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EOS7C Version 1.0: TOUGH2 Module for Carbon Dioxide or Nitrogen in Natural Gas
(Methane)
Reservoirs

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Publication Date

2004-06-29

EOS7C Version 1.0:
TOUGH2 Module for Carbon Dioxide or Nitrogen in
Natural Gas (Methane) Reservoirs

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March 2004

This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems through the National Energy Technology Laboratory, and by Lawrence Berkeley National Laboratory under Department of Energy Contract No. DE-AC03-76SF00098.

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Abstract

EOS7C is a TOUGH2 module for multicomponent gas mixtures in the systems methane-carbon dioxide ($\text{CH}_4\text{-CO}_2$) or methane-nitrogen ($\text{CH}_4\text{-N}_2$) with or without an aqueous phase and H_2O vapor. EOS7C uses a cubic equation of state and an accurate solubility formulation along with a multiphase Darcy's Law to model flow and transport of gas and aqueous phase mixtures over a wide range of pressures and temperatures appropriate to subsurface geologic carbon sequestration sites and natural gas reservoirs. EOS7C models supercritical CO_2 and subcritical CO_2 as a non-condensable gas, hence EOS7C does not model the transition to liquid or solid CO_2 conditions. The components modeled in EOS7C are water, brine, non-condensable gas, gas tracer, methane, and optional heat. The non-condensable gas (NCG) can be selected by the user to be CO_2 or N_2 . The real gas properties module has options for Peng-Robinson, Redlich-Kwong, or Soave-Redlich-Kwong equations of state to calculate gas mixture density, enthalpy departure, and viscosity. Partitioning of the NCG and CH_4 between the aqueous and gas phases is calculated using a very accurate chemical equilibrium approach. Transport of the gaseous and dissolved components is by advection and Fickian molecular diffusion. We present instructions for use and example problems to demonstrate the accuracy and practical application of EOS7C.

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1. Introduction

Interest in geologic carbon sequestration involving the direct injection of carbon dioxide (CO₂) into depleted natural gas (i.e., methane, CH₄) reservoirs (e.g., Oldenburg et al., 2001; Oldenburg, 2003) prompted the development of the simulation capabilities provided in TOUGH2/EOS7C. The new module EOS7C is the latest enhancement of a series of modules derived from the EOS3 module as shown in Table 1. The starting point for development of EOS7C was the radionuclide transport module EOS7R (Oldenburg and Pruess, 1995; Pruess et al., 1999), to which we added capabilities for modeling real gas mixtures such as CO₂ and CH₄, and N₂ and CH₄, and including the capability of modeling supercritical CO₂. This report describes EOS7C, the TOUGH2 module for simulating CO₂ or N₂ injection and mixing processes in natural gas reservoirs and gas storage reservoirs (Oldenburg et al., 2001; Oldenburg, 2003). The sample problems and input format descriptions in the present report along with the TOUGH2 User's Guide (Pruess et al., 1999) provide sufficient information for using EOS7C. The effect of brine (i.e., salinity) on gas solubility has not been implemented in EOS7C v. 1.0.

Table 1. Module progression and enhancement.

TOUGH2 Module	Components	Added Capability
EOS3	Water, air, heat	
EOS7	Water, brine, air, heat	Dense brine
EOS7R	Water, brine, parent radionuclide, daughter radionuclide, air, heat	Decay, adsorption, volatilization, of radionuclides in trace concentrations.
EOS7C	Water, brine, non-condensable gas, tracer, methane, heat	Real gas properties module with option of CO ₂ or N ₂ as non-condensable gas.

2. Mathematical Formulation

2.1 General

The general conservation equations solved in TOUGH2 for simulating multicomponent and multiphase flow and transport in porous media are presented in Pruess et al. (1999) along with a complete description of the theory and use of TOUGH2 which will not be repeated here. In this report, we focus on EOS7C and its specific methods and capabilities for modeling two phases and five components plus heat. The symbols and index numbers for these phases and components in EOS7C are shown in Table 2. The non-condensable gas (NCG) can be chosen by the user as either carbon dioxide (CO₂) or nitrogen (N₂) (see input parameter IE(16)). Density, viscosity, and temperature- and pressure-dependent solubility for gas mixtures are included in EOS7C through the use of a real gas properties module as described below.

Table 2. Phases and components in EOS7C (NCG = non-condensable gas).

Phases (β)	Components (κ)				
1 – gas (g)	1 – water	2 – brine	3 – NCG	4 – tracer	5 – methane
2 – aqueous (w)	1 – water	2 – brine	3 – NCG	4 – tracer	5 – methane

2.2 Real Gas Mixture Properties

Density

EOS7C makes use of a set of subroutines contained within a submodule called ZEVSREAL, where ZEVS stand for Z factor, Enthalpy, Viscosity, and Solubility, and REAL refers to the fact that the module calculates properties of real gas mixtures. ZEVSREAL calculates mixture properties using cubic equations of state, so-named because the volume terms are raised to either

the first, second, or third power (Reid et al., 1987). The most common two-parameter equations of state can be written as

$$P = \frac{RT}{V - b} - \frac{a}{V^2 + ubV + wb^2} \quad (1)$$

where the parameters and functions u , w , b , and a take on different values depending on the particular cubic equation of state being used, and T here is in degrees K. Other symbols are defined in Nomenclature. EOS7C provides the option for Peng-Robinson, Redlich-Kwong, or Soave-Redlich-Kwong depending on user input (see input parameter IE(15)). However, our experience is that the Peng-Robinson equation of state is very accurate for CO₂-CH₄ systems and N₂-CH₄ systems, and therefore the remaining discussion and test problems all employ the Peng-Robinson equation of state. Readers interested in more detail in the range of applicability of Eq. 1 and recommendations on the use of various equations of state should consult Reid et al. (1987) and Poling et al. (2000) for more information.

The approach taken in EOS7C is to use the Peng-Robinson equation of state to calculate the Z factor of the mixture, where

$$PV = ZnRT \quad (2)$$

From this value, the density of the gas mixture can be calculated using

$$\rho = \frac{MW n}{V} = \frac{P MW}{Z R T} \quad (3)$$

where the molecular weight (MW) is the molecular weight of the real gas mixture.

Enthalpy

The enthalpy of the real-gas mixtures is calculated using an ideal gas value with an added enthalpy departure to account for real gas effects. Real gas mixtures depart from ideality in ways that can be modeled with cubic equations of state. In ZEVSREAL, we calculate enthalpy as

$$H = (H - H^{ig}) + H^{ig} = (H - H^{ig}) + \sum_i X^i H^{i,ig} \quad (4)$$

where $(H - H^{ig})$ is the enthalpy departure. ZEVSREAL uses cubic equations of state (e.g., Peng-Robinson) to calculate the enthalpy departures and ideal gas enthalpy change to come up with the total enthalpy change of the real gas mixture.

Standard TOUGH2 (Pruess et al., 1999) uses real-gas properties (steam tables) for steam enthalpy, and thus produces more accurate steam enthalpies than the cubic equations of state can provide. At user discretion (see input parameter IE(14)), the user can choose to use the steam tables (subroutine SUPST) to calculate the enthalpy of the steam (water vapor) fraction in the gas, and ZEVSREAL to calculate the enthalpy of the NCG and CH₄ mixture fraction. The total gas mixture enthalpy is then calculated as a weighted combination of the SUPST and ZEVSREAL contributions. The reference state for enthalpy calculations in EOS7C is normalized to agree with TOUGH2 and the NIST Chemistry Web Book (NIST, 2003), i.e., internal energy is zero for saturated liquid at 273.16 K (0 °C).

Viscosity

Another important transport property for gas flow and transport is the viscosity of the real gas mixture. ZEVSREAL uses the method of Chung et al. (1988) as described in Reid et al. (1987) and Poling et al. (2000). This method is accurate to within 5-10% for the range of conditions expected in subsurface natural gas reservoirs.

