The Modeling of 3D Compositional Grading and Plus Fraction Molecular Weight Change in Non-isothermal Petroleum Reservoirs

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Published online: 10 Dec 2012.

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Composition and physical properties vary within hydrocarbon reservoirs, even in well connected ones; it is of crucial interest to model this change in order to initialize the reservoir simulator. In this work, a non-isothermal model is used to depict changes in plus fraction molecular weight and it will be integrated into another non-isothermal model describing fluid compositional changes within a 3D reservoir. Previously, the model has been validated versus 1D real reservoir data. It will be used to model compositional change of real hydrocarbon in a synthetic 3D reservoir subjected to temperature gradient in x, y, and z directions.

Keywords: compositional grading, concentration distribution function, plus fraction, stability analysis

1. INTRODUCTION

Several factors may lead to compositional variation within the reservoir, some of which are: gravity (Sage and Lacey, 1939), thermal diffusion (Dougherty and Drickamer, 1955), incomplete hydrocarbon migration/mixing (Gibson et al., 2006), natural convection (Ghorayeb and Firoozabadi, 2000), dynamic flux of water aquifer contacting only a part of a reservoir (Hoier and Whitson, 2000), asphaltene precipitation (tar mat) at the lower parts of a reservoir (Riemens et al., 1988), biodegradation (Temeng et al., 1998), reservoir compartmentalization (Elshahawi et al., 2005), genesis (Smalley and England, 1992), and capillary forces (Lee, 1989; Wheaton, 1991).

The model used in this study considers only effects of gravity and temperature gradient, assuming steady-state conditions and zero net mass flux (stationary state).

2. THEORY

The formulation for calculating compositional variation under the force of gravity for an isothermal system was first given by Gibbs (1961).

Based on stationary system assumption and theory of irreversible processes, Faissat et al. (1994) proposed the following model for non-isothermal compositional grading:

$$\nabla \mu_k = M_k g - Q_k^{net} \frac{gradT}{T}.$$ (1)

In this model, $gradT$ is temperature gradient, Q_k^{net} is called the net heat of transport (NHT) of component k in the mixture, M is molecular mass, and μ is chemical potential. From this equation another, more useful relationship can be derived, as given in Eq. (2):

$$\nabla \ln(f_k) = \frac{M_k g}{RT} - Q_k^{net} \frac{\nabla T}{RT^2}.$$ (2)

Apparently this model can be used in 3D systems as it is written in vector form and can be used in any direction in any coordinate system; writing this equation in an arbitrary direction of h:

$$\frac{\partial \ln(f_k)}{\partial h} = \frac{M_k g_h}{RT} - Q_k^{net} \frac{\partial T/\partial h}{RT^2},$$ (3)

where g_h is the component of g, the gravitational acceleration, in the direction of h. Here, integration of both parts needs M_k and Q_k^{net} to be constant in the direction of h; these parameters are defined in the following sections.

3. NET HEAT OF TRANSPORT (NHT)

An appropriate multicomponent expression for NHT is needed, and some expressions have been proposed by Haase (1969), Kempers (1989), and Belery and da Silva (1990). Here the model proposed by Firoozabadi et al. (2000) is used. It is given in Eq. (4):

$$Q_i^{net} = -\frac{\Delta \overline{U}_i}{\tau_i} + \left[\sum_{j=1}^{n} \frac{x_j \Delta \overline{U} j}{\tau_j} \right] \frac{\overline{v}_i}{\sum_{j=1}^{n} x_j \overline{v}_j},$$ (4)

where ΔU is the partial molar internal energy departure from that of ideal gas mixture obtained from equation of state (EOS), τ_i is an irreversible factor, which is 4.0 as proposed by authors for binaries, and for multicomponent liquid mixtures at low pressures it varies from 3–5; thus, 4.0 will be taken for all components.

