04 0.00000000E+00
*************************************************************

               COMPONENT MASS IN PLACE (KG)
***************************************************************************
 PHASES     *    GAS          AQUEOUS        ADSORBED        TOTAL
***************************************************************************
 COMPONENTS *
 WATER      * 0.51964683E-01 0.22368834E+04 0.00000000E+00 0.22369354E+04
 BRINE      * 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
 NCG        * 0.13558726E+00 0.66337131E-01 0.00000000E+00 0.20192439E+00
 TRC        * 0.41526950E+00 0.35130708E+00 0.00000000E+00 0.76657658E+00
 CH4        * 0.34208324E+01 0.12965252E-01 0.00000000E+00 0.34337976E+01
***************************************************************************

**********************************************************************************************************************************
```

Figure E-2. Selected Capillary Fringe Problem Output