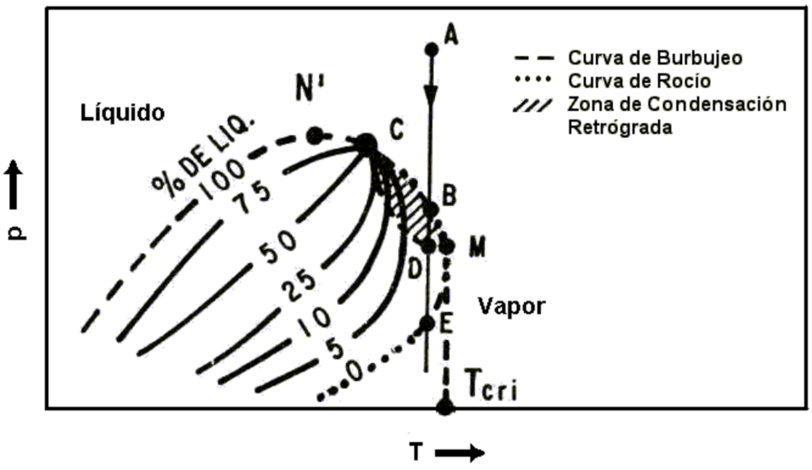
1

Problema Composicional Térmico

1.1. Ejemplo a resolver térmico 1

1.2. Ejemplo a resolver térmico 2

El conocer el diagrama de fases para el yacimiento de interés, es una forma cuantitativa de determinar el tipo de fluido y las condiciones de producción (características) del yacimiento.



1.3. Datos y ecuaciones constitutivas: extraídos del artículo Smith-Perkins y la entrada/salida de STARS

La presión parcial de cada componente p_j en la fase aceite es obtenida mediante la Ley de Raoults.

(Si un soluto tiene una presión de vapor medible, la presión de vapor de su disolución siempre es menor que la del disolvente puro. De esta forma la relación entre la presión de vapor de la disolución y la presión de vapor del disolvente depende de la concentración del soluto en la disolución. Esta relación entre ambos se formula mediante la Ley de Raoult. Es decir que la presión de vapor del soluto crece linealmente con su fracción molar)

$$p_j = x_j p_{vj}$$

donde x_i es la fracción molar del componente j en el aceite y p_{vj} es la presión del vapor.

Aplicando la Ley de Dalton de presiones parciales y haciendo la suma de estas igual a la presión media total del bloque.

$$p = \sum_j p_j + p_{vw} + p_{air}$$

donde p_{vw} es la presión del vapor del agua a la temperatura del bloque, y p_{air} es la diferencia de la presión parcial del aire o del gas de combustión.

El cálculo de vaporización anterior se debe ajustar, dos situaciones se plantean. Para ver mas detalle véase Smith-Perkins, Experimental and numerical simulation of ISC.

(La ley de las presiones parciales (conocida también como ley de Dalton) fue formulada en el a?o 1803 por el físico, químico y matemático británico John Dalton. Establece que la presión de una mezcla de gases, que no reaccionan químicamente, es igual a la suma de las presiones parciales que ejercería cada uno de ellos si solo uno ocupase todo el volumen de la mezcla, sin cambiar la temperatura. La ley de Dalton es muy útil cuando deseamos determinar la relación que existe entre las presiones parciales y la presión total de una mezcla de gases.)

Se supone una mezcla uniforme para cada bloque (simplificación, el calculo se encuentra dentro de los rangos).

