

FULL COMPOSITIONAL SIMULATION OF TWO-PHASE FLOWS

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ABSTRACT

The simulation of multiphase flow, considered in the case of coexisting vapor and liquid phases, is a very important topic in the development and production oil and gas reservoirs. The present work presents the development of a general approach for the calculation of single and multiphase flows in pipelines. This approach can be defined as ‘full compositional, since the vapour and liquid phases are described taking into account the chemical composition. This approach is interesting and valuable both from the theory and practical point of view. The physical properties required are calculated at each time step using the actual composition instead of relying on property tables generated from a single constant fluid composition. From this point of view the congruency between the dynamic pressure generated by the solution of the Navier-Stokes equations at constants temperature and thermodynamic pressure of the system is a critical constraint in the numerical solution of the system. An example related to fast pipeline depressurization is presented and discussed. Another example shows the pressurization of a pipeline, initially filled with nitrogen, by means of well-produced hydrocarbon stream.

1. INTRODUCTION

The simulation of multiphase flow in pipelines has become a very important topic in research and engineering along the past 20 years. This fact has been promoted mainly by the exploitation of oil and gas reservoirs in off-shore fields and the transportation to onshore treatment facilities. In these cases, technical and economic problems posed by the installation of separation equipment, the multiphase transport in a single pipeline has posed itself as the only practical solution. So multiphase flow, which is considered in the case of coexisting vapour and liquid phases, is a very important theme in the exploitation of oil and gas reservoirs. The term flow-assurance has been introduced to define the technology applied for the design of pipeline systems, prevention and the solution of problems related to fluid flow that can arise during their operations. To this scope, along the years, a number of simulation programs and tools have been developed starting from the needs of nuclear industry where LOCA simulations have assumed a pre-eminent aspect. It was from these needs of the nuclear industry that some simulation tools (e.g. RELAP, CATHARE) have been developed for the evaluation of mixed steam-water flows. These tools have been the starting point for the development of new gas-liquid flow simulators, with the scope of solving the problems faced by the oil and gas industry particularly for the development of offshore fields. These needs have fed a large number of researches in the two-phase flow with a particular accent on slug-flow calculation. Today commercial tools such as Olga, Tacite and LedaFlow are well known and are probably the most used simulators for steady state and transient multi-phase flow modelling. Within the enormous amount of published papers in the field of fluid flow in pipelines, practically all experimental data and simulated cases deal with fluid of constant composition. Most experiments use very simple and safe two-component systems such as: air-water, nitrogen-water, nitrogen-naphtha and very few more. These two-components systems have no resemblance to real cases where the oil-gas mixture is described by tens of hydrocarbon components (from C1 to C80), light gases (N₂, CO₂, H₂S, mercaptanes) and

water. The thermodynamic approach used is greatly approximated: physical properties of the phases are pre-calculated and stored in tables which are the sources where the simulator picks property values when required by the solution algorithm. Within the numerous problems arising in the design and operation of pipelines (start-up, shut-down and restart), the calculation depressurization which can arise from both planned or unplanned events is a central point in the evaluation of safety consequences. As unplanned events are concerned, fast pipeline depressurization due to their rupture is probably the most severe effect that requires accurate simulation. The calculation of the outflow of highly flammable gas and oil is very important to assess the safety consequences in the nearby environment. Since these effects are usually connected to remarkable fluid cooling from Joule-Thomson effects, the prediction of the minimum temperature reached by the pipeline material is critical for the possible metal fragility. In the simulation of fast depressurization the results obtained by commercial tools are not always reliable. In the following chapters, a different and more complete approach is presented. Fluid flow equation are strictly coupled with thermodynamic equation of state for the evaluation of fluid properties taking into account all the possible changes in pressure, temperature and fluid compositions. The numerical method used for the calculation of the fluid temperature is analysed in detail in terms of thermodynamic constraints. In the last part two cases exhibiting compositional changes are presented and discussed. Due to the limits this presentation must comply with, themes such as the type of flow (stratified, bubble, slug, etc.) are not analysed in the proposed examples and only the importance of composition changes during the dynamic of the two-phase flow are presented.