Solubility of Real Gas Mixture Components

The method of computing the partitioning of the NCG between aqueous and gas phases is presented here assuming CO₂ is the NCG, but the same treatment is used in the case that N₂ is the NCG. Note that the effects of brine on aqueous phase solubility are not included in the present EOS7C v. 1.0 formulation. We begin by writing the equation for the dissolution and exsolution of CO₂ in the aqueous phase as



the equilibrium constant for which is given by

$$K_{CO_2(g)} = \frac{a_{CO_2}}{f_{CO_2}} \quad (6)$$

where a is the activity which refers to the aqueous phase and f is the fugacity which refers to the gas phase. The Poynting Correction accounts for the change in equilibrium constant due to pressure change (Prausnitz et al., 1986) and can be written as

$$K_{T,P} = K_{T,P^0}^0 \exp\left(\frac{(P - P^0)\bar{V}_i}{RT}\right) \quad (7),$$

where the equilibrium constant (K_{T,P^0}^0) at reference pressure (P^0) of 1 bar can be taken from the literature or fitted to experimental data (Spycher et al., 2003). We define the activity of CO₂ in the aqueous phase as a function of activity coefficient and molality as

$$a_{CO_2} = \gamma m_{CO_2} \quad (8)$$

Assuming the activity coefficient to be equal to one, the mole fraction of CO₂ in the aqueous phase is given by

$$x_{aq}^{CO_2} = \frac{a_{CO_2}}{55.508} \quad (9)$$

assuming there are 55.508 moles H₂O per kg of aqueous phase. The fugacity of CO₂ can be written

$$f_{CO_2} = \phi_{CO_2} y_g^{CO_2} P^t = \frac{a_{CO_2}}{K_{CO_2(g)}} \quad (10)$$

where ϕ is the fugacity coefficient, y_g is the mole fraction in the gas phase, and P^t is the total gas pressure. Combining Eqs. 6, 9, and 10, we have an expression for the equilibrium constant

$$K_{CO2(g)} = \frac{55.508 x_{aq}^{CO2}}{\phi_{CO2} y_g^{CO2} P^t} \quad (11).$$

For CO₂, if $T < 100$ °C, we use partial molar volumes of Spycher et al. (2003) for calculating the equilibrium constant of Eq. 11 in the ZEVSREAL subroutines. For other components and temperatures, we use SUPCRT92 (Johnson et al., 1992) and the slop98 database of Shock and Plyasunov (2004) to calculate equilibrium constants.

From the definition of partial pressure, the equilibrium constant of Eq. 11, and a Henry's Law-type relation, we can define an effective Henry's coefficient from

$$P^{CO2} = y_g^{CO2} P_t = \frac{55.508 x_{aq}^{CO2}}{K_{CO2(g)} \phi_{CO2}} = Kh_{CO2} x_{aq}^{CO2} \quad (12)$$

where the effective Henry's coefficient (Kh) is given by

$$Kh_{CO2} = \frac{55.508}{K_{CO2(g)} \phi_{CO2}} \quad (13).$$

In EOS7C, the accurate Henry's coefficients given by Eq. 13 are used to calculate partitioning of the NCG and CH₄ components in the gas and aqueous phases. Because ZEVSREAL is called assuming gas phase mole fractions are known, and yet such mole fractions are a function of the effective Henry's coefficient, an iterative approach is used wherein the first guess of Kh is taken from the approach used in EWASG (Battistelli et al., 1997), specifically the models of Cramer (1982), and D'Amore and Truesdell (1988). This iteration converges quickly.

2.3 Molecular Diffusion

The current EOS7C v. 1.0 uses a simplified model for binary diffusion of the chemical components dissolved in aqueous and gas phases as discussed in the TOUGH2 User Guide (Pruess et al., 1999). For gas-phase diffusion, TOUGH2 includes pressure and temperature effects. Specifically, pressure (P) is assumed to be inversely proportional to pressures by the factor $1.0 \times 10^5/P$ (Pruess et al., 1999). For example, if pressure is 2×10^5 Pa, the corresponding effective molecular diffusivity for the gas is one-half the input value which is referenced to 1.0×10^5 Pa. This approach overpredicts diffusivity for CO₂ mixtures above approximately 20 bars (Poling et al., 2000, p. 11.16), with a total overprediction of a factor of two at $P = 100$ bars. Temperature also affects gas diffusivity in TOUGH2 by the factor $((T + 273.15)/273.15)^{\text{TEMP}}$ (see TOUGH2 User Guide (Pruess et al., 1999)). If molecular diffusivity is input as a negative number in TOUGH2, the absolute value of this number is used for the phase molecular diffusivity without modification by S and τ (saturation and tortuosity) and without pressure or temperature effects. However, no diffusive fluxes are calculated for grid blocks where τ is input as zero or blank regardless of the phase molecular diffusivity. Interested readers are referred to Pruess et al. (1999), Appendix D, pp. 155-156 for further details. More sophisticated molecular diffusion capabilities (e.g., the dusty gas model) will be implemented in future versions of EOS7C.

3. Implementing Real Gas Components

Users familiar with TOUGH2 equation of state modules will notice from Table 1 that we developed EOS7C by replacing the air in EOS7R with CH₄, and changing the volatile radionuclide components of EOS7R into gas components with real gas properties appropriate to CO₂ or N₂ as specified by the user. Unlike the early version of EOS7R (Oldenburg and Pruess,

1995), single-phase gas conditions are allowed in EOS7C consistent with the revised EOS7R in TOUGH2 Version 2 (Pruess et al., 1999). However, EOS7C is designed for two-phase conditions (i.e., gas and aqueous phases present) and very limited testing has been done for single-phase conditions. In two-phase conditions, vapor pressure is independent of salinity of the aqueous phase. As the brine component is nonvolatile, continued vaporization could increase brine mass fractions in the aqueous phase beyond unity which is not physically reasonable. Users need to be aware of this possibility, which arises from the fact that EOS7C, like EOS7R, represents the aqueous phase as a mixture of water and brine, not as a mixture of water and salt. Therefore, EOS7C cannot be used for processes in which solubility limits would be reached, at which point solid salt would precipitate. The tracer component in EOS7C is similar to the radionuclide components in EOS7R in that this component does not affect gas properties and is expected to exist only in trace concentrations (e.g., mass fractions of order 10^{-6}). A summary of EOS7C specifications is printed upon execution and is reproduced here in Fig. 1.

```

*****
*           EOS7C: EQUATION OF STATE FOR MIXTURES OF WATER/BRINE/NON-CONDENSIBLE GAS/TRACER/METHANE           *
*****
ENTHALPY OPTION:   SUPST (IE(14) = 1)           EQUATION OF STATE: PR (IE(15) = 1)           NON-CONDENSIBLE GAS: CO2 (IE(16) = 1)

OPTIONS SELECTED ARE: (NK,NEQ,NPH,NB,NKIN) = (5,6,2,8,5)

      NK = 5 - NUMBER OF COMPONENTS
      NEQ = 6 - NUMBER OF EQUATIONS PER GRID BLOCK
      NPH = 2 - NUMBER OF PHASES THAT CAN BE PRESENT
      NB = 8 - NUMBER OF SECONDARY PARAMETERS (OTHER THAN' COMPONENT MASS FRACTIONS)
      NKIN = 5 - number of components for initializing thermodynamic conditions (default is NKIN = NK)

      For NB = 6, diffusion is "off", for NB = 8, diffusion is "on"

AVAILABLE OPTIONS for (NK,NEQ,NPH,NB):
      (5,5,2,6 or 8) - WATER, BRINE, NCG, TRC, CH4; ISOTHERMAL;           VARIABLES (P, XB, XNCG, XTRC, X OR S+10, T)
      (5,6,2,6 or 8) - WATER, BRINE, NCG, TRC, CH4; NON-ISOTHERMAL;       VARIABLES (P, XB, XNCG, XTRC, X OR S+10, T)
      (4,4,2,6 or 8) - WATER, BRINE, NCG, TRC, NO CH4; ISOTHERMAL;       VARIABLES (P, XB, XNCG, XTRC, T)
      (4,5,2,6 or 8) - WATER, BRINE, NCG, TRC, NO CH4; NON-ISOTHERMAL;   VARIABLES (P, XB, XNCG, XTRC, T)

NKIN = NK or NKIN = NK-2. Default options are (5,5,2,8) - isothermal, diffusion "on", NKIN=NK

THE NK = 4 ("NO CH4") OPTIONS MAY ONLY BE USED FOR PROBLEMS WITH SINGLE-PHASE LIQUID CONDITIONS THROUGHOUT.

THE NORMAL NUMBER OF SECONDARY PARAMETERS OTHER THAN MASS FRACTIONS IS 6 PER PHASE. IN EOS7C, WE OPTIONALLY ADD TO THIS A
SATURATION-DEPENDENT TORTUOSITY FOR EACH PHASE, AS WELL AS TEMPERATURE AND PRESSURE DEPENDENCE OF THE DIFFUSION COEFFICIENT.
*****

NKIN = 5   *** ALLOWS INITIALIZATION WITH DIFFERENT SETS OF PRIMARY VARIABLES. ***
          *** THIS IS USEFUL FOR STARTING EOS7C SIMULATIONS FROM EOS7 INITIAL CONDITIONS. ***
          = NK (default): (P,XB,XNCG,XTRC,XCH4,T) FOR SINGLE PHASE, (P,XB,XNCG,XTRC,S+10,T) FOR TWO-PHASE. (EOS7C FORMAT).
          = NK-2: (P,XB,XCH4,T) FOR SINGLE PHASE, (P,XB,S+10,T) FOR TWO-PHASE. (EOS7 FORMAT). WILL INITIALIZE XNCG = XTRC = 0.
*****

```

Figure 1. Example of self-documenting printout for EOS7C.