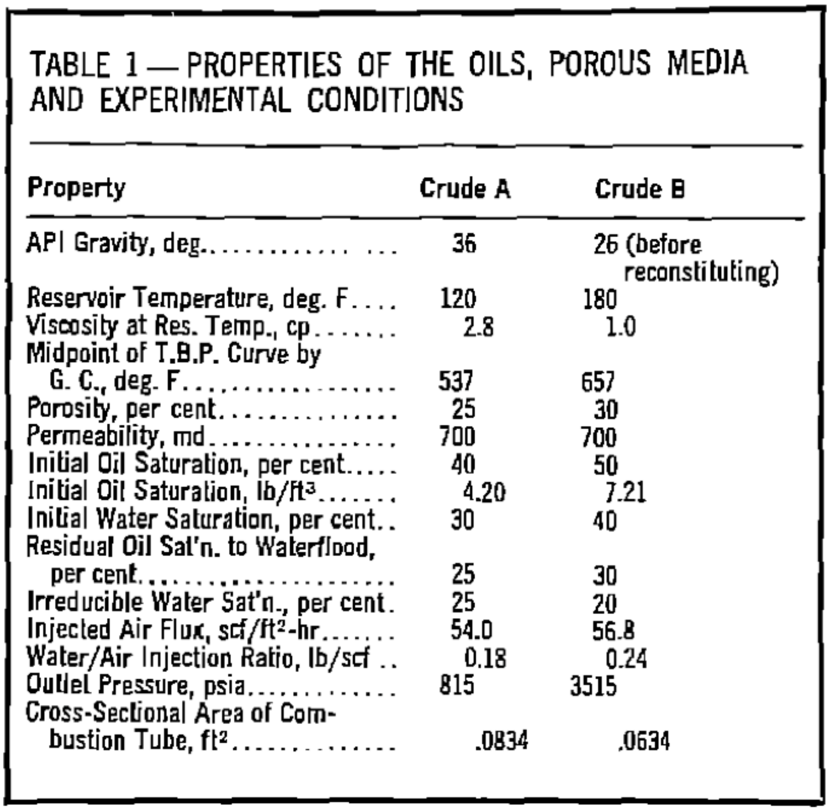


TABLE 1 — PROPERTIES OF THE OILS, POROUS MEDIA AND EXPERIMENTAL CONDITIONS

Property	Crude A	Crude B
API Gravity, deg.	36	26 (before reconstituting)
Reservoir Temperature, deg. F	120	180
Viscosity at Res. Temp., cp	2.8	1.0
Midpoint of T.B.P. Curve by G. C., deg. F	537	657
Porosity, per cent	25	30
Permeability, md	700	700
Initial Oil Saturation, per cent	40	50
Initial Oil Saturation, lb/ft^3	4.20	7.21
Initial Water Saturation, per cent	30	40
Residual Oil Sat'n. to Waterflood, per cent	25	30
Irreducible Water Sat'n., per cent	25	20
Injected Air Flux, scf/ft^2-hr	54.0	56.8
Water/Air Injection Ratio, lb/scf	0.18	0.24
Outlet Pressure, psia	815	3515
Cross-Sectional Area of Combustion Tube, ft^2	.0834	.0634

Datos STARS

1.4. Descripción del problema

A laboratory experiment illustrating the forward wet combustion experiment is matched. The experiment and another simulation matching attempt is described by F.W. Smith T.K. Perkins in JCPT, vol. 12, no. 3, 1973, pp.44

and by K.H. Coats in SPE 8394.

The experiment took place in a vertical adiabatic combustion tube, with 8.8 cm inside diameter and 1.753 m long. Air was injected at the top of the tube for 28.8 min, followed by the injection of water and air at constant rate and water-air ratio.

Special Features:

1) Wet combustion process: no solid fuel deposition. 2) Co-injection of water and air. 3) One hydrocarbon component: liquid; nonvolatile. 4) Two non-condensible gases: oxygen and inert gases. 5) One chemical reactions: combustion of HEVY oil components. Reaction products are water, CO and CO2 (CO2/CO = 1.079). 6) Temperature of injection end is raised initially from 49 C to 267 C using external heaters. 7) Injection of air, followed by water-air co-injection.

