GVD - Gas, Volatile Oil and Dead Oil

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1. Physical Model

The pores of the rock are filled by two phases, a gaseous phase and a liquid oleic phase. There are three chemical components, an insoluble gas A, a volatile hydrocarbon B and a non-volatile (or "dead") hydrocarbon D. The insoluble gas exists only in the gaseous phase, the volatile hydrocarbon exists both in the liquid and gaseous phases, while the dead oil exists only in the liquid phase.

2. Thermodynamical Equilibrium

2.1. Thermodynamical assumptions

We assume that the temperature (T) is contant and that the pressure (P) can be considered constant as far as thermodynamical properties are concerned. The equation of state for the oleic phase expresses that the sum of all volume fractions is equal to one (the ideal liquid approximation)

$$\frac{\varrho_{ob}}{\varrho_{oB}} + \frac{\varrho_{od}}{\varrho_{oD}} = 1,\tag{1}$$

where each ϱ_{oI} denote idealized density¹ of pure component I at the prevailing temperature and pressure; ϱ_{oi} are actual the molar densities of component I in the oleic mixture.

Let ϱ_o and ϱ_g be the molar densities of the oleic and gaseous phases, respectively; let \mathcal{Y}_i and \mathcal{X}_i be the molar fractions of each component in the oleic and gaseous phase, respectively; and let ϱ_{gi} be the molar densities of component I in the gaseous phase². We have

$$\varrho_o = \varrho_{ob} + \varrho_{od}, \quad \mathcal{Y}_b = \frac{\varrho_{ob}}{\varrho_o}, \quad \mathcal{Y}_d = \frac{\varrho_{od}}{\varrho_o}, \quad \text{and} \quad \mathcal{Y}_b + \mathcal{Y}_d = 1.$$
(2)

$$\varrho_g = \varrho_{gb} + \varrho_{gd}, \quad \mathcal{X}_a = \frac{\varrho_{ga}}{\varrho_g}, \quad \mathcal{X}_b = \frac{\varrho_{gb}}{\varrho_g}, \quad \text{and} \quad \mathcal{X}_a + \mathcal{X}_b = 1,$$
(3)

Let P_B^* be the vapor pressure of the pure oleic component B at the current temperature. From Raoult's law, the actual vapor pressure of component B is

$$P_{ob} = P_B^* \mathcal{Y}_b. \tag{4}$$

For gaseous phase we use the ideal gas law:

$$P_{ga} = \varrho_{ga} R T, \quad P_{gb} = \varrho_{gb} R T, \quad P = P_{ga} + P_{gb}. \tag{5}$$

¹The molar density ϱ is the number of moles per unit volume. Therefore, ϱ is the inverse of the molar volume, V_m ; we keep ϱ for density, *i.e.* volumetric mass density.

²We use boldface math letters to represent the state variables of the problem. As we will see, we choose s, y and u.

In thermodynamical equilibrium, the partial pressure of component B in the oleic and the gaseous phases are equal; using (4), the partial pressures are

$$P_{ob} = P_{qb} \Leftrightarrow P_B^* \mathcal{Y}_b = RT \,\varrho_{qb}. \tag{6}$$

2.2. Thermodynamical relations

From (1) to (6) we write oleic the molar density ϱ_{ob} as affine function of ϱ_{od} , and gaseous molar densities as the ratio of two affine functions on ϱ_{od} :

$$\varrho_{ob} = -\frac{\varrho_{oB}}{\varrho_{oD}} \varrho_{od} + \varrho_{oB}, \tag{7a}$$

$$\varrho_{ga} = \frac{1}{RT} \frac{(\delta_B - \delta_D) \,\varrho_{od} - \delta_B \,\varrho_{oD}}{Q(\varrho_{od})}, \quad \varrho_{gb} = \frac{P_B^* \,\varrho_{oB}}{RT} \,\frac{\varrho_{od} - \varrho_{oD}}{Q(\varrho_{od})}$$
(7b)

where

$$\delta_D = P \varrho_{oD}, \quad \delta_B = (P - P_B^*) \varrho_{oB}.$$
 (8)

and

$$Q(\varrho_{od}) = (\varrho_{oB} - \varrho_{oD})\varrho_{od} - \varrho_{oB}\varrho_{oD}. \tag{9}$$

The relations between the molar densities may be rewritten as relations between molar fractions depending on \mathcal{Y}_d , see (2.c):

$$\mathcal{Y}_d = \boldsymbol{y}, \quad \mathcal{Y}_b(\boldsymbol{y}) = 1 - \boldsymbol{y}, \quad \mathcal{X}_a(\boldsymbol{y}) = 1 - \frac{P_b^*}{P} (1 - \boldsymbol{y}), \quad \mathcal{X}_b(\boldsymbol{y}) = \frac{P_b^*}{P} (1 - \boldsymbol{y}).$$
 (10)

Lemma 1. The model has molar fractions between 0 and 1 for $\mathbf{y} \ge 1 - P/P_B^*$. Therefore, if $P \ge P_B^*$ the model is valid for all $\mathbf{y} \in [0,1]$.

The molar densities are related to y:

$$\varrho_{od} = \boldsymbol{y} \,\varrho_o(\boldsymbol{y}), \quad \varrho_{ob} = (1 - \boldsymbol{y}) \,\varrho_o(\boldsymbol{y}),$$
(11a)

$$\varrho_{ga} = \varrho_g - \varrho_* (1 - \boldsymbol{y}), \quad \varrho_{gb} = \varrho_* (1 - \boldsymbol{y}).$$
(11b)

where

$$\varrho_o(\mathbf{y}) = \frac{BD}{D(1-\mathbf{y}) + B\mathbf{y}},\tag{12}$$

and

$$\varrho_g = P/RT, \quad \varrho_* = P_B^*/RT, \quad \varrho_{oD} = D, \quad \varrho_{oB} = B.$$
(13)

3. Molar Balance in the Flow

We use the porous media notation s_i and f_i for saturation and fractional flow of each phase; the subscript o stands for oleic and g for gaseous. We assume usual the normalization:

$$s_o + s_g = 1, \quad f_o + f_g = 1,$$
 (14)

where the fractional flux functions depend on viscosities, μ_o and μ_g , and relative permeability, k_o and k_g ,

$$f_o = \frac{k_o/\mu_o}{k_o/\mu_o + k_g/\mu_g}, \quad f_g = \frac{k_g/\mu_g}{k_o/\mu_o + k_g/\mu_g}.$$
 (15)