2. FLUID DYNAMIC MODELS

The equations required for the description of single phase and multiphase flows are well known and their derivation is presented in many text-books and almost all the publications related to multi-phase flow dynamic. Among available documentation we can quote two of them: the historically relevant and brilliant text book on fluid dynamics of Landau and Lifchitz [1], and the more recent text of Ishii and Ibiki [2]. So, conservation equations for mass, momentum and energy are presented here without any derivation and with no particular comments. We will consider a fluid system formed by NC chemical components (e.g. methane, ethane, nitrogen, etc.) whose relative amount is defined by the number of moles or mass units. The composition is described by a vector \mathbf{z} of dimension NC and each individual chemical component is identified by an upper index. Two possible approaches are currently used to describe a two-phase system: (1) the drift-flux model or (2) the two-fluid model. In the first case momentum balance equations of the vapour and liquid phases are coupled together and the phases different velocities are described by *drift* relations. Separate equations are instead used in the two-fluid model. In the following presentation the two-fluid model is used. The conservation of mass is expressed by the differential equation:

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla(\alpha_k \rho_k u_k) = m_k \quad (1)$$

Here the subscript k is used to indicate the vapour or the liquid phase: usually the vapour phase (V) takes the value 1 whereas the liquid phase (L) has the index 2. In the case of a fluid mixture, volumetric and thermodynamic properties, which are usually considered functions of the pressure and temperature only, are dependent on the phase compositions as well. The phase composition is denoted by the vector \mathbf{z} whose components z_i denote the molar or weight fraction of the i -th chemical component. In some cases the symbol \mathbf{y} is used to identify the vapour composition vector and the symbol \mathbf{x} is used for the liquid phase. So in general, the following relations hold:

$$\rho_k = \rho(T, P, \mathbf{z}_k) \quad (2)$$

$$\rho_V = \rho(T, P, \mathbf{y}) \quad (3)$$

$$\rho_L = \rho(T, P, \mathbf{x}) \quad (4)$$

For a two-phase system, the vapour and liquid volume fractions α_k sum to 1.

$$\alpha_V + \alpha_L = 1 \quad (5)$$

The momentum balance equation of phase k can be written as:

$$\frac{\partial \alpha_k \rho_k u_k}{\partial t} + \nabla(\alpha_k \rho_k u_k u_k + \alpha_k P) = P_k \nabla \alpha_k + \alpha_k \rho_k g \sin \vartheta + M_k^i \quad (6)$$

Besides mass balance equations, when dealing with vapour-liquid two-phase flow a 'conservation volume' equation must be added to the previous equations. This equation expresses the fact that the sum of volume fractions of the phases must be equal one. We avoid the derivation of the equation, that can be found in a number of text-books or references, and write it as:

$$\frac{\alpha_V}{\rho_V} \frac{\partial \rho_V}{\partial t} + \frac{\alpha_L}{\rho_L} \frac{\partial \rho_L}{\partial t} = -\frac{1}{\rho_V} \frac{\partial}{\partial z} (\alpha \rho u)_V - \frac{1}{\rho_L} \frac{\partial}{\partial z} (\alpha \rho u)_L \quad (7)$$

The conservation of energy can be derived in the form:

$$\frac{\partial}{\partial t} \alpha_k \rho_k \left(E_k + \frac{u_k^2}{2} \right) + \nabla \left[\alpha_k \rho_k \left(E_k + \frac{u_k^2}{2} \right) u_k \right] = -\nabla q_k + \nabla P \cdot u_k \quad (8)$$

By introducing the phase enthalpy defined as:

$$H_k = E_k + \frac{P_k}{\rho_k} \quad (9)$$

the energy equation is written as:

$$\frac{\partial \rho_k H_k}{\partial t} + \nabla(\rho_k H_k u_k) = -\nabla q_k + \frac{DP_k}{Dt} + \dot{q} \quad (10)$$