La longitud del tubo de combustión es de 1.7526 m dividido en 20 secciones de igual DZ, se tiene $\frac{1,7526m}{20} = 0,08763cm$, la porosidad es constante en todo el tubo de combustiń con valor de 0.25 y permeabilidad de μm^2

Datos STARS

————————GRID AND RESERVOIR DEFENITION——————————

GRID VARI
1 1 20
-Indica como se secciona el dominio

KDIR DOWN
-Indica que la dirección en z es positiva en sentido hacia abajo

DI IVAR
0.0880234 cm
-Indica el valor del Δi

DJ IVAR
0.0880234 cm
-Indica el valor del Δj

DK IVAR
20*0.08763 cm
-Indica el valor del Δk, que en este caso es igual en todas las celdas

DTOP
0
-Indica la profundidad a la que se encuentra el yacimiento

POR CON
0.25
-Indica la porosidad constante en todo el dominio

PERMI CON = PERMJ CON = PERMK CON
0.6908 mum^2
-Indica el valor de la permeabilidad, el cual es constante e igual en todas las direcciones

-Propiedades térmicas de la roca
ROCKCP 1.607E+6 2700
THCONR 4.4861E+5
THCONW 4.4861E+5
THCONO 4.4861E+5
THCONG 4.4861E+5
THCONMIX *TEMPER -Da un valor de temperatura efectiva

——————FLUID DEFINITIONS———————

MODEL 4 4 2 1
-Indica las componentes y las fases (agua, aceite pesado, gas inerte, oxigeno) no hay componente solidas

CMM
0.018 0.5089 0.038 0.032

-Molecular Weight (Required) *CMM PURPOSE: Assign molecular weights. FORMAT: *CMM cmm(1) ... cmm(ncomp) DEFINITIONS: cmm Molecular mass of component (kg/gmol — lb/lbmol). The unit is (mass/mole), even if *MASSBASIS was specified. DEFAULTS: Enter cmm(k) = 0 for aqueous component k to get the water default of 0.01802 kg/gmole (18.02 lb/lbmole). EXPLANATION: Since many fluid properties are on a per-mole basis, cmm is very important. For example, liquid density, which determines the hydrostatic head of each phase, will depend directly on the mass density, that is, the product mole density times mass/mole. The molecular masses of some common pure substances are: Water Nitrogen Oxygen 0.01802 kg/gmole (18.02 lb/lbmole) 0.02801 kg/gmole (28.01 lb/lbmole) 0.03199 kg/gmole (31.99 lb/lbmole) Very frequently a hydrocarbon component is actually a pseudo- component, representing a group of pure components over a range of C numbers. For example, a heavy oil pseudo- component may cover the range C15 to C30, as suggested by a distillation analysis. The mass density of this fraction can be measured directly, but its molecular mass usually is postulated or estimated using a mathematical model. The value of the cmm is, in itself, not critical. However, it is crucial that the mass density used in the simulator be equal to the measured mass density, in which case the *MASSDEN density input option may be preferred. A table of molecular masses for selected components is in Table 6.

PCRIT
22110 349.6 5171.1 5033.2
-Presión critica para cada componente

TCRIT
647.4 887.8 194.4 154.4
-Temperatura critica de cada componente

KV1
0 0
-Valor por default en STARS

KV4
0 0
-Valor por default en STARS

K Value Correlations *KV1, *KV2, *KV3, *KV4, *KV5 PURPOSE: Specify gas-liquid K value correlations. FORMAT: *KV1 kv1(1) ... kv1(numx) *KV2 kv2(1) ... kv2(numx) *KV3 kv3(1) ... kv3(numx) *KV4 kv4(1) ... kv4(numx) *KV5 kv5(1) ... kv5(numx) DEFINITIONS: kv1 First coefficient in the correlation for gas-liquid K value (kPa — psi). kv2 Second coefficient in the correlation for gas-liquid K value (1/kPa — 1/psi). kv3 Third coefficient in the correlation for gas-liquid K value. kv4 Fourth coefficient in the correlation for gas-liquid K value (C — F). This coefficient has the unit of temperature difference. It has the same value for temperature scales C and K, and has the same value for temperature scales F and R. kv5 Fifth coefficient in the correlation for gas-liquid K value (C — F). This coefficient has the unit of temperature, and is different for each temperature scale. Often this coefficient is quoted in other sources in absolute degrees K or R, even though all other temperatures are quoted in C or F. Here, this coefficient is quoted in the same unit as all other temperatures, so it may be necessary to convert it from absolute to C or F.