We also assume that

TO DO: Relative permeabilities; Darcy's law; Viscosity.

$$k_o = s_o^2$$
, $k_g = s_q^2 = (1 - s_o)^2$, (16a)

$$\mu_o(\mathbf{y}) = \mu_{oD} \mathbf{y} + \mu_{oB} (1 - \mathbf{y}), \quad \text{constant } \mu_g = \mu_G. \tag{16b}$$

Taking the viscosity ratios

$$\mathcal{R}(\boldsymbol{y}) = \frac{\mu_o(\boldsymbol{y})}{\mu_G} = \mathcal{D}\,\boldsymbol{y} + \mathcal{B}\,(1 - \boldsymbol{y}) = \mathcal{B} + (\mathcal{D} - \mathcal{B})\boldsymbol{y},\tag{17}$$

where

$$\mathcal{B} = \mu_{oB}/\mu_{oG},\tag{18a}$$

$$\mathcal{D} = \mu_{oD}/\mu_{oG}.\tag{18b}$$

We define

$$f_o(\mathbf{s}, \mathbf{r}) = \frac{s_o^2}{s_o^2 + \mathbf{r}(1 - s_o)^2}, \quad f_g(\mathbf{s}, \mathbf{r}) = \frac{\mathbf{r}(1 - s_o)^2}{s_o^2 + \mathbf{r}(1 - s_o)^2},$$
 (19a)

$$f(s, y) = f_o(s, \mathcal{R}(y)). \tag{19b}$$

The molar balance of each component in each phase is given by the following equations

$$\frac{\partial}{\partial t}(\varphi \varrho_{ga} s_g) + \frac{\partial}{\partial x}(\varrho_{ga} u_g) = 0$$
(20a)

$$\frac{\partial}{\partial t}(\varphi \varrho_{gb} s_g) + \frac{\partial}{\partial x}(\varrho_{gb} u_g) = q_b$$
(20b)

$$\frac{\partial}{\partial t}(\varphi \varrho_{ob} s_o) + \frac{\partial}{\partial x}(\varrho_{ob} u_o) = -q_b \tag{20c}$$

$$\frac{\partial}{\partial t}(\varphi \varrho_{od} s_o) + \frac{\partial}{\partial x}(\varrho_{od} u_o) = 0 \tag{20d}$$

where the source term q_b represent the rate of mole transfer of oil b from the oleic to the gaseous phase; it is very large. In (20) u_o and u_g are the Darcy velocities of the oleic and gaseous phases. Defining the total velocity $\mathbf{u} = u_o + u_g$, using Darcy's law one can show that $u_o = f_o \mathbf{u}$ and $u_g = f_g \mathbf{u}$. Using the expressions for u_o and u_g , adding (20b) and (20c), we obtain conservation equations for A, B and D.

$$\varphi \frac{\partial}{\partial t} (\varrho_{ga} s_g) + \frac{\partial}{\partial x} (\varrho_{ga} f_g) \boldsymbol{u} = 0$$
 (21a)

$$\varphi \frac{\partial}{\partial t} (\varrho_{gb} s_g + \varrho_{ob} s_o) + \frac{\partial}{\partial x} (\varrho_{gb} f_g + \varrho_{ob} f_o) \boldsymbol{u} = 0$$
 (21b)

$$\varphi \frac{\partial}{\partial t} (\varrho_{od} s_o) + \frac{\partial}{\partial x} (\varrho_{od} f_o) \boldsymbol{u} = 0$$
 (21c)

or, using (14) and representing s_o as s

$$\varphi \frac{\partial}{\partial t} (\varrho_{ga} - \varrho_{ga} \mathbf{s})) + \frac{\partial}{\partial x} (\varrho_{ga} - \varrho_{ga} f_o) \mathbf{u} = 0$$
 (22a)

$$\varphi \frac{\partial}{\partial t} (\varrho_{gb} + (\varrho_{ob} - \varrho_{gb}) \mathbf{s}) + \frac{\partial}{\partial x} (\varrho_{gb} + (\varrho_{ob} - \varrho_{gb}) f_o) \mathbf{u} = 0$$
 (22b)

$$\varphi \frac{\partial}{\partial t} (\varrho_{od} \mathbf{s}) + \frac{\partial}{\partial r} (\varrho_{od} f_o \mathbf{u}) = 0$$
 (22c)

The Gibbs' phase rule, F = C - P + 2, for three components (C = 3) and two phases (P = 2) leads to three degrees of freedom. We assume that temperature and pressure are constants and we set the remaining thermodynamical two variables: the oil saturation s and other variable y (this variable will be taken as the dead oil molar fraction in Section B). The system (22) may be rewritten as

$$\frac{\partial}{\partial t}\mathfrak{S}(\boldsymbol{s}, \boldsymbol{y}) + \frac{\partial}{\partial x}(\boldsymbol{u}\mathcal{F}(\boldsymbol{s}, \boldsymbol{y})) = 0$$
(23)

where

$$\mathfrak{S}(\boldsymbol{s}, \boldsymbol{y}) = \varphi \begin{bmatrix} \varrho_{ga}(1 - \boldsymbol{s}) \\ \varrho_{gb}(1 - \boldsymbol{s}) + \varrho_{ob} \, \boldsymbol{s} \\ \varrho_{od} \, \boldsymbol{s} \end{bmatrix}, \quad \mathcal{F}(\boldsymbol{s}, \boldsymbol{y}) = \begin{bmatrix} \varrho_{ga} \, (1 - f) \\ \varrho_{ob} \, f + \varrho_{gb}(1 - f) \\ \varrho_{od} \, f \end{bmatrix}$$
(24)

or as

$$\frac{\partial}{\partial t}G(\boldsymbol{s},\boldsymbol{y},\boldsymbol{u}) + \frac{\partial}{\partial x}(F(\boldsymbol{s},\boldsymbol{y},\boldsymbol{u})) = 0$$
(25)

where

$$G(s, \mathbf{y}, \mathbf{u}) = \varphi \begin{bmatrix} \varrho_{ga}(1 - \mathbf{s}) \\ \varrho_{gb}(1 - \mathbf{s}) + \varrho_{ob} \mathbf{s} \\ \varrho_{od} \mathbf{s} \end{bmatrix}, \quad F(s, \mathbf{y}, \mathbf{u}) = \mathbf{u} \begin{bmatrix} \varrho_{ga} (1 - f) \\ \varrho_{ob} f + \varrho_{gb} (1 - f) \\ \varrho_{od} f \end{bmatrix}$$
(26)