4. CHANGES OF PLUS FRACTION MOLECULAR WEIGHT WITH LOCATION THROUGH THE HYDROCARBON SYSTEM

There are two works aiming at modeling changes of plus fraction molecular weight in the system: the first, published by Galeana et al. (1994), which deals with isothermal case, and the second by Bakhtiari Nia and Movagharnejad (2007), which deals with a non-isothermal case but simplified to do so; the authors use the latter in this work, and it is described as follows.

The change of plus fraction molecular weight with location will be described and then using empirical correlations other physical properties of this fraction will be found. First, a concentration distribution function (CDF) that describes the concentration distribution of sub-fractions in the plus fraction will be introduced. The CDF is usually shown by $F(I)$, where I is the distribution variable ($MW, T_b, \ldots$) and satisfies:

$$\int F(I)dI = 1. \tag{5}$$

The most widely used variables are molecular weight and carbon number; the authors use molecular weight. It is usually desirable to define the fluid by a semi-continuous scheme where light fractions are shown discretely while heavies are defined by a CDF.

As a result, mole fraction of constituents having MW less than or equal to i is calculated from:

$$x_{qi} = \int_{\eta}^{i} F(M)dM. \tag{6}$$

Here, η is MW of the lightest component within the CDF. Average MW of components having MW between j and i is calculated from:

$$\overline{M_{j-i}} = \frac{\int_{j}^{i} MF(M)dM}{x_{j-i}}. \tag{7}$$

In this relation, x_{j-i} is the total mole fraction of those components:

$$x_{j-i} = \int_{j}^{i} F(M)dM. \tag{8}$$

That is the area under the curve of $F(M)$ restricted between $M = i$ and $M = j$. Equation (3) can be integrated with respect to h as:

$$RT \ln \left(\frac{f_i^h}{f_i^{h_0}} \right) = M_i g(h - h_0) - Q_i^{net} \frac{\nabla T}{T}. \tag{9}$$

In this relation, f_i^h shows fugacity of component i, h and h_0 show current and the reference depths.

The CDF used in this work is as follows (Manafi et al., 1999):

$$F(M) = \frac{B^2 MW}{\eta^A MW} \left[\frac{M - \eta}{\eta} \right]^{(B_{MW}^{-1})} \times \exp \left[-\frac{B_{MW}}{A_{MW}} \left[\frac{M - \eta}{\eta} \right]^{B_{MW}} \right]. \tag{10}$$

If the heavy fraction under study is C_{7+}, and if there is no information about η, it can be assumed as 84. A_{MW} and B_{MW} are distribution parameters; they adjust the shape of the CDF and can be found by matching the CDF to the real composition distribution. B_{MW} can be assumed unity (Manafi et al., 1999) to reach the following equation:

$$\overline{M} = \eta(A_{MW} + 1). \tag{11}$$

To expand the above equation in all M intervals, a method called "Method of Moments" is used (Galeana et al., 1994). In this method, the moment of order "r" is calculated as:

$$m^r = \int_{\eta}^{\infty} M^r F(M) dM. \tag{12}$$

The first moment obviously gives average molecular weight of heavies (MW of the plus fraction), considering Eq. (11):

$$\eta(A_{MW} + 1) = \left\{ \left[\frac{\eta A_{MW}}{(b\eta A_{MW} + 1)^2} + \frac{\eta}{b\eta A_{MW} + 1} \right] \exp(b\eta) \exp(c) \right\}_{h^0} \times \frac{x_h^0}{x_h} - 1, \tag{13}$$

where x shows mole fraction of the plus fraction and

$$b = \frac{g_h(h - h^0)}{RT}, \text{ and, } c = -\frac{Q_i^{net} \nabla T (h - h^0)}{RT^2} \tag{14}$$

As a result, the variable distribution parameter (A_{MW}) can be calculated at each step and can also have changes of plus fraction molecular weight, whatever the fraction is, but the important point is that η is different for different plus fractions. The authors have found that for any C_{n+} fraction with $n > 6$, one can take η as the molecular weight of C_{n-1} fraction, but in general it should be found by regression over compositional data of MW vs. concentration of chemicals within the plus fraction range. It can clearly be seen that, again, this model is a 3D one.