PRSR
5620
-Presión de referencia

prsr -Reference pressure (kPa — psi) corresponding to the densities entered by *MOLDEN, *MASSDEN or *MOLVOL, and *SOLID$_{D}EN$.

TEMR
322.2
-Temperatura de referencia
(temr -Reference temperature used by many T-dependent and thermal properties (C — F). See EXPLANATION, below.)

TEMR is used in conjunction with the following input data:

1. Liquid density data (*MOLDEN, *MASSDEN or *MOLVOL),

2. Liquid and gas phase enthalpy data (*CPL1, *CPG1, etc.),

3. Formation heat capacity (*ROCKCP),

4. Reaction enthalpy data (*RENTH). Most reaction enthalpy data is referred to 25 C, so the default value is recommended for combustion simulations.

5. Wellbore heatloss othe steam boiler.

CPL1
0 1278.1 30.27 32.15
(Liquid and gas phase enthalpy data)

HVR
0 0
(hvr -First coefficient in vapourization enthalpy correlation (J/gmol-Cev — Btu/lbmol-Fev)) DEFAULTS: If none of these keywords is present, the fluid heat capacities will be: a) Aqueous components: liquid and vapour from internal water table, b) Oleic components: vapour is 0.25 Btu/lb-F; liquid is 0.5 Btu/lb-F for liquid-based enthalpy options, 0.25 Btu/lb-F for gas-based enthalpy option, c) All other components: vapour is 0.25 Btu/lb-F. These defaults usually are quite adequate, and are recommended unless you have specific values to use. When the gas-based enthalpy option is used, for a ?dead? component assign a liquid value to the gas keyword *CPG1, etc. Defaulting is done on a per-component basis. Therefore, if you want to over-ride the default for a particular component, enter zeroes in that component?s position for each enthalpy definition keyword that appears in the data. It is necessary to do this since the enthalpy keywords require a number for each component. For example, to over-ride the default of only component 3 out of 5 components, and only for liquid heat capacity, use the following: *CPL1 0 0 30.5 0 0 Here components 1, 2, 4 and 5 each will end up with zero for all enthalpy data, which indicates that the defaults above are to be used. The absence of *EV results in ev = 0.38. (pag. 312)

EV
0 0
ev -Second coefficient in vapourization enthalpy correlation.

PURPOSE: Over-ride defaults for fluid heat capacities.

DEFAULTS: If none of these keywords is present, the fluid heat capacities will be: a) Aqueous components: liquid and vapour from internal water table, b) Oleic components: vapour is 0.25 Btu/lb-F; liquid is 0.5 Btu/lb-F for liquid-based enthalpy options, 0.25 Btu/lb-F for gas-based enthalpy option, c) All other components: vapour is 0.25 Btu/lb-F. These defaults usually are quite adequate, and are recommended unless you have specific values to use. When the gas-based enthalpy option is used, for a ?dead? component assign a liquid value to the gas keyword *CPG1, etc. Defaulting is done on a per-component basis. Therefore, if you want to over-ride the default for a particular component, enter zeroes in that component?s position for each enthalpy definition keyword that appears in the data. It is necessary to do this since the enthalpy keywords require a number for each component. For example, to over-ride the default of only component 3 out of 5 components, and only for liquid heat capacity, use the following: *CPL1 0 0 30.5 0 0 Here components 1, 2, 4 and 5 each will end up with zero for all enthalpy data, which indicates that the defaults above are to be used. The absence of *EV results in ev = 0.38. (pag 312)

MASS DEN
979.5 906.6 719.2 [kg/m^3]
12.8 24.4 65.1 [api]