THE PRIMARY VARIABLES ARE

P - PRESSURE T - TEMPERATURE XB - BRINE MASS FRACTION
 XNCG - MASS FRACTION OF NON-CONDENSIBLE GAS XTRC - MASS FRACTION OF VOLATILE TRACER
 S+10. - (GAS PHASE SATURATION + 10.) X - CH4 MASS FRACTION IN GAS T - TEMPERATURE

```

*****
*                               *
*          COMPONENTS          *
*                               *
*          # 1 - WATER         *
*                               *
*          # 2 - BRINE         *
*                               *
*          # 3 - NCG          *
*                               *
*          # 4 - TRC          *
*                               *
*          # 5 - CH4          *
*                               *
*          # 6 - HEAT         *
*                               *
*****

*****
*                               *
*          FLUID PHASE CONDITION      PRIMARY VARIABLES      *
*                               *
*          SINGLE-PHASE GAS (#)      P, XB, XNCG, XTRC,      X, T *
*                               *
*          SINGLE-PHASE LIQUID (*)      P, XB, XNCG, XTRC,      X, T *
*                               *
*          TWO-PHASE (*)      P, XB, XNCG, XTRC, S+10., T *
*                               *
*****
*          (#) XB, XNCG, XTRC AND X ARE MASS FRACTIONS IN THE GAS PHASE.
*          (*) XB, XNCG, XTRC AND X ARE MASS FRACTIONS IN THE AQUEOUS PHASE.
*****

NEGATIVE REFERENCE PRESSURE OF - .100000E+06 PA WAS SPECIFIED, THUS BRINE PROPERTIES ARE IDENTICAL TO WATER FOR ALL SALINITIES.

PROPERTIES OF NCG AND TRACER:      DOMAIN      NCG      TRC
    HALF-LIFE (SECONDS):      -ALL-      NO DECAY      0.1000E+51
    MOLECULAR WEIGHT (GM/MOLE):      -ALL-      0.4400E+02      0.2300E+03
    INVERSE HENRY CONST. (1/PA):      -ALL-      VARIABLE      0.5700E-10
    HEAT CAPACITY (J/(KG K)):      -ALL-      VARIABLE      NEGLIGIBLE
GAS PHASE DIFFUSIVITY (M**2/S):      -ALL-      0.1000E-04      0.1000E-04
AQ. PHASE DIFFUSIVITY (M**2/S):      -ALL-      0.1000E-09      0.1000E-09
DISTRIBUTION COEFF. (M**3/KG):      rock      0.0000E+00      0.0000E+00

MOLECULAR DIFFUSIVITY OF WATER, BRINE, NCG, TRC, AND CH4 THROUGH THE GASEOUS AND AQUEOUS PHASES, (FDDIAG(PHASE,COMP)) [M**2/S]:
PHASE 1 = GAS; PHASE 2 = AQUEOUS
    PHASE COMP    PHASE COMP    PHASE COMP    PHASE COMP    PHASE COMP    PHASE COMP    PHASE COMP    PHASE COMP    PHASE COMP
    -1-    -1-    -1-    -2-    -1-    -3-    -1-    -4-    -1-    -5-    -2-    -1-    -2-    -2-    -2-    -3-    -2-    -4-    -2-    -5-
    0.1000E-04 0.00000E+00 0.10000E-04 0.10000E-04 0.10000E-04 0.10000E-09 0.00000E+00 0.10000E-09 0.10000E-09 0.10000E-09 0.10000E-09

```

Figure 1. Example of self-documenting printout for EOS7C (continued).

4. Using EOS7C

4.1 Compilation of EOS7C

As an extension of TOUGH2, EOS7C consists of all of the TOUGH2 subroutines, some with modifications, and the new equation of state module EOS7C with its new subroutines. The program units and changes are given in Appendix 1. Typical compilation on a LINUX workstation with the Portland Group Fortran compiler, for example, would be as follows:

```
pgf77 -c -r8 -i8 t2cg22.f meshm.f eos7cv1.f zevsreald.f t2f.f ma28.f t2solv.f
```

The italics indicate the new program units of EOS7C.

4.2 Input Formats

Below we describe the input formats for specifying EOS7C-specific input. Other TOUGH2 input parameter formats are given in Pruess et al. (1999). EOS7C-specific input parameters are provided through the SELEC block and PARAM block.

MULTI	format(4I5)
	NK, NEQ, NPH, NB, NKIN
NK	Set NK = 5 for water, brine, NCG, gas tracer, and CH ₄ .
NEQ	Number of equations per grid block. Set NEQ = NK for isothermal problems. Set NEQ = NK + 1 for nonisothermal problems.
NPH	Number of phases. Set NPH = 2.
NB	Number of secondary parameters. Set NB = 6 for no-diffusion, NB = 8 for diffusion on.
NKIN	Number of mass components in INCON (default is NKIN = NK). This parameter can be used to initialize EOS7C run (NK = 4 or 5)

with EOS7 (NK = 2 or 3) INCON data, in which case NCG and trace gases (components 3 and 4) are initialized with $X_{g,l}^k = 0$.

PARAM.1 format(2I2, 3I4, 24I1, 2E10.4)

NOITE, KDATA, MCYC, MSEC, MCYPR, (MOP(I), I = 1, 24), DIFF0, TEXP

See TOUGH2 User Guide (Pruess et al., 1999), TOUGH2 informative printout for description of all of the above parameters except the following:

MOP(20)

Option for resetting variables.¹

0: Variables are not reset if partial pressures exceed total pressure.

1: Pressure is reset to sum of partial pressures if partial pressures exceed total pressure.

2: NCG mass fraction is reset if sum of partial pressures exceeds total pressure.

¹This option is needed because in some cases, the sum of partial pressures exceeds the total pressure, e.g., if temperature changes cause rapid exsolution of dissolved gases. When this occurs, erroneous negative mass fractions can arise. In this case, setting MOP(20) = 1 or 2 can alleviate the problem. However, as a default, we recommend setting MOP(20) = 0, as this problem is not often encountered.

PARAM.4 primary variables used for default conditions for all gridblocks that are not assigned by means of data blocks INDOM or INCON. Option START is necessary to use default INCON (see Pruess et al., 1999). Two lines will be read for the six primary variables in EOS7C. See INCON description for primary variable description.

PARAM.4 format(4E20.14)

DEP(I), I = 1,6

INCON introduces gridblock-specific initial conditions. Two lines will be read per gridblock for the six primary variables in EOS7C.

INCON.1 format(4E20.14)

DEP(I), I = 1,6

DEP(I) are the primary variables as follows:

Single-phase conditions

$(P, X^{brine}, X^{ncg}, X^{trc}, X^{CH_4}, T)$ where P is pressure, X^{brine} is always brine mass fraction in the liquid phase, other X 's are mass fractions in gas or liquid phase, and T is temperature in °C.

Two-phase conditions

$(P, X^{brine}_{liq}, X^{ncg}_{liq}, X^{trc}_{liq}, S + 10, T)$ where P is gas-phase pressure, X 's are brine, NCG, TRC mass fractions in the liquid, S is gas saturation, and T is temperature in °C

SELEC keyword to introduce a data block with reference brine and NCG input data.

SELEC.1 format(8I5)

IE(1), NGBINP(1), NGBINP(2), NGBINP(3), NFBL, NFBR, NFBT, NFBB

IE(1) Set equal to 6 to read six additional data records.

IE(14) Set equal to 0 to use ZEVSREAL for enthalpy of gas mixture,
Set equal to 1 to use SUPST for water vapor, and ZEVSREAL for
NCG and CH₄, with a weighted sum used for the mixture enthalpy.

IE(15) Set equal to 1 for Peng-Robinson (PR) equation of state;
Set equal to 2 for Redlich-Kwong (RK) equation of state;
Set equal to 3 for Soave-Redlich-Kwong (SRK) equation of state.

IE(16) Set equal to 1 for CO₂,
Set equal to 2 for N₂.