5. CHARACTERIZATION OF THE PLUS FRACTION AND IMPORTANT EQUATION OF STATE (EOS) PARAMETERS

As mentioned, it is necessary for the plus fraction to be characterized in each step in order to run the EOS in the calculations. The EOS chosen by the authors is that proposed by Peng and Robinson (1976), with volume shift parameter and binary interaction parameters from Chou-Prausnitz (1989) and Chueh-Prausnitz (1967) relations, respectively, and will be dealt with as constants (Cheuh-Prausnitz coefficient is considered to be 0.15 as default) as calculated by the Eclipse Reservoir Simulator developed by Schlumberger Co. (2005). Pure component properties come from Katz-Firoozabadi property tables (Schlumberger Co., 2005), while the plus fractions are characterized using Kesler-Lee relationships (1978) for critical temperature and pressure and acentric properties; the critical volume and also normal boiling point needed in Kesler-Lee correlations will come from Riazi-Daubert correlation (1980). K-values (K_i) used as a first guess in flash calculations will be calculated using Wilson correlation (1964).

6. NUMERICAL ALGORITHM

The numerical algorithm used here is that proposed by Whitson and Belery (1994) modified for a non-isothermal effect as follows:

$$\overline{f}_i = f_i^0 \times \exp\left(-\frac{c_i P}{RT} + \frac{c_i^0 P^0}{RT^0} \right) \times \exp\left(-\frac{M_i g(z - z^0)}{RT} - \frac{Q_i^{net}(T - T^0)}{RT^2} \right), \tag{15}$$

$$Y_i = Z_i \frac{\overline{f}_i}{f_i}, \tag{16}$$

$$Q(P, Z) = 1 - \sum_{i=1}^{n_c} Y_i, \tag{17}$$

$$r_i = \frac{\overline{f}_i}{f_i} \left(\sum_{i=1}^{n_c} Y_i \right)^{-1}, \tag{18}$$

$$Y_i^{(n+1)} = Y_i^{(n)} \times r_i, \tag{19}$$

$$P^{(n+1)} = P^{(n)} - \frac{Q^{(n)}}{\left[\frac{\partial Q}{\partial P} \right]^{(n)}}, \tag{20}$$

where c_i shows volume correction parameter ($v_i^{corrected} = v_i - c_i$), z shows elevation, Z is the composition, n is iteration counter, and n_c is number of components present in the mixture.

Convergence criteria are:

$$\left| 1 - \sum_{i=1}^{n_c} Y_i \right| < 10^{-13}, \left[\sum_{i=1}^{n_c} \frac{\ln(r_i Y_i)}{\ln(Z_i)} \right]^2 < 10^{-8}. \tag{21}$$

At each step a stability check should be performed, which is, here, executed by direct minimization of the tangent plane distance introduced by Baker et al. (1982) to find local minima using a Newton-Raphson scheme and global search for a minimum using a tunneling method outlined by Cetin et al. (1993). A flowchart of the calculation is given in Figure 1.

The model has been validated elsewhere versus measured data of 1D type (Nikpoor et al., 2011).