MOLDEN
55500 1924.8

For each adsorbed/trapped condensable component, if *SOLID$_DENisabsentthen = k0, cp, ctandcptareobtainedfrom*$ $MASSDEN(orequivalent), *CP, *CT1and*CPT, forthatcomponent?sliquidreferencephase.If*SOLID_CPisabsentthencps1$ $CPL1and*CPL2whenthefluidenthalpyisreferencedtotheliquidphase; otherwisethedefaultisthesameasforsolidcomponent.(p$

prsr Reference pressure (kPa — psi) corresponding to the densities entered by *MOLDEN, *MASSDEN or *MOLVOL, and *SOLID$_DEN.(pag,$307)

The value of the cmm is, in itself, not critical. However, it is crucial that the mass density used in the simulator be equal to the measured mass density, in which case the *MASSDEN density input option may be preferred. A table of molecular masses for selected components is in Table 6. (pag. 305) (Tabla 6 pag.875)

CP
1.45e-6 1.45e-6

cp -Compressibility (1/kPa — 1/psi) at constant temperature. (DUDA)

CT1
0 6.84e-4

ct1 -First coefficient of the thermal expansion correlation (1/C — 1/F). ct1 is the thermal expansion coefficient when ct2 = 0. (pag. 321)

Liquid Densities (Required) *MOLDEN, *MASSDEN, *MOLVOL, *CP, *CT1, *CT2, *CPT, *GASSYLIQ PURPOSE: Assign component liquid densities. FORMAT: *MOLDEN *MASSDEN *MOLVOL *CP *CT1 *CT2 *CPT *GASSYLIQ den(1) denm(1) vol(1) cp(1) ct1(1) ct2(1) cpt(1) comp$_name....................den(numx)denm(numx)vol(numx)cp(nur$

ct1 -First coefficient of the thermal expansion correlation (1/C — 1/F). ct1 is the thermal expansion coefficient when ct2 = 0. (pag. 321)

DEFAULTS: The absence of *CP implies that all cp(k) = 0. The absence of *CT1 implies that all ct1(k) = 0. The absence of *CT2 implies that all ct2(k) = 0. The absence of *CPT implies that all cpt(k) = 0. (pag. 322)

AVG
2.435e-16 0 3.719e-15 3.883e-15

avg(i) -First coefficient in correlation for temperature dependence of viscosity of component i in the gas phase (cp/K**bvg(i) — cp/R**bvg(i)). avg(i) must be non-negative, and may be zero only if (a) bvg(i) = 0 or (b) the component does not appear in the gas phase.

Gas Phase Viscosities *AVG, *BVG, *GVISCOR PURPOSE: Override the internal gas phase viscosity with a composition-dependent, and possibly pressure- dependent, calculation. FORMAT: *AVG avg(1) ... avg(numy) *BVG bvg(1) ... bvg(numy) *GVISCOR (pag. 330)

BVG
1.075 0 0.702 0.721

(véase el keyword anterior)

AVISC
0 1.157e-13

avisc(i), bvisc(i) Coefficients of the correlation for temperature dependence of component viscosity in the liquid phases. The unit of avisc(i) is cp (viscosity). The unit of bvisc(i) is temperature difference which has the same value if the temperature unit is C or K and the same value if the temperature unit is F or R. The correlation for component i viscosity viso(i) is viso(i) = avisc(i) · exp[bvisc(i) / T] where T is in absolute degrees. Neither avisc(i) nor bvisc(i) may be negative. See Table 4 for suggested coefficient values for selected components. For an aqueous component, enter zero to get the internal water table (water phase only). For a component not found in the phase in question, enter a zero value for avisc. A zero value for bvisc(i) results in viso(i) = avisc(i).