4. Characteristic analysis

therefore we have the following matrix

$$J = [uD\mathcal{F} - \lambda D\mathfrak{S}, \mathcal{F}] \tag{27}$$

where the first two columns are

$$[uD\mathcal{F} - \lambda D\mathfrak{S}] = \tag{28}$$

$$\begin{bmatrix} -\varrho_{ga} \left(\boldsymbol{u}\partial_{s}f - \lambda\varphi \right) & \left(\boldsymbol{u} - \boldsymbol{u}f - \lambda\varphi + \lambda\varphi s \right) \partial_{\boldsymbol{y}}\varrho_{ga} + \left(\boldsymbol{u}f - \lambda\varphi s \right) \partial_{\boldsymbol{y}}\varrho_{oa} - \boldsymbol{u}\varrho_{ga}\partial_{\boldsymbol{y}}f \\ \left(\varrho_{ob} - \varrho_{gb} \right) \left(\boldsymbol{u}\partial_{s}f - \lambda\varphi \right) & \left(\boldsymbol{u} - \boldsymbol{u}f - \lambda\varphi + \lambda\varphi s \right) \partial_{\boldsymbol{y}}\varrho_{gb} + \left(\boldsymbol{u}f - \lambda\varphi s \right) \partial_{\boldsymbol{y}}\varrho_{ob} + \boldsymbol{u}\left(\varrho_{ob} - \varrho_{gb} \right) \partial_{\boldsymbol{y}}f \\ \varrho_{od} \left(\boldsymbol{u}\partial_{s}f - \lambda\varphi \right) & \left(\boldsymbol{u}f - \lambda\varphi s \right) \partial_{\boldsymbol{y}}\varrho_{od} + \boldsymbol{u}\varrho_{od}\partial_{\boldsymbol{y}}f \end{bmatrix} \end{bmatrix}$$

$$(29)$$

which lead to the following two generalized eigenvalues

$$\lambda_s(s, y, u) = \frac{u}{\varphi} \, \partial_s f(s, y) \tag{30a}$$

$$\lambda_e(\mathbf{s}, \mathbf{y}, \mathbf{u}) = \frac{\mathbf{u}}{\varphi} \frac{f(\mathbf{s}, \mathbf{y}) - \Omega(\mathbf{y})}{\mathbf{s} - \Omega(\mathbf{y})}$$
(30b)

with corresponding eigenvectors multiples of (if no denominators vanish)

$$(1, 0, 0),$$
 $(31a)$

$$(1, v_{\boldsymbol{y}}, v_{\boldsymbol{u}}), \tag{31b}$$

with

$$v_{\mathbf{y}} = \frac{\varphi}{\mathbf{u}} \frac{(s-\Omega)(\lambda_s - \lambda_e)}{(f-\mathbf{s})(\varpi f - \omega) - (s-\Omega)\,\partial_{\mathbf{u}} f},\tag{32a}$$

$$v_{\mathbf{u}} = \frac{\varphi}{\mathbf{u}} \frac{\mathbf{u} \,\varpi(f - \mathbf{s})(\lambda_{s} - \lambda_{e})}{-\omega \,\mathbf{s} + (\varpi \,\mathbf{s} + \omega)f - \varpi f^{2} + (\mathbf{s} - \Omega)\,\partial_{\mathbf{u}}f},\tag{32b}$$

where we have the following dimensionless quantities

$$\Omega(\mathbf{y}) = \Gamma(\mathbf{y})/\Psi(\mathbf{y}),\tag{33a}$$

$$\omega(\mathbf{y}) = \gamma(\mathbf{y})/\Psi(\mathbf{y}),\tag{33b}$$

$$\varpi(\mathbf{y}) = \psi(\mathbf{y})/\Psi(\mathbf{y}),\tag{33c}$$

depending on

$$\gamma(\mathbf{y}) = -\varrho_g \,\varrho_* \,\varrho_o(\mathbf{y})/\varrho_{oB},\tag{34a}$$

$$\psi(\mathbf{y}) = \gamma(\mathbf{y}) + \rho_* \, \rho_o(\mathbf{y}), \tag{34b}$$

$$\Gamma(\mathbf{y}) = \varrho_q \, \varrho_* \, \mathbf{y},\tag{34c}$$

$$\Psi(\mathbf{y}) = \Gamma(\mathbf{y}) - (\varrho_g - \varrho_* (1 - \mathbf{y})) \varrho_o(\mathbf{y}). \tag{34d}$$

4.1. Behavior of $\Omega(y)$.

We assume $\varrho_* < \varrho_g < \varrho_{oD} < \varrho_{oB}$.

Taking

$$a = \varrho_g \, \varrho_* \, \varrho_{oB}, \quad b = \varrho_g \, \varrho_* \, \varrho_{oD}, \quad c = \varrho_* \, \varrho_{oB} \, \varrho_{oD}, \quad d = \varrho_g \, \varrho_{oB} \, \varrho_{oD},$$
 (35)

we have

$$\Omega(\mathbf{y}) = \frac{p(\mathbf{y})}{q(\mathbf{y})},\tag{36}$$

where

$$p(\mathbf{y}) = (a-b)\mathbf{y}^2 + b\mathbf{y}$$
, and $q(\mathbf{y}) = p(\mathbf{y}) - c\mathbf{y} + c - d$. (37)

We have

$$p(\mathbf{y}) = 0 \Leftrightarrow \mathbf{y} = 0 \lor \mathbf{y} = -\frac{b}{a-b} = -\frac{\varrho_{oD}}{\varrho_{oB} - \varrho_{oD}} < 0;$$
 (38a)

$$p(0) = 0$$
 and $p(1) = a = \varrho_g \, \varrho_* \, \varrho_{oB} > 0.$ (38b)

Therefore, p increases monotonically from 0 to a > 0 as y goes from 0 to 1.