7.   CASE STUDY 1: SINGLE PHASE

The fluid system is a 12-component heavy Iranian oil at Azadegan oil field, southwest of Iran. It contains acidic gases and is fractioned up to C_{7+}. Pressure and temperature at the reference point are 175 BARSA and 370 K, respectively (reference depth is 3,000 m subsea at $x = 0$ and $y = 0$ location, the end of the reservoir is a depth of 3,100 m, $x = 100$ m and $y = 100$ m). Temperature gradients at x, y, and z directions are 0.003, 0.004, and -0.035 K/m, respectively. The synthetic reservoir under study is a 100 m $\times$ 100 m $\times$ 100 m cube. The code runs with step sizes $\Delta x = \Delta y = \Delta h = 10$ m and at each step it calculates composition, pressure, and molecular weight of the plus fraction and updates all of its other characterization properties needed in EOS calculations in an iterative mode, verifies stability of the fluid at reservoir temperature and pressure, then if the fluid is stable, it calculates solution gas oil ratio and formation volume factor of the fluid using a single step flash. It also calculates isothermal compressibility factor and isobaric thermal expansion of the mixture at the reservoir pressure. If the mixture is unstable (which is not the case in the authors' study) the code continues with calculation of the gas-oil-contact with accuracy of 1 m and then goes to the gas column. Reference fluid is given in Table 1 and some of the outputs are shown in Figure 2.
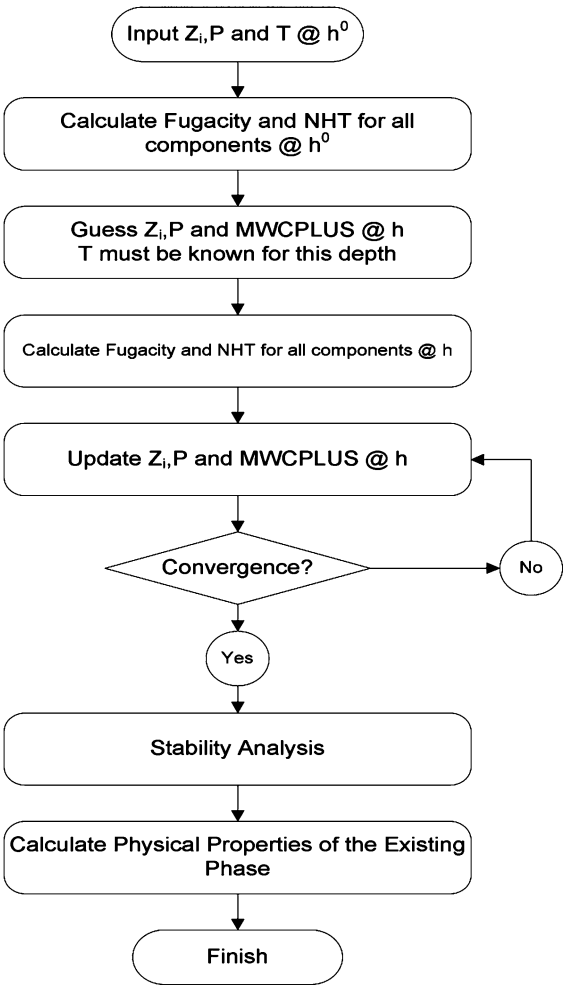
FIGURE 1   Numerical algorithm of compositional grading calculation.