When a compositional approach is used the mass balance of the chemical component contained in the vapor and liquid phases must be considered. Taking into account a control volume, the mass balance of the i -th component of the mixture (e.g. methane) can be written as:

$$\frac{\partial m_k^i}{\partial t} + \nabla(m_k^i u_k) = 0 \quad (11)$$

where the index i applies to all chemical components existing in the fluid system (from 1 to NC). Excluding the existence of reactions between the chemical components, the change of the local composition of mass contained in a control volume V is the effect of convective flow and vapour-liquid equilibrium. Diffusivity effects related to chemical components are not considered. When the differential equations are integrated, by assuming the temperature is

constant across one time step Δt , then the change of the phase density can be associated to the change of pressure and equation (8) can be rewritten as:

$$\left(\frac{\alpha_v}{\rho_v} \frac{\partial \rho_v}{\partial P} + \frac{\alpha_L}{\rho_L} \frac{\partial \rho_L}{\partial P} \right) \frac{\partial P}{\partial t} = - \frac{1}{\rho_v} \frac{\partial}{\partial z} (\alpha \rho u)_v - \frac{1}{\rho_L} \frac{\partial}{\partial z} (\alpha \rho u)_L \quad (12)$$

The complete set of the Navier-Stokes equations are solved using a mixed implicit-explicit integration scheme. The material and momentum balance equations are integrated using an implicit scheme. The energy balance equations are combined and solved using an explicit Euler integration. Details of the applied integration method are not given and a valuable reference is the text of Ferziger and Peric [3]. The component balance equation (11) is integrated based on the new phase velocities and densities obtained in the previous steps.

3. EQUATIONS OF STATE AND TEMPERATURE CALCULATION

Thermodynamic equations of state realize the integration between fluid-mechanics and the constraints existing, between vapour and liquid phases, in a two-phase fluid flow. When a compositional approach is used, fluid properties (which are dependent on the system composition, local temperature and pressure) are connected with the solution of the Navier-Stokes equations. For example, the pressure must satisfy (or can be the result) the thermodynamic equation of state and the momentum balance equation. The result of the numerical solution of the flow equations (momentum and mass balance) over a time increment dt produces new values of the density and fluid pressure. Similarly the solution of the energy equations generates new values of the energy contained in a control volume V_0 . So at the new time t' new values of the internal energy are derived and should be connected to local temperature, pressure and densities as $E = E(T, V)$, $E = E(T, P)$ or $E = E(T, \rho)$. When an equation of state for a multicomponent chemical system is applied, the pressure, temperature and density (or volume) should also satisfy the equation of state. In an abstract form the latter can be written as:

$$\Phi(T, P, V, \mathbf{z}) = 0 \quad (13)$$

If we suppose to use one of the cubic equation of state, which are used extensively in the oil&gas simulation world, the above equation of state takes the form:

$$P = \frac{RT}{(V-b)} - \frac{a(T)}{V(V-b)} \quad (14)$$

for the Soave-Redlich-Kwong equation [4], or

$$P = \frac{RT}{(V-b)} - \frac{a(T)}{V(V+b)+b(V-b)} \quad (15)$$

for the Peng-Robinson equation [5]. In the above two equations we have dropped, for simplicity, the dependence of the a and b parameters from the vapour phase composition y or liquid phase composition x .

$$b = \sum_i^{NC} z_i b_i \quad (16)$$

$$a = \sum_{i,j}^{NC} z_i z_j a_i a_j (1 - k_{ij}) \quad (17)$$

In addition, at equilibrium, vapour and liquid phase compositions must satisfy the equality of the chemical potentials in the two phases. Avoiding, also in this case, a detailed derivation of the equations, the equilibrium constraint is described by the *K-value* relations as:

$$\frac{y_i}{x_i} = K_i(T, P, \mathbf{x}, \mathbf{y}) \quad (18)$$

In detail the K_i function has a mathematical expression which is highly non-linear and is dependent on the equation of state selected for the description of the system to be simulated. One of the relevant points for the dynamic simulation of fluid flow is the evaluation of the temperature of the fluid with time. This becomes very important for multi-phase flow when additional evaporation or condensation affecting vapour and liquid phases must be considered. In this respect the temperature is usually calculated after fluid pressure and phase velocities have been updated as results of the integration though a time step . A link between pressure and temperature of vapour and liquid in equilibrium can be expressed using the well-known Clausius-Clapeyron equation:

$$\frac{dP}{dT} = \frac{\Delta H}{T\Delta V} \quad (19)$$

Strictly speaking, this equation is valid for two phases in equilibrium of the same composition, or in other terms, only when the system is formed by a single chemical component. If the system is formed by two or more chemical components, temperature and pressure are related by a more complex equation since the variation of the chemical potentials must be taken into account:

$$VdP - SdT - \sum_i m^i d\mu^i = 0 \quad (20)$$

After the energy equation has been integrated, the new value of the total energy per unit mass is obtained. This value E can be compared with the value of the previous time t_0 . To compute the new temperature a number of possible paths can be used, all based on new value of the energy obtained from the integration of the balance equation. For a vapour-liquid system, the energy of the unit mass can be written as:

$$E = E_v w_v + E_L w_L \quad (21)$$

Where w_i indicates the weight fraction of the phase. By taking the differential of the above equation and considering the constraints:

$$w^v + w^L = 1 \quad (22)$$

$$dw^v + dw^L = 0 \quad (23)$$

we can write, assuming the vapour fraction as independent variable:

$$dE = w_v dE_v + (1 - w_v) E_L + (E_v - E_L) dw_v \quad (24)$$

The differentials of the vapour and liquid internal energy terms can be expanded in terms of the partial derivatives with respect to pressure and temperature as:

$$dE_i = \left(\frac{\partial E_i}{\partial T} \right)_P dT + \left(\frac{\partial E_i}{\partial P} \right)_T dP \quad (25)$$

Finally by substituting the expansion (25) into eq. (24), a final expression which relates the change of pressure and temperature to the change of the energy is obtained. This relation can be symbolically expressed as:

$$\Delta E = f(\Delta T, \Delta P) \quad (26)$$

At this stage, we have one equation with two independent variables, i.e. the changes of pressure and temperature; one must be eliminated and more than one option is possible. One solution is to relate the pressure and temperature changes using the Clausius-Clapeyron equation. A second one uses the pressure change obtained by the previous integration of the momentum and mass balance equations.

4. TWO EXAMPLES OF PIPELINE SIMULATION

The above equations have been implemented within a process simulation software [6] which provides the thermodynamic framework required for the definition of the chemical components, the calculation of thermodynamic properties, as function of the equations of state, and the evaluation of the equilibrium between vapour and liquid phases. Since fluid properties are not derived and interpolated from predefined tables but are calculated at each time step as functions of phase compositions, the simulation time required to solve a given problem is much higher. However a deeper insight of how compositions change and have effect on the evolution of the fluid-dynamics can be obtained. Two examples related to problems concerning the transport of oil&gas through pipelines are presented. The first describes the pressurization of a pipeline containing pure nitrogen with a hydrocarbon fluid and the change of the nitrogen concentration is followed. The second example shows compositional changes found during the fast depressurization of a pipeline filled with a 3-component hydrocarbon mixture.

4.1 Pipeline pressurization

The first example is a real case taken from offshore plant design. The problem to be simulated is the pressurization of a pipeline PL1, connecting two offshore facilities, as required by start-up procedures. The line, with internal diameter equal to 0.2679 m, is 500 m long and is initially filled with nitrogen at 20 bar. The pipeline PL1 is connected to another production line PL0 filled with hydrocarbon fluid produced by a nearby reservoir. The hydrocarbon fluid is received at 80 bar and is used to pressurize the pipeline before subsequent start-up operations are initiated. To this purpose a control valve is opened in a time period of about 3 minutes allowing the fluid to fill the PL1 pipeline. The composition of the hydrocarbon fluid is given by Table 1.

Table 1. Fluid Composition used for pipeline pressurization case

No	Component	Molar Fraction, %
1	H2O	0.0172
2	N2	0.6984
3	CO2	4.5054
4	H2S	6.6298
5	C1	39.1120
6	C2	23.4063
7	C3	22.2626
8	IC4	0.8409
9	NC4	1.4369
10	IC5	0.3492
11	NC5	0.3753
12	C6	0.2604
13	C7	0.0716
14	C8	0.0263
15	C9	0.0063
16	C10	0.0013

As shown by Figure 1, the initial flow of the hydrocarbon fluid from 80 bar to 20 produces a large temperature decrease generated by the Joule-Thompson effect.