We have

$$q(0) = c - d = -\varrho_{oB} \,\varrho_{oD}(\varrho_q - \varrho_e) < 0, \tag{39a}$$

$$q(1) = a - d = -\varrho_{oB} \,\varrho_g(\varrho_{oD} - \varrho_e) < 0. \tag{39b}$$

$$\partial_{yy}^2 q(y) = 2(a-b) = 2 \varrho_g \varrho_*(\varrho_{oB} - \varrho_{oD}) > 0.$$
(39c)

Therefore, in the [0,1] interval, q(y) is negative with maximum max $\{c-d,a-d\}$.

Finally, $\Omega(\boldsymbol{y})$ is negative and well defined in the interval [0,1].

5. Hugoniot

Given $W_{-} = (s_{-}, y_{-}, u_{-})$ the Hugoniot curve from W_{-} is:

$$\mathcal{H}(W_{-}) = \{ W_{+} = (\mathbf{s}_{+}, \mathbf{y}_{+}, \mathbf{u}_{+}) : \exists \sigma \in \mathbb{R}, F(W_{+}) - F(W_{-}) - \sigma(G(w_{+}) - G(W_{-})) = 0 \}. \tag{40}$$

5.1. Extension and Secondary Bifurcation.

Lemma 2. The Hugoniot curve $\mathcal{H}(W_{-})$ contains the horizontal straight line, with constant composition and speed, $\mathbf{y}_{-} = \mathbf{y}_{+}$, $\mathbf{u}_{-} = \mathbf{u}_{+}$:

$$\mathcal{H}_s(W_-) = \{ (s_+, y_-, u_-) : s_+ \in [0, 1] \}. \tag{41}$$

Proof. Assuming that $W_+ = (s_-, y_+, u_-) \neq W_-$ in (40) we obtain – we recall (26) –

$$\boldsymbol{u}\,\varrho_{qa}\left(f_{-}-f_{+}\right)-\varphi\,\sigma\,\varrho_{qa}\left(\boldsymbol{s}_{-}-\boldsymbol{s}_{+}\right)=0\tag{42a}$$

$$\mathbf{u} \, \rho_{ob} \, (f_{+} - f_{-}) + \mathbf{u} \, \rho_{ab} \, (f_{-} - f_{+}) - \varphi \, \sigma \, \rho_{ob} \, (\mathbf{s}_{+} - \mathbf{s}_{-}) - \varphi \, \sigma \, \rho_{ab} \, (\mathbf{s}_{-} - \mathbf{s}_{+}) = 0$$
 (42b)

$$\boldsymbol{u}\,\rho_{od}\left(f_{+}-f_{-}\right)-\varphi\,\sigma\,\rho_{od}\left(\boldsymbol{s}_{+}-\boldsymbol{s}_{-}\right)=0\tag{42c}$$

where $\boldsymbol{u} = \boldsymbol{u}_- = \boldsymbol{u}_+$, $f_+ = f(\boldsymbol{s}_+, \boldsymbol{y}_-)$, $f_- = f(\boldsymbol{s}_-, \boldsymbol{y}_-)$ and $\varrho_{ga} = \varrho_{ga}(\boldsymbol{y}_-) = \varrho_{ga}(\boldsymbol{y}_+)$ – idem for ϱ_{gb} , ϱ_{ob} and ϱ_{od} – then

$$\sigma = \frac{u}{\varphi} \frac{f_+ - f_-}{s_+ - s_-} \tag{43}$$

is a trivial solution of each equation in (42).

Lemma 3. On the branch $\mathcal{H}_s(W_-)$, as in Lemma 2, the exists a left-characteristic shock associated to λ_e , that is, a shock with speed $\lambda_e(W_-)$, if and only if

$$a s_{+}^{2} + b s_{+} + c = 0, (44)$$

where

$$a = \lambda_e (1 + r_-) \left((1 + r_-) \mathbf{s}_-^2 - 2 r_- \mathbf{s}_- + r_- \right)$$
(45a)

$$b = -r_{-} \left(2 \lambda_{e} (1 + r_{-}) s_{-}^{2} - 2 (1 + 2 r_{-} \lambda_{e}) s_{-} + 1 + 2 r_{-} \lambda_{e} \right)$$

$$(45b)$$

$$c = r_{-} \left(\lambda_{e} (1 + r_{-}) \mathbf{s}_{-}^{2} - (1 + 2 r_{-} \lambda_{e}) \mathbf{s}_{-} + r_{-} \lambda_{e} \right)$$

$$\left(b = -2c - r_{-} \right).$$
(45c)

has solutions for $s \in [0, 1]$.

Proof. On $\mathcal{H}_s(W_-)$ we look for a *left-characteristic shock* associated to λ_e , that is, a $W_+ \neq W_-$ such that

$$\sigma = \lambda_e(W_-) \Leftrightarrow \frac{u}{\varphi} \frac{f_+ - f_-}{s_+ - s_-} = \lambda_e(W_-) \Leftrightarrow f_+ = f_- + \hat{\lambda}_e (s_+ - s_-), \tag{46}$$

where

$$\hat{\lambda}_e = \varphi \, \lambda_e(W_-)/\boldsymbol{u}. \tag{47}$$

From (46) we obtain the third degree equation on s_+ (where $\mathcal{R}(y_-) = \mathcal{R}(y_+) = r_-$)

$$\frac{s_{+}^{2}}{s_{+}^{2} + r_{-}(1 - s_{+})^{2}} = \frac{s_{-}^{2}}{s_{-}^{2} + r_{-}(1 - s_{-})^{2}} + \hat{\lambda}_{e}(s_{+} - s_{-})$$
(48)

which may be divided by $s_+ - s_-$ to obtain (44).

Lemma 4. A left-characteristic shock on \mathcal{H}_s associated to λ_e is also a right-characteristic shock on \mathcal{H}_s associated to λ_e ; therefore, it is a doubly-characteristic shock (or doubly-sonic shock).