TABLE 1
Case Study 1: Composition of the Reference Fluid

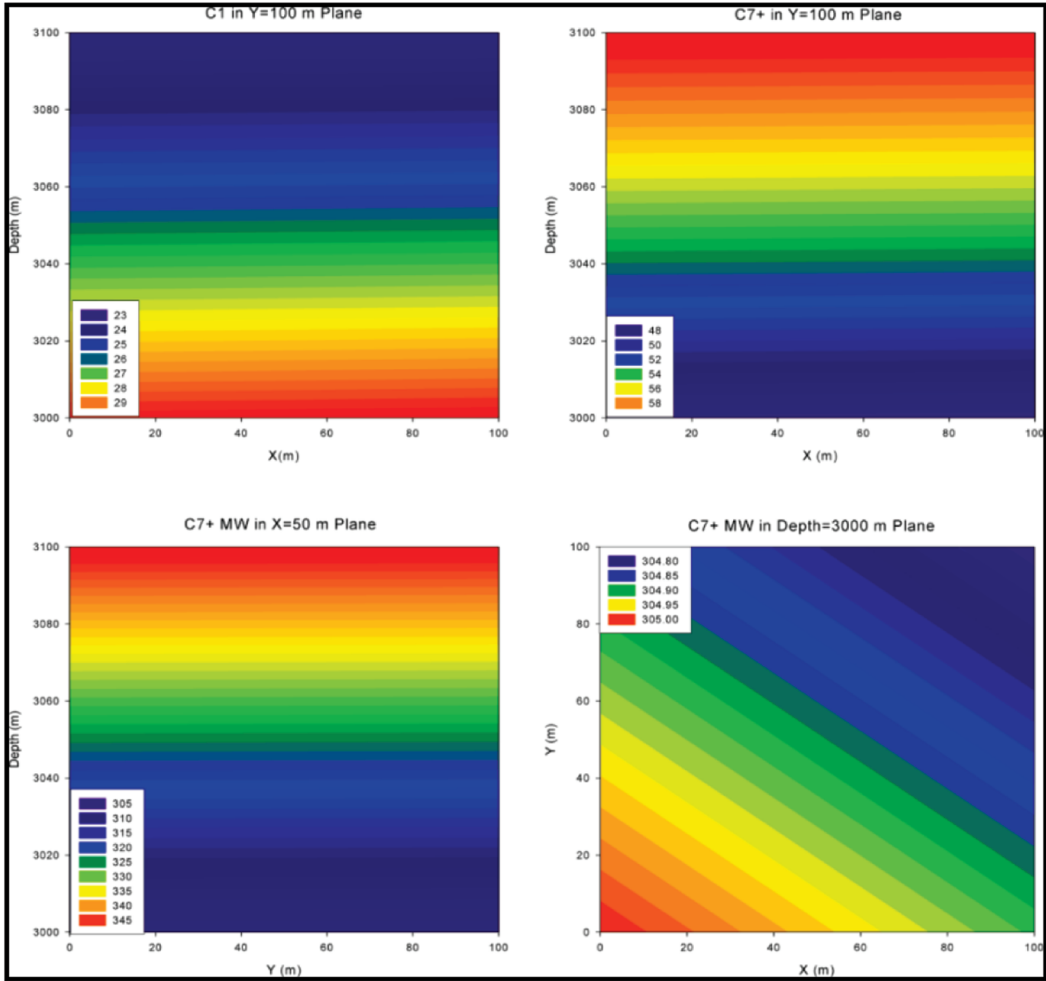| Component	Mole%	MW	SPgr
H_2S	0.04		
N_2	0.4		
CO_2	1.44		
C_1	29.59		
C_2	7.36		
C_3	5.39		
iC_4	0.91		
nC_4	2.98		
iC_5	1.43		
nC_5	1.78		
C_6	1.4		
C_{7+}	47.28	305	0.9643

FIGURE 2   Case study 1: Some outputs of running the model code. (color figure available online)

As is apparent from the graphs, temperature increase in horizontal directions causes a decrease in heavy fractions and molecular weight of the plus fraction and the opposite in the case of light components; from here it can be concluded how solution gas-oil ratio, density, formation volume factor, and other physical properties of oil change. Gravity acts opposite to the temperature gradient in the vertical direction; gravity effect in this case is stronger than that of thermal diffusion and the consequence is opposite to what has been seen in horizontal directions. The results of 3D compositional grading simulation are completely consistent with what is observed in normal 1D case.