DEFAULTS: If *AVISC is present but *BVISC is absent, the component viscosities are viso(i) = avisc(i). If zero data is entered at all temperatures for an aqueous component, internal water data will be used for that component in the water phase only. There is no default for aqueous component data in the oil phase, even if the data is assigned with *LIQPHASE in force. If *XNACL is absent, xnacl = 0 is assumed. (pag. 333)

BVISC
0 2726.7

(véase keyword anterior)

**Reaction specification

STOREAC
0 1 0 45.2915

Critical Chemical Reaction Data *STOREAC, *STOPROD, *FREQFAC, *FREQFACP PURPOSE: Assign critical reaction data for a number of reactions. FORMAT: *STOREAC sto1(1) ... sto1(ncomp) *STOPROD sto2(1) ... sto2(ncomp)

*FREQFAC rrf or *FREQFACP $p_r$rfrrfDEFINITIONS : sto1Stoichiometriccoefficientofreactingcomponent.Itmustbeno
negative.Enterzeroforcomponentswhicharenotreacting.Normally,thestoichiometriccoefficientsarebasedononemoleofoneo
negative.Enterzeroforcomponentswhicharenotbeingproducedinthisreaction.Normally,thestoichiometriccoefficientsarebase

STOPROD
29.71 0 37.46 0

(véase keyword anterior)

RORDER
0 2 0 1

Noncritical Chemical Reaction Data

*RORDER Enrr(1) ... enrr (ncomp)

enrr -Order of reaction with respect to each reacting component's concentration factor. It must be non-negative. Enter zero for non-reacting components. Normally, enrr = 1. If enrr = 0, the reaction rate will be independent of that component's concentration.

FREQFAC
3.0837E5

Critical Chemical Reaction Data

*STOREAC, *STOPROD, *FREQFAC, *FREQFACP

PURPOSE:

Assign critical reaction data for a number of reactions.

FORMAT:

*STOREAC sto1(1) ... sto1(ncomp)

*STOPROD sto2(1) ... sto2(ncomp)

*FREQFAC rrf

or

*FREQFACP

$p_r$rfrrf

DEFINITIONS:

rrf -Reaction frequency factor (unit is variable). It must be non-negative. This is the constant factor in the expression for reaction rate (see below). The unit depends upon data entered via *STOREAC, *RORDER, *O2PP *O2CONC.

$p_r$rf−Pressure(kPa|psi)correspondingtofrequencyfactorrrfintable.$p_r$rfentriesmustbeincreasingandevenlyspaced.Interpol
FREQFACPonlytoprovidereactionratedependenceonpressurebeyondthatnaturallyoccurringthroughconcentrationfactorsvia
FREQFACPreplaceskeyword ∗ FREQFAConaper − reactionbasis.

RENTH
5.E7

4. Reaction enthalpy data (*RENTH). Most reaction enthalpy data is referred to 25 C,so the default value is recommended for combustion simulations.(pag. 309)

renth Reaction enthalpy (J/gmol — Btu/lbmol). It is positive for exothermic reactions and negative for endothermic reactions. The default is 0. Reaction enthalpy is referenced to temperature TEMR and the enthalpy base phase given by the choice of CPL's and CPG's entered elsewhere. In most cases, the reaction enthalpy is based on gas phase at 25 deg C. (pag. 342)

EACT
50000.0

One exception is the definition of molecular weight, which must retain the unit (mass/mole), i.e., (kg/gmole) in SI units and (lb/lbmole) in field units. The other exception is reaction activation energy *EACT which retains its per-mole unit. (pag. 109)

eact -Activation energy (J/gmol — Btu/lbmol), which determines the dependence of the reaction rate on grid block temperature (see below). For chemical reactions (e.g., combustion) this quantity is non-negative. However, negative values are allowed, with a warning, to accommodate advanced options like non-equilibrium interphase mass transfer. Activation energies are often given in cal/gmole, so be sure that the units are converted correctly. (pag. 343)

————————-ROCK-FLUID PROPERTIES————————

ROCKFLUID

Rock-Fluid Property Identifier (Required)

*ROCKFLUID

PURPOSE:

*ROCKFLUID indicates the start of the rock-fluid data.

FORMAT:

*ROCKFLUID

DEFAULTS:

Required keyword. No default.