Proof. Let Ω be equal to $\Omega(\boldsymbol{y}_{-}) = \Omega(\boldsymbol{y}_{+})$. From (46), that is, from $\frac{\boldsymbol{u}}{\varphi} \frac{f_{+} - f_{-}}{s_{+} - s_{-}} = \frac{\boldsymbol{u}}{\varphi} \frac{f_{-} - \Omega}{s_{-} - \Omega}$ we obtain $\frac{\boldsymbol{u}}{\varphi} \frac{f_{+} - f_{-}}{s_{+} - s_{-}} = \frac{\boldsymbol{u}}{\varphi} \frac{f_{+} - f_{-} + f_{-} - \Omega}{s_{+} - s_{-} + s_{-} - \Omega} = \frac{\boldsymbol{u}}{\varphi} \frac{f_{+} - \Omega}{s_{+} - \Omega} = \lambda_{e}^{+}.$

Appendix A. Parameters of the model.

In this definitions we need to know the following parameters:

Constant	Code	Description
φ	phi	Porosity
ϱ_g	rg	Gas molar density, P/RT
ϱ_*	re	Gas molar density in absence of components A and D, P_B^*/RT
$B = \varrho_{oB}$	В	Molar density of pure (oleic) component B.
$D = \varrho_{oD}$	D	Molar density of pure component D.
$\mathcal{B} = \mu_{oB}/\mu_G$	mB	Ratio of (oleic) component B viscosity to gas viscosity
$\mathcal{D} = \mu_{oD}/\mu_G$	mD	Ratio of component D viscosity to gas viscosity

Approximate values at temperature 310 K.

Name	Formula	M(g/mol)	ρ (g/cm3)	$\varrho \; (mol/m^3)$	$\mu \ (m/s^2)$	$P^*(kPa)$
Propane	C_3H_8	44	-	-	-	≈ 1000
Hexane	$C_6 H_{14}$	86	0.64	7.44e3	0.4e6	44
Hexadecane	$C_{16}H_{34}$	226	0.74	3.27e3	2.9e6	< 0.01

Appendix B. Molar densities depending on \mathcal{Y}_{od} for the thermodynamic of Sec. 2.

Where we set the parameter y as the molar fraction of dead oil in the oleic phase, \mathcal{Y}_{od} , therefore the equations (11) and (12) hold:

$$\varrho_{od} = \boldsymbol{y} \, \varrho_o(\boldsymbol{y}), \quad \varrho_{ob} = (1 - \boldsymbol{y}) \, \varrho_o(\boldsymbol{y}),$$

$$\varrho_{ga} = \varrho_g - \varrho_* \, (1 - \boldsymbol{y}), \quad \varrho_{gb} = \varrho_* \, (1 - \boldsymbol{y}).$$

where

$$\varrho_o(\boldsymbol{y}) = \frac{BD}{D(1-\boldsymbol{y}) + B\boldsymbol{y}}.$$

B.1. Expressions for oil molar density, $\varrho_o(y)$.

We recall (12) and we define the auxiliary quantities which depend on B and D, we recall (13).

$$L = D(1 - \boldsymbol{y}) + B\boldsymbol{y} = D + (B - D)\boldsymbol{y}; \tag{49a}$$

$$P = \frac{D - B}{L}. (49b)$$

$$L = D + (B - D) * y;$$

 $P = (D - B) / L;$

Then we have

$$\varrho_o = \frac{BD}{L} \tag{50a}$$

$$\partial_{\boldsymbol{y}}\varrho_o = P\,\varrho_o \tag{50b}$$

$$\partial_{yy}^2 \varrho_o = 2 P \, \partial_y \varrho_o \tag{50c}$$

B.2. Molar densities and its derivatives

Two of the molar densities depend on $\varrho_o(y)$ of Sec. B.1.

$$\varrho_{ga} = \varrho_g - \varrho_* \left(1 - \boldsymbol{y} \right). \tag{51}$$

$$\varrho_{gb} = \varrho_* \left(1 - \boldsymbol{y} \right). \tag{52}$$

$$\varrho_{ob} = (1 - \mathbf{y}) \,\varrho_o(\mathbf{y}),\tag{53}$$

Rob =
$$(1.0 - y) * Ro;$$

 $dRob_dy = - Ro + (1.0 - y) * dRo_dy;$
 $d2Rob_dy2 = -2.0 * dRo_dy + (1.0 - y) * d2Ro_dy2$

$$\varrho_{od} = \boldsymbol{y} \,\varrho_o(\boldsymbol{y}),\tag{54}$$

Appendix C. Fractional Flow, f(s, y), as function of composition.

C.1. Expressions for viscosity ratios, $\mathcal{R}(y)$.

The function $\mathcal{R}(y)$ models the dependence of the fluid viscosity on the fluid composition y. We recall (17) and (18).

$$\mathcal{R}(\mathbf{y}) = \mathcal{D} + (\mathcal{B} - \mathcal{D})\mathbf{y} \tag{55a}$$

$$\partial_{\mathbf{y}} \mathcal{R}(\mathbf{y}) = \mathcal{B} - \mathcal{D} \tag{55b}$$

$$\partial_{\boldsymbol{u}\boldsymbol{v}}^2 \mathcal{R}(\boldsymbol{y}) = 0 \tag{55c}$$

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R = mD + (mB - mD) * y;

dR_dy = mB - mD;

d2R_dy2 = 0.0;
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C.2. Expressions for the fractional flow $f_o(s,r)$

We start defining an auxiliary quantity, M(s, r), the denominator of f_o . We recall (17) and (19b).

$$M = s^2 + r \left(1 - s\right)^2 \tag{56a}$$

$$\partial_{\mathbf{s}} M = 2\,\mathbf{s} - 2\,\mathbf{r}\,(1-\mathbf{s}) \tag{56b}$$

$$\partial_{\mathbf{r}} M = (1 - \mathbf{s})^2 \tag{56c}$$

$$\partial_{ss}^2 M = 2 + 2 \, r \tag{56d}$$

$$\partial_{sr}^2 M = -2\left(1 - s\right) \tag{56e}$$

$$\partial_{rr}^2 M = 0 \tag{56f}$$

We define also the auxiliary quantities (where F stands for fraction)