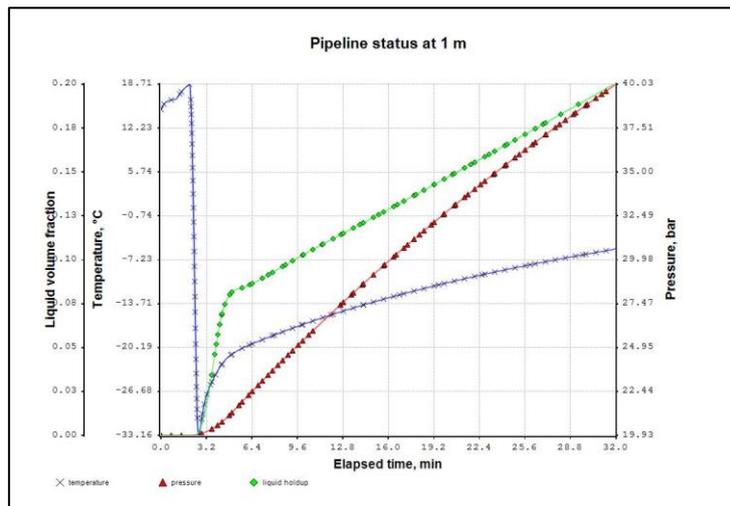


Figure 1. Pressure, temperature and liquid holdup evolution at 1 m after pipeline entry

On the contrary at the final closed end of the pipeline PL1, the temperature increases due to the compression of the pre-existing nitrogen fluid by the incoming fluid. The pipeline is not thermally insulated, external temperature is set at 20°C and nitrogen is initially flowing at 15 °C. So the initial temperature increase is the results of the heat flux caused by temperature difference. The next Figure 2 shows the time variation of pressure and composition at the end of the pipeline. Pressure increases steadily, as the hydrocarbon fluid flow reaches the final point of the closed pipeline and the nitrogen molar fraction rapidly decreases, due to the same factor.

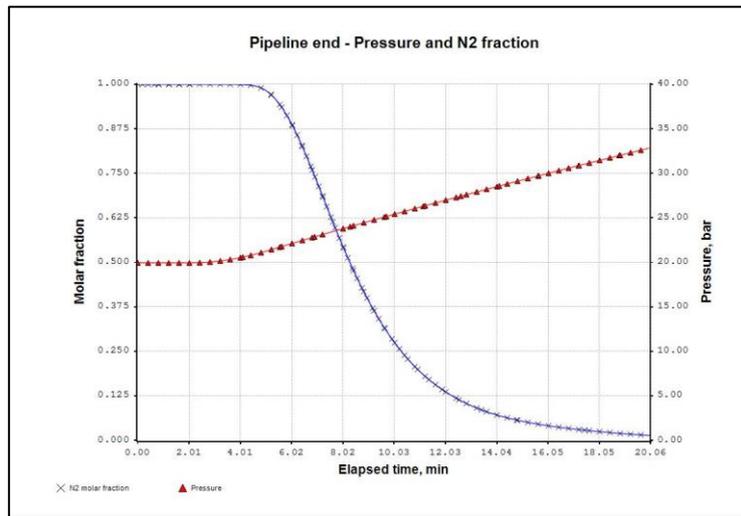


Figure 2. Nitrogen molar fraction change and pressure build-up at pipeline end

4.2 Pipeline Depressurization

This second example presents the simulation of the fast depressurization of a pipeline due to a rupture. Pipeline ruptures are well known problems which are usually difficult to be reliably simulated. The calculation of the rapid pressure and temperature changes is recognized as a ‘stress test’ of the numerical algorithm implemented for the solution of the fluid flow equations. From the engineering design point of view the knowledge of the temperature profile and the minimum value obtained during the depressurization is a very important information required to assure that the material does not enter into the unwanted region of brittle fragility. In the field of pipeline depressurization, the experiments performed some year ago by BP and Shell and known as ‘Isle of Grain experiments’ [7] are often mentioned and their results are reported and discussed. However, the simulation of these experiments are not suitable to picture the change of fluid composition during the depressurization since the fluid used was nearly pure propane (95 % propane, 5 % n-butane) and the change of the overall composition is very small. To illustrate a larger composition change, a different mixture is used as shown in Table 2.