CONDITIONS:

This keyword must be the first keyword in the ROCK-FLUID DATA keyword group. ROCK-FLUID DATA must follow immediately after component properties. (pag. 372)

RPT 1 -Tipo de roca

SWT (Water-oil relative permeabilities)

Sw	Krw	Krow
0.25	0.0	1.0
0.30	0.005	0.81
0.35	0.02	0.64
0.40	0.045	0.49
0.45	0.08	0.36
0.50	0.125	0.25
0.55	0.18	0.16
0.60	0.245	0.09
0.65	0.32	0.04
0.70	0.405	0.01
0.75	0.5	0.0
1.0	1.0	0.0

SLT *NOSWC (Oil-gas relative permeabilities)

Liquid-Gas Relative Permeability Table

*SLT

PURPOSE:

Define the liquid-gas relative permeability table.

TABLE:

SLT (*NOSWC) (smooth)

Sl krg krog (Pcog (Pcogi)) -or-

*SLT (*NOSWC) (smooth) *WATERGAS

Sl krg krog krwg (Pcog (Pcogi))

smooth = *SMOOTHEND *LINEAR — *QUAD — *CUBIC

DEFINITIONS:

*NOSWC

Table liquid saturation Sl does not contain connate water saturation Swc, and therefore is all oil. The *STONE1 option is unavailable with *NOSWC.

(pag. 390)

```
Sl Krg Krog
—- ——- ——-
0.34 1.0 0.0
0.40 0.826 0.008
0.45 0.694 0.028
0.50 0.574 0.059
0.55 0.465 0.101
0.60 0.367 0.155
0.65 0.281 0.221
0.70 0.207 0.298
0.75 0.143 0.386
0.80 0.092 0.486
0.85 0.052 0.597
0.90 0.023 0.72
0.95 0.006 0.854
1.0 0.0 1.0
```

————————-INITIAL CONDITIONS————————

*INITIAL

Initial Conditions Identifier (Required)

*INITIAL

PURPOSE:

*INITIAL indicates the beginning of initial condition values.

FORMAT:

*INITIAL

DEFAULTS:

Required keyword.

CONDITIONS:

This keyword must be the first keyword in the INITIAL CONDITIONS keyword group, which must come immediately after the ROCK-FLUID DATA keyword group. The only required keywords in this section are those which define the initial pressure distribution. (pag. 435)

VERTICAL OFF

13. Saturation over-ride via *SW, *SO, *SG is now honoured when*DWOC and *DGOC are used with *VERTICAL *OFF. (pag. 6)

INITREGION 1

(*INITREGION key

Introduces an initialization region to which data is assigned. The numerical key is an integer from 1 to the maximum number of initialization regions. All regions from 1 to the maximum must be specified and may appear in any order.) (pag. 346)

Property: Pressure (kPa)

Max: 5620 Min: 5620

PRES CON

5620

Property: Water Saturation Max: 0.3 Min: 0.3

SW CON 0.3

** Initial gas saturation = 0.3

** Property: Oil Saturation Max: 0.4 Min: 0.4

SO CON 0.4

** Property: Temperature (K) Max: 322 Min: 322

TEMP CON 322

** Property: Gas Mole Fraction(INRT GAS) Max: 0.71 Min: 0.71

MFRAC_GAS ÍNRT GAS'CON 0.71

** Property: Gas Mole Fraction(OXYGEN) Max: 0.29 Min: 0.29

MFRAC_GAS ÓXYGEN'CON 0.29

** Property: Oil Mole Fraction(HEVY OIL) Max: 0.084 Min: 0.084

MFRAC_OIL 'HEVY OIL'CON 1.0

-Indica el valor de los diferentes parámetros en la condiciones iniciales

————————NUMERICAL CONTROL————————

*NUMERICAL ** All these can be defaulted. The definitions

** here match the previous data.

*NORM *PRESS 500 *SATUR .2 *TEMP 30 *Y .2 *X .2

===================== SUMMARY (from subroutine: INDATA) =========

Reading of initial data is complete.

Simulation will stop if there were error messages.

0 Warning messages. 0 Error messages.

==