InvM = 1.0 / M; $FMs = dM_ds * InvM;$ $FMr = dM_dr * InvM;$ $FMss = d2M_ds2 * InvM;$ FMsr = d2M_dsdr * InvM; // The derivative Drrf could contain the term FMrr (= 0)

We have $-\sec(56)$

$$f_o(\boldsymbol{s}, \boldsymbol{r}) = \frac{\boldsymbol{s}^2}{M},\tag{57a}$$

$$\partial_{\mathbf{s}} f_o(\mathbf{s}, \mathbf{r}) = \frac{2 \mathbf{s}}{M} - \frac{\partial_{\mathbf{s}} M}{M} f_o$$
 (57b)

$$\partial_{\mathbf{r}} f_o(\mathbf{s}, \mathbf{r}) = -\frac{\partial_{\mathbf{r}} M}{M} f_o \tag{57c}$$

$$\partial_{ss}^{2} f_{o}(s, \mathbf{r}) = \frac{2}{M} - 2 \frac{\partial_{s} M}{M} \partial_{s} f_{o} - \frac{\partial_{ss}^{2} M}{M} f_{o}$$
(57d)

$$\partial_{sr}^{2} f_{o}(s, r) = -\frac{\partial_{s} M}{M} \partial_{r} f_{o} - \frac{\partial_{r} M}{M} \partial_{s} f_{o} - \frac{\partial_{sr}^{2} M}{M} f_{o}$$
(57e)

$$\partial_{rr}^{2} f_{o}(s, r) = \left(2\left(\frac{\partial_{r} M}{M}\right)^{2} - \frac{\partial_{rr}^{2} M}{M}\right) f_{o} = 2\left(\frac{\partial_{r} M}{M}\right)^{2} f_{o}$$
(57f)

```
fo = s * s * InvM;
df_{dso} = 2.0 * s * InvM - FMs * fo;
dfo_dr = - FMr * fo;
d2f_ds2o = 2.0 * InvM - 2.0 * FMs * dfo_ds - FMss * fo;
d2fo_dsdr = - FMs * dfo_dr - FMr * dfo_ds - FMsr * fo;
d2fo_dr2 = 2.0 * FMr * FMr * fo;
                                               // Since d2M_dr2 = 0 for all R(y)
```

C.3. Expressions for fractional flow, f(s, y).

The composition of function

$$f(s, y) = f_o|_{(s, \mathcal{R}(y))}$$
(58a)

$$\partial_{\mathbf{s}} f(\mathbf{s}, \mathbf{y}) = \partial_{\mathbf{s}} f_o|_{(\mathbf{s}, \mathcal{R}(\mathbf{y}))}$$
 (58b)

$$\partial_{y} f(s, y) = \partial_{r} f_{o}|_{(s, \mathcal{R}(y))} \partial_{y} \mathcal{R}|_{(y)}$$
(58c)

$$\partial_{ss}^2 f(s, y) = \partial_{ss}^2 f_o|_{(s, \mathcal{R}(y))}$$
 (58d)

$$\partial_{sy}^{2} f(s, y) = \partial_{sr}^{2} f_{o}|_{(s, \mathcal{R}(y))} \partial_{y} \mathcal{R}|_{(y)}$$
(58e)

$$\partial_{yy}^{2} f(s, y) = \partial_{rr}^{2} f_{o}|_{(s, \mathcal{R}(y))} \left(\partial_{y} \mathcal{R}|_{(y)}\right)^{2} + \partial_{r} f_{o}|_{(s, \mathcal{R}(y))} \partial_{yy}^{2} \mathcal{R}|_{(y)}$$
(58f)

Remark: In Eq. (58f) the term $\partial_{\boldsymbol{v}\boldsymbol{v}}^2 \mathcal{R}|_{(\boldsymbol{y})} \partial_{\boldsymbol{r}} f_o|_{(\boldsymbol{s},\mathcal{R}(\boldsymbol{y}))}$ vanishes since \mathcal{R} is linear in \boldsymbol{y} .

```
f = fo;
df_ds = dfo_ds;
df_dy = dfo_dr * dR_dy;
d2f_ds2 = d2fo_ds2;
d2f_dsdy = d2fo_dsdr * dR_dy;
d2f_dy2 = d2f_dr2 * dR_dy * dR_dy + df_dr * d2R_dy2;
```

Appendix D. Expressions for the Accumulation $\mathfrak{S}(s,y)$ and G(s,y,u) on s and an abstract y.

In this section ϱ_{ga} , ϱ_{gb} , ϱ_{ob} and ϱ_{od} depend on parameter \boldsymbol{y} . The fractional flow f depend on \boldsymbol{s} and \boldsymbol{y} .

D.1. Accumulation Jet of $\mathfrak{S}(s,y)$.

D.1.1. Expressions of the Accumulation, $\mathfrak{S}(s,y)$. We recall left-hand-side of (24).

$$\mathfrak{S}(oldsymbol{s},oldsymbol{y}) = arphi \left[egin{array}{c} arrho_{ga} \left(1-oldsymbol{s}
ight) \ arrho_{ob} \, oldsymbol{s} + arrho_{gb} (1-oldsymbol{s}) \ arrho_{od} oldsymbol{s} \end{array}
ight]$$

```
GG[0] = phi * Rga * (1 - s);
GG[1] = phi * ( Rob * s + Rgb (1 - s) );
GG[2] = phi * Rod * s;
```

D.1.2. Expressions of the Derivative of the Accumulation, $D\mathfrak{S}(s,y)$.

$$D\mathfrak{S} = \varphi \begin{bmatrix} -\varrho_{ga} & \partial_{\boldsymbol{y}}\varrho_{ga} \ (1-\boldsymbol{s}) \\ \varrho_{ob} - \varrho_{gb} & \boldsymbol{s} \, \partial_{\boldsymbol{y}}\varrho_{ob} + (1-\boldsymbol{s}) \, \partial_{\boldsymbol{y}}\varrho_{gb} \\ \varrho_{od} & \boldsymbol{s} \, \partial_{\boldsymbol{y}}\varrho_{od} \end{bmatrix}$$

$$(59)$$

```
DGG[0][0] = -phi * Rga;
DGG[0][1] = phi * dRga_dy (1 - s);
DGG[1][0] = phi * (Rob - Rgb);
DGG[1][1] = phi * ( dRob_dy * s + dRgb_dy * (1 - s) );
DGG[2][0] = phi * Rod;
DGG[2][1] = phi * dRod_dy * s;
```

D.1.3. Expressions of the Hessian of the Accumulation, $D^2\mathfrak{S}(s,y)$.