Table 2. Fluid Composition for pipeline leak simulation

No	Component	Molar Fraction, %
1	C1	50
2	NC4	40
3	NC8	10

The pressure and temperature region where vapour and liquid phases are in equilibrium, is described by the phase-envelope shown by Figure 3. The pipeline is 1 km long (internal diameter 0.154 m) filled with the fluid defined by the above fluid stored at 120 bar and 20 °C. Allowing an initial time interval for stabilization, at 3 s a rupture event is initiated. The fluid is discharged through a hole of 50 mm diameter.

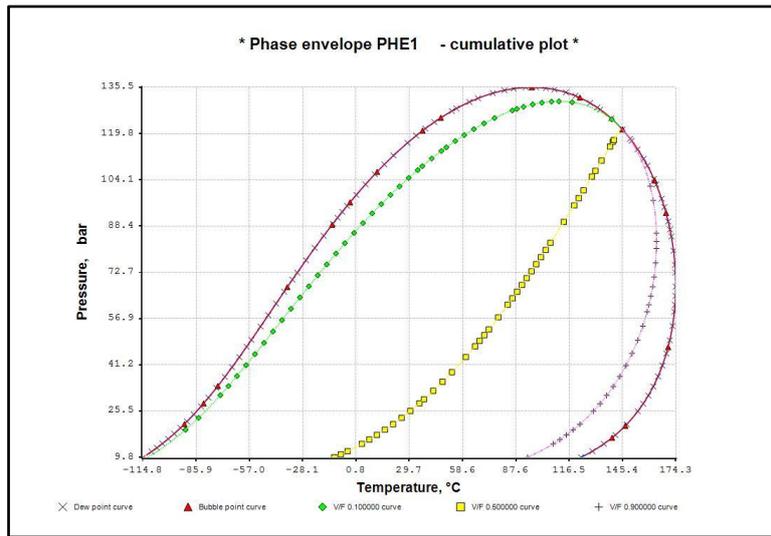


Figure 3. Phase envelope of the methane, n-butane and n-octane mixture defined in Table 2

At the temperature of the mixture flowing in the line, its bubble point pressure is slightly below 120 bar, so during the depressurization the fluid enters very soon the two-phase region. Figure 4 gives the change of the pressure at the final pipeline point where the rupture is located and the change of the mixture composition (as measured by a virtual analyser) is presented by Figure 5. Finally one example of the pressure and temperature profile along the pipeline is represented in Figure 6.

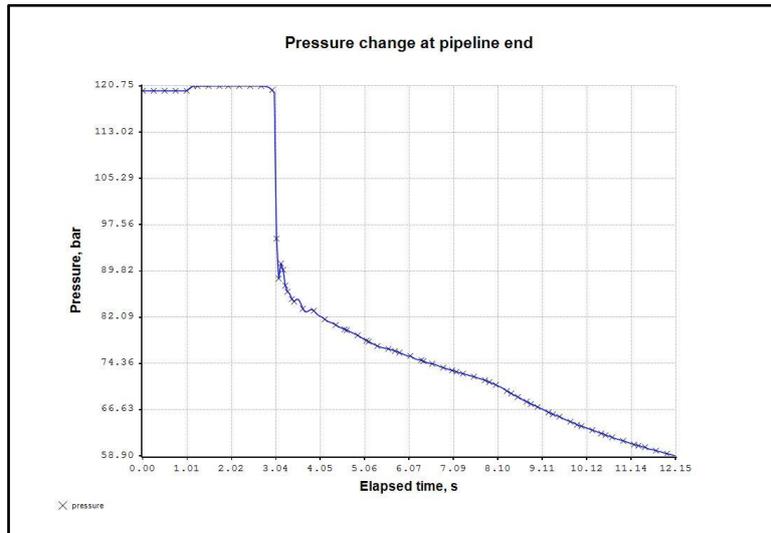


Figure 4 Pressure change at leak position (pipeline end point)

The pipeline is initialized allowing the mixture flowing through and by closing inlet and outlet valves at 1 s with a pressure stabilization effect. The leak is initiated by an event starting at 3.00 s and completed in 0.02 s. The pressure curve, presented by Figure 4, shows the internal value of the final segment which contains the leak hole. Initially the fluid discharged is liquid, so the pressure drop is very fast and becomes slower with the increase of the vapour fraction. Small pressure oscillations can be related to the existence of reverse pressure waves.