SELEC.2 format(3E10.4) (unchanged from standard EOS7)

P0, T0, ρ0

P0 Reference pressure, in Pa

T0 Reference temperature, in °C

ρ_0 Brine density at (P0, T0), in kg m⁻³.
 For P0, T0, ρ_0 equal to zero or blank, default values of P0 = 1 x 10⁵ Pa, T0 = 25 °C, and $\rho_0 = 1185.1$ kg m⁻³ will be used. For P0 < 0, brine will be assumed to be pure water. This allows modeling of flow with two waters that differ only in trace constituents, but have identical thermophysical properties.

SELEC.3 format(3E10.4) (unchanged from standard EOS7)
 v(i), i = 1,3
 v(i) Coefficients for salinity correction in aqueous phase viscosity (see Pruess et al., 1999, p. 41). If v(i) =0 for I = 1, 2, 3, default values will be used: v(1) = 0.4819, v(2) = -0.2774, v(3) = 0.7814. Specification of brine as pure water in record SELEC.2 will override viscosity specifications, and will always result in viscosity of pure water being used.

SELEC.4 format(7E10.4)
 Leave this line blank.

SELEC.5 format(7E10.4)
 Leave this line blank.

SELEC.6 format(7E10.4)
 Leave this line blank.

SELEC.7 format(7E10.4)
 blank, XMW(4), blank, blank, blank, blank, HCTRC
 XMW(4) Molecular weight of tracer component 4, in g/mole.
 HCTRC Inverse Henry's constant for gas tracer (component 4), Pa⁻¹ .

DIFFU format(2E10.4)

FDDIAG(1,1),FDDIAG(2,1)

FDDIAG(1,2),FDDIAG(2,2)

FDDIAG(1,3),FDDIAG(2,3)

FDDIAG(1,4),FDDIAG(2,4)

FDDIAG(1,5),FDDIAG(2,5)

Molecular diffusivity of components 1–5 in phases 1, 2 (gas and liquid) in $\text{m}^2 \text{s}^{-1}$. If FDDIAG(NP,NK) is input as a negative number, the absolute value is used for the phase molecular diffusivity (d_{β}^k) without modification by S and τ (saturation and tortuosity) and without pressure or temperature effects in the case of gas diffusivity.

Table 3. Molecular diffusivities for two phases and five components.

Phase	Component	(NP,NK)	Input	Units
Gaseous	Water	(1,1)	DIFFU(1,1)	$\text{m}^2 \text{s}^{-1}$
	Brine	(1,2)	DIFFU(1,2)	$\text{m}^2 \text{s}^{-1}$
	NCG	(1,3)	DIFFU(1,3)	$\text{m}^2 \text{s}^{-1}$
	Tracer	(1,4)	DIFFU(1,4)	$\text{m}^2 \text{s}^{-1}$
	Methane	(1,5)	DIFFU(1,5)	$\text{m}^2 \text{s}^{-1}$
Aqueous	Water	(2,1)	DIFFU(2,1)	$\text{m}^2 \text{s}^{-1}$
	Brine	(2,2)	DIFFU(2,2)	$\text{m}^2 \text{s}^{-1}$
	NCG	(2,3)	DIFFU(2,3)	$\text{m}^2 \text{s}^{-1}$
	Tracer	(2,4)	DIFFU(2,4)	$\text{m}^2 \text{s}^{-1}$
	Methane	(2,5)	DIFFU(2,5)	$\text{m}^2 \text{s}^{-1}$

5. Example Problems

5.1 SAM7C1: Density, Viscosity, Solubility, and Enthalpy of Real Gas Mixtures

In this section, we present a simple test problem designed to demonstrate the gas mixture property calculations of EOS7C v. 1.0 through comparison of computed properties with independent reference values. This is an extension of the gas-mixture property comparison done in an earlier code comparison study using an early version of EOS7C (Oldenburg et al., 2002). The problem is a series of gridblocks arranged in 10 columns with three rows. The various conditions are shown in Tables 4–6 in a manner suggestive of the two-dimensional layout of the gridblocks.

The input file for SAM7C1 is shown in Figure 2. A partial output file is shown in Figures 3 and 4. Note the first three letters of the gridblock name suggests the compositions in each gridblock, while the last two numbers give the row and column, respectively. In Tables 7-12, we present a summary of the results and comparisons to standard reference values.

The first comparison we present is for density (ρ), viscosity (μ), and solubility of CO₂ and CH₄ gas mixtures (Tables 7 and 8). Carbon dioxide undergoes large changes in density and viscosity as it passes from subcritical to supercritical conditions. The critical pressure and temperature of CO₂ (73.8 bars, 31.0 °C) will be reached in the subsurface at depths greater than approximately 800 m. Thus CO₂ will most commonly be supercritical in subsurface carbon sequestration sites. Therefore, we present estimates of physical properties at both subcritical (40 bars, 40 °C) and supercritical (100 bars, 40 °C) conditions. For brevity, we present in Tables 7 and 8 physical properties only for the end members and 50-50 mole fraction mixtures. We have included

reference values either from published data or from more detailed estimation methods as noted. Note that EOS7C gives compositions in terms of mass fraction (X), whereas the compositions in the tables are specified in terms of mole fractions in the gas (x_g) or in the liquid (x_l) phases. The conversions from mass fraction to mole fraction are given by the equations

$$x^i = \frac{\frac{X^i}{MW^i}}{\sum_i \frac{X^i}{MW^i}} \quad (14)$$

$$X^i = \frac{x^i MW^i}{\sum_i x^i MW^i} \quad (15).$$

Note further in Tables 7 and 8 that for two-phase conditions, there is a small amount of water vapor in the gas phase that is not present in the reference calculations. This small amount of water has little effect on the given properties as shown by comparing the two-phase gridblocks with the single-phase gas gridblocks. As shown in Tables 7 and 8, EOS7C approximates gas mixture properties very well.

In Tables 9–12, we present comparisons of enthalpy calculations using the IE(14) = 1 option, i.e., SUPST for steam fraction and ZEVSREAL for CO₂ and CH₄ fractions. This approach appears to be quite accurate as shown by comparing EOS7C estimates against NIST Chemistry Web Book values.

Table 4. SAM7C1 multicomponent gas mixture conditions.

Two-Phase P = 40 bars T = 40 °C	Two-Phase P = 100 bars T = 40 °C	Single-Phase Gas P = 40 bars T = 40 °C	Single-Phase Gas P = 100 bars T = 40 °C
$x_g^{CO_2} = 1.0$ $x_g^{CH_4} = 0.0$ $x_g^{H_2O} = \text{trace}$	$x_g^{CO_2} = 1.0$ $x_g^{CH_4} = 0.0$ $x_g^{H_2O} = \text{trace}$	$x_g^{CO_2} = 1.0$ $x_g^{CH_4} = 0.0$ $x_g^{H_2O} = 0.0$	$x_g^{CO_2} = 1.0$ $x_g^{CH_4} = 0.0$ $x_g^{H_2O} = 0.0$
$x_g^{CO_2} = 0.5$ $x_g^{CH_4} = 0.5$ $x_g^{H_2O} = \text{trace}$	$x_g^{CO_2} = 0.5$ $x_g^{CH_4} = 0.5$ $x_g^{H_2O} = \text{trace}$	$x_g^{CO_2} = 0.5$ $x_g^{CH_4} = 0.5$ $x_g^{H_2O} = 0.0$	$x_g^{CO_2} = 0.5$ $x_g^{CH_4} = 0.5$ $x_g^{H_2O} = 0.0$
$x_g^{CO_2} = 0.0$ $x_g^{CH_4} = 1.0$ $x_g^{H_2O} = \text{trace}$	$x_g^{CO_2} = 0.0$ $x_g^{CH_4} = 1.0$ $x_g^{H_2O} = \text{trace}$	$x_g^{CO_2} = 0.0$ $x_g^{CH_4} = 1.0$ $x_g^{H_2O} = 0.0$	$x_g^{CO_2} = 0.0$ $x_g^{CH_4} = 1.0$ $x_g^{H_2O} = 0.0$

Table 5. SAM7C1 pure steam conditions.

Steam P = 1.013 bar	Steam P = 2 bars
T = 150 °C	T = 150 °C
T = 200 °C	T = 200 °C
T = 250 °C	T = 250 °C

Table 6. SAM7C1 pure CO₂ and CH₄ gas conditions.