 $D2GG1[1][1] = phi * (s * d2Rob_dy2 + (1 - s) * d2Rgb_dy2);$

$$D^{2}\mathfrak{S}_{0} = \varphi \begin{bmatrix} 0 & -\partial_{\boldsymbol{y}}\varrho_{ga} \\ -\partial_{\boldsymbol{y}}\varrho_{ga} & \partial_{\boldsymbol{y}\boldsymbol{y}}^{2}\varrho_{ga} & (1-\boldsymbol{s}) \end{bmatrix}$$

$$(60)$$

$$D^{2}\mathfrak{S}_{2} = \begin{bmatrix} 0 & \varphi \,\partial_{\boldsymbol{y}}\varrho_{od} \\ \varphi \,\partial_{\boldsymbol{y}}\varrho_{od} & \varphi \,\boldsymbol{s} \,\partial_{\boldsymbol{y}\boldsymbol{y}}^{2}\varrho_{od} \end{bmatrix}$$
(62)

```
D2GG2[0][0] = 0;
D2GG2[0][1] = phi * dRod_dy;
D2GG2[1][0] = D2GG2[0][1];
D2GG2[1][1] = phi * d2Rod_dy2 * s
```

D.2. Accumulation Jet of G(s, y, u)

D.2.1. Expressions for the Accumulation G(s, y). In order to calculate the accumulation we need the expressions of Section B.1. We define:

$$G(s, y, u) = \mathfrak{S}(s, y) \tag{63}$$

```
G[0] = GG[0];
G[1] = GG[1];
G[2] = GG[2];
```

D.2.2. Expressions for the Jacobian of Accumulation, DG.

$$DG(s, y, u) = \begin{bmatrix} D\mathfrak{S} & 0 \end{bmatrix}$$
 (64)

```
DG[0][0] = DGG[0][0];
DG[0][1] = DGG[0][1];
DG[0][2] = 0.0;
//
DG[1][0] = DGG[1][0];
DG[1][1] = DGG[1][1];
DG[1][2] = 0.0;
//
DG[2][0] = DGG[2][0];
DG[2][1] = DGG[2][1];
DG[2][2] = 0.0;
```

Expressions for the Hessian of Accumulation, D^2G .

$$D^{2}G_{i}(\boldsymbol{s},\boldsymbol{y}) = \varphi \begin{bmatrix} \partial_{\boldsymbol{s}\boldsymbol{s}}^{2}\mathfrak{S}_{i} & \partial_{\boldsymbol{s}\boldsymbol{y}}^{2}\mathfrak{S}_{0} & 0\\ \partial_{\boldsymbol{s}\boldsymbol{y}}^{2}\mathfrak{S}_{i} & \partial_{\boldsymbol{y}\boldsymbol{y}}^{2}\mathfrak{S}_{i} & 0\\ 0 & 0 & 0 \end{bmatrix}$$

$$(65)$$

```
D2G[0][0][0] = D2GG[0][0][0];
D2G[0][0][1] = D2GG[0][0][1];
D2G[0][0][2] = 0.0;
//
D2G[0][1][0] = D2GG[0][1][0];
D2G[0][1][1] = D2GG[0][1][1];
D2G[0][1][2] = 0.0;
//
D2G[0][2][1] = 0.0;
D2G[0][2][2] = 0.0;
D2G[0][2][3] = 0.0;
D2G[1][0][0] = D2GG[1][0][0];
D2G[1][0][1] = D2GG[1][0][1];
D2G[1][0][2] = 0.0;
//
D2G[1][1][0] = D2GG[1][1][0];
D2G[1][1][1] = D2GG[1][1][1];
D2G[1][1][2] = 0.0;
//
D2G[1][2][0] = 0.0;
D2G[1][2][1] = 0.0;
```

Appendix E. Expressions for the Partial Flux $\mathcal{F}(s,y)$ and for the Total Flux F(s,y,u) on s and an abstract y.

E.1. Partial Flux Jet, $\mathcal{F}(s,y)$.

E.1.1. Expressions for the Partial Flux, $D\mathcal{F}(s,y)$ **.** See right-hand-side of (24).

$$\mathcal{F}(\boldsymbol{s}, \boldsymbol{y}) = \begin{bmatrix} \varrho_{ga} (1 - f) \\ \varrho_{ob} f + \varrho_{gb} (1 - f) \\ \varrho_{od} f \end{bmatrix}$$

$$\tag{66}$$

```
PF[0] = Rga - Rga * f;
PF[1] = Rgb + (Rob - Rgb) * f;
PF[2] = Rod * f;
```

E.1.2. Expressions for the Derivative of the Partial Flux, $D\mathcal{F}(s,y)$.

$$D\mathcal{F} = \begin{bmatrix} -\varrho_{ga}\partial_{\mathbf{s}}f & (1-f)\partial_{\mathbf{y}}\varrho_{ga} - \varrho_{ga}\partial_{\mathbf{y}}f \\ (\varrho_{ob} - \varrho_{gb})\partial_{\mathbf{s}}f & f\partial_{\mathbf{y}}\varrho_{ob} + (1-f)\partial_{\mathbf{y}}\varrho_{gb} + (\varrho_{ob} - \varrho_{gb})\partial_{\mathbf{y}}f \\ \varrho_{od}\partial_{\mathbf{s}}f & f\partial_{\mathbf{y}}\varrho_{od} + \varrho_{od}\partial_{\mathbf{y}}f \end{bmatrix}$$
(67)

```
PF[0][0] = -Rga * df_ds;
PF[0][1] = (1 - f) * dRga_dy - Rga * df_dy;
PF[1][0] = (Rob - Rgb) * df_ds;
PF[1][1] = f * dRob_dy + (1 - f) * dRgb_dy + (Rob - Rgb) * df_dy;
PF[2][0] = Rod * df_ds;
PF[2][1] = f * dRod_dy + Rod * df_dy;
```