8.   CASE STUDY 2: TWO PHASE

The fluid system is a 17-component heavy oil at Azadegan oil field, southwest of Iran. It contains acidic gases and is fractioned up to C_{12+}. Pressure and temperature at the reference point are 85
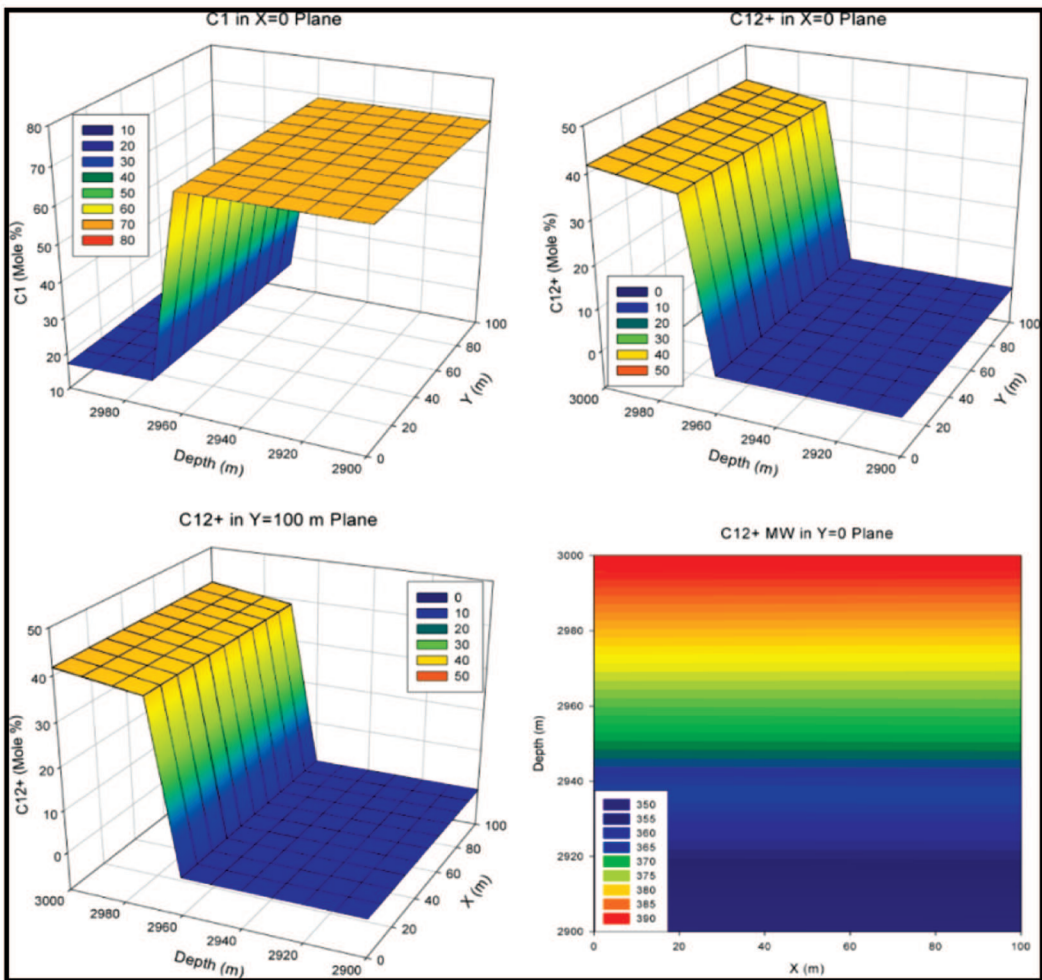
FIGURE 3   Case study 2: Some outputs of running the model code. (color figure available online)

BARSA and 370 K, respectively (reference depth is 3,000 m subsea at $x = 0$ and $y = 0$ location, end of the reservoir is a depth of 2,900 m, $x = 100$ m and $y = 100$ m). Temperature gradients at x, y, and z directions are 0.003, 0.004, and −0.05 K/m, respectively. The synthetic reservoir under study is a 100 m × 100 m × 100 m cube. Reference fluid is given in Table 2 and some of the outputs are shown in Figure 3.