Single-Phase Gas $x_g^{CO_2} = 1.0$	Single-Phase Gas $x_g^{CO_2} = 1.0$	Single-Phase Gas $x_g^{CH_4} = 1.0$	Single-Phase Gas $x_g^{CH_4} = 1.0$
P = 1.013 bars T = 20 °C	P = 100 bars T = 20 °C	P = 1.013 bars T = 20 °C	P = 100 bars T = 20 °C
P = 1.013 bars T = 100 °C	P = 100 bars T = 100 °C	P = 1.013 bars T = 100 °C	P = 100 bars T = 100 °C
P = 1.013 bars T = 180 °C	P = 100 bars T = 180 °C	P = 1.013 bars T = 180 °C	P = 100 bars T = 180 °C

```

*SAM7C1* ... Verification problem for EOS7C.
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
rock      2      2600.      .20      1.e-12      1.e-12      1.e-12      2.51      1000.
          7          0.20      .27          1.          0.01
          7          0.20      .25      .00084      1.e5          1.

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
5         6         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      1          110 000000020000400 13
          -1.          9.8066
          1.e-9
          1.e-5
          1.000e5          0.          0.e-1          0.e-4
          10.500          40.

IE(14) = 1, use SUPST & ZEVSREAL for enthalpy. IE(14) = 0, use ZEVSREAL only.
IE(15) = 1, use Peng-Robinson eqn. of state. IE(15) = 2,3 use RK,SRK, resp.
IE(16) = 1, NCG is CO2. IE(16) = 2, NCG is N2.
SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
6
-1.e5          1      1      1

1.e50      230.00          0.0          0.0          0.0          0.0      5.70e-11

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-5      1.e-10
0.e-6      0.e-6
1.e-5      1.e-10
1.e-5      1.e-10
1.e-5      1.e-10

```

Figure 2. Input file for SAM7C1.

INCON	1	2	3	4	5	6	7	8
CO211	4.000e6 10.50		0. 40.		0.0320		0.e-4	
MIX21	4.000e6 10.50		0. 40.		0.0165		0.e-4	
CH431	4.000e6 10.50		0. 40.		0.0000		0.e-4	
CO212	1.000e7 10.50		0. 40.		0.0505		0.e-4	
MIX22	1.000e7 10.50		0. 40.		0.0290		0.e-4	
CH432	1.000e7 10.50		0. 40.		0.0000		0.e-4	
CO213	4.000e6 0.0		0. 40.		1.0000		0.e-4	
MIX23	4.000e6 0.2667		0. 40.		0.7333		0.e-4	
CH433	4.000e6 1.00		0. 40.		0.0000		0.e-4	
CO214	1.000e7 0.00		0. 40.		1.0000		0.e-4	
MIX24	1.000e7 0.2667		0. 40.		0.7333		0.e-4	
CH434	1.000e7 1.00		0. 40.		0.0000		0.e-4	
H2O15	1.013e5 0.00		0. 150.		0.0000		0.e-4	
H2O25	1.013e5 0.00		0. 200.		0.0000		0.e-4	
H2O35	1.013e5 0.00		0. 250.		0.0000		0.e-4	
H2O16	2.000e5 0.00		0. 150.		0.0000		0.e-4	
H2O26	2.000e5 0.00		0. 200.		0.0000		0.e-4	
H2O36	2.000e5 0.00		0. 250.		0.0000		0.e-4	
CO217	1.013e5 0.00		0. 20.		1.0000		0.e-4	
CO227	1.013e5 0.00		0. 100.		1.0000		0.e-4	
CO237	1.013e5 0.00		0. 180.		1.0000		0.e-4	
CO218	1.000e7 0.00		0. 20.		1.0000		0.e-4	
CO228	1.000e7 0.00		0. 100.		1.0000		0.e-4	
CO238	1.000e7 0.00		0. 180.		1.0000		0.e-4	
CH419	1.013e5 1.00		0. 20.		0.0000		0.e-4	

Figure 2. Input file for SAM7C1 (continued).


```

CH429      1.013e5      0.      0.0000      0.e-4
           1.00      100.
CH439      1.013e5      0.      0.0000      0.e-4
           1.00      180.
CH410      1.000e7      0.      0.0000      0.e-4
           1.00      20.
CH420      1.000e7      0.      0.0000      0.e-4
           1.00      100.
CH430      1.000e7      0.      0.0000      0.e-4
           1.00      180.

ELEME-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
CO211      10.1000E+010.1000E+01      0.5000E+000.5000E+00-.5000E+00
MIX21      10.1000E+010.0000E+00      0.5000E+000.5000E+00-.1500E+01
CH431      10.1000E+010.1000E+01      0.5000E+000.5000E+00-.2500E+01
CO212      10.1000E+010.1000E+01      0.5000E+000.1500E+01-.5000E+00
MIX22      10.1000E+010.0000E+00      0.5000E+000.1500E+01-.1500E+01
CH432      10.1000E+010.1000E+01      0.5000E+000.1500E+01-.2500E+01
CO213      10.1000E+010.1000E+01      0.5000E+000.2500E+01-.5000E+00
MIX23      10.1000E+010.0000E+00      0.5000E+000.2500E+01-.1500E+01
CH433      10.1000E+010.1000E+01      0.5000E+000.2500E+01-.2500E+01
CO214      10.1000E+010.1000E+01      0.5000E+000.3500E+01-.5000E+00
MIX24      10.1000E+010.0000E+00      0.5000E+000.3500E+01-.1500E+01
CH434      10.1000E+010.1000E+01      0.5000E+000.3500E+01-.2500E+01
H2O15      10.1000E+010.1000E+01      0.5000E+000.4500E+01-.5000E+00
H2O25      10.1000E+010.0000E+00      0.5000E+000.4500E+01-.1500E+01
H2O35      10.1000E+010.1000E+01      0.5000E+000.4500E+01-.2500E+01
H2O16      10.1000E+010.1000E+01      0.5000E+000.5500E+01-.5000E+00
H2O26      10.1000E+010.0000E+00      0.5000E+000.5500E+01-.1500E+01
H2O36      10.1000E+010.1000E+01      0.5000E+000.5500E+01-.2500E+01
CO217      10.1000E+010.1000E+01      0.5000E+000.6500E+01-.5000E+00
CO227      10.1000E+010.0000E+00      0.5000E+000.6500E+01-.1500E+01
CO237      10.1000E+010.1000E+01      0.5000E+000.6500E+01-.2500E+01
CO218      10.1000E+010.1000E+01      0.5000E+000.7500E+01-.5000E+00
CO228      10.1000E+010.0000E+00      0.5000E+000.7500E+01-.1500E+01
CO238      10.1000E+010.1000E+01      0.5000E+000.7500E+01-.2500E+01
CH419      10.1000E+010.1000E+01      0.5000E+000.8500E+01-.5000E+00
CH429      10.1000E+010.0000E+00      0.5000E+000.8500E+01-.1500E+01
CH439      10.1000E+010.1000E+01      0.5000E+000.8500E+01-.2500E+01
CH410      10.1000E+010.1000E+01      0.5000E+000.9500E+01-.5000E+00
CH420      10.1000E+010.0000E+00      0.5000E+000.9500E+01-.1500E+01
CH430      10.1000E+010.1000E+01      0.5000E+000.9500E+01-.2500E+01

CONNE

ENDCY-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
MESHMAKER1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
XYZ
      0.
NX      1      1.
NY      10     1.
NZ      3      1.

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

```

Figure 2. Input file for SAM7C1 (continued).

Table 7. Properties of CO₂-CH₄-H₂O gas mixtures at 40 bars and 40 °C.

	gas phase				aqueous phase	
	x _g ^{CH4}	x _g ^{CO2}	ρ (kg m ⁻³)	μ (Pa s)	x _l ^{CH4}	x _l ^{CO2}
EOS7C	2.62 x 10 ⁻³	0.996	85.12	1.70 x 10 ⁻⁵	2.05 x 10 ⁻⁶	1.33 x 10 ⁻²
Reference	0.	1.	83.79 [1]	1.73 x 10 ⁻⁵ [1]	0.	1.37 x 10 ⁻² [2]
EOS7C	0.501	0.497	51.85	1.44 x 10 ⁻⁵	3.66 x 10 ⁻⁴	6.82 x 10 ⁻³
Reference	0.5	0.5	51.33 [1]	1.67 x 10 ⁻⁵ [1]	3.66 x 10 ⁻⁴ [3,4,5,6]	6.74 x 10 ⁻³ [3,4,5,6]
EOS7C	0.998	0.	26.48	1.21 x 10 ⁻⁵	7.15 x 10 ⁻⁴	0.
Reference	1.	0.	26.10 [1]	1.23 x 10 ⁻⁵ [1]	7.22 x 10 ⁻⁴ [3,4,5,6]	0.

See Table 8 for references.