E.1.3. Expressions for the Hessian of the Partial Flux, $D^2\mathcal{F}(s,y)$.

$$D^{2}\mathcal{F}_{0} = \begin{bmatrix} -\varrho_{ga} \partial_{ss}^{2} f & -\partial_{y}\varrho_{ga} \partial_{s} f - \varrho_{ga} \partial_{sy}^{2} f \\ -\partial_{y}\varrho_{ga} \partial_{s} f - \varrho_{ga} \partial_{sy}^{2} f & (1-f) \partial_{yy}^{2} \varrho_{ga} - 2 \partial_{y} \varrho_{ga} \partial_{y} f - \varrho_{ga} \partial_{yy}^{2} f \end{bmatrix}$$

$$PF[0][0][0] = -Rga * d2f_ds2;$$
(68)

```
PF[0][0][1] = -dRga_dy * df_ds - Rga * d2f_dsdy;

PF[0][1][0] = PF[0][0][1];

PF[0][1][1] = (1 - f) * d2Rga_dy2 - 2 * dRga_dy * df_dy - Rga * d2f_dy2;
```

$$D^{2}\mathcal{F}_{1} = \begin{bmatrix} (\varrho_{ob} - \varrho_{gb}) \, \partial_{ss}^{2}f & (\partial_{y}\varrho_{ob} - \partial_{y}\varrho_{gb}) \, \partial_{s}f + (\varrho_{ob} - \varrho_{gb}) \, \partial_{sy}^{2}f \\ \dots & f \, \partial_{yy}^{2}\varrho_{ob} + (1-f) \, \partial_{yy}^{2}\varrho_{gb} + 2 \, (\partial_{y}\varrho_{ob} - \partial_{y}\varrho_{gb}) \, \partial_{y}f + (\varrho_{ob} - \varrho_{gb}) \, \partial_{yy}^{2}f \end{bmatrix}$$
(69)
$$PF[1][0][0] = (Rob - Rgb) * d2f_ds2;$$

$$PF[1][0][1] = (dRob_dy - dRgb_dy) * df_ds + (Rob - Rgb) * d2f_dsdy;$$

$$PF[1][1][0] = PF[1][0][1];$$

$$PF[1][1][1] = f*d2Rob_dy2 + (1-f)*d2Rgb_dy2 + 2*(dRob_dy - dRgb_dy)*df_dy + (Rob - Rgb)*d2f_dy2;$$

$$D^{2}\mathcal{F}_{3} = \begin{bmatrix} \varrho_{od} \, \partial_{ss}^{2}f & \partial_{y}\varrho_{od} \, \partial_{s}f + \varrho_{od} \, \partial_{sy}^{2}f \\ \partial_{y}\varrho_{od} \, \partial_{s}f + \varrho_{od} \, \partial_{sy}^{2}f & f \, \partial_{yy}^{2}\varrho_{od} + 2 \, \partial_{y}\varrho_{od} \, \partial_{y}f + \varrho_{od} \, \partial_{yy}^{2}f \end{bmatrix}$$
(70)
$$PF[2][0][0] = Rod * d2f_ds2;$$

$$PF[2][0][1] = dRod_dy * df_ds + Rod * d2f_dsdy;$$

$$PF[2][1][0] = PF[2][0][1];$$

$$PF[2][1][1] = f * d2Rod_dy2 + 2 * dRod_dy * df_dy + Rod * d2f_dy2;$$

E.2. Total Flux Jet, F(s, y, u).

In order to calculate the Flux we need the expressions of sections B.1, C.1 and C.2, as well as the derivatives of the partial flux function F(s, y) and its derivatives are useful. We have:

$$F(s, y, u) = \mathcal{F}(s, y).$$

```
F[0] = u * PF[0];
F[1] = u * PF[1];
F[2] = u * PF[2];
```

Expressions for the Derivative of the Flux, $D\mathcal{F}(s,y,u)$

$$D\mathcal{F} = [\mathbf{u}DF, F] \tag{71}$$

```
F[0][0] = u * PF[0][0];

F[0][1] = u * PF[0][1];

F[0][2] = PF[0];

//

F[1][0] = u * PF[1][0];

F[1][1] = u * PF[1][1];

F[1][2] = PF[1];

//

F[2][0] = u * PF[2][0];

F[2][1] = u * PF[2][1];

F[2][1] = PF[2];
```

Expressions for the Hessian of the Flux, $D\mathcal{F}(s, y, u)$

$$D^{2}\mathcal{F}_{i} = \begin{bmatrix} \mathbf{u}\partial_{ss}^{2}F_{i} & \mathbf{u}\partial_{sy}^{2}F_{i} & \partial_{s}F_{i} \\ \mathbf{u}\partial_{sy}^{2}F_{i} & \mathbf{u}\partial_{yy}^{2}F_{i} & \partial_{y}F_{i} \\ \partial_{s}F_{i} & \partial_{y}F_{i} & 0 \end{bmatrix}$$

$$(72)$$

```
F[0][0][0] = u * PF[0][0][0];

F[0][0][1] = u * PF[0][0][1];

F[0][0][2] = PF[0][0];

//

F[0][1][0] = F[0][0][1];

F[0][1][1] = u * PF[0][1][1];

F[0][1][2] = PF[0][1];

//
```

```
F[0][2][0] = F[0][0][2];
F[0][2][1] = F[0][1][2];
F[0][2][2] = 0.0;
// -----
F[1][0][0] = u * PF[1][0][0];
F[1][0][1] = u * PF[1][0][1];
F[1][0][2] = PF[1][0];
//
F[1][1][0] = F[1][0][1];
F[1][1][1] = u * PF[1][1][1];
F[1][1][2] = PF[1][1];
//
F[1][2][0] = F[1][0][2];
F[1][2][1] = F[1][1][2];
F[1][2][2] = 0.0;
// -----
F[2][0][0] = u * PF[2][0][0];
F[2][0][1] = u * PF[2][0][1];
F[2][0][2] = PF[2][0];
//
F[2][1][0] = F[2][0][1];
F[2][1][1] = u * PF[2][1][1];
F[2][1][2] = PF[2][1];
//
F[2][2][0] = F[2][0][2];
F[2][2][1] = F[2][1][2];
F[2][2][2] = 0.0;
```

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