5. CONCLUSION

The development of algorithms for the simulation of vapour-liquid two-phase flow through pipelines taking into account the chemical composition of the fluid is an important topic for the analysis of multiphase transport. This development extends the usual two-fluids model algorithms with chemical components mass balances. In performing the numerical integration, chemical equilibrium and thermodynamic fluid properties (density, energy and viscosity) are calculated at each time step without any loss of details which would arise from the use of pre-calculated property tables. The validity of this approach is demonstrated by two cases taken from flow-assurance design practices in the on-shore and off-shore engineering.

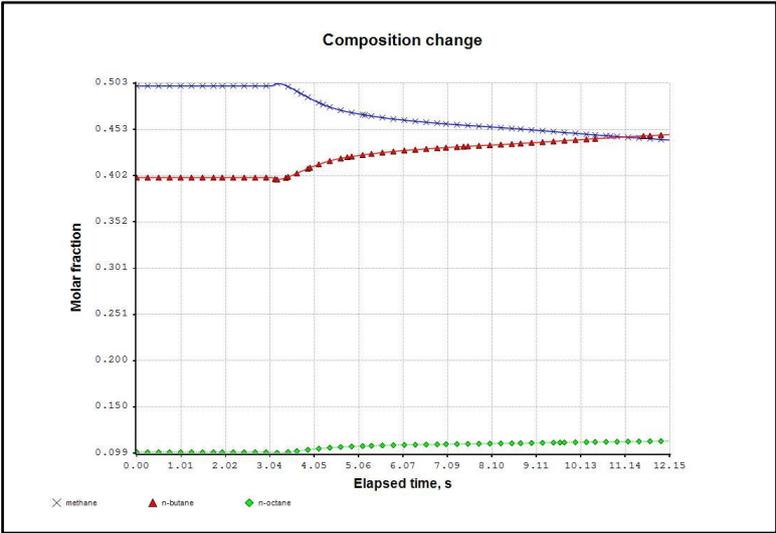


Figure 5 Methane, n-butane and n-octane composition at leak position

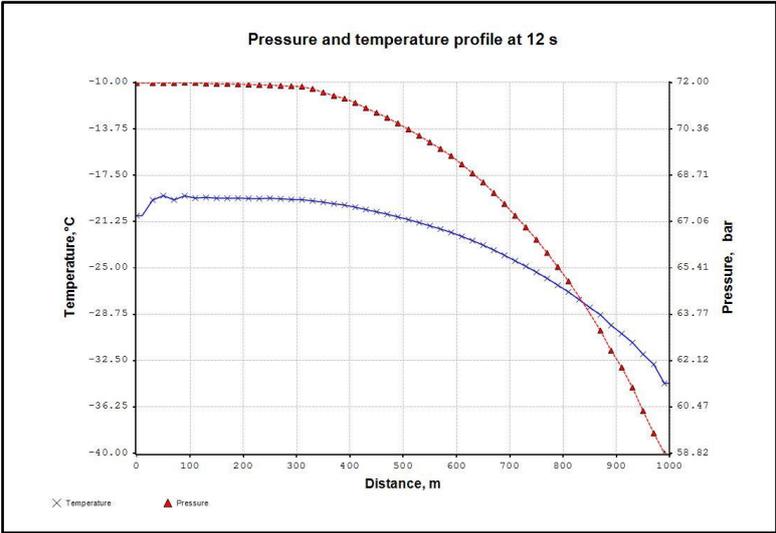


Figure 6 Pressure and temperature profile - 9 seconds after leak event.

NOTATION

Variables

g	gravitational acceleration, m/s^2
m	mass flux
u	phase velocity, m/s
w	phase weight fraction
E	internal energy, J/kg
H	phase enthalpy, J/kg
P	pressure, Pa
T	absolute temperature, K
V	volume, m^3
x	liquid composition
y	vapour composition
z	generic phase composition

Greek symbols

α	phase volume fraction
ρ	phase density, kg/m^3
μ	chemical potential

Sub-scripts & super-scripts

k	phase index
i	chemical component index

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