Table 8. Properties of CO₂-CH₄-H₂O gas mixtures at 100 bars and 40 °C.

	gas phase				aqueous phase	
	x _g ^{CH4}	x _g ^{CO2}	ρ (kg m ⁻³)	μ (Pa s)	x _l ^{CH4}	x _l ^{CO2}
EOS7C	6.98 x 10 ⁻³	0.992	544.96	4.18 x 10 ⁻⁵	2.18 x 10 ⁻⁵	2.13 x 10 ⁻²
Reference	0.	1.	631.90 [1]	5.04 x 10 ⁻⁵ [1]	0.	2.19 x 10 ⁻² [2]
EOS7C	0.503	0.497	154.59	1.80 x 10 ⁻⁵	7.93 x 10 ⁻⁴	1.21 x 10 ⁻²
Reference	0.5	0.5	153.97 [1]	1.94 x 10 ⁻⁵ [1]	7.95 x 10 ⁻⁴ [3,4,5,6]	1.21 x 10 ⁻² [3,4,5,6]
EOS7C	0.999	0.	71.72	1.42 x 10 ⁻⁵	1.49 x 10 ⁻³	0.
Reference	1.	0.	70.03 [1]	1.41 x 10 ⁻⁵ [1]	1.54 x 10 ⁻³ [3,4,5,6]	0.

¹NIST, 1992

²Wiebe and Gaddy, 1940.

³Spycher and Reed, 1988.

⁴Johnson et al., 1992.

⁵Shock et al., 1989.

⁶Wagman et al., 1982.

Table 9. Enthalpy of pure steam.

	1.013 bar 150 °C	1.013 bar 200 °C	1.013 bar 250 °C	2 bar 150 °C	2 bar 200 °C	2 bar 250 °C
EOS7C	2.776×10^6	2.875×10^6	2.974×10^6	2.768×10^6	2.871×10^6	2.971×10^6
Reference [1]	2.776×10^6	2.875×10^6	2.974×10^6	2.769×10^6	2.871×10^6	2.971×10^6

¹NIST Standard Reference Database 69 – March 2003 Release: NIST Chemistry Web Book.

Table 10. Enthalpy of pure CO₂ gas.

	1.013 bar 20 °C	1.013 bar 100 °C	1.013 bar 180 °C	100 bar 20 °C	100 bar 100 °C	100 bar 180 °C
EOS7C	4.985×10^5	5.730×10^5	6.533×10^5	2.437×10^5	4.999×10^5	6.087×10^5
Reference [1]	5.016×10^5	5.723×10^5	6.484×10^5	2.427×10^5	5.041×10^5	6.086×10^5

¹NIST Standard Reference Database 69 – March 2003 Release: NIST Chemistry Web Book.

Table 11. Enthalpy of pure CH₄ gas.

	1.013 bar 20 °C	1.013 bar 100 °C	1.013 bar 180 °C	100 bar 20 °C	100 bar 100 °C	100 bar 180 °C
EOS7C	9.050×10^5	1.092×10^6	1.298×10^6	7.911×10^5	1.022×10^6	1.251×10^6
Reference [1]	8.988×10^5	1.085×10^6	1.291×10^6	7.943×10^5	1.023×10^6	1.251×10^6

¹NIST Standard Reference Database 69 – March 2003 Release: NIST Chemistry Web Book.

Table 12. Enthalpy of 50-50 mole fraction CO₂-CH₄ mixture.

	40 bar 40 °C	100 bar 40 °C
EOS7C	6.157×10^5	5.132×10^5
Reference [1]	6.040×10^5 *	5.500×10^5 *

¹NIST 14 Database 1992. *normalized to NIST Chemistry Web Book reference condition.

5.2 SAM7C2: CO₂ Injection into a Depleted Gas Reservoir

In this sample problem, we demonstrate the use of EOS7C for the injection of CO₂ into a simplified two-dimensional depleted natural gas (CH₄) reservoir. This problem is modeled after the case shown in Oldenburg et al. (2001). In the problem, a two-dimensional depleted natural gas reservoir lies above a water table in a cross-sectional tilted system. The upper right-hand corner gridblock is held at constant pressure while CO₂ is injected in the middle-left of the reservoir. As CO₂ is injected, the pressure increases and injected CO₂ displaces CH₄ toward the upper right-hand corner. The input file is shown in Fig. 5. The initial conditions are provided in the INCON file. To compare the iteration sequence and provide a benchmark against which to check EOS7C installation, we present in Fig. 6 the beginning iteration printouts with residuals and in Fig. 7 the final iteration printouts. These numbers may vary slightly for different computers, but they should not differ greatly if EOS7C is installed correctly.

We show in Fig. 8 the liquid saturation field and the mass fraction of CO₂ in the gas after ten years. As shown, CO₂ fills the reservoir and drives CH₄ out through the constant-pressure gridblock. More details on Carbon Sequestration with Enhanced Gas Recovery (CSEGR) and the use of CO₂ as a cushion gas for natural gas storage can be found in Oldenburg et al. (2001), and Oldenburg (2003).

```

*SAM7C2* ... Rio Vista CSEGR.
ROCKS-----1-----2-----3-----4-----5-----6-----7-----8
domen 2 2600. .35 1.e-12 1.e-12 1.e-14 2.51 1000.
1.e-10 0.25
7 0.20 .27 1. 0.01
7 0.20 .25 .00084 1.e5 1.
wattb 2 2600. .35 1.e-12 1.e-12 1.e-12 2.51 2.e4
0.25
5
1 0.e5 .0 1.
bdrys 2 2600. .35 1.e-12 1.e-12 1.e-14 2.51 2.e4
0.25
7 0.20 .27 1. 0.01
7 0.20 .25 .00084 1.e5 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
3 400 40010 030000020000400 13
1.00e02 3.15600e08 -1. 2.0e9 9.8066
1.e-5
5.300e6 0. 0.e-1 0.e-4
10.500 65.
TIMES-----1-----2-----3-----4-----5-----6-----7-----8
2
3.156e7 6.312e7 3.156e8

IE(14) = 1, use SUPST & ZEVSREAL for enthalpy. IE(14) = 0, use ZEVSREAL only.
IE(15) = 1, use Peng-Robinson eqn. of state. IE(15) = 2,3 use RK,SRK, resp.
IE(16) = 1, NCG is CO2. IE(16) = 2, NCG is N2.
SELEC-----1-----2-----3-----4-----5-----6-----7-----8
6 1 1
-1.e5

1.e50 4.00 0.e-6 0.e-6 0.e-6 0.e-6 1.000e-10

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-5 1.e-10
0.e-6 1.e-10
1.e-5 1.e-10
1.e-5 1.e-10
1.e-5 1.e-10

GENER-----1-----2-----3-----4-----5-----6-----7-----8
A3A 1CO2 COM3 8.2E-00 5.356e4

FOFT -----1-----2-----3-----4-----5-----6-----7-----8
A2W 1

xNCON-----1-----2-----3-----4-----5-----6-----7-----8
A11 1
1.260e7 0. 0.e-1 0.e-4
10.50 65.

ENDCY-----1-----2-----3-----4-----5-----6-----7-----8
MESHMAKER1-----*-----2-----3-----4-----5-----6-----7-----8
XYZ
-.78
NX 1 1.e3
NY 33 200.
NZ 1 5.0