9.   CASE STUDY 3: SINGLE PHASE

This reference fluid is taken from Table 4 of work by Jaubert et al. (2002), here the 25-component system is a light oil at 190 BARSA pressure and 325 K temperature at a location of (0, 0, 0). The synthetic reservoir under study is a 100 m × 100 m × 100 m cube and temperature gradients
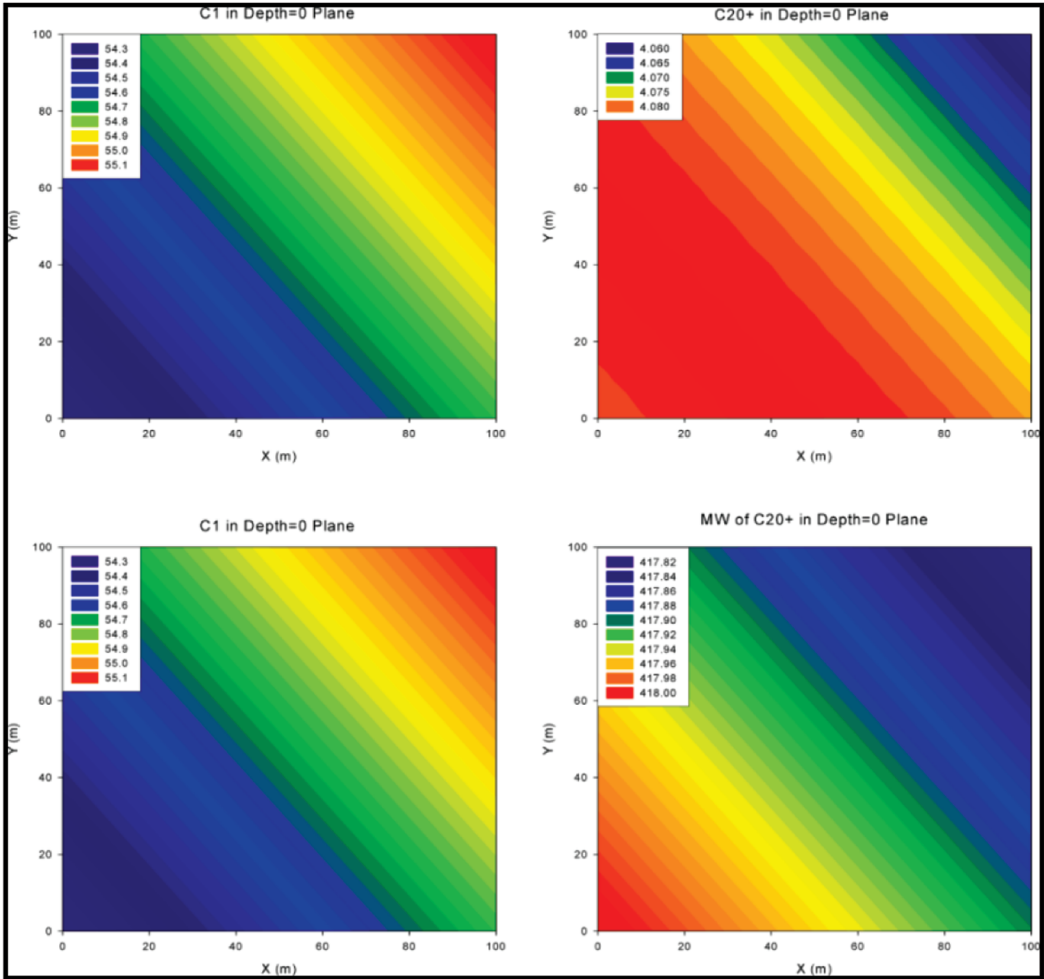
FIGURE 4   Case study 3: Some outputs of running the model code. (color figure available online)

at x, y, and h ($h = -z$) directions are 0.01, 0.012, and -0.05 K/m, respectively. The code runs with step sizes $\Delta x = \Delta y = \Delta h = 10$ m. The code with step sizes of 20 and 5 m have been tested and the same results produced; this shows that the implicit scheme of the algorithm is quite strong and stable. Some of the outputs are shown in Figure 4.

10.   CONCLUSIONS

A 3D method for calculation of compositional grading in non-isothermal three-dimensional reservoir fluid systems is introduced. It incorporates modeling of molecular weight change of the plus fraction with location in the system. Stability tests are used to predict the location of gas-oil contact in the reservoir.

TABLE 2
Case Study 2: Composition of the Reference Fluid

Component	Mole%	MW	SPgr
H_2S	0.0228		
N_2	0.1336		
CO_2	2.0700		
C_1	17.0642		
C_2	8.0545		
C_3	6.8799		
iC_4	1.3279		
nC_4	4.4268		
iC_5	2.3771		
nC_5	2.7859		
C_6	3.3485		
C_7	3.0268		
C_8	1.5953		
C_9	0.8068		
C_{10}	1.6686		
C_{11}	2.6221		
$C_{12}+$	41.7894	390	0.9634

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