```

Figure 5. Input file for SAM7C2, CO₂ injection into gas reservoir.

```

***** VOLUME- AND MASS-BALANCES *****
***** [KCYC,ITER] = [ 0, 0] ***** THE TIME IS 0.000000E+00 SECONDS, OR 0.000000E+00 DAYS

      PHASES PRESENT
*****
      PHASES *      GAS      AQUEOUS
*****
      VOLUME (M^3) * 0.69750655E+08 0.16089934E+09
      MASS (KG) * 0.16446265E+10 0.15805386E+12
*****

      COMPONENT MASS IN PLACE (KG)
*****
      PHASES *      GAS      AQUEOUS      ADSORBED      TOTAL
*****
      COMPONENTS *
      WATER * 0.11776724E+08 0.15803280E+12 0.00000000E+00 0.15804458E+12
      BRINE * 0.15159424E-09 0.19854241E-05 0.00000000E+00 0.19855757E-05
      NCG * 0.76983088E-21 0.13123056E-20 0.00000000E+00 0.20821365E-20
      TRC * 0.12892203E-19 0.13581595E+01 0.00000000E+00 0.13581595E+01
      CH4 * 0.16328497E+10 0.21055095E+08 0.00000000E+00 0.16539048E+10
*****

*****

...ITERATING... AT [ 1, 1] --- DELTEX = 0.100000E+03 MAX. RES. = 0.820000E-03 AT ELEMENT A3A 1 EQUATION 3
A3A 1( 1, 2) ST = 0.100000E+03 DT = 0.100000E+03 DX1= 0.145844E+03 DX2= -.627571E-24 T = 65.000 P = 3925142. S = 0.729421E+00
...ITERATING... AT [ 2, 1] --- DELTEX = 0.200000E+03 MAX. RES. = 0.163999E-02 AT ELEMENT A3A 1 EQUATION 3
A3A 1( 2, 2) ST = 0.300000E+03 DT = 0.200000E+03 DX1= 0.249230E+03 DX2= -.125143E-23 T = 65.000 P = 3925391. S = 0.729420E+00
...ITERATING... AT [ 3, 1] --- DELTEX = 0.400000E+03 MAX. RES. = 0.327991E-02 AT ELEMENT A3A 1 EQUATION 3
A3A 1( 3, 2) ST = 0.700000E+03 DT = 0.400000E+03 DX1= 0.385830E+03 DX2= -.249442E-23 T = 65.000 P = 3925777. S = 0.729419E+00
...ITERATING... AT [ 4, 1] --- DELTEX = 0.800000E+03 MAX. RES. = 0.655926E-02 AT ELEMENT A3A 1 EQUATION 3
A3A 1( 4, 2) ST = 0.150000E+04 DT = 0.800000E+03 DX1= 0.537215E+03 DX2= -.497038E-23 T = 65.000 P = 3926314. S = 0.729417E+00
...ITERATING... AT [ 5, 1] --- DELTEX = 0.160000E+04 MAX. RES. = 0.131155E-01 AT ELEMENT A3A 1 EQUATION 3
A3A 1( 5, 2) ST = 0.310000E+04 DT = 0.160000E+04 DX1= 0.709155E+03 DX2= -.990817E-23 T = 65.000 P = 3927023. S = 0.729413E+00
...ITERATING... AT [ 6, 1] --- DELTEX = 0.320000E+04 MAX. RES. = 0.262169E-01 AT ELEMENT A3A 1 EQUATION 3
A3A 1( 6, 2) ST = 0.630000E+04 DT = 0.320000E+04 DX1= 0.974776E+03 DX2= -.197579E-22 T = 65.000 P = 3927998. S = 0.729404E+00
...ITERATING... AT [ 7, 1] --- DELTEX = 0.640000E+04 MAX. RES. = 0.523751E-01 AT ELEMENT A3A 1 EQUATION 3
...ITERATING... AT [ 7, 2] --- DELTEX = 0.640000E+04 MAX. RES. = 0.298503E-04 AT ELEMENT A3A 1 EQUATION 3
A3A 1( 7, 3) ST = 0.127000E+05 DT = 0.640000E+04 DX1= 0.141534E+04 DX2= -.393480E-22 T = 65.000 P = 3929413. S = 0.729387E+00
...ITERATING... AT [ 8, 1] --- DELTEX = 0.128000E+05 MAX. RES. = 0.104511E+00 AT ELEMENT A3A 1 EQUATION 3
...ITERATING... AT [ 8, 2] --- DELTEX = 0.128000E+05 MAX. RES. = 0.108988E-03 AT ELEMENT A3A 1 EQUATION 3
A3A 1( 8, 3) ST = 0.255000E+05 DT = 0.128000E+05 DX1= 0.202145E+04 DX2= -.781711E-22 T = 65.000 P = 3931435. S = 0.729354E+00
...ITERATING... AT [ 9, 1] --- DELTEX = 0.256000E+05 MAX. RES. = 0.208045E+00 AT ELEMENT A3A 1 EQUATION 3
...ITERATING... AT [ 9, 2] --- DELTEX = 0.256000E+05 MAX. RES. = 0.404018E-03 AT ELEMENT A3A 1 EQUATION 3
A25 1( 9, 3) ST = 0.511000E+05 DT = 0.256000E+05 DX1= 0.533981E+02 DX2= -.576303E-24 T = 65.000 P = 3927407. S = 0.452492E+00
...ITERATING... AT [ 10, 1] --- DELTEX = 0.512000E+05 MAX. RES. = 0.412122E+00 AT ELEMENT A3A 1 EQUATION 3
...ITERATING... AT [ 10, 2] --- DELTEX = 0.512000E+05 MAX. RES. = 0.148003E-02 AT ELEMENT A3A 1 EQUATION 3
...ITERATING... AT [ 10, 3] --- DELTEX = 0.512000E+05 MAX. RES. = 0.127906E-03 AT ELEMENT A35 1 EQUATION 5
A36 1( 10, 4) ST = 0.102300E+06 DT = 0.512000E+05 DX1= 0.802834E+03 DX2= 0.628686E-24 T = 65.000 P = 3928795. S = 0.339701E+00

```

Figure 6. Beginning of iteration sequence for SAM7C2.

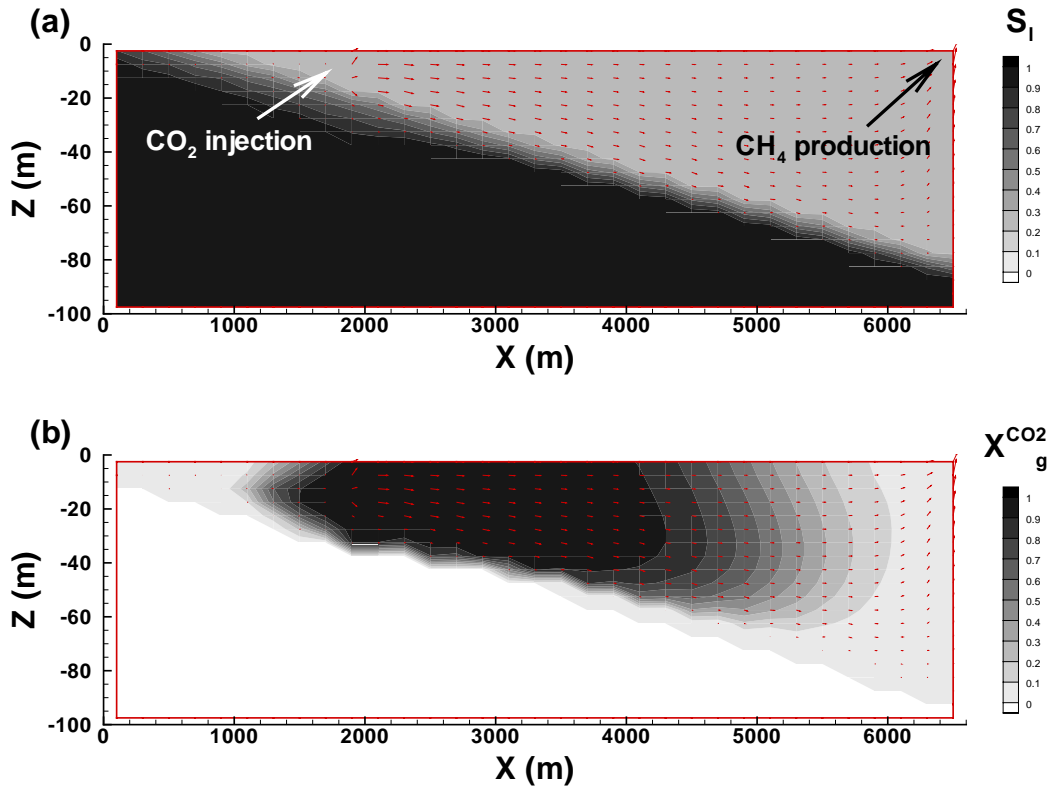


Figure 8. Tilted two-dimensional gas reservoir after 10 years of CO₂ injection showing (a) liquid saturation and gas velocity vectors, and (b) mass fraction of CO₂ in the gas phase and gas velocity vectors.

5.3 SAM7C3: CO₂ Injection into a Saturated System

This sample problem demonstrates the capabilities of EOS7C for modeling CO₂ injection into saturated systems such as aquifers. The geometry consists of a one-dimensional radial system 10 m thick with CO₂ injection at a rate of 8.4 kg s⁻¹. The outer boundary is held at constant pressure and liquid saturated conditions. The input file is shown in Fig. 9. Note a small amount of CH₄ is co-injected with CO₂ to improve the numerical behavior of the simulation. The initial pressure is uniform at 150 bars with temperature set at 65 °C. As shown in Fig. 10, after two days (1400 tonnes of CO₂ injected), the CO₂ gas plume reaches gridblock A1 7, 26 m from the injection point.

```

*SAM7C3* ... one-d radial injection into saturated region.
ROCKS-----1-----2-----3-----4-----5-----6-----7-----8
dome      2      2600.      .35      1.e-12      1.e-12      1.e-12      2.51      1000.
1.e-10
7          0.20          0.16          1.          .01
7          0.20          .15          .00084      1.e5          1.
bndry     2      2600.      .35      1.e-12      1.e-12      1.e-12      2.51      2.e4
0.25
5
1          0.e5          0.0          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
3 500      50010 030000020000400 23
1.7280E+05      -1.      1.0e9          9.8066
1.00e01
1.e-5
1.500e7          0.          0.e-6          0.e-6
0.0e-0          65.

IE(14) = 1, use SUPST and GASEOS for enthalpy. IE(14) = 0, use GASEOS only.
IE(15) = 1, use Peng-Robinson eqn. of state. IE(15) = 2,3 use RK,SRK, resp.
IE(16) = 1, NCG is CO2. IE(16) = 2, NCG is N2.
SELEC-----1-----2-----3-----4-----5-----6-----7-----8
6
-1.e5
1 1 1

1.e50      4.00      0.e-6      0.e-6      0.e-6      0.e-6 1.000e-10

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-5      1.e-10
0.e-6      1.e-10
1.e-5      1.e-10
1.e-5      1.e-10
1.e-5      1.e-10

GENER-----1-----2-----3-----4-----5-----6-----7-----8
A1 1CO2      COM3      8.4E+00      5.356e4
A1 1CH4      COM5      8.4E-03      5.356e4

INCON
A1 12      0.35000000E+00
0.150000000000000E+08 0.000000000000000E+00 0.000000000000000E+00 0.000000000000000E+00
0.000000000000000E+01 0.650000000000000E+02

```

Figure 9. Input file for one-dimensional saturated-zone radial injection problem.

```

ELEME ---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
A1 1      10.1257E+030.2513E+02      0.1000E+01      -.5000E+01
A1 2      10.3770E+030.7540E+02      0.3000E+01      -.5000E+01
A1 3      10.6283E+030.1257E+03      0.5000E+01      -.5000E+01
A1 4      10.2011E+040.4021E+03      0.8000E+01      -.5000E+01
A1 5      10.4901E+040.9802E+03      0.1300E+02      -.5000E+01
A1 6      10.7163E+040.1433E+04      0.1900E+02      -.5000E+01
A1 7      10.1307E+050.2614E+04      0.2600E+02      -.5000E+01
A1 8      10.1973E+050.3946E+04      0.3454E+02      -.5000E+01
A1 9      10.1551E+060.3102E+05      0.5975E+02      -.5000E+01
A1 10     10.2056E+070.4112E+06      0.1743E+03      -.5000E+01
A1 11     10.3726E+080.7451E+07      0.6948E+03      -.5000E+01
A1 12     20.7459E+590.1492E+09      0.3061E+04      -.5000E+01

CONNE
A1 1A1 2      10.1000E+010.1000E+010.1257E+03
A1 2A1 3      10.1000E+010.1000E+010.2513E+03
A1 3A1 4      10.1000E+010.2000E+010.3770E+03
A1 4A1 5      10.2000E+010.3000E+010.6283E+03
A1 5A1 6      10.3000E+010.3000E+010.1005E+04
A1 6A1 7      10.3000E+010.4000E+010.1382E+04
A1 7A1 8      10.4000E+010.4545E+010.1885E+04
A1 8A1 9      10.4545E+010.2066E+020.2456E+04
A1 9A1 10     10.2066E+020.9388E+020.5052E+04
A1 10A1 11    10.9388E+020.4267E+030.1685E+05
A1 11A1 12    10.4267E+030.1939E+040.7047E+05

ENDCY-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
MESHMAKER1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
RZ2D
RADII
8
0.      2.      4.      6.      10.     16.     22.     30.
LOGAR
5      5.e3      2.
LAYER
1
10.

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

```

Figure 9. Input file for one-dimensional saturated-zone radial injection problem (continued).

6. Final Notes

Summary of important points to remember in using EOS7C:

- For successful use of EOS7C, users should be experienced with TOUGH2 and have access to the TOUGH2 User's Guide (Pruess et al., 1999) for supplementary information.
- NKIN controls the type of INCON file or block to be read from. For NKIN = NK, the INCON file is expected to be in the EOS7C format with up to six primary variables. For NKIN = 2 or 3, the INCON is expected to be in standard EOS7 format with up to four primary variables.
- MOP(20) selects whether to reset variables to ensure that negative mass fractions do not occur (see p. 18 of this report or EOS7C informative printout for details).
- The SELEC parameters IE(14), IE(15), and IE(16) control the enthalpy calculation, the equation of state, and the choice of NCG, respectively.
- The effects of brine (i.e., salinity) on gas solubility are neglected in EOS7C v. 1.0.
- Although the gas mixture densities are very accurate in EOS7C v. 1.0, no effects of dissolved gas components on liquid density are included.

- The intended application area of EOS7C is natural gas (methane, CH₄) reservoirs. As such, whatever part of the gas phase that is not made up of water vapor, CO₂, or gas tracer is assumed to be made up of CH₄.
- If molecular diffusivity is input as a negative number, the absolute value of this number is used for the phase molecular diffusivity without modification by S and τ (saturation and tortuosity) and without pressure or temperature effects. However, no diffusive fluxes are calculated for domains where τ is input as zero or blank regardless of the phase molecular diffusivity.
- Pressure (P) affects gas diffusivity by the factor $1.0 \times 10^5/P$ (Pruess et al., 1999). For example, if pressure is 2.0×10^5 Pa, the corresponding effective molecular diffusivity for the gas is one-half the input value. This can result in overestimation of molecular diffusivity at high pressures (see p. 15 of this report for details).
- Temperature affects gas diffusivity by the factor $((T + 273.15)/273.15)^{\text{TEXP}}$ (Pruess et al., 1999). If TEXP is input as zero, temperature effects on gas diffusivity are neglected.

Appendix 1. Program units in EOS7C.

SUBROUTINE EOS
SUBROUTINE PP7R
SUBROUTINE HENRYINV
SUBROUTINE OUT
SUBROUTINE SOLIT
SUBROUTINE ZEVSREAL

Table A1. Summary of changes for program units in EOS7C.

Program unit	Basic changes for adding NCG and CH ₄ .
EOS	Changed to handle NCG and CH ₄ . Calls ZEVSREAL
PP7R	Changed to handle NCG and gas tracer instead of radionuclides.
HENRYINV	Calculates inverse Henry's coefficients as function of temperature.
OUT	Changed to print out properties and headings relevant to gas simulations.
SOLIT	Calls HENRYINV and ZEVSREAL iteratively to find solubility.
ZEVSREAL	Calculates real-gas mixture properties.

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Acknowledgments

This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems through the National Energy Technology Laboratory, and by Lawrence Berkeley National Laboratory under Department of Energy Contract No. DE-AC03-76SF00098. We thank Chao Shan and Jonny Rutqvist (LBNL) for internal reviews, and Alfredo Battistelli for a very thorough external review.

Nomenclature

<i>a</i>	activity	-
<i>d</i>	molecular diffusivity	$\text{m}^2 \text{ s}^{-1}$
<i>f</i>	fugacity	Pa
<i>H</i>	enthalpy	J kg^{-1}
<i>K</i>	equilibrium constant	-
<i>Kh</i>	Henry's coefficient	Pa^{-1}
<i>MW</i>	molecular weight	kg mole^{-1}
NCG	non-condensable gas	
NEQ	number of equations per grid block	
NK	number of mass components (species)	
NKIN	number of mass components (species) in INCON file or block	
NPH	maximum number of phases present	
<i>P</i>	pressure	Pa
<i>q</i>	source term	$\text{kg m}^{-3} \text{ s}^{-1}$
<i>R</i>	gas constant ($8.31433 \text{ J kg}^{-1} \text{ }^\circ\text{C}^{-1}$)	$\text{J kg}^{-1} \text{ K}^{-1}$
<i>S</i>	phase saturation	-
<i>t</i>	time	sec.

T	Temperature	°C, K
U	internal energy	J kg ⁻¹
V	volume	m ³
\bar{V}_i	partial molar volume	m ³ mol ⁻¹
x	mole fraction in the liquid phase	-
X	mass fraction	-
y	mole fraction in the gas phase	-
Y	Y-coordinate	m
Z	Z-coordinate	m
Z	Z factor	-

Greek symbols

γ	activity coefficient	-
μ	dynamic viscosity	kg m ⁻¹ s ⁻¹
ϕ	porosity, fucacity coefficient	-
ρ	density	kg m ⁻³
τ	tortuosity	-

Subscripts and superscripts

aq	aqueous phase
g	gas phase
l	liquid
0	reference value
β	phase
κ	mass components